Supporting Information

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SI Text

A. Directed Networks

We can easily extend the multiscale mixing measure r_{α} described in the main text to directed networks. The main change is to incorporate two sets of marginals *a* and *b* that describe the proportion of edges starting from and ending at each of the attribute types. Then the directed global assortativity of a network with respect to a particular categorical node attribute y_i is

$$r_{\text{global}} = \frac{\sum_g e_{gg} - \sum_g a_g b_g}{1 - \sum_g a_g b_g},$$
[S1]

where a_g and b_g represent the total number of outgoing and incoming links of all nodes of type g,

$$a_g = \sum_h e_{gh}, \qquad b_h = \sum_g e_{gh}.$$
 [S2]

Then we can update our definition of local assortativity accordingly,

$$r(\ell) = \frac{1}{Q_{\max}} \sum_{g} (e_{gg}(\ell) - a_g b_g).$$
 [S3]

B. Scalar Attributes

For scalar attributes, we can simply calculate the Pearson's correlation across edges. Using x_i and x_j to indicate the scalar attribute value of the nodes in edge A_{ij} , then we can write the global assortativity as

$$r_{\text{global}} = \frac{\text{cov}(x_i, x_j)}{\sigma_i \sigma_j}$$
[S4]

$$=\frac{\sum_{ij}A_{ij}(x_{i}-\bar{x})(x_{j}-\bar{x})}{\sum_{i}k_{i}(x_{i}-\bar{x})^{2}},$$
 [S5]

where $\bar{x} = 1/2m \sum_{i} k_i x_i$ is the mean value of x weighted by node degree k and σ_i is the SD of the attribute values. If we standardize the scalar values using the linear transformation $\tilde{x}_i = \frac{x_i - \bar{x}}{\sigma_i}$, then we can simplify this further as

$$r_{\text{global}} = \sum_{ij} \frac{A_{ij}}{2m} \tilde{x}_i \tilde{x}_j.$$
 [S6]

Then we can calculate the local assortativity $r_{\alpha}(\ell)$ for scalar variables as

$$r_{\alpha}(\ell) = \sum_{ij} w_{\alpha}(i;\ell) \frac{A_{ij}}{k_i} \tilde{x}_i \tilde{x}_j.$$
 [S7]

Fig. S1 gives some examples of distributions of r_{multi} for scalar attributes in the food web network.

C. Categorical Assortativity as a Correlation

The assortativity coefficient r_{global} for categorical attributes can be interpreted as a normalized Pearson's correlation. To see this, we start by observing that the Pearson's correlation of two binary variables is equivalent to the Phi coefficient for binary contingency tables (31). Table S1 shows a contingency table using the same notation as the directed assortativity, i.e., *a* and *b* give the marginal proportions and *e* gives the joint proportions.

Then the Pearson product–moment correlation of these variables is known as ϕ , which we derive using the moments of a Bernoulli distribution,

$$\phi = \frac{\mathbb{E}[y_i, y_j] - \mathbb{E}[y_i]\mathbb{E}[y_j]}{\sigma_{y_i}\sigma_{y_j}}$$
[S8]

$$=\frac{e_{11}-a_1b_1}{\sqrt{a_1a_0}\sqrt{b_1b_0}}.$$
 [S9]

Note that it is only necessary to calculate this in terms of e_{11} , since $e_{11} - a_1b_1 = e_{00} - a_0b_0$. We can see this using the identity $e_{00} = b_0 - a_1 + e_{11}$,

$$e_{00} - a_0 b_0 = b_0 - a_1 + e_{11} - (1 - a_1)(1 - b_1)$$
[S10]

$$= (1 - b_1) - a_1 + e_{11} - (1 - a_1 - b_1 + a_1 b_1)$$
 [S11]

$$= e_{11} - a_1 b_1.$$
 [S12]

A well-known issue with ϕ is that the extreme values of +1 and -1 are typically unobtainable, which can cause issues with its interpretation. In fact, $\phi = 1$ can only occur if $a_1 = b_1$, e.g., when the network is undirected, while $\phi = -1$ can only occur if $a_1 = b_2 = 0.5$ (32, 33). To address this issue, there have been a number of proposed normalizations to ensure the $\phi = 1$ is obtainable (34). One such normalization is the ϕ/ϕ_{max} proposed by Cureton (35),

$$\frac{\phi}{\phi_{\max}} = \frac{e_{11} - a_1 b_1}{\beta - a_1 b_1},$$
[S13]

where β is the maximum possible value that e_{11} can take, i.e., $\min(a_1 b_1)$. Note that, for undirected networks,

$$\sqrt{a_1 b_1 a_2 b_2} = \sqrt{a_1^2 a_2^2}$$
 [S14]

$$= a_1 a_2$$
 [S15]

$$= a_1(1 - a_1)$$
 [S16]

$$=a_1-a_1^2,$$
 [S17]

which equals ϕ_{\max} when $a_1 \leq a_2$.

Then we can generalize ϕ/ϕ_{max} from binary to multicategory variables by treating each distinct value as a binary variable and taking their sum. If we set $\beta = 1$, then we obtain Eq. **S1**, and thus we recover Newman's assortativity (13). We also note that Eq. **S1** also corresponds to Cohen's κ that is frequently used to assess interrater agreement (36).

The normalization of the assortativity coefficient means that $r_{\min} \leq r \leq 1$ and

$$r_{\min} = -\frac{\sum_g a_g b_g}{1 - \sum_g a_g b_g},$$
[S18]

which lies in the range $-1 \le r_{\min} < 0$.

D. Assortativity as Autocorrelation of a Time Series

Assume a scalar attribute x_i on each node *i* of an undirected network. As mentioned in the main text, the probability of being at node *i* is stationary and proportional to the degree, $\pi_i = k_i/2m$. Given that a random walker is currently at node *i*, it moves to node *j* with probability A_{ij}/k_i .

We define a random time series, using the simple random walker, as the sequence of attributes of the nodes visited in the random walk, i.e., the value of the time series at time t is the attribute value x of the node visited at time t in the random walk. Asymptotically, the average value observed by the random walker is $\bar{x} = \sum_i \pi_i x_i = \sum k_i x_i/2m$, and the variance is $\sigma^2 = \sum_i \pi_i x_i^2 - \bar{x}^2$.

Likewise, the autocovariance between the attribute observed at two consecutive steps (time lag of 1) is $R_x = \sum_{ij} \pi_i A_{ij} / k_i x_i x_j - \bar{x}^2$. Replacing x by $\tilde{x} = \frac{x-\bar{x}}{\sigma}$, we obtain the autocorrelation $R_{\bar{x}} = \sum_{ij} \pi_i A_{ij} / k_i \tilde{x}_i \tilde{x}_j$, which coincides with r_{global} as defined in Eq. **S6**.

When faced with categorical data, we proceed as in *SI Text*, section C. We consider, for each type g of nodes, the scalar attribute x_g valued at 1 for nodes with type g and zero elsewhere. The modularity Q is therefore the sum for each type g of the autocovariance, $Q = \sum_g R_g$. As in *SI Text*, section C, this can be normalized in various ways, one of which is Newman's global assortativity as used in this article, which therefore represents a sort of categorical autocorrelation of the time series process of the categorical attributes observed by the stationary simple random walker.

E. Disconnected Networks

By using the personalized PageRank as a neighborhood function, it means that only nodes within the same connected component contribute to r_{multi} . Consequently, r_{multi} for each node is insensitive to whether multiple connected components are included.

F. Missing Values

It is common, when dealing with real datasets, that some values may be missing. This is the case for the Facebook 100 data, where a number of node attributes are missing. When considering the global assortativity, previous work has simply ignored contributions from missing data values (3). That is, only edges that connect nodes for which both the attribute values are known are considered when calculating e_{gh} . This treatment works fine for the global assortativity, because each edge counts equally. However, simply omitting missing values when calculating the local assortativity can cause a bias in the distribution. For example, consider the case when node ℓ and its immediate neighbors have missing values but, beyond those, the attribute values are known. For small values of α , the weight $w_{\alpha}(i; \ell)$ is largest for nodes with missing attribute values. Simply ignoring their edges would mean reassigning more weight to edges farther away from ℓ when normalizing to ensure that $\sum_{gh} e_{gh}(\ell) = 1$, a necessary step in calculating the assortativity. Then, when we examine the distribution of $r(\ell)$ across all nodes in the network, the resulting distribution will be a biased representation. To deal with this issue, we calculate each of the local assortativities as normal, but assign each a weight $z_{\ell} = \sum_{gh} e_{gh}(\ell)$, i.e., the sum of local edge counts before normalization. The weight z_{ℓ} describes our confidence in the local assortativity estimate from $z_{\ell} = 0$, indicating no confidence, to $z_{\ell} = 1$ when all node attributes within the neighborhood are known. We adjust for these weights when plotting the histograms in the main text.

G. Calculating the Personalized PageRank Vector

The personalized PageRank vector is the stationary distribution of a random walk with restarts. We calculate it by direct simulation of the random walk process using the power method:

$$w_{\alpha}(i;\ell)_{s+1} = \alpha \sum_{j} \frac{A_{ij}}{k_i} w_{\alpha}(j;\ell)_s + (1-\alpha)\delta_{i,\ell}, \quad [S19]$$

and, at convergence, yields a distribution $w(i; \ell)$ with a mode at ℓ .

H. Integrating over α

To integrate over all values of α , we take advantage of the fact that we can equivalently write the η th approximation the power method in Eq. **S19** as the η th degree truncation of the power series (37),

$$w_{\alpha}(i;\ell)_{\eta} = \delta_{i,\ell} + \sum_{s=1}^{\eta} \alpha^{s} \left[\left(\frac{A_{i\ell}}{k_{i}} \right)^{s} - \left(\frac{A_{i\ell}}{k_{i}} \right)^{(s-1)} \right].$$
 [S20]

By taking advantage of the relationship between α and the sequence of approximations computed by the power method, we can calculate the distribution $w_{\alpha}(i; \ell)$ for a given $\alpha = \alpha_0$ and use the sequence of approximations to calculate the distribution for any other α (37),

$$w_{\alpha}(i;\ell)_{\eta} = \delta_{i,\ell} + \sum_{s=1}^{\eta} \frac{\alpha^{s}}{\alpha_{0}^{s}} \left(w(i;\ell,\alpha_{0})_{s} - w(i;\ell,\alpha_{0})_{s-1} \right).$$
 [S21]

We can then integrate over all possible values of α (23),

$$w_{\text{multi}}(i;\ell)_{\eta} = \int_{0}^{1} w_{\alpha}(i;\ell)_{\eta} \,\mathrm{d}\alpha \qquad [S22]$$

$$= \delta_{i,\ell} + \sum_{s=1}^{\eta} \frac{\left(w_{\alpha_0}(i;\ell)_s - w_{\alpha_0}(i;\ell)_{s-1}\right)}{(s+1)\alpha_0^s}.$$
 [S23]

I. Null Model Network Generation

We created a null model to generate networks with the same global assortativity as the observed network to compare the distributions of r_{multi} . For a fair comparison, we decided to keep the node degree and metadata label fixed while randomly rewiring the network. We do so using a modified version of the Markov chain Monte Carlo (MCMC) sampling of the configuration model for stub-labeled simple graphs (38) [for simple graphs, sampling from the space of stub-labeled graphs is equivalent to sampling from the space of vertex-labeled graphs (38)]. The modification is to ensure that we sample a graph with (approximately) the same global assortativity as the observed network. We achieve this by adding a rejection sampling step based on the binomial likelihood of observing the number of edges between nodes of the same type $m_{in} = m \sum_{g} e_{gg}$ given the proportion of edges required to maintain the global assortativity $\omega_{\rm in} = \sum_{g} e_{gg},$

$$L(G_i) = \log \binom{m}{m_{\rm in}} (\omega_{\rm in})^{m_{\rm in}} (1 - \omega_{\rm in})^{m - m_{\rm in}}.$$
 [S24]

The modified MCMC algorithm is shown in Algorithm 1.

Algorithm 1: stub-labeled MCMC. Require: initial simple graph G_0 , initial temp. t_0 Ensure: sequence of graphs G_i for i < number of graphs to sample do choose two edges at random randomly choose one of the two possible swaps if edge swap would create a self-loop or multiedge then resample current graph: $G_i \leftarrow G_{i-1}$ else if $Unif(0,1) < \exp(L(G_i) - L(G_{i-1})/t_i)$ then swap the chosen edges, producing G_i else reject G_i $t_{i+1} \leftarrow$ update (t_i) .

J. Datasets

Weddell Sea Food Web. The food web of the Antarctic Weddell Sea (4) consists of 488 species and 15,885 consumer relations. For each of the nodes in this network, we have five categorical attributes: Metabolic Category {*Plant, Ectotherm vertebrate, Endotherm vertebrate, Invertebrate*}, Feeding Type {*Carnivorous/necrovorous, Herbivorous/detrivorous, Detrivorous, Omnivorous, Primary producer, Carnivorous*}, FeedingMode {*Pelagic predator, Predator/scavenger, Primary producer, Predator, Deposit-feeder, Grazer, Suspension-feeder*}, Mobility {1, 2, 3, 4}, Environment {*Bathydemersal, Land-based, Resource, Pelagic,* *Benthopelagic, Benthic, Demersal*}. For scalar attributes, we use the mean mass of the species, mobility (although discrete, the values are ordinal), and node degree.

Facebook 100. The Facebook 100 dataset (3) contains an anonymized snapshot of the friendship connections among 1,208,316

users affiliated with the first 100 colleges admitted to Facebook. The dataset contains a total of 93,969,074 friendship edges between users of the same college. Each node has a set of categorical social variables: status {*undergraduate*, *graduate* stu*dent*, *summer student*, *faculty*, *staff*, *alumni*}, dorm, major, gender {*male*, *female*}, and graduation year.



Fig. S1. Multiscale assortativity for different scalar attributes in the Weddell Sea Food Web: node degree, average species mass, and mobility. Note that mobility is a discrete ordinal variable (taking integer values in Eqs. 1 and 4), and, in the main text, we treat it as an unordered discrete variable.





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Fig. 53. Distributions of the local assortativity by residence (dorm) separated into first years and the rest of the students for each school. Schools are ordered by increasing proportion of first years that are more assortative than the rest of the students. In general, first-year students are more assortative than the rest, one schools in which the difference between first year and the rest is negligible. In a few schools, we observe that the first-year students are less assortative than the rest.

DNA C

Table S1. Binary contingency table

	$y_j = 0$	$y_j = 1$	
$y_i = 0$	e ₀₀	e ₀₁	a 0
<i>y</i> _{<i>i</i>} = 1	e ₁₀	e ₁₁	a 1
	b_0	b_1	

Table S2. List of schools ordered by global assortativity

1 Amherst 41 0.081 51 William 77 0.203 2 Princeton 12 0.087 52 Emory 27 0.205 3 Trinity 100 0.109 54 Tennessee 95 0.208 4 Stanford 3 0.109 55 Wake 73 0.212 6 Johns Hopkins 55 0.110 56 MIT 8 0.2219 7 Hamilton 46 0.113 57 UMass 92 0.2222 8 Bowdoin 47 0.118 58 Berkeley 13 0.2222 9 Harvard 1 0.120 59 USC 35 0.224 10 Brown 11 0.126 61 UVA 16 0.230 12 Wellesley 22 0.127 62 Penn 94 0.231 13 Haverford 76 0.128 63 Northwestern 25 0.235 14 Wesleyan 43 0.130 66 Michigan 23 0.236 17 Williams 40 0.133 67 FSU 53	No.	School	<i>r</i> _{global}	No.	School	<i>r</i> _{global}
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