Evolution of robust network topologies: Emergence of central backbones

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We model the robustness against random failure or intentional attack of networks with arbitrary large-scale structure. We construct a block-based model which incorporates both connectivity and interdependence links, as well as arbitrary degree distributions and block correlations. By optimizing the percolation properties of this general class of networks, we identify a simple core-periphery structure as the topology most robust against random failure. In such networks, a distinct and small “core” of nodes with higher degree is responsible for most of the connectivity, functioning as a central “backbone” of the system. This centralized topology remains optimal under certain conditions, such as given fraction of interdependence links and fixed degree distributions. This distinguishes simple centralised topologies as the most likely to emerge, when robustness against failure is the dominant evolutionary force.

One of the most important characteristics of large networked systems is their capacity to function reliably. Perhaps the simplest paradigm employed in the study of robustness of network systems is the theory of percolation [1], which describes the conditions for the formation of a system-spanning connected component. Arguably, if a system is not connected to begin with, it is unlikely to remain optimal when other constraints are imposed other than those defined previously [2].

In this Letter, we investigate analytically and numerically the most fundamental large-scale structures [3] which results in robustness against random failure and malicious attack. By constructing a general block-based model, and analytically deriving its percolation properties, we obtain the topological configuration which optimizes a well-defined robustness criterion. In the case of random failure, we find that a remarkably simple core-periphery (CP) topology [4] emerges as the most optimal, when no other constraints are imposed other than the overall cost in realizing the system. This topology remains optimal when one introduces interdependence links, and it can entirely suppress the catastrophic failure present in fully random topologies. However, in the case of targeted attacks, the fully random configuration turns out to be the most robust. We also consider the scenario where degree constraints are present, and find that the bimodal core-periphery structure is replaced by strongly assortative and dissortative block topologies, for random and targeted attacks, respectively.

Here we consider a stochastic blockmodel [5,7] which defines an ensemble of networks composed of B discrete node blocks, where \( n_r \) is the number of nodes in block \( r \) and \( e_{rs} \) is the number of edges between blocks \( r \) and \( s \) (or twice that number if \( r = s \)). Each block is allowed its own degree distribution, \( p_k^r \). We also consider interdependence edges by defining a distinct matrix \( \hat{e}_{rs} \) and degree distributions \( p_k^r \), in an analogous fashion. As in [2], if a node \( u \) is dependent on another node \( v \), \( u \) fails automatically when \( v \) fails, and vice-versa. In the case of multiple dependencies [8], all support nodes must fail in order for the dependent node to fail (i.e., they are redundant). Assuming that the values of \( n_r \) are large enough, this ensemble becomes locally tree-like [9], thus it is possible to adapt the epidemics-based generating function formalism [10,12], which becomes exact in the limit of large networks. If we define \( u_r \) as the probability that a node belonging to block \( r \) is not in a macroscopic component via one of its neighbors, the dilution variable \( \phi_k^r \) as the fraction of nodes belonging to block \( r \) and with degree \( k \) which are not removed from the network, and additionally the interdependence dilution \( \phi_r \), defined as the fraction of nodes from block \( r \) which were not removed due to the failure of the support nodes, we can write the following self-consistency equations (see Supplemental Material for a derivation):

\[
\hat{u}_r = \sum_s m_{rs} \left[ 1 - \hat{\phi}_s f'_s(1) + \hat{\phi}_s f'_s(u_s) \right] \tag{1}
\]

\[
\hat{\phi}_r = 1 - f'_r(1 - \sum_s m_{rs} S_0^s) + f'_r(0), \tag{2}
\]

where \( m_{rs} = e_{rs}/n_r k_r \) is the asymmetric matrix defining the fraction of edges adjacent to vertices of block \( r \) which are also adjacent to block \( s \), where \( k_r = \sum_s e_{rs}/n_r \) is the average degree of block \( r \). \( S_r = \phi_r S_0^r \) is the fraction of nodes of block \( r \) which belong to a macroscopic component, and \( S_0^r = f'_r(1) - f'_r(u_r) \), given as a function of the diluted degree generating function \( f'_0(z) = \sum_k p_k^r \phi_k^r z^k \). Furthermore, \( f'_r(z) = \sum_k g_k^r \phi_k^r z^k \) generates the diluted excess degree distribution of block \( r \), with \( g_k^r = p_{k+1}^r(k+1)/k_r \). Note that we have \( f'_r(z) = f'_0(z)/g'_0(1) \) where \( g'_0 = \sum_k p_k^r z^k \) generates the undiluted degree distribution of block \( r \). The generating function \( f'_r(z) = \sum_k p_k^r z^k \) describes the degrees corresponding to interdependent edges alone. The total fraction of nodes which belong to a macroscopic component is simply \( S = \sum_r w_r S_r \), where \( w_r = n_r/N \) is the fraction of nodes belonging to a macroscopic component.
nodes belonging to block $r$, and the total dilution in the network is likewise $\phi = \sum_{r,k} w_{r,k} \phi^e_{r,k}$.

Although quite straightforward, this parametrization is a generalization of many scenarios considered in the literature, such as two fully interdependent networks [2], the single networks with mixed connectivity and interdependence edges [17,19], as well as networks with only connectivity edges and arbitrary degree distribution and correlations [20], all of which correspond to specific choices of the parameters defined here. In Fig. 1 is shown an example of a block structure with both support and interdependence links, as described in the legend. It also shows a comparison with the empirical percolation profile of networks realized from this ensemble, which is in excellent agreement with the theoretical prediction.

We are interested in obtaining the block topologies for which the robustness against failure or attack are optimal. Following [21] we will consider the total robustness of a network ensemble to be given by

$$R = 2 \int_0^1 S(\phi) d\phi, \quad (3)$$

where the factor 2 is chosen so that $R \in [0, 1]$, with $R = 1$ being possible only in the hypothetical scenario $S(\phi) = \phi$, attainable only for infinitely dense networks. Thus our ultimate task is to find the parametrization of the blockmodel ensemble which maximizes Eq. 3 under suitable constraints. In the following, we focus on the special case with uniform failure of nodes within a single block, $\phi_k^e \equiv \phi$; hence $f^e_d(z) = \phi g^e_d(z)$. The total dilution becomes simply $\phi = \sum_r w_r \phi_r$. Without loss of generality, since heterogeneous degree-based dilution can still be achieved if nodes of different degrees belong implicitly to different blocks. In the case of random failure we have simply, $\phi_r = \phi$. In the case of targeted attacks we will use $\phi_r \propto e^{\kappa_r(1-b)/b}$, where $b \in [0, 1]$ must be so chosen to achieve a desired total $\phi$.

Instead of directly finding the network topology parametrization which maximizes $R$, we proceed by obtaining the configuration which delivers a specified value of $R$, and is otherwise maximally random. We do so in order to identify network structures with a varied degree of robustness, and to isolate the most fundamental characteristic responsible for its increase. Hence, we consider a null model of robust networks, where superfluous characteristics are explicitly discarded. More specifically, we maximize the entropy of network ensemble [22], subject to the constraint that the average robustness is fixed [23]. This amounts to finding the critical points of the Lagrangian $\Lambda = \Sigma - \tilde{\beta}(R - R^*)$, where $\Sigma = \ln \Omega$ is the microcanonical entropy (with $\Omega$ being the number of different network realizations for a specific ensemble parametrization), $R$ and $R^*$ are the actual and desired average robustness respectively, and $\tilde{\beta}$ is a Lagrange multiplier. Instead of fixing $R^*$, one may fix $\beta$, and this becomes equivalent to minimizing the free energy of the ensemble,

$$F = -NR - \Sigma/\beta, \quad (4)$$

since $\Lambda \equiv \tilde{\beta}(F/N + R^*)$, and $\beta \equiv -\tilde{\beta}/N$. In Eq. 4 the value $-NR$ plays the role of average energy, and $\beta$ is the inverse temperature, which can also be interpreted as a “selective pressure” [24], since for $\beta = 0$ the entropy is strictly maximized (i.e. all networks occur with...
equal probability), and conversely for $\beta \to \infty$ the average robustness is strictly maximized. In our case we have $\Sigma = S + \hat{S}$, where $\hat{S}$ is the stochastic blockmodel entropy \[^{26}\].

$$S = -\sum_r n_r \sum_k p^*_k \left( \ln p^*_k + \ln k! \right) - \frac{1}{2} \sum_{rs} e_{rs} \ln \left( \frac{e_{rs}}{e_r e_s} \right),$$

which includes the entropy of the degree distributions of the individual blocks, and $\hat{S}$ is equivalently defined as a function of $\hat{e}_{rs}$ and $p^*_r$ \[^{26}\].

Solving the system given by Eqs. 1 and 2 cannot be performed analytically, and thus the same holds for obtaining $R$ and $\mathcal{F}$. Hence we must resort to solving Eqs. 1 and 2 numerically (by simple iteration), in order to obtain Eqs. 3 and 4. The minimization of Eq. 3 can then be performed within arbitrary precision with any suitable minimization algorithm (see Supplemental Material for details).

The ensemble can have additional constraints, which must be imposed when minimizing $\mathcal{F}$. One such constraint we will consider throughout this paper is that the average degree $\langle k \rangle$ will be fixed at a given value, which represents the putative cost of adding extra edges to the network, compared to simply replacing them. Furthermore, in order to restrict the number of degrees of freedom of the model to a manageable size, we will assume that all blocks have the same type of degree distribution, which can be different only in their average value, $\kappa_r$. This does not alter very strongly the type of networks which are ultimately attainable, since in principle one can construct many different topologies by composing a larger number of such blocks. We will also forbid nodes with degree zero, since these never belong to a macroscopic component. The degree distribution we use is a modified Poisson distribution $p^*_k = (1 - \delta_{k,0}) e^k_k / (e^k - 1) k!$ [identical to a regular Poisson, but with support $k \geq 1$], which is generated by $g^*_k(z) = z e^{(\kappa_r - 1)(z - 1)}$, which of course implies that $\kappa_r \geq 1$ for all $r$. The same distribution will also be used for the interdependence degrees, $p^*_r$. Note that this simplifies the entropy to $S = \sum_r n_r \ln(e^{\kappa_r n_r} - 1) - \frac{1}{2} \sum_{rs} e_{rs} \ln(e_{rs}/n_r n_s)$, and equivalently for $\hat{S}$. Finally, the total number of blocks $B$ will also remain fixed during the minimization of $\mathcal{F}$.

In absence of any further constraints, we start with the case of random failures, and no interdependence links ($\kappa_r = 0$). We observe that increasing $\beta$ leads from a fully random graph ($\beta = 0$) to a topology which can be significantly more robust (see Fig. 2a). For $B = 2$ blocks, this topology is a core-periphery (CP) structure \[^{4, 5}\], where one block is much smaller and has a much larger average degree, $\kappa_r$, and attracts a large portion of the edges. One might expect this to be a special case when one imposes $B = 2$, and that different robust topologies may arise for $B > 2$. However, this turns out not to be the case, and we find exactly the same CP topology for any value of $B$ larger than two, in the sense that two or more blocks may be merged together, with the ensemble remaining equivalent, until only $B = 2$ blocks are left. In Fig. 2b, are shown two resulting ensembles for different $\beta$ and with $B = 3$, for $\langle k \rangle = 2$. The size and average degree of the core block become smaller and larger, respectively, for larger values of $\beta$. Examples of how such networks can look like are shown in Fig. 2c.

For sufficiently large $\beta$, the vast majority of periphery nodes are connected exclusively to core nodes, which are much smaller in number (infinitesimally so for $\beta \to \infty$), and which are connected among themselves, forming a central backbone \[^{27}\].

Observing how the value of $R$ changes with $\beta$ exposes a structural phase transition at a critical value of $\beta = \beta^*$, below which the networks are fully random ($e_{rs} \propto e_r e_s$, and $\kappa_r = \langle k \rangle$), and above which the CP topology is observed (see Fig. 3a). The value of $\beta^*$ becomes smaller for larger $\langle k \rangle$, close to two, and larger for either sparser or denser graphs. The CP topology is particularly advantageous for sparse graphs, with lower $\langle k \rangle$, but is less so for denser graphs, as can be seen in Fig. 3b, which shows a comparison between the $\beta = 0$ (random) and $\beta = \infty$ (optimal) cases, as a function of $\langle k \rangle$.

When node interdependence is enforced ($\kappa_r \geq 1$ \[^{28}\]), the same CP structure emerges for larger values of $\beta$, as shown in Fig. 4b. For $\beta \to \infty$, the percolation tran-
sions and (b) targeted attacks. In both cases the values \( w_r \) and \( \kappa_r \) are kept fixed. (c, d) Ensemble samples with \( N = 10^6 \) nodes, \( \beta \to \infty \), for (c) random failures and (d) targeted attacks.

The average interdependence degrees, \( \kappa_r \), become correlated with the connectivity degrees, \( \kappa_s \), with most interdependence edges lying between two core nodes, which therefore benefit more from the extra redundancy, to the indirect benefit of the periphery nodes as well. In comparison to the \( \langle k \rangle = 0 \) case, denser networks benefit more from the CP topology, since it removes the abrupt phase transition. The benefit diminishes for larger \( \langle k \rangle \), since the larger redundancy already provides an inherent robustness to random networks. A special case is \( \langle k \rangle = 1 \), which shows a lower improvement, because it strictly forbids intra-core redundancy.

As seen in Figs. 2a and 3a, the CP topology is excellent against random failure, but is extremely fragile against targeted attacks, in which the core nodes are removed before the rest (the value of \( S \) vanishes for an infinitesimal value of \( 1 - \phi \)). Instead, if one optimizes \( \tilde{R} \) against targeted attacks, one obtains that the random block topology is the most robust. The only exceptions are very sparse networks with \( \langle k \rangle \lesssim 2 \) (see Fig. 3b). Since these networks are close or below the percolation threshold even for \( \phi = 1 \), the CP topology is still an improvement over the fully random case, even if gets destroyed very quickly by a targeted attack.

In some realistic situations there are degree constraints restricting the accessible topologies [21]. Here we introduce this by forcing that the blocks have prescribed sizes and average degrees (see Supplemental material for details). As can be seen in Fig. 3b, in the case of random failure, the optimal topology approaches the CP configuration as much as the imposed constraints allow, and the inter-block connectivity becomes strongly dissonative, with the nodes with largest degrees serving as intermediaries between the nodes with the lowest degrees and an innermost “core” composed of more of such alternating layers. For targeted attacks the resulting topology is quite different: The blocks with higher \( \kappa_r \) are “expelled” from the network, since they are the first to be removed in an attack. The resulting topology is highly assortative, with blocks with similar \( \kappa_r \) connecting preferentially to themselves. This is qualitatively equivalent to the “onionlike” topology found empirically in [21]. An exception to this are the blocks with small \( \kappa_r \). These do form a CP structure, since an assortative connectivity would have very weak percolation properties even when no nodes are removed, i.e. \( \phi = 1 \) (similarly to the case \( \langle k \rangle \lesssim 2 \) discussed previously). Very similar results are obtained when interdependence is introduced (see Supplemental material).

The topologies described above arise when no constraint other than those considered is being imposed, and the ensemble entropy is maximized. This is not often the case for real systems, since they may be subject to competing selective pressures, with robustness being only one of them, as well as other topological restrictions, frozen accidents, etc. Nevertheless, the analysis presented here suggests that a simple core-periphery structure is the most natural configuration which achieves robustness against random failure (and that a random, non-centralized topology works best against targeted attacks). Therefore, it not a surprise that a CP topology is indeed found to some extent in many real systems [4], such as the Internet [29], and gene regulation networks [24]. Also, our results indicate that other features found in real systems, such as scale-free degree distributions, are not a strict necessity for robustness, and do not arise naturally for this purpose, and thus may be simply a byproduct of a non-equilibrium organization process.

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\[\text{[26]}\] Eq. 5 omits constant terms which are not relevant to the optimization parameters, and is valid in the sufficiently sparse case (see \[\text{[25]}\]), which is also assumed for Eqs. \[\text{[1]}\] and \[\text{[2]}\].

\[\text{[27]}\] This is reminiscent of the random graphs with bimodal degree distribution in \[\text{[31]}\]. However, these do not possess a CP topology, since all nodes are forced to be randomly connected.

\[\text{[28]}\] We could also allow autonomous nodes, i.e. $\hat{\kappa}_r < 1$ \[\text{[34]}\]. But allowing this leads to trivial block structures where all interdependence edges are confined to an isolated block of insignificant size. We therefore focus on the harder case where autonomous nodes are not allowed.

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Supplemental Material: Evolution of robust network topologies

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GENERATING FUNCTION PERCOLATION
FORMALISM

Following [1–3], we derive self-consistency equations for the percolation properties of stochastic blockmodel ensembles as follows. If we let $u_r$ describe the probability that a node belonging to block $r$ is not in a macroscopic component via one of its neighbors, the dilution variable $\hat{\phi}_r^s$ as the fraction of nodes belonging to block $r$ and with degree $k$ which are not removed from the network, and additionally the interdependence dilution $\phi_r$, defined as the fraction of nodes from block $r$ which were not removed due to the failure of the support nodes, we can write,

$$u_r = \sum_k m_{rs} \left( 1 - \hat{\phi}_r \hat{\phi}_{k+1}^s + \hat{\phi}_r \hat{\phi}_{k+1}^s u_s \right) q_k,$$

where $m_{rs} = e_{rs}/n_r \kappa_r$ is the asymmetric matrix defining the fraction of edges adjacent to vertices of block $r$ which are also adjacent to block $s$, and $q_k = p_{k+1}^s (k+1)/\kappa_r$ is the excess degree distribution of block $r$, and $\kappa_r = \sum_s e_{rs}/n_r$ is the average degree of block $r$. This can be rewritten in compact form as

$$u_r = \sum_s m_{rs} \left[ 1 - \phi_r f_1(1) + \phi_r f_1(u_s) \right],$$

where $f_1(z) = \sum_k q_k \phi^r_{k+1} z^k$ is the generating function of the excess degree distribution. Note that we have $f_1(z) = f_1^r(z)/g_0^r(1)$ where $g_0^r = \sum_k p^r_k z^k$ and $f_0^r(z) = \sum_k p^r_k \phi^r_k z^k$ are the generating functions of the original and diluted degree distributions, respectively.

The fraction of nodes of block $r$ which belong to a macroscopic component is given by $S_r = \phi_r S^0_r$, where $S^0_r = f_0^r(1) - f_0^r(u_r)$. The total fraction of nodes which belong to a macroscopic component, or if its dependence neighbors is also dependent on $u$, will be removed from the network in the likewise $\phi = \sum_k w_r p^r_k \phi^r_k$.

In the case of no interdependence edges, we have simply $\phi = 1$, and Eq. 2 describes $S_r$ completely. Otherwise, an additional fraction of nodes will be removed from the macroscopic components, if the nodes to which they depend do not belong to the component. The fraction $\hat{\phi}_r$ of nodes which are not removed in this way can be obtained by

$$\hat{\phi}_r = \sum_k p^r_k \left[ 1 - (1 - \sum_s m_{rs} S^0_s)^k \right] + p^r_0,$$

where $\hat{k}$ are the interdependence degrees, and $p^r_0$ is the interdependence degree distribution of block $r$. Here it is assumed that the interdependence is undirected (if node $u$ is dependent on $v$, then $v$ is also dependent on $u$), and that at least one dependency must not fail in order for the dependent node not to fail (i.e. redundant interdependence), and furthermore that a node with $k = 0$ is autonomous (see below for variations of these rules). We may write this equation in a more compact form as

$$\phi_r = 1 - \hat{f}_0^r (1 - \sum_s m_{rs} S^0_s) + \hat{f}_0^r(0),$$

where $\hat{f}_0^r(z) = \sum_k p^r_k z^k$ is the interdependence degree generating function. Note that the right hand side of Eq. 4 depends only on $u_r$ variables (via $S^0_r$), and thus may be included directly into Eq. 2, resulting in a total of only $B$ equations. Similarly to [3], here we omit the detailed description of the failure cascades as done in e.g. [2], however these correspond simply to repeated iterations of Eqs. 2 and 4, where one must first obtain the convergence of the $u_r$ variables, and then of the $\phi_r$ variables, in succession. However, if one is only interested in the steady state, simultaneously iterating Eqs. 2 and 4 is more straightforward.

One may also consider different interdependence rules by slightly modifying Eq. 4. For instance, in the case of non-redundant interdependence, where all dependencies are essential, so that if any one of them fails, the dependent node fails as well, can be described by replacing Eq. 4 by

$$\hat{\phi}_r = \hat{f}_0^r \left( \sum_s m_{rs} S^0_s \right) + \hat{f}_0^r(0).$$

Furthermore, one may also consider the situation where the interdependence is directed, i.e. if node $u$ depends on node $v$, $v$ does not necessarily depend on $u$ (in this situation it assumed that $e_{rs}$ is also directed, and thus asymmetric, and the variables $k$ describe the dependence in-degree). This can be implemented by an almost trivial modification, simply by replacing $S^0_r \rightarrow S_r$ in Eq. 4 or 5, where we have, as before, $S_r = \hat{\phi}_r S^0_r$. This is simply because a node will fail either if it does not belong to a macroscopic component, or if its dependence neighbors fail. However, in the case of directed interdependence, the likelihood that two nodes are mutually interdependent is vanishingly small, and thus the support node will depend exclusively on other nodes, which will themselves not fail with probability given by $\phi_r$. This introduces a direct coupling between the variables $\phi_r$ (which is only indirect in the undirected case). Although seemingly innocuous, this modification can drastically change the percolation properties of the system, in particular when the
FIG. 1. Robustness $R$ to uniform node removal of random networks with one block $B = 1$, as a function of $k$, and different values of $\langle k \rangle$, for (a) undirected interdependence and (b) directed dependence; (c) Relative size of the largest component $S$ as a function of the dilution $\delta$, for a random graph with $\langle k \rangle = 5$, directed dependencies and different $\langle k \rangle$ values. The solid lines are results obtained via Eqs. 2 and 4 (with $S_0^s \to S_\ast$), and the filled symbols are obtained empirically with a network realization with $N = 10^6$ nodes.

average degrees $\bar{k}_r$ are close to one. Indeed if all nodes have $\bar{k} = 1$, the failure of an infinitesimal fraction of nodes will always cause a global cascade, independently of how well connected the network is. This is easy to understand, since the removal of a single node will necessarily cause the failure of another node, which will trigger the failure of a third one, and so on, until a loop is reached. The average size of these cascades diverges, and thus the values of $S_r$ will drop to zero. The robustness of random networks (B=1) with different values of $\langle k \rangle$ and $\langle k \rangle$ are shown in Fig. 1, for both connectivity and interdependence degree distributions given in the main text if $\langle k \rangle \geq 1$ or $p_k = (\langle k \rangle)\delta_{k,1} + (1 - \langle k \rangle)\delta_{k,0}$ if $\langle k \rangle < 1$. For undirected interdependence, we have that $R$ approaches one for $\langle k \rangle \to \infty$, for all values of $\langle k \rangle$. However for directed dependence, we have $R$ dropping to zero as $\langle k \rangle$ approaches one, independently of $\langle k \rangle$.

In all cases, the percolation threshold can be obtained by examining the Jacobian $J = \{\partial(u_r^e|\bar{\phi}_r^e)/\partial(u_s|\bar{\phi}_s)\}$, where $u_r^e$ and $\bar{\phi}_r^e$ correspond to the right-hand side of Eqs. 2 and 4, respectively. If the largest eigenvalue $\lambda$ of $J$ at the fixed point $u_r = 1$ and $\bar{\phi}_r = f_0^e(0)$ exceeds one, this solution is unstable, and thus some value of $S_r$ must be finite, and hence the condition $\lambda = 1$ marks the percolation transition.

MINIMIZATION OF THE FREE ENERGY, $\mathcal{F}$

As mentioned in the main text, the computation of $R$ and thus $\mathcal{F}$ must be done numerically, by iterating Eqs. 2 and 4 until convergence within some desired precision is reached. This means that the minimization of $\mathcal{F}$ must also be performed numerically. We used different algorithms, depending on the set of constraints used. In the case of $\langle k \rangle = 0$, the L-BFGS-B quasi-Newton method [4], with gradient obtained with finite differences, delivered fast and reliable results if the number of degrees of freedoms were not very large ($B = 2$ or 3). For larger number of blocks, the non-gradient COBYLA algorithm [5] performed better. In the case $\langle k \rangle > 0$, the discontinuity in $S(\phi)$ makes the gradient estimation unreliable, and the COBYLA algorithm is a better choice. In both cases, when improved precision was necessary, a repeated sequential one-dimensional minimization over all variables using Brent’s method [6] was performed, at the expense of longer computational time. In the case of very large values of $B$, an initial estimation using the ALPSO stochastic swarm-based algorithm [7] was used, which was then improved upon, whenever possible, with COBYLA.

In all cases, the constrained optimization problem was transformed into an unconstrained one, via appropriate transformations. The normalization constraints, $\sum_r w_r = 1$ and $\sum_{rs} e_{rs} = N(\langle k \rangle)$ can be imposed simply by transforming $w_r = C \exp(\tilde{w}_r)$, and $e_{rs} = D \exp(\tilde{e}_{rs})$ with $C^{-1} = \sum_r w_r$ and $D^{-1} = \sum_{rs} e_{rs}/N(\langle k \rangle)$, and solving for $\tilde{w}_r$ and $\tilde{e}_{rs}$. Note that we can set, e.g. $\tilde{w}_0 = 0$ and $\tilde{e}_{00} = 0$ so that only $2B + B(B - 1)/2 - 2$ free variables remain. The degree constraints $\kappa_r \geq 1$ can be imposed via the transformations $\kappa_r = \tilde{\kappa}_r$ if $\kappa_{\min} \equiv \min(\{\kappa_r\}) \geq 1$ otherwise $\kappa_r = a_r\tilde{\kappa}_r + 1$ where $a_r = (\kappa_r - 1)/\sum_s w_s(\kappa_s - \kappa_{\min})$. The new row and column sums of $e_{rs}$ given by $\sum_s e_{rs} = \sum_s e_{sr} = N w_r\kappa_r$, can then be enforced in the $e_{rs}$ matrix via a Sinkhorn scaling [8]. The same transformations can be used for the $\tilde{e}_{rs}$ matrix. With all these transforms in place, the optimization problem becomes fully unconstrained, with $\tilde{w}_r$, $\tilde{e}_{rs}$ and $\tilde{e}_{sr}$ lying in the interval $[-\infty, \infty]$. Note that the variable $N$ is only included in the text to slightly simplify the notation, but it is entirely unnecessary during the optimization, since one needs to work only with normalized variables.

In all minimizations performed, the same solutions were found, regardless of the algorithm used or the initial configuration. Although the different methods have different precision and convergence speed, the results were always mutually consistent. Additionally, the independence of the results on the initial configuration implies the results obtained were always a global minimum of the free energy.
FIG. 2. (a, c) Fraction $S$ of nodes in the macroscopic component as function of the dilution $\phi$, for different $\beta$ values, fixed values of $w_r$ and $\kappa_r$, and $\langle \kappa \rangle = 1.2$, for random failures (a) and targeted attacks (c). The solid lines are results obtained via Eqs. 2 and 4, and the filled symbols are obtained empirically with a network realization of size $N = 10^6$; (b, d) Correlation matrices $e_{rs}/e_r e_s$ (black) and $\hat{e}_{rs}/\hat{e}_r \hat{e}_s$ (red), block size $w_r$ and average degrees $\kappa_r$ (black) and $\hat{\kappa}_r$ (red), for $\beta \to \infty$, for random failures (b) and targeted attacks (d).

IMPOSING DEGREE CONSTRAINTS

As mentioned in the main text, in some realistic situations there are degree constraints restricting the accessible topologies [9]. Here we introduce it by forcing that the blocks have prescribed sizes and average degrees, following $w_r \propto \kappa_r^{-\gamma}$ and $\kappa_r = e^c r$, with $r \in [0, B-1]$ and $c = \ln \kappa_{\text{max}}/(B-1)$. This allows us to have a very broad range of degrees, similar to what is found in scale-free networks. In Fig. 5 of the main text are shown the results for $B = 6$, $\gamma = 2$ and $\kappa_{\text{max}} = 10^3$. Very similar results are found by varying $B$, $\gamma$ and $\kappa_{\text{max}}$ (not shown).

Here we expand briefly on these results by introducing interdependence, i.e. $\langle \hat{k} \rangle \geq 1$. We do so in slightly different way than before, by imposing a separation of the network into two parts of equal size, such that connectivity (interdependence) edges are only allowed between nodes in the same (different) part. This is to mimic, e.g. the situation of computer and electricity infrastructure, where interdependence is only meaningful between the two different types of nodes. With this constraint, we obtain a configuration very similar to the case without interdependence (see Fig. 2), with dissortative and assortative connectivity for the random and targeted removal, respectively. However, the interdependence connectivity is slightly more elaborate: For random failures, the values of $\hat{\kappa}_r$ are correlated with $\kappa_r$, and the $\hat{e}_{rs}$ matrix displays a more assortative connectivity, with blocks depending on other blocks with similar average degree. In the case of targeted attacks, the interdependence shows a CP structure for blocks with low degree, but otherwise follows the same segregated pattern as the connectivity edges.

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