

# Supplementary Information: Network dismantling

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We provide in this Supplementary Information further technical details and additional results in support of the main text. It is organized as follows. In Section I we prove the NP-completeness of the dismantling decision problem. In Sec. II we extend the analytic results of the main text, presenting the details of the cavity method computation of the decycling number of random graphs (II A), a lower bound on the decycling number valid for all graphs (II B), and an expansion of the decycling number for Erdős-Rényi random graphs close to their percolation threshold and for large average degrees (II C). Section III is then devoted to several algorithmic aspects: in III A, III B and III C we detail the three stages of our main algorithm (derivation of the Min-Sum equations, tree dismantling and greedy reintroduction of cycles respectively), while in III D we give further details on the other dismantling algorithms we have studied. Finally in Section IV we provide further results on other real-world and artificial scale-free networks.

## I. PROOF OF NP-COMPLETENESS OF THE DISMANTLING PROBLEM

For our proof, we will employ the decisional (minimum) Vertex Cover problem, which is NP-Complete, and is defined as follows. Remember that a vertex cover is a subset of vertices  $W \subset V$  such that for each  $(i, j)$  in  $E$ ,  $i \in W$  or  $j \in W$ .

VERTEX COVER: Given a graph  $G = (V, E)$  and  $F \in \mathbb{N}$ , does a vertex cover  $W \subset V$  with  $|W| \leq F$  exist?

The VERTEX COVER problem is NP-Complete.

$C(N)$ -DISMANTLING: Given a graph  $G' = (V', E')$  and  $F \in \mathbb{N}$ , does a  $C(|V'|)$ -dismantling set  $S$  with  $|S| \leq F$  of  $G'$  exist?

**Theorem 1.** *Assume  $C : \mathbb{N} \rightarrow \mathbb{N}$  to be a non-decreasing (polynomially computable) function with  $C(N) < N^a$  for  $N \geq N_0$  with  $0 \leq a < 1$ . Then the  $C(N)$ -DISMANTLING problem is NP-Complete.*

*Proof.*  $C(N)$ -DISMANTLING belongs clearly to NP. If  $C \equiv 1$ , one can see that  $C$ -DISMANTLING is identical to VERTEX COVER and is thus NP-Complete. Otherwise, take  $N_1$  such that  $C(N_1) \geq 2$  and consider  $N \geq \max\{N_0, N_1\}$ . Define

$$C' = C'(N) = \min \left\{ k \in \mathbb{N} : \frac{C(kN)}{k} < 2 \right\}. \quad (1)$$

*Remark.* For constant  $C(N) \equiv C \geq 2$ , then  $C'(N) \equiv \frac{C+1}{2}$  if  $C$  is odd, and  $C'(N) \equiv \frac{C}{2} + 1$  if  $C$  is even.

Note that  $C' \geq 2$  and  $C'$  is polynomial in  $N$ : the value  $k = \lceil \frac{1}{2} N^a \rceil^{\frac{1}{1-a}}$  belongs to the set in the RHS of (1), as  $k \geq (\frac{1}{2} N)^{\frac{a}{1-a}}$  so  $k^{a-1} \leq (\frac{1}{2} N)^{-a}$  and then  $\frac{C(kN)}{k} < \frac{(kN)^a}{k} = k^{a-1} N^a \leq 2$ ; so  $C' \leq k = \lceil \frac{1}{2} N^a \rceil^{\frac{1}{1-a}}$ . We will prove that

$$C' \leq C(C'N) < 2C'. \quad (2)$$

The second inequality in (2) follows from (1). For the first inequality,

$$C(C'N) \geq C((C' - 1)N) \quad (3)$$

$$\geq 2(C' - 1) \quad (4)$$

$$\geq C', \quad (5)$$

where (3) follows from the fact that  $C$  is non-decreasing, (4) follows from the minimality of  $C'$  in its definition (1) and (5) from the fact that  $C' \geq 2$ .

Now, take a graph  $G$  with  $|V| = N$ , and construct  $G'$  by adding  $C' - 1$  leaves to any vertex of  $G$ . Precisely, let  $G' = (V', E')$  with  $V' = V \cup \{\ell_{v,i} : v \in V, i \in \{1, \dots, C' - 1\}\}$  and  $E' = E \cup \{(v, \ell_{v,i}) : v \in V, i \in \{1, \dots, C' - 1\}\}$  where we assume the two unions to be disjoint. The number of vertices of  $G'$  is  $|V'| = N' = NC'$  (which is polynomial in  $N$ ). The construction of  $G'$  is clearly polynomial.

Take any vertex cover  $W$  of  $G$ . Then  $W$  is a  $C'$ -dismantling of  $G'$ : thanks to the vertex cover property, each  $v \in V \setminus W$  can only be connected to the  $C' - 1$  extra leaves  $\ell_{v,i}$ . As  $C' \leq C(N')$ , then  $W$  is also a  $C(N')$ -dismantling of  $G'$ .

Conversely, take any  $C(N')$ -dismantling set  $S$  of  $G'$ . Define  $\pi : V' \rightarrow V$  by  $\pi(v) = v$  for  $v \in V$  and  $\pi(\ell_{v,i}) = v$  for  $v \in V, 1 \leq i \leq C' - 1$ . Consider the set  $W = \pi(S)$ . In short,  $W$  is constructed from  $S$  by replacing all occurrences  $\ell_{v,i}$  by  $v$ . Then clearly  $|W| = |\pi(S)| \leq |S|$  and  $W$  is still a  $C(N')$ -dismantling of  $G'$ : replacing  $\ell_{v,i}$  by  $v$  introduces a new component  $\{\ell_{v,i}\}$  of size 1 but can only reduce the size of the other components. Moreover,  $W$  is also a vertex cover of  $G$ : suppose on the contrary that it is not, and take an edge  $(i, j) \in E$  such that  $i, j \notin W$ . Then both vertices belong to a connected component of  $G' \setminus W$  of size  $2C' > C(N')$ , which contradicts the fact that  $W$  was a  $C(N')$ -dismantling of  $G'$ . Thus,  $W$  must be a vertex cover of  $G$  with size no greater than  $|S|$  and that proves the result.  $\square$

**Corollary 2.** For  $C(N) = \text{const}$ ,  $C(N) = \log N$ , and  $C(N) = N^a$  with  $0 \leq a < 1$ ,  $C(N)$ -DISMANTLING is NP-Complete.

*Remark.*  $(N - k)$ -DISMANTLING is polynomial for any constant  $k$ .

## II. ANALYTIC RESULTS

### A. Details on the cavity equations for the decycling number of random graphs

We give here some more details on the cavity method computation of the decycling number of sparse random graphs, in particular on the derivation and solution of the BP equations. A full derivation in a more general context can be found in [1].

When computing the typical free-energy of a large random graph with degree distribution  $q$  one has to determine the probability law  $P(\eta)$  of the messages  $\eta$ , which is the solution of an integral equation of the form:

$$P(\eta) = \sum_{k=0}^{\infty} \tilde{q}_k \int dP(\eta^{(1)}) \dots dP(\eta^{(k)}) \delta(\eta - f_k(\eta^{(1)}, \dots, \eta^{(k)})), \quad (6)$$

where  $\tilde{q}_k = (k+1)q_{k+1} / \sum_k kq_k$  is the size-biased distribution associated to  $q$  (i.e. the probability of finding a vertex of degree  $k+1$  when choosing an edge uniformly at random), and  $f_k$  the function encoding the local BP equation, eq. (9)

in the main text, between messages around a vertex of degree  $k + 1$ . This type of equation can be efficiently solved numerically via a population dynamics procedure, in which  $P$  is approximated by a large sample of representative values of  $\eta$ , updated according to (6) until convergence to a fixed point. The free-energy density of the model can then be computed as the average with respect to  $P$  of suitable functions of the messages. In the present model these messages are real vectors of a dimension which grows linearly with the parameter  $T$  introduced above as a cutoff on the allowed times in the leaf-removal dynamics.

In the Replica Symmetric version of the cavity method a message (or field)  $\eta$  of (6) corresponds to a  $2T$  dimensional vector of components denoted  $(a_0, a_1, \dots, a_T, b_{T-1}, \dots, b_1)$ . The function  $f_k$  which gives  $\eta$  as a function of  $\eta^{(1)}, \dots, \eta^{(k)}$  reads explicitly:

$$\begin{aligned} e^{-\mu b_t} &= 1 + e^{-\mu + \mu \sum_{i=1}^k (a_0^{(i)} - b_{t-1}^{(i)})} , \\ e^{-\mu a_t} - e^{-\mu a_{t+1}} &= e^{-\mu + \mu \sum_{i=1}^k (a_0^{(i)} - b_t^{(i)})} \sum_{i=1}^k \left( e^{\mu (b_t^{(i)} - a_{t+1}^{(i)})} - e^{\mu (b_t^{(i)} - a_{t+2}^{(i)})} \right) , \end{aligned} \quad (7)$$

with the conventions used to have more compact expressions:  $b_0 = 0$ ,  $b_T = a_T$ ,  $a_{T+1} = b_{T-1}$ . Once the self-consistent equation on  $P(\eta)$  is solved the thermodynamic quantities are obtained as follows. The limit of  $(\ln Z)/N$  reads

$$\phi = \mu + \mathbb{E}[\ln z_{\text{site}}(\eta^{(1)}, \dots, \eta^{(k)})] - \frac{d}{2} \mathbb{E}[\ln z_{\text{edge}}(\eta^{(1)}, \eta^{(2)})] ,$$

where  $\mathbb{E}[\cdot]$  denotes the average over the i.i.d. copies  $\eta^{(i)}$  drawn from  $P(\eta)$  and over the integer  $k$  drawn from the degree distribution  $q$ , and  $d$  is the mean of  $q$ . The two functions  $z_{\text{site}}$  and  $z_{\text{edge}}$  arise from the local contributions to the Bethe free-energy of sites and edges respectively, and read

$$z_{\text{site}} = 1 + e^{-\mu + \mu \sum_{i=1}^k a_0^{(i)}} \left[ e^{-\mu \sum_{i=1}^k b_{T-1}^{(i)}} + \sum_{t=1}^T e^{-\mu \sum_{i=1}^k b_{t-1}^{(i)}} \sum_{i=1}^k \left( e^{\mu (b_{t-1}^{(i)} - a_t^{(i)})} - e^{\mu (b_{t-1}^{(i)} - a_{t+1}^{(i)})} \right) \right] , \quad (8)$$

$$z_{\text{edge}} = e^{\mu (a_0^{(1)} + a_0^{(2)})} \left[ e^{-\mu (b_T^{(1)} + b_T^{(2)})} + \sum_{t=0}^{T-1} \left\{ (e^{-\mu a_t^{(1)}} - e^{-\mu a_{t+1}^{(1)}}) e^{-\mu b_t^{(2)}} + (e^{-\mu a_t^{(2)}} - e^{-\mu a_{t+1}^{(2)}}) e^{-\mu b_t^{(1)}} \right\} \right] . \quad (9)$$

The fraction  $\theta$  of vertices included in the decycling sets selected by the conjugated chemical potential  $\mu$  and the entropy  $s$  (the Legendre transform of  $\phi$ ) then read:

$$\theta = \mathbb{E} \left[ \frac{1}{z_{\text{site}}(\eta^{(1)}, \dots, \eta^{(k)})} \right] , \quad s = \phi - \mu \theta . \quad (10)$$

Varying the parameter  $\mu$  one can compute in this way the entropy  $s(\theta)$  counting the exponential number of decycling sets containing a fraction  $\theta$  of vertices. The RS estimate of the decycling number  $\theta_{\text{dec}}$  is then obtained as the point where  $s$  vanishes.

This estimate is, however, only a lower bound to the true value of  $\theta_{\text{dec}}$  because of the effects of the replica symmetry breaking. A more precise estimate is obtained by using the (energetic) cavity method at the first level of replica symmetry breaking (1RSB), in which the parameter  $\mu$  is replaced by the Parisi breaking parameter  $y$ ; the message  $\eta$  of (6) is then a vector  $(p_0, \dots, p_{T-1}, r_T, \dots, r_0)$  constrained by the normalization  $p_0 + \dots + p_{T-1} + r_T + \dots + r_0 = 1$

(hence the number of independent parameters is again  $2T$ ). These are updated according to

$$p_t = \frac{1}{Z} e^y \tilde{p}_t, \quad (11)$$

$$r_t = \frac{1}{Z} e^y \tilde{r}_t \text{ for } t \geq 1, \quad (12)$$

$$r_0 = \frac{1}{Z} \left( 1 - \sum_{t=0}^{T-1} \tilde{p}_t - \sum_{t=1}^T \tilde{r}_t \right), \quad (13)$$

$$Z = 1 + (e^y - 1) \left( \sum_{t=0}^{T-1} \tilde{p}_t + \sum_{t=1}^T \tilde{r}_t \right), \quad (14)$$

$$\tilde{p}_t = \sum_{i=1}^k p_{t+1}^{(i)} \prod_{j \neq i} \left( \sum_{t'=0}^t r_{t'}^{(j)} \right), \quad (15)$$

$$\tilde{r}_t = \prod_{i=1}^k \left( \sum_{t'=0}^{t-1} r_{t'}^{(i)} \right) - \prod_{i=1}^k \left( \sum_{t'=0}^{t-2} r_{t'}^{(i)} \right), \quad (16)$$

with  $p_T = r_T$  by convention. One computes then a thermodynamic potential  $\Phi(y)$  with a formula similar to the one yielding  $\phi(\mu)$  at the RS level, namely

$$\Phi = -y + \mathbb{E}[\ln \mathcal{Z}_{\text{site}}(\eta^{(1)}, \dots, \eta^{(k)})] - \frac{d}{2} \mathbb{E}[\ln \mathcal{Z}_{\text{edge}}(\eta^{(1)}, \eta^{(2)})],$$

with

$$\mathcal{Z}_{\text{site}} = 1 + (e^y - 1) \left[ \prod_{i=1}^k \left( \sum_{t=0}^{T-1} r_t^{(i)} \right) + \sum_{i=1}^k \sum_{t=1}^T p_t^{(i)} \prod_{j \neq i} \left( \sum_{t=0}^{t-1} r_t^{(j)} \right) \right], \quad (17)$$

$$\mathcal{Z}_{\text{edge}} = e^{-y} + (1 - e^{-y}) \left[ \left( \sum_{t=0}^T r_t^{(1)} \right) \left( \sum_{t=0}^T r_t^{(2)} \right) + \sum_{t=0}^{T-1} \left\{ p_t^{(1)} \left( \sum_{t'=0}^t r_{t'}^{(2)} \right) + p_t^{(2)} \left( \sum_{t'=0}^t r_{t'}^{(1)} \right) \right\} \right]. \quad (18)$$

The energetic complexity function (the equivalent of the entropy at the 1RSB level) is then obtained by an inverse Legendre transform with respect to  $\Phi$ , namely

$$\Sigma = \Phi + y\theta, \quad \theta = 1 - \mathbb{E} \left[ \frac{\mathcal{Z}'_{\text{site}}}{\mathcal{Z}_{\text{site}}} \right] + \frac{d}{2} \mathbb{E} \left[ \frac{\mathcal{Z}'_{\text{edge}}}{\mathcal{Z}_{\text{edge}}} \right],$$

where the prime denotes the derivative with respect to the explicit dependence in  $y$  of the expressions of  $\mathcal{Z}_{\text{site}}$  and  $\mathcal{Z}_{\text{edge}}$  given above. The 1RSB estimate of the decycling number is then obtained from the criterion of cancellation of the complexity  $\Sigma$ . Both the replica symmetric and 1RSB results for a range of values of  $T$  are reported in Table 1 in the main text. Extrapolating the 1RSB estimate of the decycling number in the limit  $T \rightarrow \infty$  leads to the values reported in Table 1 in the main text.

The replica symmetric and 1RSB computations yield improving lower bounds on the decycling number of light-tailed random graphs, in the sense that  $\theta^{\text{RS}}(q) \leq \theta^{\text{1RSB}}(q) \leq \theta_{\text{dec}}(q)$ . For some degree distributions  $q$  these inequalities become equalities (see [1] for details on random regular graphs), for others the 1RSB estimate is strictly tighter than the RS one. It is probable that for some choices of  $q$  the 1RSB estimate is not equal to the decycling number, whose exact determination would require the use of the so-called full RSB computation. The latter is not tractable numerically for models of sparse random graphs, we expect in any case the quantitative difference between the 1RSB and full RSB results to be rather small.

## B. A simple lower bound

We present here a lower bound on the decycling number  $\theta_{\text{dec}}(G)$  valid for any graph  $G$  (a similar reasoning can be found in [2]), generalizing the bound  $\theta_{\text{dec}}(G) \geq \frac{d-2}{2(d-1)}$  for  $d$ -regular graphs.

TABLE I: The  $T$ -dependence of the RS and 1RSB cavity predictions for the decycling number of Erdős-Rényi random graphs of average degree  $d = 3.5$ . The decycling numbers reported in table 1 in the main text are obtained by interpolation of the 1RSB results to  $T \rightarrow \infty$ .

$T$	$\theta^{\text{RS}}(T)$	$\theta^{\text{1RSB}}(T)$
3	0.22714	0.22797
5	0.20042	0.20077
9	0.18507	0.18515
13	0.18046	0.18051
19	0.17795	0.17797
30	0.17638	0.17638
40	0.17590	0.17590
50	0.17569	0.17569

We denote  $k_i$  the degree of vertex  $i$  and  $M$  the number of edges. With

$$\langle k \rangle = \frac{1}{N} \sum_{i \in V} k_i \quad (19)$$

the empirical average degree, one has  $M = N \frac{\langle k \rangle}{2}$ .

Consider now a subset  $S$  of the vertices, and its complement  $S^c = V \setminus S$ . One can divide the edges in three categories, with  $M = M_1 + M_2 + M_3$ , where  $M_1$  is the number of edges between two vertices of  $S$ ,  $M_2$  counting the edges between  $S$  and  $S^c$ , and  $M_3$  the edges inside  $S^c$ . One has

$$\sum_{i \in S} k_i = 2M_1 + M_2, \quad \sum_{i \in S^c} k_i = 2M_3 + M_2, \quad (20)$$

and in particular

$$M_1 + M_2 \leq \sum_{i \in S} k_i. \quad (21)$$

Suppose now that  $S$  is a decycling set of the graph, in such a way that  $S^c$  induces a forest. Hence one has

$$M_3 \leq |S^c| - 1 = N - |S| - 1. \quad (22)$$

Summing these two inequalities, and expressing  $M$  in terms of the average degree, yields

$$\frac{1}{N} \sum_{i \in S} (k_i - 1) \geq \frac{\langle k \rangle}{2} - 1 + \frac{1}{N}. \quad (23)$$

This inequality constrains the possible decycling sets. To obtain a simpler lower bound on the size of the decycling sets, consider a permutation  $\sigma$  from  $\{1, \dots, N\}$  to  $V$  that orders the vertices according to their degrees:  $k_{\sigma(1)} \geq k_{\sigma(2)} \geq \dots$ . The inequality above can then be continued to get

$$\frac{1}{N} \sum_{i=1}^{|S|} (k_{\sigma(i)} - 1) \geq \frac{\langle k \rangle}{2} - 1 + \frac{1}{N}. \quad (24)$$

Let us call the left hand side of this inequality  $l(\theta = |S|/N, G)$ , which is an increasing function of  $\theta$ , and define  $\theta_{\text{lb}}(G)$  as the smallest value of  $\theta$  such that the inequality is fulfilled. Then the decycling number  $\theta_{\text{dec}}(G)$  of this graph is certainly lower-bounded by  $\theta_{\text{lb}}(G)$ .

The shape of  $l(\theta)$  can be described in terms of the empirical degree distribution of the graph,

$$\hat{q}_k = \frac{1}{N} \sum_{i \in V} \delta_{k, k_i}. \quad (25)$$

As the graph is finite so is its maximal degree, let us call it  $K$ . One realizes easily that  $l(\theta, G)$  is a piecewise linear continuous increasing function, starting from 0 in  $\theta = 0$ , linearly increasing on  $\theta \in [0, \hat{q}_K]$  with slope  $K - 1$ , then again

with a constant slope  $K - 2$  on the interval  $\theta \in [\widehat{q}_K, \widehat{q}_K + \widehat{q}_{K-1}]$ , and so on and so forth. It is thus more convenient to introduce two integrated quantities:

$$\widehat{Q}_k = \sum_{k'=k}^{\infty} \widehat{q}_{k'} , \quad \widehat{T}_k = \sum_{k'=k}^{\infty} \widehat{q}_{k'}(k' - 1) , \quad (26)$$

the summations being cut off at  $K$  in this finite graph case. Indeed for all  $k$  one has  $l(\widehat{Q}_k, G) = \widehat{T}_k$ , and the function  $l(\theta, G)$  is the linear interpolation between this discrete set of points. One can thus determine its intersection with the right hand side of (24) to compute the lower bound  $\theta_{\text{lb}}(G)$ .

In the case of random graphs drawn with a degree distribution  $q$  the typical decycling number  $\theta_{\text{dec}}(q)$  can be lower-bounded as above by replacing the empirical distribution  $\widehat{q}$  by  $q$ :  $\theta_{\text{lb}}(q) = l^{-1} \left( \frac{\langle k \rangle}{2} - 1 \right)$ , where  $\langle k \rangle$  is now averaged with respect to  $q_k$ , and  $l$  is defined by replacing  $\widehat{Q}_k$  and  $\widehat{T}_k$  by their counterparts

$$Q_k = \sum_{k'=k}^{\infty} q_{k'} , \quad T_k = \sum_{k'=k}^{\infty} q_{k'}(k' - 1) . \quad (27)$$

The numerical evaluation of this lower bound for a Poissonian random graph of average degree  $d = 3.5$  yields  $\theta_{\text{lb}} = 0.141084$ , not that far from the 1RSB prediction  $\theta_{\text{dec}} = 0.175$ . The lower bound matches the asymptotic expansion presented below when  $d \rightarrow 1$  (i.e. close to the percolation threshold), while it reaches the limit  $1/2$  when  $d$  diverges (the large  $d$  limit of  $\theta_{\text{dec}}$  being  $1$ ).

### C. Decycling close to the percolation threshold and for large degrees

In addition to the numerical results obtained by the cavity method let us state analytical asymptotic expansions for the decycling number of Poissonian random graphs with average degree close to the percolation threshold ( $d = 1 + \epsilon$ ) or very large ( $d \rightarrow \infty$ ). Close to the percolation a random graph is essentially made of a 3-regular kernel of vertices joined by paths of degree 2 nodes; decycling the kernel is sufficient to decycle the whole graph, and the decycling number of a random 3-regular is known [3], which yields

$$\theta_{\text{dec}}(d = 1 + \epsilon) = \frac{1}{3}\epsilon^3 + O(\epsilon^4) . \quad (28)$$

On the other hand when  $d$  is very large the Poissonian random graph behaves like a regular graph (the degree distribution being concentrated around its average), an asymptotic expansion in this case was obtained in [1] (in agreement with the rigorous bounds of [4]), hence

$$\theta_{\text{dec}}(d) = 1 - \frac{2 \ln d}{d} - \frac{2}{d} + O\left(\frac{1}{d \ln d}\right) . \quad (29)$$

## III. ALGORITHMS

### A. The Min-Sum algorithm and its implementation

In this section we derive the Min-Sum (MS) algorithm introduced in eqs. (10-12) of the main text, that aims at finding decycling sets of the smallest possible size. As explained in the main text this amounts to find the unique minimum of the cost function  $\sum_i \psi_i(t_i)$ , with  $\psi_i(t_i) = \mathbb{I}[t_i = 0] + \varepsilon_i(t_i)$ , over the feasible configurations of the activation times  $\{t_i\} \in \{0, \dots, T\}^V$ . These variables have to fulfill the constraint that for all vertices  $i$  either  $t_i = 0$  (when  $i$  belongs to the decycling set) or it is determined by the adjacent variables according to  $t_i = 1 + \max_2(\{t_j\}_{j \in \partial i})$ . We recall that the  $\varepsilon_i(t_i)$  are infinitesimally small random variables that are introduced to ensure the uniqueness of the minimum of the cost function, and its closeness to one of the minima of the original cost function. In practice we took  $\varepsilon_i$  to be uniformly random between 0 and  $10^{-7}$ .

It turns out to be easier to study a slight modification of this optimization problem, with a relaxed constraint

$$t_i \geq 1 + \max_2(\{t_j\}_{j \in \partial i}) \quad \text{if } 0 < t_i \leq T \quad (30)$$

that corresponds to a lazy version of the leaf removal algorithm, in which a node can be removed once it became a leaf, but it is not necessarily removed as soon as it could be. Thanks to the monotonicity of the leaf removal procedure its

final outcome, the 2-core of the graph, is independent of the order in which the leaves are removed, and of the parallel or sequential character of these updates. Hence the optimization problem with the strict or relaxed constraints are completely equivalent if  $T \geq N$ , the maximal number of possible steps of the leaf removal. For smaller values of  $T$  this equivalence is not ensured, but the optimum with the relaxed constraints still provides a valid decycling set. It will be useful in the following to use the following logical equivalent of (30),

$$\sum_{j \in \partial i} \mathbb{I}[t_j \geq t_i] \leq 1 \quad \text{if } 0 < t_i \leq T . \quad (31)$$

Our goal now is to compute the field  $h_i(t_i)$  defined as the minimum of the cost function over feasible configurations with a given value of  $t_i$ , as indeed the unique minimum can be deduced from the fields through  $t_i^* = \operatorname{argmin} h_i(t_i)$ , and then the corresponding decycling set is identified with the vertices  $i$  where  $t_i^* = 0$ . To justify the MS heuristics for the approximate computation of the fields  $h_i$  on any graph it is simpler to consider first a tree graph, on which the MS approach is exact for any local cost function. The function under consideration here is the sum of local terms  $\psi_i(t_i)$  on each vertex,  $h_i(t_i)$  can thus be decomposed as a sum of its own contribution  $\psi_i$  and of the contributions of the vertices in each of the subtrees rooted at one of its neighbor  $j \in \partial i$ . Taking into account the constraint (31) for the positive times, denoted  $\mathcal{C}$  in the following, it yields

$$h_i(t_i) = \psi_i(t_i) + \min_{\{t_j\}_{j \in \partial i} : \mathcal{C}} \sum_{j \in \partial i} h_{ji}(t_j, t_i) \quad \text{for } 0 < t_i \leq T , \quad (32)$$

$$h_i(0) = \psi_i(0) + \sum_{j \in \partial i} \min_{t_j} h_{ji}(t_j, 0) , \quad (33)$$

where  $h_{ji}(t_j, t_i)$  are messages defined on each directed edge  $j \rightarrow i$  of the graph, that give the minimum cost of the variables in the subtree rooted at  $j$  and excluding  $i$ , over the feasible configurations with prescribed values of  $t_j$  and  $t_i$ . Thanks to the recursive structure of a tree these messages obey themselves similar equations,

$$h_{ij}(t_i, t_j) = \psi_i(t_i) + \min_{\{t_k\}_{k \in \partial i \setminus j} : \mathcal{C}} \sum_{k \in \partial i \setminus j} h_{ki}(t_k, t_i) \quad \text{for } 0 < t_i \leq T , \quad (34)$$

$$h_{ij}(0, t_j) = \psi_i(0) + \sum_{k \in \partial i \setminus j} \min_{t_k} h_{ki}(t_k, 0) . \quad (35)$$

These Min-Sum equations involve  $O(T^2)$  quantities for each edge of the graph because of the two time indices of the messages  $h_{ij}$ . Fortunately this quadratic dependence on  $T$  can be reduced to a linear one by some further simplifications that we now explain.

As can be readily seen from (34) and (31), the dependence of  $h_{ij}$  on  $t_j$  is only through  $\mathbb{I}[t_j < t_i]$ . We will thus define

$$h_{ij}(t_i, t_j) = \begin{cases} h_{ij}^1(t_i) & \text{if } t_j < t_i , \\ h_{ij}^0(t_i) & \text{if } t_j \geq t_i , \end{cases} \quad (36)$$

which gives a parametrization of each message with  $O(T)$  real numbers.

Calling  $\mathcal{T}_{ij}^s = \{\{t_k\}_{k \in \partial i \setminus j} : \sum_{k \in \partial i \setminus j} \mathbb{I}[t_k \geq t_i] = s\}$ , Eq. (34) can be rewritten as follows for  $0 < t_i \leq T$ :

$$\begin{aligned} h_{ij}^0(t_i) &= \psi_i(t_i) + \min_{\mathcal{T}_{ij}^0} \sum_{k \in \partial i \setminus j} h_{ki}(t_k, t_i) \\ &= \psi_i(t_i) + \sum_{k \in \partial i \setminus j} \min_{t_k < t_i} h_{ki}(t_k, t_i) \\ &= \psi_i(t_i) + \sum_{k \in \partial i \setminus j} \min_{t_k < t_i} h_{ki}^0(t_k) , \end{aligned} \quad (37)$$

as indeed  $t_j \geq t_i$  in the definition of  $h_{ij}^0$  all the other removal times  $t_k$  for  $k \in \partial i \setminus j$  have to be strictly smaller than  $t_i$  for the condition (31) to be fulfilled. On the other hand in the situation described by  $h_{ij}^1$  at most one of the removal

times  $t_k$  for  $k \in \partial i \setminus j$  can be greater or equal than  $t_i$ , hence for  $0 < t_i \leq T$ :

$$\begin{aligned}
h_{ij}^1(t_i) &= \psi_i(t_i) + \min_{\mathcal{T}_{ij}^0 \cup \mathcal{T}_{ij}^1} \sum_{k \in \partial i \setminus j} h_{ki}(t_k, t_i) \\
&= \psi_i(t_i) + \min \left\{ \sum_{k \in \partial i \setminus j} \min_{t_k < t_i} h_{ki}^0(t_k), \min_{\mathcal{T}_{ij}^1} \sum_{k \in \partial i \setminus j} h_{ki}(t_k, t_i) \right\} \\
&= \psi_i(t_i) + \min \left\{ \sum_{k \in \partial i \setminus j} \min_{t_k < t_i} h_{ki}^0(t_k), \min_{k \in \partial i \setminus j} \left[ \min \left\{ h_{ki}^0(t_i), \min_{t_k > t_i} h_{ki}^1(t_k) \right\} + \sum_{\ell \in \partial i \setminus j, k} \min_{t_\ell < t_i} h_{\ell i}^0(t_\ell) \right] \right\} \\
&= \psi_i(t_i) + \sum_{k \in \partial i \setminus j} \min_{t_k < t_i} h_{ki}^0(t_k) + \min \left\{ 0, \min_{k \in \partial i \setminus j} \left[ \min \left\{ h_{ki}^0(t_i), \min_{t_k > t_i} h_{ki}^1(t_k) \right\} - \min_{t_k < t_i} h_{ki}^0(t_k) \right] \right\}. \quad (38)
\end{aligned}$$

The equations (10-12) of the main text can now be readily obtained by defining the following quantities:

$$L_{ki}(t_i) = \min_{t_k < t_i} h_{ki}^0(t_k), \quad (39)$$

$$R_{ki}(t_i) = \min \left\{ h_{ki}^0(t_i), \min_{t_k > t_i} h_{ki}^1(t_k) \right\}, \quad (40)$$

$$M_{ij}(t_i) = \min \left\{ 0, \min_{k \in \partial i \setminus j} \{ R_{ki}(t_i) - L_{ki}(t_i) \} \right\}, \quad (41)$$

$$(42)$$

in terms of which the equations (37,38) can be rewritten

$$h_{ij}^0(t_i) = \psi_i(t_i) + \sum_{k \in \partial i \setminus j} L_{ki}(t_i) \quad \text{for } 0 < t_i \leq T, \quad (43)$$

$$h_{ij}^1(t_i) = \psi_i(t_i) + \sum_{k \in \partial i \setminus j} L_{ki}(t_i) + M_{ij}(t_i) \quad \text{for } 0 < t_i \leq T, \quad (44)$$

$$h_{ij}^0(0) = \psi_i(0) + \sum_{k \in \partial i \setminus j} R_{ki}(0), \quad (45)$$

the last equation corresponding to the unconstrained minimization over the removal times of the neighbors of a vertex  $i$  included in the decycling set.

Let us give a more explicit interpretation of the quantities  $L, R$  and of the last equations.  $L_{ki}(t_i)$  is the minimum feasible cost in the subtree of  $G \setminus i$  rooted in  $k$  with the only condition that  $t_k < t_i$  (see Eq. (39)). On the other hand, in Eq. (40) we define  $R_{ki}(t_i)$  to be the minimum feasible cost in the subtree of  $G \setminus i$  rooted in  $k$  with  $t_k \geq t_i$ . As the message  $h_{ij}^1(t_i)$  corresponds to a situation in which  $j$  has already been removed at time  $t_i$ , one of the neighbors  $k \in \partial i \setminus j$  can be removed after  $i$ . It follows that for  $t_i > 0$  the minimum feasible cost is given by the cost  $\psi_i(t_i)$  plus the minimum between the minimum feasible cost when all neighbors  $k \in \partial i \setminus j$  is removed before  $i$  and the same quantity when one of the neighbors is allowed to be removed at a later time.

The field  $h_i(t_i)$  is then obtained from the messages (see Eqs. (32,33)) according to

$$h_i(t_i) = \psi_i(t_i) + \sum_{k \in \partial i} L_{ki}(t_i) + M_i(t_i), \quad (46)$$

$$h_i(0) = \psi_i(0) + \sum_{k \in \partial i} R_{ki}(0), \quad (47)$$

$$M_i(t_i) = \min \{ 0, \min_{k \in \partial i} \{ R_{ki}(t_i) - L_{ki}(t_i) \} \}. \quad (48)$$

Finally a more efficient implementation can be devised, noting that common quantities can be pre-computed in order to obtain the  $h_{ij}$  for all the outgoing edges around a given vertex  $i$ . One indeed obtains an implementation



which runs in linear time both in  $T$  and in the degree  $k_i$  of  $i$  by defining

$$S_i^0(t_i) = \sum_{k \in \partial i} L_{ki}(t_i) , \quad (49)$$

$$S_i^1 = \sum_{k \in \partial i} R_{ki}(0) \quad (50)$$

$$k_i(t_i) \in \arg \min_{k \in \partial i} \{R_{ki}(t_i) - L_{ki}(t_i)\} \quad (51)$$

$$Q_i(t_i) = \min \left\{ 0, \min_{k \in \partial i \setminus k_i(t_i)} \{R_{ki}(t_i) - L_{ki}(t_i)\} \right\} \quad (52)$$

$$M_{ij}(t_i) = \begin{cases} M_i(t_i) & \text{if } j \neq k_i(t_i) \\ Q_i(t_i) & \text{if } j = k_i(t_i) \end{cases} \quad (53)$$

which can all be computed in time  $O(Tk_i)$ ; we can then express the different values of the messages  $h_{ij}$  as

$$h_{ij}^0(t_i) = \psi_i(t_i) + S_i^0(t_i) - L_{ji}(t_i) \quad (54)$$

$$h_{ij}^1(t_i) = \psi_i(t_i) + S_i^0(t_i) - L_{ji}(t_i) + M_{ij}(t_i) \quad (55)$$

$$h_{ij}^0(0) = \psi_i(0) + S_i^1 - R_{ji}(0) \quad (56)$$

which can be also computed in time  $O(T)$  for each  $j \in \partial i$ . The computation time for a complete iteration on all vertices  $i$  is thus  $O(\sum_i k_i T) = O(|E|T)$ . The computation of the field  $h_i(t_i)$  in (46)-(47) is similar:

$$h_i(t_i) = \psi_i(t_i) + S_i^0(t_i) + M_i(t_i) \quad \text{for } 0 < t_i \leq T , \quad (57)$$

$$h_i(0) = \psi_i(0) + S_i^1 . \quad (58)$$

This derivation of the Min-Sum equations shows that the algorithm is exact on a tree: the recurrence equations on  $h_{ij}$  are guaranteed to converge, and the configuration  $t_i^*$  obtained from the MS expression of  $h_i$  is the unique minimum of the cost function over feasible configurations. One can, however, iterate the recurrence equations on  $h_{ij}$  for any graph, and use the MS formalism as an heuristic algorithm that provides a good approximation to the optimum, in particular when there are not many short loops. There are, however, two issues with the convergence of the message passing equations on  $h_{ij}$ :

- the  $h_{ij}$  defined above are extensive energies, that would grow indefinitely in presence of loops in the graph. This problem is easily cured by adding a constant value  $C_{ij}$  to all fields  $h_{ij}(t_i, t_j)$ , in such a way to keep the maximum entry of this matrix equal to a constant, for instance zero. This does not spoil the validity of the algorithm, as we only need informations about the relative energies of configurations to construct the decycling set: the optimum  $t_i^* = \operatorname{argmin} h_i(t_i)$  is obviously invariant by a shift of the reference energy.
- even with this normalization the message passing equations are not guaranteed to converge. When they did not we enforced their convergence by employing a reinforcement procedure, that consists in taking  $\psi_i(t_i) = \mathbb{I}[t_i = 0] + \varepsilon_i(t_i) + \tau \gamma h_i(t_i)$  where  $h_i$  is the local field computed with (57)-(58) in the previous iteration,  $\gamma$  is a small real value and  $\tau$  is the iteration time. Typically we use in our simulation  $\gamma = 10^{-3}$ .

## B. Tree-breaking in decycled graphs

We explain now the second stage of our algorithm, namely the dismantling of the acyclic graph obtained using MS in the first stage.

### 1. Optimal tree breaking

The computation of the  $C$ -dismantling number of a tree  $G$  can be performed in a time growing polynomially with  $C$  and with the size  $N$  of the graph, by the following dynamic programming approach.

Let us denote  $G_{i \rightarrow j}$  the connected component of the vertex  $i$  in the graph obtained from  $G$  by removing one of its neighbors  $j$ , and call  $S_{ij}(c)$  the minimum number of vertices to be removed from  $G_{i \rightarrow j}$  to have that no component

of the reduced graph is larger than  $C$  and that the component of  $i$  is no larger than  $c$ . These quantities satisfy the following recursion:

$$S_{ij}(c) = \min_{\substack{\{c_k\}_{k \in \partial i \setminus j} \\ \sum_{k \in \partial i \setminus j} c_k \leq c-1}} \sum_{k \in \partial i \setminus j} S_{ki}(c_k) \text{ if } 0 < c \leq C ,$$

$$S_{ij}(0) = 1 + \sum_{k \in \partial i \setminus j} S_{ki}(C) .$$

Using max-convolutions (see e.g. [5]) these quantities can be computed on all directed edges of the tree in time  $O(NC^2)$ . By adding an extra leaf  $i'$  attached to a node  $i$  on the tree, the quantity  $S_{ii'}(C)$  gives the decycling number. A small modification can be used to also find optimal dismantling sets in time  $O(NC^2)$ . Even though polynomial, this complexity is often too expensive in practice even for moderate values of  $C$ . Fortunately we will see below a greedy strategy that achieves almost the same performance.

## 2. Greedy tree-breaking

An alternative approach to the dismantling of a forest is to follow a greedy heuristic, removing iteratively the node in the largest connected component of the forest (i.e. a tree) that leaves the smallest largest component. This procedure is guaranteed to  $C$ -dismantle the forest by removing  $S = N/C$  vertices or less. This ensures the dismantling to a sublinear size of the largest component  $C \leq N/\log N$  by removing a sublinear number of vertices  $S \leq \log N$ . Moreover, it can be implemented in time  $O(N(\log N + T))$  where  $T$  is the maximal diameter of the trees inside this forest. The worst case in terms of number of removed nodes is reached in the case of a one-dimensional chain, in which one needs to remove  $S = 2^k - 1$  nodes to obtain components of size  $C(S) \leq N/2^k$ .

For a given tree  $G$  on  $N$  vertices, let us call  $F$  the subset of vertices  $i$  which are optimal in the above sense, namely such that the removal of  $i$  from  $G$  minimizes the size of the largest component of  $G \setminus i$ . The elements of  $F$  can be characterized in a very simple way. Denote by  $C(i)$  the size of the largest component of  $G \setminus i$ , so  $C(i) = \max_{j \in \partial i} |G_{j \rightarrow i}|$  and  $F = \arg \min_{i \in V} C(i)$ . Then  $i^* \in F$  if and only if  $C(i^*) \leq N/2$ . Suppose indeed that for  $i^* \in F$ ,  $C(i^*) > N/2$  and take  $j \in \partial i^*$  such that  $|G_{j \rightarrow i^*}| = C(i^*)$ . Then, as  $|G_{i^* \rightarrow j}| + |G_{j \rightarrow i^*}| = N$ , we have that  $C(j) < \max\{N/2, C(i^*)\} = C(i^*)$  which is absurd. Conversely, suppose that  $C(i) \leq N/2$  and take  $i^* \in F \setminus i$ . Consider the unique path  $(i, k_1, \dots, k_n, i^*)$  in  $G$ . Then  $|G_{k_1 \rightarrow i}| \leq C(i)$ , and  $|G_{i \rightarrow k_1}| \geq N - C(i) \geq N/2$ . But  $G_{i \rightarrow k_1} \subseteq G_{k_n \rightarrow i^*}$  so  $C(i^*) \geq N/2$ .

This characterization of  $F$  can be used constructively to find an  $i^* \in F$  efficiently. Pick for each connected component of the initial forest a ‘‘root’’ vertex  $i_0 \in V$ . For each  $i$  compute  $w_i = |G_{i \rightarrow j}|$  where  $j$  is the unique neighbor of  $i$  on the path between  $i$  and the root  $i_0$ , starting from the leaves and exploiting the relation  $w_i = 1 + \sum_{k \in \partial i \setminus j} w_k$ ; note that  $C(i_0) = \max_{j \in \partial i_0} w_j$ . Place  $i_0$  into a priority queue with priority given by the component size  $K(i_0) = 1 + \sum_{j \in \partial i_0} w_j$ . Iteratively pick the largest component from the queue. Then construct the sequence  $i_t$  as follows: for every  $t$ , if  $C(i_t) \leq N/2$ , then  $i^* = i_t \in F$  and the process stops. Otherwise, iteratively choose  $i_{t+1}$  such that  $w_{i_{t+1}} = C(i_t) > N/2$ .

Once  $i^*$  is chosen and removed, the component is broken into  $|\partial i^*|$  components, each one rooted at  $k \in \partial i^*$ . From these, only the component rooted at  $i_{t-1}$  needs to have its  $w$  values updated, as its orientation changed. The only needed adjustments are along the path  $i_0, i_1, \dots, i_t$  and can be computed in time proportional to  $t$ , which is bounded by the diameter of the tree, which is in turn bounded by  $T$ .

As the cost of the priority queue updates scale as  $O(\log N)$ , the total number of operations for each vertex removal is thus  $O(\log N + T)$ , hence the total number of operations for greedily dismantling a forest scales as  $O(N \cdot (\log N + T))$ , as claimed above.

We performed an extensive comparison of the optimal and greedy procedure for values of  $C$  sufficiently small for the optimal one to be doable in a reasonable time, using as a benchmark the forest output by the MS algorithm applied to an Erdős-Rényi random graph of 78125 nodes and average degree 3.5. As shown in Fig. 1 we found the greedy strategy to have very close to optimal performances, therefore we used this much faster procedure in all other numerical simulations.

## C. Greedy reintroduction of cycles

The initial condition for the reverse greedy procedure is the graph obtained after the removal from  $G$  of a set  $S^0$  of nodes (dismantling set) and characterized by largest connected components of size  $C$ . Let us consider a target value  $C' > C$  for the size of the largest connected components. As long as the size of the largest connected components

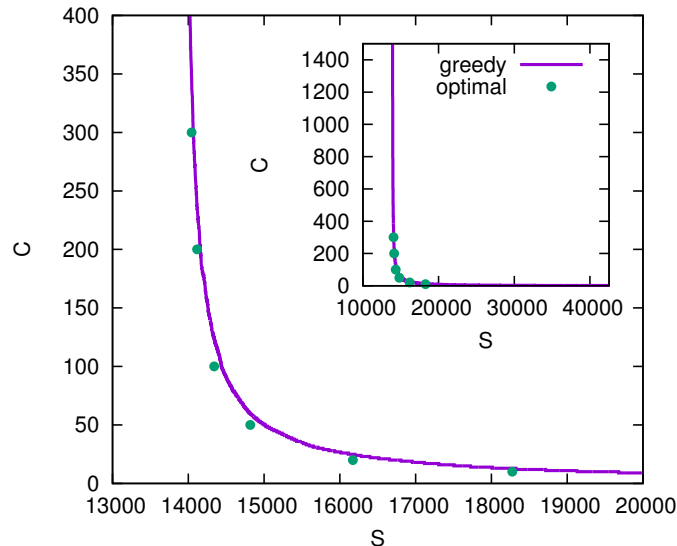


FIG. 1: Comparison between greedy and optimal forest-breaking on the output of the MS algorithm for an Erdős-Rényi random graph with 78,125 vertices and average degree 3.5.

in the graph is smaller than  $C'$ , the removed nodes are reintroduced one at a time by means of the following greedy strategy: at each iteration step  $t$ , we choose for reinsertion the node  $i \in S^t$  (and the edges to vertices in  $V \setminus S^t$ ) such that the connected component  $V_i^t$  the node  $i$  ends up in is the smallest possible. An efficient implementation of the greedy reinsertion is easily obtained by maintaining a priority queue of the removed vertices with priority given by the size  $|V_i^t|$ . When a vertex  $i$  is reintroduced in the graph, the number of connected components that get merged is at most equal to the degree  $k_i$  of the vertex (in the original graph  $G$ ). The number of elements in the priority queue that have to be modified after the reinsertion of  $i$  is bounded by the number of nodes  $j \in S^t$  that are connected to the new component in the original graph  $G$ . As the size of the largest component is at most  $C'$ , this number is at most  $k_{\max}C'$ , where  $k_{\max}$  is the maximal degree of the graph. The computational cost of reintroducing a vertex in the graph is entirely given by the one of updating the queue, which is thus bounded by  $k_{\max}C' \log(k_{\max}C')$ . In a sparse graph, the update cost is thus typically sublinear in  $N$ , making the reverse greedy strategy very efficient.

#### D. Competing algorithms

##### 1. Simulated Annealing

Besides our main algorithm based on the Min-Sum procedure we have studied the network dismantling problem using simulated annealing, i.e. building a Monte Carlo Markov Chain that makes a random walk in the space of configurations of the subsets  $S \subset V$  of removed vertices. We assign an energy to each configuration according to

$$\mathcal{E} = |S|\nu + C, \quad (59)$$

in which  $|S|$  is the number of removed nodes,  $C$  the size of the largest connected component in the graph obtained by removing  $S$ , and  $\nu$  is a free parameter. Note indeed that a set  $S$  of removed vertices can be considered “good” for two reasons: either because it is small, or because its removal fragments the graph into small components. These two figures of merits obviously contradict each other and cannot be optimized simultaneously,  $\nu$  thus controls the balance between these two frustrating goals.

As usual in simulated annealing algorithms we introduce an inverse temperature  $\beta$  that is slowly increased during the evolution of the Markov Chain, and at each time step  $t$  we consider a move from the current configuration  $S^t$  to a new configuration  $S_{\text{new}}$ , that is accepted according to a standard Metropolis criterion, i.e. with probability

$$\min \left[ 1, e^{-\beta[\mathcal{E}_{\text{new}} - \mathcal{E}^t]} \right], \quad (60)$$

where  $\mathcal{E}_{\text{new}}$  and  $\mathcal{E}^t$  are the energies of  $S_{\text{new}}$  and  $S^t$  respectively. If the move is accepted we set  $S^{t+1} = S_{\text{new}}$ ,  $\mathcal{E}^{t+1} = \mathcal{E}_{\text{new}}$ , otherwise the Markov Chain remains in the same configuration. The proposed configuration  $S_{\text{new}}$  is

constructed in the following way at each time step: a node  $i$  is chosen uniformly at random among all the  $N$  vertices of the graph, and its status is reversed (if  $i \in S^t$  then  $S_{\text{new}} = S^t \setminus i$ , if  $i \notin S^t$  then  $S_{\text{new}} = S^t \cup \{i\}$ ). We then need to compute the energy  $\mathcal{E}_{\text{new}}$  of this proposed configuration; the first term is easily dealt with as  $|S|$  varies by  $\pm 1$  depending on whether  $i \in S^t$  or not. We thus only need to compute the size  $C_{\text{new}}$  of the largest component in the new configuration, facing three possible cases:

1. if  $i \notin S^t$  and  $i$  belongs to the largest component of  $G \setminus S^t$  the size  $C_{\text{new}}$  of the largest component is recomputed;
2. if  $i \notin S^t$  but  $i$  does not belong to the largest component of  $G \setminus S^t$  then  $C_{\text{new}} = C^t$  does not change;
3. if  $i \in S^t$  then it is only necessary to compute the size  $C_i$  of the cluster  $i$  belongs to once it is reintroduced in the graph and compare the latter with the current largest component, i.e.  $C_{\text{new}} = \max(C^t, C_i)$ .

The Markov chain is irreducible, recurrent and aperiodic, thus ergodic and the Metropolis criterion ensures detailed balance, therefore the SA algorithm would sample correctly the probability measure  $\propto e^{-\beta\mathcal{E}}$  if run with an infinitesimally small annealing velocity. Unlike standard applications of simulated annealing, such as spin systems with short-range interactions, in the present problem a single move (node removal/reintroduction) can produce energy variations over a large range of scales, with the consequence that there is no natural criterion to choose the annealing protocol. We tested several different annealing protocols and we adopted one in which the inverse temperature  $\beta$  is increased linearly from  $\beta_{\text{min}}$  to  $\beta_{\text{max}}$  (thus concentrating the measure on close to ground-state configurations), with an increment of  $d\beta$  at each time step (i.e. after each one attempted move). Protocols in which the inverse temperature is varied only after  $O(N)$  attempted moves were also considered, with no relevant difference in the results. Similarly, there is no natural choice of the initial conditions. We tested the cases in which the initial set  $S^0$  is empty and in which nodes are randomly assigned to  $S^0$  independently with probability 1/2, but for sufficiently small values of  $\beta_{\text{min}}$ , different choices had no relevant effects on the optimization process.

Fig. 2 displays the minimum energy achieved using the SA algorithm (with  $\nu = 0.6$ ) on Erdős-Rényi random graphs of average degree  $d = 3.5$  and increasing sizes from  $N = 1024$  to  $N = 16384$ . For comparison we also plot the results obtained using the Min-Sum algorithm (horizontal lines). For small sizes, the SA algorithm outperforms Min-Sum when the annealing scheme is sufficiently slow ( $d\beta$  very small). Increasing  $N$ , the quality of the results obtained with SA degrades, as it would require an increasingly slower annealing protocol in order to achieve the same results obtained using Min-Sum. These results show that, even though the SA implementation proposed is simple and relatively fast even on large networks, the necessity of an increasingly slower annealing protocol prevents SA from reaching optimal results in a reasonable computational time.

The results for simulated annealing presented in Fig. 1 and Fig. 4 of the main text are obtained with parameters  $d\beta = 10^{-8}$ ,  $\beta_{\text{min}} = 0.5$  for both,  $\beta_{\text{max}} = 20$ ,  $\nu = 1.2$  for Fig. 1, and  $\beta_{\text{max}} = 10$ ,  $\nu = 2.0$  for Fig. 4.

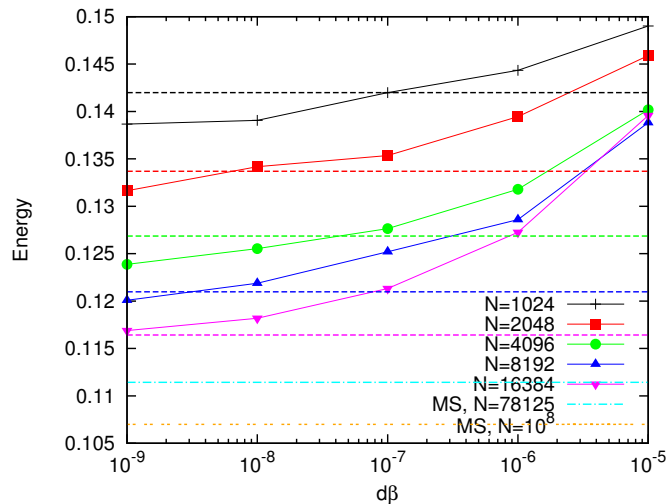


FIG. 2: Energy  $\mathcal{E}$  as function of the rate  $d\beta$  used to increase  $\beta$  from  $\beta_{\text{min}} = 0.5$  to  $\beta_{\text{max}} = 30$  in the SA algorithm ( $\nu = 0.6$ ) used to dismantle Erdős-Rényi random graphs of average degree  $d = 3.5$  and increasing size from  $N = 1024$  (top) to  $N = 16384$  (bottom). We also report the minimum energy achieved with the Min-Sum (MS) algorithm on the same graphs and for graphs of larger sizes  $N = 78125$  (cyan line) and  $N = 10^8$  (orange line).

## 2. Score-based algorithms

Let us give here more details about the other dismantling algorithms to which we compared our own proposals. They all proceed by the (irreversible) removal of nodes from the graphs to be dismantled, the differences between them relying in the choice of a score function that assigns to each vertex  $i$  of the graph a score  $e_i$ , the vertices being removed in the order of decreasing scores (with random choices in case of ties). This quantity  $e_i$  should be an heuristic measure of the importance, or centrality, of the vertex  $i$ , in the sense that more central nodes should lead to a larger decrease in the size of the largest component when  $i$  is removed. We have investigated the following score functions, the names corresponding to the key in the figures:

- RND,  $e_i = 1$  for all  $i$ ; this leads to a random choice of the removed vertices, i.e. to classical site percolation.
- DEG,  $e_i = k_i$  the degree of node  $i$ , this corresponds to removing the highest degree nodes first.
- EC, for eigenvector centrality, uses as a score the eigenvector  $e_i$  associated to the largest eigenvalue  $\lambda$  of the adjacency matrix  $A_{ij} = \mathbb{I}[\langle i, j \rangle \in E]$  of the graph, in other words the solution of the linear system of equations

$$\lambda e_i = \sum_{j \in \partial i} e_j . \quad (61)$$

For a connected graph the Perron-Frobenius theorem ensures that this eigenvector is unique and that it can be chosen positive.

- $\text{CI}_\ell$ , for collective influence at level  $\ell$ , is a centrality measure introduced by Morone and Makse [6] to provide a heuristic measure of the influence that a node has on the neighbors within a certain distance  $\ell$  from it. The collective influence of node  $i$  at level  $\ell$  is defined as

$$\text{CI}_\ell(i) = (k_i - 1) \sum_{j \in \partial B(i, \ell)} (k_j - 1) \quad (62)$$

where  $\partial B(i, \ell)$  denotes the set formed by all the nodes that are at distance  $\ell$  from node  $i$  [6]. The CI value of node  $i$  takes two contributions, the degree of node  $i$  and the number of edges emerging at distance  $\ell$  from a ball surrounding  $i$ . On expander graphs, such as random graphs, the number of nodes contained in a ball  $B(i, \ell)$  grows exponentially with  $\ell$ , hence the calculation of the collective influence scores for all nodes of the graph becomes computationally demanding already for moderately small distance values ( $\ell = 4, 5$ ).

We also made some tests with the score function defined as the betweenness centrality and as the non-backtracking centrality [7], but for the graphs we considered the results we obtained were both qualitatively and quantitatively similar (or worse) to those obtained using EC, hence we do not report them.

For a given score function one can envision different ways to implement the dismantling algorithm; the simplest would be to compute the scores for all vertices of the original graph, and then to remove the vertices in the order defined by this ranking. We used instead an adaptive version, which gives much better results, that consist in recomputing the scores of all remaining vertices after each removal of the node with highest score in the current graph; all the results presented in the main text and the SI have been obtained in this way. Even if it performs better this adaptive strategy is also much more computationally demanding; an intermediate compromise between these two extreme strategies would be to recompute the scores only after a finite fraction  $x$  of nodes is removed. Another implementation twist consists in recomputing the scores only for the vertices belonging to the currently largest connected components, as the removal of a vertex outside it would not decrease the size of the largest component. This is useful in particular if one tries to compute the EC scores by the power method (multiplying several times an initial guess by the adjacency matrix); instead of the full adjacency matrix one can consider only the submatrix corresponding to the vertices in the largest component. By construction this submatrix is irreducible and the power method will converge, hence solving the possible convergence issues encountered by the power method in the case of coexistence of several connected components in the graph. The restriction to the largest component modifies also the behavior of the DEG heuristic, as it avoids the removal of large degree nodes in already small components.

## IV. OTHER REAL-WORLD AND SCALE-FREE GRAPHS

We already explained in the main text that dismantling a graph by means of the decycling (plus greedy tree breaking) is guaranteed to be optimal only for sparse random graphs with locally tree-like structure. Nevertheless,

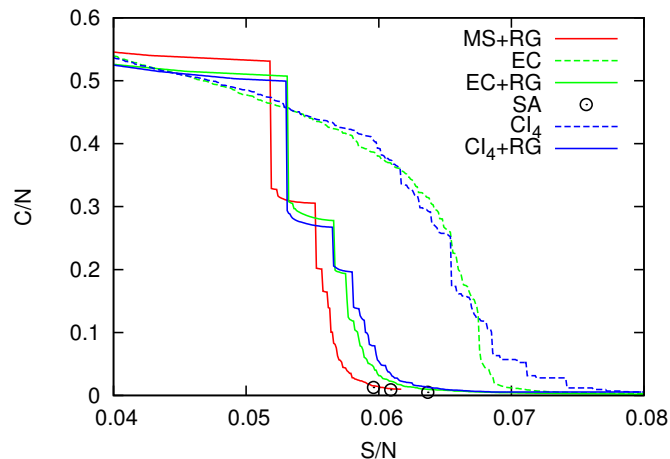


FIG. 3: Size of the largest component in scale-free random graphs, of size  $N = 10^4$  nodes and degree distribution  $P(d) \propto d^{-\gamma}$  with  $\gamma = 2.5$ , as function of the fraction of removed nodes  $S$ . The nodes are removed using adaptive Eigenvector Centrality (EC), adaptive Eigenvector Centrality plus Reverse Greedy (EC+RG), Collective Influence with diameter  $\ell = 4$  (CI<sub>4</sub>), the same plus Reverse Greedy (CI<sub>4</sub>+RG), Min-Sum plus Reverse Greedy (MS+RG), and Simulated Annealing (SA) with  $d\beta = 10^{-8}$  and  $\beta_{\min} = 0.5, \beta_{\max} = 20$  (and several values of  $\nu$ ).

we observed that when the algorithm is complemented by a simple reverse greedy (RG) strategy the final result is usually very good also on networks in which many small loops are present, such as in the case of the Twitter graph in Fig. 4 in the main text. Our way to state the quality of the result is the direct comparison with the other available algorithms, that are the Simulated Annealing algorithm and the other heuristics (e.g. EC, CI) also complemented by the RG strategy.

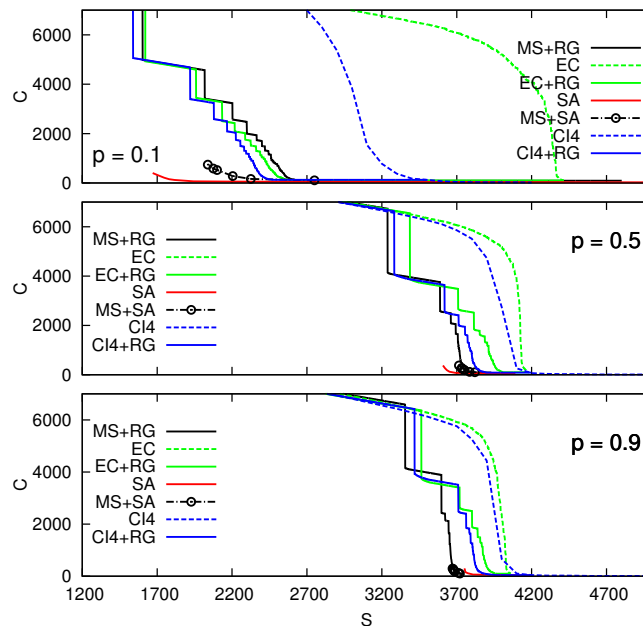


FIG. 4: Size of the largest component in WS small-world networks with rewiring probability  $p = 0.1, 0.5, 0.9$  achieved by removing a fraction of nodes using Eigenvector Centrality (EC), Eigenvector Centrality plus Reverse Greedy (EC+RG), Collective Influence with diameter  $\ell = 4$  (CI<sub>4</sub>), Collective Influence with diameter  $\ell = 4$  plus Reverse Greedy (CI<sub>4</sub>+RG), Min-Sum (MS), Min-Sum plus Reverse Greedy (MS+RG), Min-Sum plus SA (MS+SA), and Simulated Annealing (SA) with  $d\beta = 10^{-8}$  and  $\beta_{\min} = 0.5, \beta_{\max} = 20$  (and several values of  $\nu$ ).

We studied dismantling in the youtube network [8] with 1.13 million nodes and concluded that the reverse greedy is of immense importance here. Specifically we obtained that in order to dismantle the network into components smaller than  $C = 1000$  nodes the CI methods removes 5.12%, the ER removes 4.97%, the MS removes 5.67% nodes. The reverse greedy procedure improves all these methods and gets dismantling sizes 4.03% for CI+RG, 4.07% for EC+RG, and 3.97% for MS+RG.

We also studied dismantling on an example of a synthetic scale-free network. Results reported in Fig. 3, are qualitatively comparable to the ones for real networks.

In order to better quantify the effect of a large clustering coefficient on the different algorithmic methods under study, we considered a well-known class of random graphs with tunable clustering coefficient, the small-world network model introduced by Watts and Strogatz [9]. The WS network is generated starting from a one-dimensional lattice in which every node is connected with  $d/2$  nearest-neighbors on both sides, then each edge  $(i, j)$  with  $i > j$  is rewired to a randomly chosen node  $k \neq j$  with probability  $p$ . Fig. 4 shows the result of dismantling WS networks of size  $N = 10^4$ ,  $d = 6$  and rewiring probability  $p = 0.1, 0.5, 0.9$ . For  $p = 0.9$  the WS network is topological similar to a random graph, with very small clustering coefficient, because almost all edges have been rewired. On this network, Min-Sum plus reverse greedy outperforms centrality-based heuristics (EC+RG and CI+RG) and gives results that are comparable with the best obtained using SA. For  $p = 0.5$ , MS+RG still gives a very good result, only slightly worse than SA. We also replaced the reverse greedy procedure with a reverse Monte Carlo method, in which a dismantling set is sought by performing the SA algorithm from the solution of the MS algorithm, by keeping only an optimal subset of the nodes already removed. The replacement of the reverse greedy procedure with a Monte Carlo based method gives improved results for both  $p = 0.9$  and  $p = 0.5$ . We stress that this could be another useful strategy to improve heuristic results even in large networks, because the SA algorithm runs on a fraction of the original graph.

When  $p$  is further decreased, the structure of the WS network significantly departs from that of a random graph and short loops start to play a very important role, it is clear that we do not expect decycling to be a good strategy for dismantling in this regime. In this regime SA performs about 30% better than any other algorithm, even though complemented with the reverse greedy strategy. When we perform SA from the solutions obtained using MS, the results are improved but still far from the best results obtained using SA alone. This is due to the fact that, in clustered networks, the dismantling set obtained by SA is not a subset of the dismantling set obtained using any other heuristic strategy, with an overlap that is usually small.

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