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Analytical solution to the *k*-core pruning process

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ABSTRACT

k-core decomposition is a widely-used method in ranking nodes or extracting important information of complex networks. It is a pruning process in which we recursively remove the vertices with degree less than *k* to obtain the core of a complex network. The simplicity and effectiveness of this approach has led to a variety of applications in many scientific fields, including bioinformatics, neurosciences, computer sciences, economics, and network sciences. However, the analytical theory of the *k*-core pruning process is still lacking. Here we find that in every pruning step of any given network, the Non-Backtracking Expansion Branch (NBEB) is directly related to the remaining *k*-core. Using this NBEB method, we obtain the analytical results of the *k*-core pruning process and its detailed critical behaviour.

1. Introduction

The *k*-core of a network is its largest subgraph, where the vertices have at least *k* edges connected to other vertices in the subgraph. Such a *k*-core of a network is often obtained by the *k*-core pruning process, in which we recursively remove the vertices of degrees less than *k*. We repeat the process iteratively until we obtain a finite-sized subgraph, the *k*-core of the network, or the network disappears. Fig. 1 shows a simplified illustration of *k*-core decomposition. Note that a 2-core decomposition is performed on the network, and that the final 2-core is obtained after two pruning steps.

The first proposed application of *k*-core decomposition was to measure the centrality of vertices in social networks [1–8], but recently it has been applied to many disciplines, including biology [9–12], informatics [13–17], economics [18,19], and network science [20–26]. Bader and Hogue [27] developed an algorithm based on *k*-core decomposition to identify the densely connected regions in the Protein–Protein Interaction network. Altaf et al. [9] applied the *k*-core decomposition to predict the functions of several function-unknown proteins. Wuchty and Almaas [10] discovered that the ratio of proteins being essential and conserved through stages of evolution increases with the *k*-coreness of the protein. Lahav et al. [11] used *k*-core decomposition to describe the hierarchical structure of the cortical organization in the human brain. Researchers in information science, economics, and complex networks have also use *k*-core as a filter to obtain relevant information in a large system [28,29], identify the central countries during economic crises [18], and locate the most influential propagators in complex networks [30,31].

The *k*-core pruning process can also model a simple evolutionary process in which fewer connected participants gradually die out in a mutualistic system. Morone et al. [32] demonstrated that *k*-core can help predict the tipping points of dynamic systems, such as gene regulatory networks and mutualistic ecosystems.

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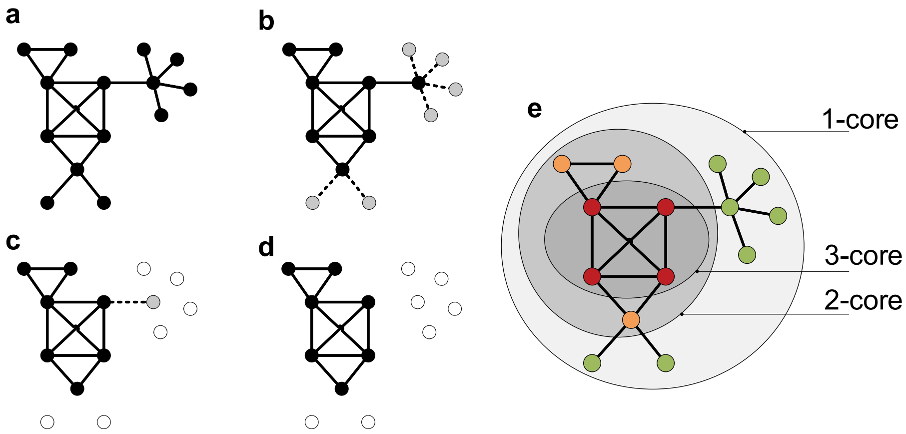

Fig. 1. The illustration of k-core pruning process and k-core. **(a–d)** the detailed pruning steps of 2-core, the discs represent vertices and the solid lines indicate the edges. Grey discs and dashed lines represent the vertices and edges that will be removed in this step. Dashed circles stand for the vertices that have been removed. **(e)** k-core decomposition result of the network. Here 1-core contains all the vertices, 2-core contains the vertices marked with red and orange, and 3-core of the network contains the red vertices.

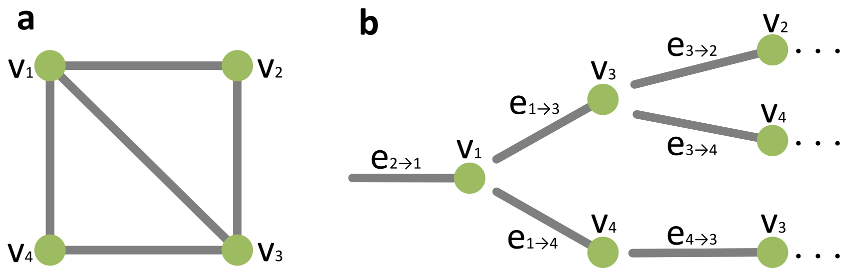

Fig. 2. An illustration of the non-backtracking expansion. **(a)** gives an example of a simple network. Here v_1's neighbouring directed edges set $S_1 = \{e_{1\to2}, e_{1\to3}, e_{1\to4}\}$, and $e_{2\to1}$'s excess neighbouring directed edges set $S_{2\to1} = \{e_{1\to3}, e_{1\to4}\}$. **(b)** shows the first three generations of the NBEB $B_{2\to1}$.

In addition to these applications in different scenarios, scientists also studied the theoretical laws of statistical behaviour of large uncorrelated random networks under k-core decomposition. The ultimate goal is to analytically find the size of the remaining k-core (if any). Fernholz and Ramachandran [33] showed that, given a value of k, increasing the density of the network will lead to the emergence of a k-core of the network. This phase transition may be continuous or discontinuous, depending on the degree distribution of the network. In 2015, Baxter et al. [34] gave a recurrence expression of the degree distribution of large uncorrelated networks during pruning. Their numerical computations reveals the critical behaviour in the process, but the analytical result is still hindered by the mathematical difficulty of the four recurrence equations.

Here we show that the NBEB can be used to analyse the k-core pruning process. We perform the non-backtracking expansion for each vertex in the network and obtain its corresponding tree structure. The topology of each tree determines at which step the corresponding vertex will be pruned, or eventually survive. This relationship enables us to directly write out the size of subgraph at each pruning step, without having to solve the recurrence relation of degree distribution. This method intuitively explains critical behaviour discovered by previous researches [33–35]. The NBEB method applies to any network topology, which is unprecedented in our knowledge. Our analytical results show that k-core pruning process is one of the few examples where we can obtain a detailed, and rigorous picture of critical behaviour.

2. Methods

Before diving into the details, let us first introduce some fundamentals to facilitate the understanding. First, in this paper, we use e for edges, v for vertices, the Greek letters α and β to denote the index of vertices, and Latin letters j, l, m to represent the degrees of vertices. $e_{2\to1}$ represents a directed edge from vertex v_2 to v_1. For a given node v_1, we define the set of directed edges from v_1 to each of its neighbours as the set of neighbouring directed edges, denoted by S_1.

Another important concept, as illustrated in Fig. 2, is the set of excess neighbouring directed edges $S_{2\to1}$, which contains all edges in S_1 except $e_{1\to2}$. We can then define an NBEB $B_{2\to1}$, which is a tree-like structure that extends from the root edge $e_{2\to1}$, to its child vertices, which here refer to excess neighbouring directed edges of $e_{2\to1}$, i.e. the elements in $S_{2\to1}$, and then continues to the "children of children", etc. Such an expansion is a recursive procedure so that an NBEB is usually infinite. A concept equivalent to our NBEB has been proposed in Ref. [36]. For convenience we use $B(S_1)$ to represent the set of all NBEBs whose root belongs to S_1. Similarly, the set of excess NBEBs, denoted by $B(S_{2\to1})$ represents the set of all NBEBs that start at $S_{2\to1}$.

For a given positive integer k, we define Y_n as the set of NBEBs that satisfies the following conditions: there exists a subbranch of the NBEB that contains the root, and the amount of child vertices of each vertex in the first n generations of this subbranch is not less than $k-1$. In addition we denote Y_0 to be the set of all the NBEBs. Obviously, $Y_0 \supset Y_1 \supset \cdots \supset Y_n \supset Y_{n+1} \supset \cdots \supset Y_\infty$. As an example, the NBEB $B_{2\to1}$ in Fig. 2**b** belongs to Y_1 when $k=3$, and it belongs to Y_∞ when $k=2$.

After the fundamentals, we introduce the following two important theorems:

Theorem 1. *An NBEB $B_{\alpha\to\beta}$ belongs to Y_n if and only if $B(S_{\alpha\to\beta})$ contains at least $k-1$ NBEBs belonging to Y_{n-1}.*

Theorem 2. *A vertex v_α survives after the nth pruning if and only if $B(S_\alpha)$ contains at least k NBEBs belonging to Y_{n-1}.*

Theorem 1 obviously stands according to the definition of Y_n, and the proof of Theorem 2 is given in Appendix.

In the following we walk through the details. Assume that the probability y_n that a randomly chosen NBEB belongs to Y_n. Obviously $y_0 = 1$, and from Theorem 1 we can directly write down the recurrence relation of y_n. Assume we randomly choose a directed edge $\alpha \to \beta$, and the set $B(S_{\alpha\to\beta})$ has j NBEBs, which means the edge $\alpha \to \beta$ has an excess degree of j. Under the condition that the network is random, for edge $\alpha \to \beta$, the probability that $B(S_{\alpha\to\beta})$ has at least $k-1$ NBEBs belonging to Y_{n-1} is a binomial probability $\sum_{m=k-1}^{j} \binom{j}{m} y_{n-1}^m (1-y_{n-1})^{j-m}$. Then y_n is the sum of all probabilities with various possible excess degrees:

$$
\begin{aligned}
y_n &= \sum_{j=k-1}^{\infty} q_j \sum_{m=k-1}^{j} \binom{j}{m} y_{n-1}^m (1-y_{n-1})^{j-m} \\
&= \sum_{m=k-1}^{\infty} \frac{y_{n-1}^m}{m!} \sum_{j=m}^{\infty} \frac{j!}{(j-m)!} q_j (1-y_{n-1})^{j-m} \\
&= \sum_{m=k-1}^{\infty} \frac{y_{n-1}^m}{m!} \cdot G_1^{(m)}(1-y_{n-1}) \\
&= 1 - \sum_{m=0}^{k-2} \frac{y_{n-1}^m}{m!} \cdot G_1^{(m)}(1-y_{n-1}) \\
&\equiv f(y_{n-1}),
\end{aligned} \tag{1}
$$

where q_j is the excess degree distribution, $G_1(z) = \sum_{j=0}^{\infty} q_j z^j$ is the probability generating function for the excess degree distribution [37], and $G^{(j)}(z)$ represents the jth derivative of $G(z)$. Similarly, from Theorem 2, the size of the remaining subgraph after the nth pruning is

$$
\begin{aligned}
r_n &= \sum_{j=k}^{\infty} p_j \sum_{m=k}^{j} \binom{j}{m} y_{n-1}^m (1-y_{n-1})^{j-m} \\
&= \sum_{m=k}^{\infty} \frac{y_{n-1}^m}{m!} \sum_{j=m}^{\infty} \frac{j!}{(j-m)!} p_j (1-y_{n-1})^{j-m} \\
&= 1 - \sum_{m=0}^{k-1} \frac{y_{n-1}^m}{m!} \cdot G_0^{(m)}(1-y_{n-1}) \\
&\equiv g(y_{n-1}),
\end{aligned} \tag{2}
$$

where p_j is the degree distribution, and $G_0(z) = \sum_{j=0}^{\infty} p_j z^j$ is the probability generating function for the degree distribution [37]. It is worthwhile to mention that r_n follows a power-law decay with respect to time near critical points, the details are shown in Appendix.

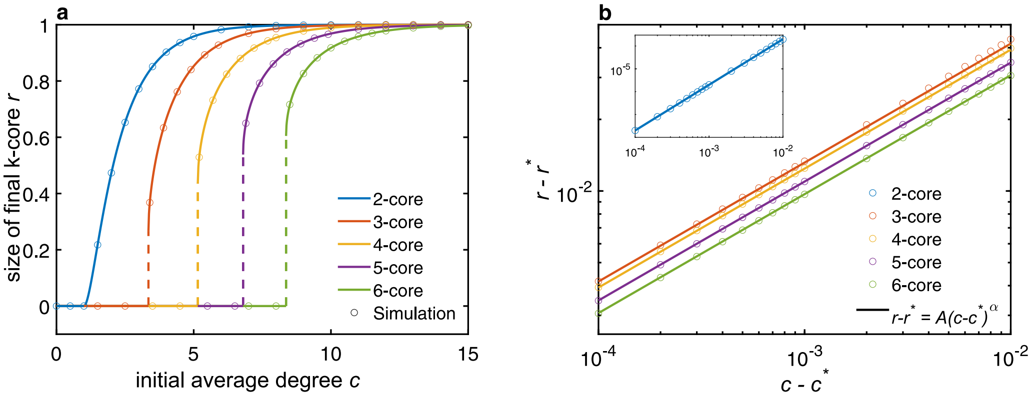

Fig. 3. The critical behaviour of the final size of k-core. **(a)** The final size of k-core r versus different initial average degrees c. The solid lines indicate our theoretical results and the circles represent the simulation results performed on 10^6 vertices. **(b)** The critical behaviours of different k-core decompositions near the critical point. The solid lines show the exact power-law relationship of $r - r^* = A(c - c^*)^\alpha$. Both the exponent α and coefficient A are obtained analytically in Appendix. The circles represent the numerical values predicted by our analytical results.

3. Results

3.1. Asymptotic result

Based on the previous introduction, here $\{y_n\}$ is a descending sequence, and $y_n \geq 0$ for all $n \in \{0, 1, 2, \dots\}$. Thus $y = \lim_{n\to\infty} y_n$ exists, and it is the largest root less than 1 of the following equation

$$y = f(y) = 1 - \sum_{m=0}^{k-2} \frac{y^m}{m!} G_1^{(m)}(1-y). \tag{3}$$

We then obtain the size of the final k-core,

$$r = \lim_{n\to\infty} r_n = 1 - \sum_{m=0}^{k-1} \frac{y^m}{m!} G_0^{(m)}(1-y). \tag{4}$$

Fig. 3**a** shows the size of the final k-core on Erdős-Rényi networks (ER networks), the transition is continuous for $k = 2$ and discontinuous for $k \geq 3$. Fig. 3**b** presents the critical behaviour of different k-core decompositions near the critical point. The figures show our results are precisely in accordance with simulations. Meanwhile, we have theoretically derived the exact critical exponents on ER networks. The critical exponent is 2 for $k = 2$, and 1/2 for $k \geq 3$. The detailed derivation is shown in Appendix.

3.2. The pruning process

The analytical results also precisely describe the transient process of the critical phenomena, i.e. the number of nodes in the remaining subgraph after each pruning step.

From Eq. (1) and (2), the computation of y_n is equivalent to a fixed-point iteration, and r_n can then be obtained because it is a function of y_{n-1}. As an example, we present an analysis of the k-core pruning process on large uncorrelated ER networks below. In this case, the generating functions of ER networks $G_0(z)$ and $G_1(z)$ happen to be the same, $e^{c(z-1)}$, where c is the average degree of the initial network. For 2-core decomposition, we obtain $f(y) = 1-e^{-cy}$, $g(y) = 1-e^{-cy}(1+cy)$, so each step of the pruning process can be represented by the corresponding iterative step of $y = f(y)$. Fig. 4 shows the process using a simple visualization method.

In 3-core decomposition, it is easy to acquire $f(y) = 1 - e^{-cy}(1 + cy)$ and $g(y) = 1 - e^{-cy}(1 + cy + (cy)^2/2)$. Unlike the result from 2-core decomposition, there is a discontinuous phase transition at the critical point $c^* = 3.3509$ (see Fig. 4**d-f**). The pruning process exhibits interesting behaviour when c approaches the critical point from the left (see Fig. 4**e**). In the first few pruning steps, r_n rapidly decreases. The pruning then reaches a bottleneck, and becomes a long transient process, followed by an avalanche of vertex removal. This phenomenon has been observed in previous numerical computations [34]. This discontinuous phase transition is intuitively explained by our analytical results. When $c \ll c^*$ the iteration rapidly converges to a stable fixed point at $y = 0$ (see Fig. 4**d**), so that no k-core remains. When $c > c^*$ the iteration stops at the largest root of $y^* = f(y^*)$. In between the two cases, as c approaches c^* from the left (see Fig. 4**e**), the curve of $f(y)$ and the diagonal line $y = f(y)$ together form a narrow channel through which the iteration process passes slowly. After passing through the narrow channel, it stops at a stable fixed point at $y = 0$, which is in accord with the critical phenomena described above.

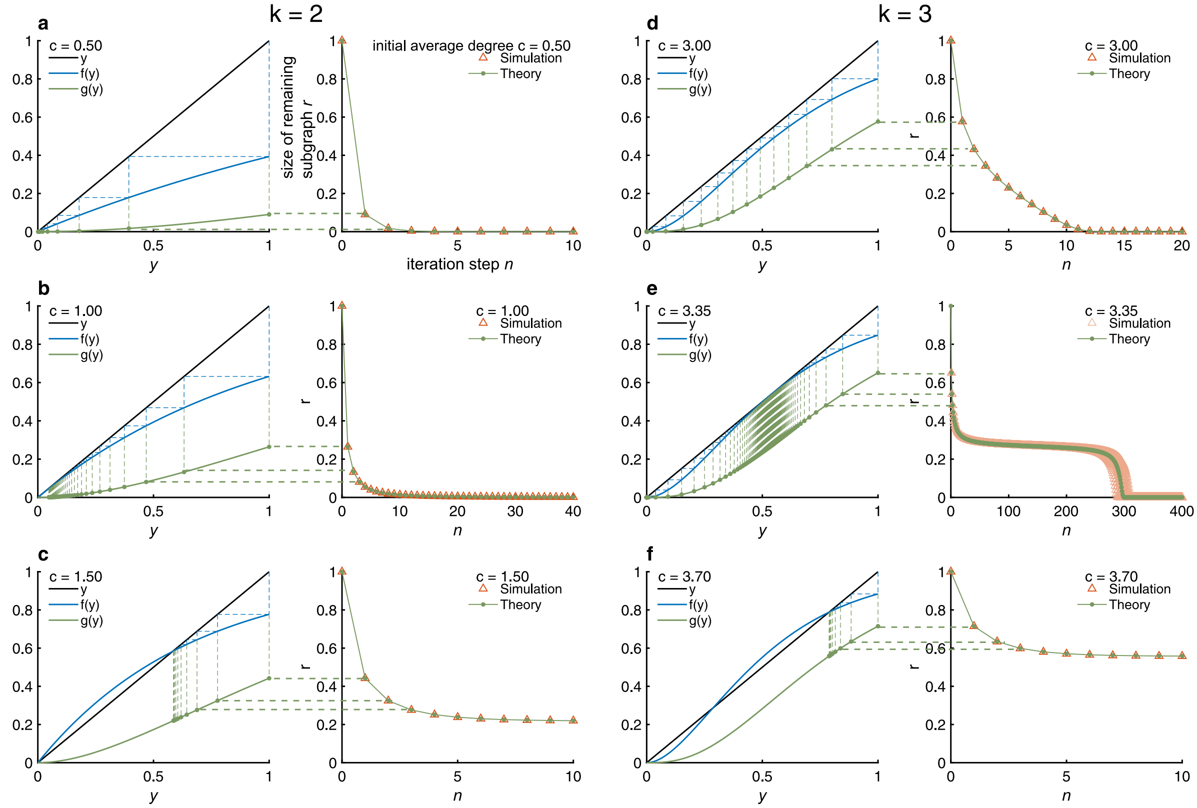

Fig. 4. The size of remaining subgraph r_n in k-core pruning process performed on ER networks. All panels consist of two parts, left and right. The left panels show $g(y)$ and the iteration of $y_n = f(y_{n-1})$ during the pruning process and the right panels show r_n from both the theoretical result and numerical simulation result. The green dashed lines in between are indications of the corresponding relationship of $r_n = g(y_{n-1})$ according to our analytical result. **(a–c)**, the result of 2-core pruning process below, at, and above the critical point $c^* = 1$, respectively. **(d–f)**, the result of 3-core pruning process below, near, and above the critical point $c^* = 3.3509$, respectively. For **a, b, c, d, f**, the numerical results are obtained from simulations on 10^6 vertices. Since the result is very sensitive to the random perturbation of the original network near the discontinuous phase transition point, the numerical results in **(e)** are obtained from 10 simulations on 5×10^8 vertices.

4. Discussion

Overall, we propose that the NBEB can be used as an intuitive way to directly present the results of k-core pruning process without solving any complex equations. Using the NBEB method, we successfully obtained the size of the remaining subgraph at any pruning step. Numerical simulations confirm that our analytical results are solid.

Our major contribution is that we have developed a new method that greatly simplifies and reforms the way we understand k-core decomposition on networks. We can specifically analyse the relationship between the behaviour of any vertex in the k-core decomposition and the NBEB, which greatly reduces the difficulty of analysis and can help us understand both this algorithm and the dynamic process. Besides, by using this theoretical solution, we precisely describe the discrete critical behaviour of the high-dimensional interacting systems, which is rare in the study of critical phenomena. In addition to the traditional degree distribution approach, this study provides new possibilities for theoretical problems of network sciences.

CRediT authorship contribution statement

Rui-Jie Wu: Performed the theoretical analysis, Writing – original draft. **Yi-Xiu Kong:** Designed the figures and performed the numerical experiments, Writing – original draft. **Zengru Di:** Designed the figures and performed the numerical experiments, Writing – original draft. **Yi-Cheng Zhang:** Designed the figures and performed the numerical experiments, Writing – original draft. **Gui-Yuan Shi:** Designed the research, Performed the theoretical analysis, Designed the figures and performed the numerical experiments, Writing – original draft.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

No data was used for the research described in the article.

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Appendix

A.1. Proof of Theorem 2

We use mathematical induction to prove the theorem. It is obvious that the theorem holds for $n = 1$. Now we prove that if the theorem is true for $n - 1$, the theorem can be established for n.

If $B_{\alpha\to\beta}$ does not belong to Y_{n-1},
$\Rightarrow B(S_{\alpha\to\beta})$ contains at most $(k-2)$ Y_{n-2} (Theorem 1),
$\Rightarrow B(S_\beta) = B(S_{\alpha\to\beta}) \cup B_{\beta\to\alpha}$ contains at most $(k-1)$ Y_{n-2},
$\Rightarrow v_\beta$ cannot survive after the $(n-1)$th pruning (induction).

Therefore, by excluding the neighbours that are bound to be removed in the $(n-1)$th pruning, if one of the remaining neighbours, v_{β^*}, survives after the $(n-1)$th pruning, $B_{\alpha\to\beta^*}$ must belong to Y_{n-1}, that is, $B(S_{\alpha\to\beta^*})$ contains at least $(k-1)$ Y_{n-2}.

Sufficiency. If $B(S_\alpha)$ contains at least k Y_{n-1},
$\Rightarrow B(S_{\beta^*\to\alpha})$ contains at least $(k-1)$ Y_{n-1},
$\Rightarrow B_{\beta^*\to\alpha}$ belongs to $Y_n \subset Y_{n-2}$ (Theorem 1),
$\Rightarrow B(S_{\beta^*}) = B(S_{\alpha\to\beta^*}) \cup B_{\beta^*\to\alpha}$ contains at least k Y_{n-2},
$\Rightarrow$ after the $(n-1)$th pruning, v_{β^*} can survive(induction),
$\Rightarrow$ in the nth pruning, v_α has degree no less than k, it can survive in this step.

Necessity. If $B(S_\alpha)$ contains at most $(k-1)$ Y_{n-1}, v_α has at most $(k-1)$ neighbours after the $(n-1)$th pruning, and will be pruned at the nth pruning. $\square$

As no assumption is adopted to prove Theorem 2, Theorem 2 can establish for any network topology.

A.2. Critical exponents on ER networks

While $k = 2$, we know that the critical point is $c^* = 1$. Assume that $c = 1 + \delta$ ($\delta > 0$), the equation $y = f(y)|_{c=1} = 1 - e^{-y}$ has the only root at $y^* = 0$. Since f is the function of both c and y: $f(c, y) = 1 - e^{-cy}$, assume the root of the function $y = 1 - e^{cy}$ is $y = y^* + \Delta y = \Delta y$, we expand f with Taylor Series at the point $(c^*, y^*) = (1, 0)$:

$$\begin{aligned} f(c,y) =& f(1+\delta, \Delta y) \\ =& f(1,0) + (\delta\frac{\partial}{\partial c} + \Delta y\frac{\partial}{\partial y})f(c,y)|_{(1,0)} \\ &+ \frac{1}{2!}(\delta\frac{\partial}{\partial c} + \Delta y\frac{\partial}{\partial y})^2 f(c,y)|_{(1,0)} + \cdots \\ =& \Delta y + \Delta y * \delta - \frac{1}{2}\Delta y^2 + o(\delta^2) + o(\Delta y^2). \end{aligned}$$

$\Delta y = y - y^* = y = f(c, y)$, we obtain $\Delta y = 2\delta + o(\delta)$. $r = g(c, y) = 1 - e^{-cy}(1 + cy)$, then take the Taylor expansion of r at point $(1, 0)$ we can obtain $\Delta r = 2\delta^2 + o(\delta^2)$. And finally we obtain the result that critical exponent equals 2, when $k = 2$.

Similarly, as $k \geq 3$, assume the critical point is (c^*, y^*), then expand $f(c, y)$ at (c^*, y^*), let $c = c^* + \delta$ ($\delta > 0$), then:

$$\begin{aligned} \Delta y =& \Delta f \\ =& \Delta y + \frac{c^{*(k-2)} y^{*(k-1)}}{(k-2)!} e^{-c^* y^*} \cdot \delta \end{aligned}$$

$$+ \frac{y^{*(k-3)}}{2\cdot(k-3)!}c^{*(k-1)}e^{-c^*y^*}(1-\frac{c^*y^*}{k-2})\cdot\Delta y^2$$
$$+ o(\delta)+o(\Delta y^2).$$

So,

$$\Delta y = \frac{\sqrt{2}y^*}{\sqrt{c^*\cdot(c^*y^*+2-k)}}\cdot\delta^{\frac{1}{2}}+o(\delta^{\frac{1}{2}}),$$

then

$$\Delta r = \frac{c^*y^*}{k-1}\cdot\frac{\sqrt{2}y^*}{\sqrt{c^*\cdot(c^*y^*+2-k)}}\cdot\delta^{\frac{1}{2}}+o(\delta^{\frac{1}{2}}).$$

We obtain the critical exponent equals 1/2, when $k \geq 3$.

A.3. Temporal decay of r_n near critical point

Similar to [38], we study the time decay of r_n near the critical point. First we study the iteration of y_n.

$$\begin{aligned} y_n - y_{n-1} &= f(y_{n-1}) - y_{n-1} \\ &= f(y^*) + f'(y^*)(y_{n-1}-y^*) + \frac{f''(y^*)}{2}(y_{n-1}-y^*)^2 + o[(y_{n-1}-y^*)^2] - y_{n-1} \\ &= \frac{1}{2}f''(y^*)(y_{n-1}-y^*)^2 + o[(y_{n-1}-y^*)^2]. \end{aligned}$$

Here, because y^* is the critical point, we use $f(y^*) = y^*$ and $f'(y^*) = 1$. Also, since f is concavity on y^*, we have $f''(y^*) < 0$ except few cases that $f''(y^*) = 0$. Then near y^*, we have

$$\frac{dy}{dn} \approx \frac{1}{2}f''(y^*)(y-y^*)^2.$$

We can easily obtain $(y_n - y^*) \sim n^{-1}$. Then the time decay of r_n is:

$$r_n - r^* = g(y_{n-1}) - g(y^*) = \sum_{i=1}^{\infty}\frac{1}{i!}g^{(i)}(y_*)(y_{n-1}-y^*)^i.$$

Since $g'(y) = \frac{y^{k-1}}{(k-1)!}G_0^{(k)}(1-y)$, for discontinuous phase transition: $1 > y^* > 0$, we have $g'(y^*) \neq 0$, so

$$r_n - r^* = g'(y_*)(y_{n-1}-y^*) + o[(y_{n-1}-y^*)].$$

That means $(r_n - r^*) \sim n^{-1}$. All the pruning process for ER network when $k \geq 3$ belong to this case.

For continuous phase transition: $y^* = 0$ and $S^* = 0$, we have $g'(y^*) = 0$, let $m = min\{i|g^{(i)}(0) \neq 0\}$, Then

$$r_n = \frac{1}{m!}g^{(m)}(0)y_{n-1}^m + o(y_{n-1}^m).$$

That means $r_n \sim n^{-m}$. In the case of 2-core pruning process of ER networks, we can easily obtain $m = 2$, so $r_n \sim n^{-2}$.

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