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Bootstrap Percolation in Living Neural Networks

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Abstract Recent experimental studies of living neural networks reveal that their global activation induced by electrical stimulation can be explained using the concept of bootstrap percolation on a directed random network. The experiment consists in activating externally an initial random fraction of the neurons and observe the process of firing until its equilibrium. The final portion of neurons that are active depends in a non linear way on the initial fraction. The main result of this paper is a theorem which enables us to find the final proportion of the fired neurons, in the asymptotic case, in the case of random directed graphs with given node degrees as the model for interacting network. This gives a rigorous mathematical proof of a phenomena observed by physicists in neural networks.

Keywords Bootstrap percolation · Phase transition · Random graphs · Neural networks

1 Introduction

Recent experimental studies of living neural networks [8, 12] reveal that their global activation induced by electrical stimulation can be explained using the concept of bootstrap percolation on a directed random network. The experiment consists in activating externally an initial random fraction of the neurons and observe the process of firing until its equilibrium. The final portion of neurons that are active depends in a non linear way on the initial fraction. The main result shown by experiments is that there exists a non-zero critical value for the fraction of initially (i.e., externally) excited neurons beyond which the global activity jumps to an almost complete activation of the network, while below this critical value the firing essentially does not spread. The main result of this paper is a theorem which enables us to find the asymptotic of final proportion of the fired neurons in the case of random directed graphs with given node degrees as the model for interacting network. This gives a rigorous mathematical proof of a phenomena observed by physicists in neural networks [10].

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In that paper, Cohen et al. find this asymptotic via mean-field assumption and they compare it to simulations and experiment. The validity of the random graph approximation to metric graphs such as the experimental neural networks is discussed in [22]. Bootstrap percolation model has been used in several related applications (see for example [15, 20, 23]). The model has a rich history in statistical physics, mostly on $G=\mathbb{Z}^d$ and finite boxes. The problem of complete occupation on $\mathbb{Z}^2$ was solved by van Enter in [13]. The existence of a sharp metastability threshold in d-dimensional lattices was proved by Holroyd [16]. More recently, bootstrap percolation has been studied on the random regular graph [5], random graphs with given vertex degrees [3], and also on infinite trees [4, 14].

A neural network is a group of interconnected neurons functioning as a circuit. The neural network is modeled as a directed graph [8] whose nodes are neurons connected by synapses. The total number of neurons is n. Let $G=(V,E)$ be a directed graph on the vertex set $V=[1,\dots,n]$. We write $i\to j$ if there is a directed link from i to j. The in-degree of a node i, denoted by $d_{in}(i)$ is the number of links that point into the node, i.e., the number of links $j\to i$ for $j\in V$. Similarly the out-degree of a node i, denoted by $d_{out}(i)$, is the number of links emanating from i, the number of links $i\to j$ for $j\in V$.

The adjacency matrix of a directed graph G on n vertices is the $n\times n$ matrix A with coordinates $A_{ij}=1$ if $j\to i$ and 0 otherwise.

We now give a precise description of the model we consider here. At the beginning of the process, and as a direct response to the externally applied electrical stimulus, a neuron has a probability α to fire. Once a neuron has fired, it stays "on" forever. A neuron will be "on" at time $t+1$ if either it was on at time t or if at least Ω of its incoming nodes were on at time t, for some Ω fixed in the model.

We denote by $X_t(i)$ the state of the neuron i at time t: i is on if $X_t(i)=1$ and off if $X_t(i)=0$. At each time step $t+1$, for the state of the node i we have

$$X_{t+1}(i)=X_t(i)+(1-X_t(i))\mathbb{1}\left(\sum_j A_{ij}X_t(j)\ge\Omega\right), \tag{1}$$

where $\mathbb{1}(\Xi)$ denotes the indicator of an event Ξ; this is 1 if Ξ holds and 0 otherwise. The dynamics is monotonic from the definition. Indeed, since a firing neuron can never turn off, we have $X_{t+1}(i)\ge X_t(i)$. When the algorithm finishes (suppose after n time steps), then the final state of a node i will be represented by $X(i)$: i.e., $X(i)=1$ if node i is active and $X(i)=0$ otherwise. Let us define $\Phi^{(n)}(\alpha)$ as

$$\Phi^{(n)}(\alpha):=n^{-1}\sum_{j=1}^{n}X(j). \tag{2}$$

In this paper, we are interested to find $\Phi(\alpha)$ the asymptotic value of $\Phi^{(n)}(\alpha)$ when $n\to\infty$ in the case of random directed graphs with arbitrary degree distribution as the underlying model for the interacting network (see for example [11, 18, 19]). Let us define $P(j,k)$ to be the probability that a randomly chosen vertex has in-degree j and out-degree k. Since every oriented edge on a directed graph must leave some vertex and enter another, $P(j,k)$ must satisfy $\sum_{j,k}(j-k)P(j,k)=0$. The next section describes this model of random digraphs.

Notation We consider the asymptotic case when $n\to\infty$ and say that an event holds w.h.p. (with high probability) if it holds with probability tending to 1 as $n\to\infty$. We shall use $\xrightarrow{p}$

for convergence in probability as $n \to \infty$. Similarly, we use o_p and O_p in a standard way. for example, if (X_n) is a sequence of random variables, then $X_n = O_p(1)$ means that "X_n is bounded in probability" and $X_n = o_p(n)$ means that $X_n/n \xrightarrow{p} 0$.

1.1 Random Graph Definition

In this section, we describe the model of random directed graphs on n vertices we consider in this paper. Let $\mathbf{d}_{in}^{(n)} = \{d_{in}^{(n)}(i), i = 1, \ldots, n\}$ and $\mathbf{d}_{out}^{(n)} = \{d_{out}^{(n)}(i), i = 1, \ldots, n\}$ be sequences of non-negative integers such that $\sum_{i=1}^{n} d_{in}^{(n)}(i) = \sum_{i=1}^{n} d_{out}^{(n)}(i)$. Sometimes, we simply write d_{in} and d_{out} instead of $d_{in}^{(n)}$ and $d_{out}^{(n)}$ if n is understood from the context. The configuration model (CM) on n vertices with degree sequences $\mathbf{d}_{in}^{(n)}$ and $\mathbf{d}_{out}^{(n)}$ is constructed as follows (e.g. see [7]):

A vertex i is represented by the set of its incoming and outgoing edges that we denote respectively by $W_{in}(i)$, and $W_{out}(i)$ with $|W_{in}(i)| = d_{in}(i)$, $|W_{out}(i)| = d_{out}(i)$. Let $W_{in} = \bigcup_i W_{in}(i)$ and $W_{out} = \bigcup_i W_{out}(i)$. A configuration is a matching of W_{in} with W_{out} and we choose the configuration at random, uniformly over all possible configurations. We denote the resulted graph by $CM(n, \mathbf{d}_{in}^{(n)}, \mathbf{d}_{out}^{(n)})$. Observe that the self-loops may occur, these become rare as $n \to \infty$ (see e.g. [11] or [17] for more precise results in this direction). It is easy to see conditional on the multigraph being simple graph, we obtain a uniformly distributed random graph with the given degree sequence.

We will let $n \to \infty$, and assume that for each n, the given sequences $\mathbf{d}_{in}^{(n)}$ and $\mathbf{d}_{out}^{(n)}$ satisfy the following regularity conditions:

Condition 1 For each $n \in \mathbb{N}$, $\mathbf{d}_{in}^{(n)} = \{d_{in}^{(n)}(i), i = 1, \ldots, n\}$ and $\mathbf{d}_{out}^{(n)} = \{d_{out}^{(n)}(i), i = 1, \ldots, n\}$ are sequences of nonnegative integers such that $\sum_{i=1}^{n} d_{in}^{(n)}(i) = \sum_{i=1}^{n} d_{out}^{(n)}(i)$, and, for some probability distribution $P(j,k)$ independent of n,

1. The degree density condition: the density of vertices of in-degree j and out-degree k tends to $P(j,k)$. i.e.,

$$\#\{i : d_{in}^{(n)}(i) = j, d_{out}^{(n)}(i) = k\}/n \to P(j,k) \quad \text{as } n \to \infty.$$

2. The finite expectation property: $\sum_{j,k} jP(j,k) = \sum_{j,k} kP(j,k) =: \lambda \in (0, \infty)$.
3. The average degree tends to the given value λ:

$$\sum_{i=1}^{n} d_{in}^{(n)}(i)/n = \sum_{i=1}^{n} d_{out}^{(n)}(i)/n \to \lambda \quad \text{as } n \to \infty.$$

In this paper, we work with the model described above, however we have to emphasize that the results of this work can be as well applied to some other random graphs models by conditioning on the vertex degrees. For example, for the Erdős-Rényi random graph $G(n, p)$, where every directed edge is present with probability p, with $np \to \lambda \in (0, \infty)$, the assumptions hold with $P(j,k) = p(j)p(k)$, where $p(.)$ is a Poisson distribution with mean λ:

$$p(k) = e^{-\lambda} \frac{\lambda^k}{k!}.$$

1.2 Statement of Result

In this section, we state the main theorem of this work.

Let D_{in} and D_{out} be random variables with the distribution $\mathbb{P}(D_{in}=j, D_{out}=k)=P(j,k)$. We define the function $f_\alpha(y)$ as follows

$$f_\alpha(y) := \lambda y - (1-\alpha)\mathbb{E}\left[D_{out}\mathbb{1}\left(\mathrm{Bin}(D_{in}, 1-y) < \Omega\right)\right].$$

Let $y^* = y^*_\alpha$ be the largest solution to $f_\alpha(y)=0$ in [0, 1], i.e.,

$$y^* = \max\{y \in [0,1] \mid f_\alpha(y) = 0\}.$$

Remark that such y^* exists because $f_\alpha(0) \le 0$, $f_\alpha(1) = \lambda\alpha > 0$ and f_α is continuous. The main result of this paper is the following theorem.

Theorem 2 *Consider the random graph $CM(n, \boldsymbol{d}_{in}^{(n)}, \boldsymbol{d}_{out}^{(n)})$ satisfying* Condition 1. *Then we have*

1. *If $y^*=0$, i.e., if $f_\alpha(y) > 0$ for all $y \in (0,1]$, then we have*

$$\Phi^{(n)}(\alpha) = 1 - o_p(1).$$

2. *If $y^* > 0$ and furthermore y^* is not a local minimum point of $f_\alpha(y)$, then*

$$\Phi^{(n)}(\alpha) = 1 - (1-\alpha)\mathbb{P}\left(\mathrm{Bin}(D_{in}, 1-y^*) < \Omega\right) + o_p(1).$$

Remark 3 By Theorem 2, one can observe that when D_{in} and D_{out} are independent, we have

$$f_\alpha(y) = \lambda\left(y - (1-\alpha)\mathbb{P}(\mathrm{Bin}(D_{in}, 1-y) < \Omega)\right),$$

and $\Phi(\alpha) := \lim_{n\to\infty}\Phi^{(n)}(\alpha)$ will depend only on the distribution of in-degree D_{in}.

Remark 4 By Theorem 2, for $\alpha < 1$, the complete percolation appears only if $f_\alpha(y) > 0$ for all $y \in (0,1]$. This will happen if $D_{in} \ge \Omega$ and

$$\alpha > 1 - \inf_{y\in(0,1)} \frac{\lambda y}{\mathbb{E}[D_{out}\mathbb{1}(\mathrm{Bin}(D_{in}, 1-y) < \Omega)]}. \tag{3}$$

Remark 5 One open question is what will happen when neither Situation 1 nor Situation 2 described in Theorem 2 take place? This will happen only if $f'_\alpha(y^*) = 0$, which is

$$\lambda = (1-\alpha)\mathbb{E}\left(D_{out}D_{in}\mathbb{1}(\mathrm{Bin}(D_{in}-1, y^*) = D_{in} - \Omega)\right). \tag{4}$$

Let us briefly explain the methods used to derive Theorem 2. The base of our approach is some standard techniques similar to those used by Balogh and Pittel [5] for the special d-regular case problem, and by Cain and Wormald [9] for the k-core problem. This means we consider the diffusion process on the random configuration model and describe the dynamics of the diffusion by a Markov chain. Our proof is mainly based on a method introduced by Wormald in [24] for the analysis of a discrete random process by using differential equations. However, our model is more general and new difficulties arise in treating the Markov chain and proving the convergence results. We refer to Sect. 3 for more details.

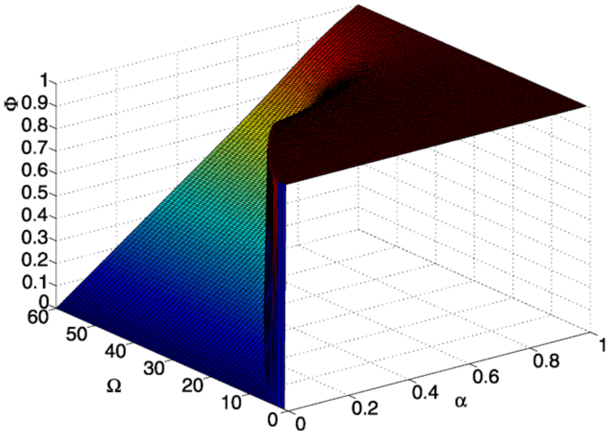

Fig. 1 (Color online) The final fraction of fired neurons as a function of α and Ω. Here $\mathbb{P}(D_{in}=k)\sim\exp(\frac{-(k-\overline{k})^2}{2\sigma^2})$ with $\overline{k}=50$ and $\sigma=15$

1.3 Simulation

Following [8, 10, 21], we assume a Gaussian distribution for in-degrees

$$\mathbb{P}(D_{in}=k)\sim\exp\left(\frac{-(k-\overline{k})^2}{2\sigma^2}\right),$$

with $\overline{k}=50$ and $\sigma=15$ based on the experimental results. Figure 1 shows the three dimensional representation of the final fraction of fired neurons, i.e., $\Phi(\alpha)$ as a function of α and Ω. This shows that both parameter Ω and α have transition values, α_c and Ω_c, where the solution changes qualitatively.

Let us assume that Ω is fixed. Then there exists a critical value for the fraction of initially excited neurons (i.e., α) beyond which the global activity jumps to an almost complete activation of the network while below this critical value the firing essentially does not spread. Indeed as we can see in Fig. 2, on the left-hand side, the map $\alpha\to\Phi(\alpha)$ exhibits a point of discontinuity. Let us define the function $g(y)$ as

$$g(y):=1-\frac{\lambda y}{\mathbb{E}[D_{out}\mathbb{1}(\mathrm{Bin}(D_{in},1-y)<\Omega)]}, \tag{5}$$

such that $y^*=y^*(\alpha)$ can be characterized as

$$y^*(\alpha)=\max\{y:\ y\in[0,1],\ g(y)=\alpha\}. \tag{6}$$

The right-hand side of Fig. 2 represents the function $g(y)$. As we can see, for $\alpha<\alpha_c$, the equation $g(y)=\alpha$ has three solutions in $[0,1]$, while for $\alpha>\alpha_c$ it has only one solution. In this case α_c can be characterized as a local maximum point of $g(y)$ in $(0,1)$.

1.4 Relation to Bootstrap Percolation in Random Regular Graphs

Bootstrap percolation in the random regular graph (non directed) $G(n,d)$ with fixed vertex degree d was studied by Balogh and Pittel in [5]. Let A_f be the final set of active vertices. The main theorem of [5] is the following

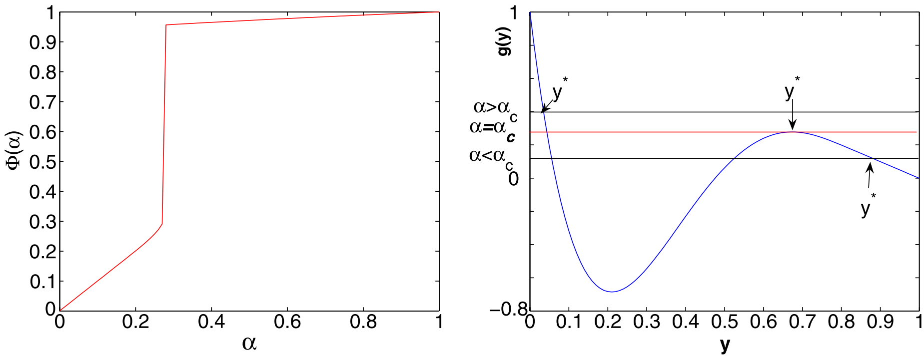

Fig. 2 (Color online) Functions $\Phi(\alpha)$ and $g(y)$ in bootstrap percolation model. Here $\mathbb{P}(D_{in}=k)\sim\exp(\frac{-(k-\overline{k})^2}{2\sigma^2})$ with $\overline{k}=50$, $\sigma=15$ and $\Omega=25$

Theorem 6 (Balogh-Pittel [5]) *Let $\Omega\le d-1$ and $\alpha\in[0,1]$ and consider the bootstrap percolation in the random d-regular graph $G(n,d)$ in which each vertex is initially active independently at random with probability α and the threshold is Ω. Let α_c be defined as follows*

$$\alpha_c := 1-\inf_{0<y\le 1}\frac{y}{\mathbb{P}(\mathrm{Bin}(d-1,1-y)\le\Omega-1)}.$$

We have

(i) *If $\alpha>\alpha_c$, then $|A_f|=n-o_p(n)$.*
(ii) *If $\alpha<\alpha_c$, then w.h.p. a positive proportion of the vertices remain inactive. More precisely, if $y^*=y^*(\alpha)$ is the largest $y\le 1$ such that*

$$\mathbb{P}(\mathrm{Bin}(d-1,1-y)\le\Omega-1)/y=(1-\alpha)^{-1},$$

then

$$\frac{|A_f|}{n}\xrightarrow{p}1-(1-\alpha)\mathbb{P}(\,\mathrm{Bin}(d,1-y^*)\le\Omega-1\,)<1.$$

In this case, Balogh and Pittel [5] have also studied the threshold in greater detail by allowing α to depend on n. They show

- if $n^{1/2}(\alpha(n)-\alpha_c)\to\infty$, then w.h.p. $|A_f|=n$;
- if $n^{1/2}(\alpha_c-\alpha(n))\to\infty$, then w.h.p. $|A_f|<n$ and furthermore

$$|A_f|=n\big(1-(1-\alpha(n))\mathbb{P}\big(\mathrm{Bin}(d,1-y^*)\le\Omega-1\big)\big)+O_p(n^{1/2}(\alpha_c-\alpha(n))^{-1/2}).$$

It would be interesting to generalize these results to our case. Note that Balogh and Pittel [5] do not use Wormald's theorem. Indeed they analyze directly the system of differential equations via exponential supermartingales by using its integrals to show that the percolation process undergoes relatively small fluctuations around the deterministic trajectory.

1.5 Organization of the Paper

In the next section we describe an approximation to the local structure of the graph by an appropriate branching process and give a heuristic argument which leads quickly to derive our result. Bootstrap Percolation is studied in detail in Sect. 3. We describe the dynamics of bootstrap percolation as a Markov chain in Sect. 3.1. The proof of out main theorem, Theorem 2, is based on the use of differential equations for solving discrete random processes. This was first introduced by Wormald [24]. We briefly discuss his method in Sect. 3.2. The proof of our main result is given in Sect. 3.3.

2 Branching Process Approximation

In this section we describe an approximation to the local structure of the graph by an appropriate branching process and give a heuristic argument which leads quickly to derive our Theorem 2. We define $P^*(j,k)$ the size biased probability mass function corresponding to P, by

$$P^*(j,k) := kP(j,k)/\lambda.$$

Indeed $P^*(j,k)$ is the probability that an incoming half-edge matches to a node with in-degree j and out-degree k. This occurs because vertices with out-degree k are k times as likely to be chosen for connections, and the outgoing edge that brings us to the new vertex uses up one of its in-degrees. Then we can approximate the local structure of a randomly chosen vertex by following branching process (see e.g. [2, 6]): with probability $P(j,k)$ the root Ø has in-degree equals to j and out-degree equals to k. Each of these vertices has in-degree equals to j and out-degree equals to k with probability $P^*(j,k)$, and so on. Let us denote this branching process by $\mathcal{X}$. Then the tree $\mathcal{X}$ describes the local structure of the graph $CM(n, \mathbf{d}_{in}^{(n)}, \mathbf{d}_{out}^{(n)})$ as n tends to infinity. We now consider the bootstrap percolation model in the infinite tree $\mathcal{X}$.

We encode the initial fired neurons by a vector χ, where $\chi_i = 1$ if the node i is fired and $\chi_i = 0$ otherwise. The random variable χ_i is Bernoulli with parameter α independent of everything else. We have

$$X_{t+1}(\emptyset) = 1 - (1 - \chi_\emptyset)\mathbb{1}\left(\sum_{i\to\emptyset} X_t(i) < \Omega)\right). \quad (7)$$

Thanks to the tree structure, the random variables $(X_t(i), i \to \emptyset)$ are independent of each other and identically distributed. Furthermore for $i \neq \emptyset$, we have:

$$X_{t+1}(i) = 1 - (1 - \chi_i)\mathbb{1}\left(\sum_{j\to i} X_t(j) < \Omega)\right). \quad (8)$$

Let D_{in}^* be a random variable with the distribution

$$\mathbb{P}(D_{in}^* = j) = \sum_k P^*(j,k) = \sum_k \frac{kP(j,k)}{\lambda}.$$

In view of (8), it is natural to introduce the following Recursive Distributional Equation (RDE):

$$X \stackrel{d}{=} 1 - (1 - \chi)\mathbb{1}\left(\sum_{l=1}^{D_{in}^*} X(l) < \Omega\right), \quad (9)$$

where χ is a Bernoulli random variable with parameter α, X and $X(l)$ are identically distributed and all random variables are independent of each others. RDE for the process X plays a similar role as the equation $\mu = K\mu$ for the stationary distribution of a Markov chain with kernel K, see [1].

Let $y = P[X = 0]$, where the distribution of X solves the RDE (9). By taking expectation in (9), we get

$$\begin{aligned} 1 - y &= 1 - (1-\alpha)\sum_j \sum_k \frac{kP(j,k)}{\lambda}\mathbb{P}(\mathrm{Bin}(j, 1-y) < \Omega) \\ &= 1 - (1-\alpha)\frac{\mathbb{E}[D_{out}\mathbb{1}(\mathrm{Bin}(D_{in}, 1-y) < \Omega)]}{\lambda}. \end{aligned}$$

We have $f_\alpha(y) = 0$. Furthermore by 7, the state of the root follows:

$$X(\emptyset) \stackrel{d}{=} 1 - (1-\chi)\mathbb{1}\left(\sum_{l=1}^{D_{in}} X(l) < \Omega\right),$$

where X_l are i.i.d. and their distribution solves the RDE (9), i.e., $f_\alpha(y) = 0$. Taking the expectation gives:

$$\mathbb{E}[X(\emptyset)] = 1 - (1-\alpha)\mathbb{P}\left(\mathrm{Bin}(D_{in}, 1-y) < \Omega\right).$$

3 Bootstrap Percolation in $CM(n, \mathbf{d}_{in}^{(n)}, \mathbf{d}_{out}^{(n)})$

This section is devoted to the proof of Theorem 2.

3.1 The Markov Chain

We first describe the dynamics of the bootstrap percolation as a Markov chain, which is perfectly tailored for asymptotic study. We consider the bootstrap percolation on $CM(n, \mathbf{d}_{in}^{(n)}, \mathbf{d}_{out}^{(n)})$. Let $m(n) := \sum_{i=1}^n d_{in}^{(n)}(i)$ denote the number of incoming edges in the graph.

At a given time step t neurons are partitioned into fired $\mathbb{F}(t)$ and non-fired $\mathbb{N}(t)$. We further partition the class of non-fired nodes according to their in- and out-degree $\mathbb{N}(t) = \bigcup_{j,k}\mathbb{N}_{j,k}(t)$. At time zero, $\mathbb{F}(0)$ contains the initial set of fired neurons. We look at the system in discrete time. At time step $t+1$ we have

$$\mathbb{F}(t+1) = \mathbb{F}(t) \cup \{v \in \mathbb{N}(t) \text{ such that } |\mathbb{F}(t) \cap \{w \in V, A_{vw} = 1\}| \geq \Omega\}.$$

We now assume the configuration model algorithm described in Sect. 1.1. One can observe that the uniform matching which constructs the graph can be obtained sequentially: choose an outgoing half edge according to any rule (random or deterministic) and then choose the corresponding incoming half edge uniformly over the unmatched incoming half edges.

We now use a different approach for the bootstrap percolation dynamics which results in a simpler Markov chain description of the system. At each step we have one interaction only between two neurons, yielding at least one fired. Our processes at each step is as follows:

- Choose an outgoing edge of a fired neuron i;
- Identify its partner j (i.e. by construction of the random graph in the configuration model, the partner is given by choosing an incoming edge randomly among all available incoming edges);
- Delete both edges. If j is currently non-fired and it is the Ω-th deleted incoming edge from j, then j fires.

Our system is described in terms of

- $N^{(n)}_{j,k,\theta}(t)$, $0 \le \theta < \Omega$, the number of non-fired neurons with in-degree j, out-degree k, and θ incoming edges from fired neurons at time t,
- $F^{(n)}_{j,k}(t)$: the number of fired neurons with in-degree j and out-degree k at time t,
- $F^{(n)}(t)$: the number of fired neurons at time t,
- $N^{(n)}_{in}(t)$: the number of incoming edges belonging to non-fired neurons at time t,
- $F^{(n)}_{in}(t)$: the number of incoming edges belonging to fired neurons at t,
- $F^{(n)}_{out}(t)$: the number of outgoing edges belonging to fired neurons at t.

Because at each step we delete one incoming edge and the number of incoming edges at time 0 is $m(n)$, the number of existing incoming edges at time t will be $m(n) - t$ and we have

$$F^{(n)}_{in}(t) + N^{(n)}_{in}(t) = m(n) - t.$$

It is easy to see that the following identities hold:

$$N^{(n)}_{in}(t) = \sum_{j,k} \sum_{\theta<\Omega} (j-\theta) N^{(n)}_{j,k,\theta}(t), \tag{10}$$

$$F^{(n)}_{out}(t) = \sum_{k,j} k F^{(n)}_{j,k}(t) - t, \tag{11}$$

$$F^{(n)}(t) = \sum_{k,j} F^{(n)}_{j,k}(t). \tag{12}$$

The process will finish at the stopping time $T^{(n)}_f$ which is the first time $t \in \mathbb{N}$ where $F^{(n)}_{out}(t) = 0$. The final number of fired neurons will be $F^{(n)}(T^{(n)}_f)$. By definition of our process $\{N^{(n)}_{j,k,\theta}, F^{(n)}_{j,k}\}_{\theta,j,k}$ represents a Markov chain. We write the transition probabilities of the Markov chain. There are three possibilities for the B, the partner of an outgoing edge of a fired neuron A.

1. B is fired, the next state is

$$N^{(n)}_{j,k,\theta}(t+1) = N^{(n)}_{j,k,\theta}(t) \quad (0 \le \theta < \Omega),$$
$$F^{(n)}_{j,k}(t+1) = F^{(n)}_{j,k}(t).$$

2. B is non-fired of in-degree j and out-degree k, and this is the $(\theta+1)$-th deleted incoming edge and $\theta + 1 < \Omega$. The probability of this event is $\frac{(j-\theta)N^{(n)}_{j,k,\theta}}{m(n)-t}$. The next state is

$$N^{(n)}_{j,k,\theta}(t+1) = N^{(n)}_{j,k,\theta}(t) - 1,$$
$$N^{(n)}_{j,k,\theta+1}(t+1) = N^{(n)}_{j,k,\theta+1}(t) + 1,$$

$$N^{(n)}_{j,k,i}(t+1) = N^{(n)}_{j,k,i}(t+1) \quad (0 \le i < \Omega,\ i \ne \theta, \theta+1),$$
$$F^{(n)}_{j,k}(t+1) = F^{(n)}_{j,k}(t).$$

3. B is non-fired of in-degree j and out-degree k, and this is the Ω-th deleted incoming edge. Then $j \ge \Omega$ and with probability $\frac{(j-\Omega+1)N^{(n)}_{j,k,\Omega-1}(t)}{m(n)-t}$, we have

$$N^{(n)}_{j,k,\theta}(t+1) = N^{(n)}_{j,k,\theta}(t) \quad (0 \le \theta < \Omega - 1),$$
$$N^{(n)}_{j,k,\Omega-1}(t+1) = N^{(n)}_{j,k,\Omega-1}(t) - 1,$$
$$F^{(n)}_{j,k}(t+1) = F^{(n)}_{j,k}(t) + 1.$$

Let P_t denote the pairing generated by time t, i.e., $P_t = \{e_{out}, e_{in}\}$ is the set of edges picked before time t. By averaging over the possible transitions, we obtain the following equations for expectation of $(N^{(n)}_{j,k,\theta}(t+1), F^{(n)}_{j,k}(t+1))$ conditioned on P_t:

$$\mathbb{E}\big[N^{(n)}_{j,k,0}(t+1) - N^{(n)}_{j,k,0}(t) | P_t\big] = -\frac{jN^{(n)}_{j,k,0}(t)}{m(n)-t},$$
$$\mathbb{E}\big[N^{(n)}_{j,k,\theta}(t+1) - N^{(n)}_{j,k,\theta}(t) | P_t\big]$$
$$= \frac{(j-\theta+1)N^{(n)}_{j,k,\theta-1}(t) - (j-\theta)N^{(n)}_{j,k,\theta}(t)}{m(n)-t} \quad (0 < \theta < \Omega),$$
$$\mathbb{E}\big[F^{(n)}_{j,k}(t+1) - F^{(n)}_{j,k}(t) | P_t\big] = \frac{(j-\Omega+1)N^{(n)}_{j,k,\Omega-1}(t)}{m(n)-t}.$$

We will show in Sect. 3.3 that the trajectory of these variables throughout the algorithm is a.a.s. (asymptotically almost surely, as $n \to \infty$) close to the solution of the deterministic differential equations suggested by these equations.

3.2 Wormald's Theorem

In this section we briefly present a method introduced by Wormald in [24] for the analysis of a discrete random process by using differential equations. In particular we recall a general purpose theorem for the use of this method. This method has been used to analyze several kinds of algorithms on random graphs and random regular graphs (e.g., [9, 18, 25]).

Recall that a function $f(u_1, \dots, u_j)$ satisfies a Lipschitz condition on $D \in \mathbb{R}^j$ if a constant $L > 0$ exists with the property that

$$|f(u_1, \dots, u_j) - f(v_1, \dots, v_j)| \le L \max_{1 \le i \le j} |u_i - v_i|$$

for all $(u_1, \dots, u_j)$ and $(v_1, \dots., v_j)$ in D. For variables $Y_1, \dots, Y_b$ and for $D \in \mathbb{R}^{b+1}$, the stopping time $T_D(Y_1, \dots, Y_b)$ is defined to be the minimum t such that

$$(t/n; Y_1(t)/n, \dots, Y_b(t)/n) \notin D.$$

This is written as T_D when $Y_1, \dots, Y_b$ are understood from the context.

The following theorem is the Theorem 5.1 of [25]. In it, "uniformly" refers to the convergence implicit in the $o()$ terms. Hypothesis (1) ensures that Y_t does not change too quickly throughout the process. Hypothesis (2) tells us what we expect for the rate of change to be, and property (3) ensures that this rate does not change too quickly.

Theorem 7 (Wormald [25]) *Let b be given (b is the number of variables). For $1 \le l \le b$, suppose $Y_l^{(n)}(t)$ is a sequence of real-valued random variables, such that $0 \le Y_l^{(n)}(t) \le Cn$ for some constant C, and H_t be the history of the sequence, i.e. the sequence $\{Y_j^{(n)}(k),\ 0 \le j \le b,\ 0 \le k \le t\}$.*

Suppose also that for some bounded connected open set $D \subseteq \mathbb{R}^{b+1}$ containing the intersection of $\{(t, z_1, \dots, z_b) : t \ge 0\}$ with some neighborhood of

$$\{(0, z_1, \dots, z_b) : \mathbb{P}(Y_l^{(n)}(0) = z_l n, 1 \le l \le b) \neq 0 \text{ for some } n\},$$

the following three conditions are verified:

1. (Boundedness) *For some function $\beta = \beta(n) \ge 1$ and for all $t < T_D$*

$$\max_{1 \le l \le b} |Y_l^{(n)}(t+1) - Y_l^{(n)}(t)| \le \beta;$$

2. (Trend) *For some function $\lambda = \lambda_1(n) = o(1)$ and for all $l \le b$ and $t < T_D$*

$$|\mathbb{E}[Y_l^{(n)}(t+1) - Y_l^{(n)}(t)|H_t] - f_l(t/n, Y_1^{(n)}(t)/n, \dots, Y_b^{(n)}(t)/n)| \le \lambda_1;$$

3. (Lipschitz) *For each l the function f_l is continuous and satisfies a Lipschitz condition on D with all Lipschitz constants uniformly bounded.*

Then the following holds

(a) *For $(0, \hat{z}_1, \dots, \hat{z}_b) \in D$, the system of differential equations*

$$\frac{dz_l}{ds} = f_l(s, z_1, \dots, z_l), \quad l = 1, \dots, b,$$

has a unique solution in D, $z_l : \mathbb{R} \to \mathbb{R}$ for $l = 1, \dots, b$, which passes through $z_l(0) = \hat{z}_l$, $l = 1, \dots, b$, and which extends to points arbitrarily close to the boundary of D.

(b) *Let $\lambda > \lambda_1$ with $\lambda = o(1)$. For a sufficiently large constant C, with probability $1 - O(\frac{b\beta}{\lambda} \exp(-\frac{n\lambda^3}{\beta^3}))$, we have*

$$Y_l^{(n)}(t) = n z_l(t/n) + O(\lambda n)$$

uniformly for $0 \le t \le \sigma n$ and for each l. Here $z_l(t)$ is the solution in (a) with $\hat{z}_l = Y_l^{(n)}(0)/n$, and $\sigma = \sigma(n)$ is the supremum of those s to which the solution can be extended before reaching within l^∞-distance $C\lambda$ of the boundary of D.

We will also use the following corollary of the above theorem, which is namely Theorem 6.1 of [25]. This theorem states that, as long as Condition 3 holds in D, the solution of the system of equations above can be extended beyond the boundary of $\hat{D}$, into D.

Corollary 8 *For any set $\hat{D} \subseteq \mathbb{R}^{b+1}$, let $T_{\hat{D}} = T_{\hat{D}}(Y_1^{(n)}, \dots, Y_b^{(n)})$ be the minimum t such that $(\frac{t}{n}, \frac{Y_1^{(n)}(t)}{n}, \dots, \frac{Y_b^{(n)}(t)}{n}) \notin \hat{D}$ (the stopping time). Assume in addition that the first two hypotheses of Theorem 7 are verified but only within the restricted range $t < T_{\hat{D}}$ of t. Then the conclusions of the theorem hold as before, after replacing $0 \le t \le \sigma n$ by $0 \le t \le \min\{\sigma n, T_{\hat{D}}\}$.*

Proof For $1 \le j \le b$, define random variables $\hat{Y}_j^{(n)}$ by

$$\hat{Y}_j^{(n)}(t+1) = \begin{cases} Y_j^{(n)}(t+1), & \text{if } t < T_{\hat{D}} \\ Y_j^{(n)}(t) + f_j(t/n, Y_1^{(n)}(t)/n, \ldots, Y_b^{(n)}(t)/n), & \text{otherwise} \end{cases}$$

for all $t \ge 0$. Then the $\hat{Y}_j^{(n)}$ satisfy the hypotheses of Theorem 7, and so the corollary follows as $\hat{Y}_j^{(n)}(t) = Y_j^{(n)}(t)$ for $0 \le t < T_{\hat{D}}$. □

3.3 Proof of Theorem 2

The proof of Theorem 2 is mainly based on Theorem 7. Indeed we will apply this theorem to show that the trajectory of $N_{j,k,\theta}^{(n)}(t)$ and $F_{j,k}^{(n)}(t)$ throughout the algorithm is a.a.s. close to the solution of the deterministic differential equations suggested by these equations.

Let (DE) be the following system of differential equations:

$$\begin{aligned} (n_{j,k,0})'(\tau) &= -\frac{j n_{j,k,0}(\tau)}{\lambda - \tau}, \\ (n_{j,k,\theta})'(\tau) &= \frac{(j-\theta+1)n_{j,k,\theta-1}(\tau) - (j-\theta)n_{j,k,\theta}(\tau)}{\lambda - \tau} \quad (\text{for } 0 < \theta < \Omega\ ), \\ (f_{j,k})'(\tau) &= \frac{(j-\Omega+1)n_{j,k,\Omega-1}(\tau)}{\lambda - \tau}, \end{aligned}$$

with $\tau \in [0, \lambda)$, and initial conditions

$$n_{j,k,0} = (1-\alpha)P(j,k), \qquad n_{j,k,\theta}(0) = 0 \quad \text{for } \ 0 < \theta < \Omega, \quad \text{and} \quad f_{j,k}(0) = \alpha P(j,k).$$

Lemma 9 *The solution of the system of differential equations* (*DE*) *is*

$$\begin{aligned} n_{j,k,\theta}(\tau) &= P(j,k)(1-\alpha)\binom{j}{i} y^{j-\theta}(1-y)^i, \\ f_{j,k}(\tau) &= P(j,k)\left[\alpha + (1-\alpha)\mathbb{P}(\mathrm{Bin}(j, 1-y) \ge \Omega)\right], \end{aligned}$$

where $y = (1 - \tau/\lambda)$.

Proof Let $u = u(\tau) = -\ln(\lambda - \tau)$. Then $u(0) = -\ln(\lambda)$, u is strictly monotone and so is the inverse function $\tau = \tau(u)$. We write the system of differential equations (DE) with respect to u:

$$\begin{aligned} (n_{j,k,0})'(u) &= -j n_{j,k,0}(u), \\ (n_{j,k,\theta})'(u) &= (j-\theta+1)n_{j,k,\theta-1}(u) - (j-\theta)n_{j,k,\theta}(u). \end{aligned}$$

Then using

$$\frac{d}{du}(n_{j,k,\theta}(u)e^{(j-\theta-1)(u-u(0))}) = e^{(j-\theta-1)(u-u(0))}(j-\theta)n_{j,k,\theta}(u),$$

and by induction, we find

$$n_{j,k,\theta}(u) = e^{-(j-\theta)(u-u(0))} \sum_{r=0}^{\theta} \binom{j-r}{i-r} \left(1 - e^{-(u-u(0))}\right)^{i-r} n_{j,k,\theta}(u(0)).$$

By going back to τ, we have

$$n_{j,k,\theta}(\tau) = y^{d-j} \sum_{r=0}^{\theta} n_{j,k,\theta}(0) \binom{j-r}{i-r} (1-y)^{i-r}, \quad y = (1-\tau/\lambda),$$

which gives

$$n_{j,k,\theta}(\tau) = P(j,k)(1-\alpha)\binom{j}{i} y^{j-\theta}(1-y)^{i}.$$

We have

$$\begin{aligned}
(f_{j,k})'(y) &= -\lambda (f_{j,k})'(\tau) \\
&= -\lambda \frac{(j-\Omega+1)n_{j,k,\Omega-1}}{\lambda y} \\
&= -(j-\Omega+1)P(j,k)(1-\alpha)\binom{j}{\Omega-1} y^{j-\Omega}(1-y)^{\Omega-1} \\
&= -P(j,k)(1-\alpha)j\mathbb{P}(\mathrm{Bin}(j-1, 1-y) = \Omega-1).
\end{aligned}$$

Then using the fact that

$$\frac{\partial}{\partial p}\mathbb{P}(\mathrm{Bin}(N,p) > K) = N\mathbb{P}(\mathrm{Bin}(N-1,p) = K),$$

and by initial condition we have

$$f_{j,k} = P(j,k)\left[\alpha + (1-\alpha)\mathbb{P}(\mathrm{Bin}(j, 1-y) \geq \Omega)\right]. \qquad \square$$

Let us fix an arbitrary constant $\epsilon > 0$. We define the operator $\wedge$ as

$$x \wedge y = \max(x,y).$$

By Condition 1, we know

$$\lambda = \sum_{j,k} kP(j,k) = \sum_{j} P(j,k) \in (0,\infty).$$

Then, there exist a constant K_ϵ, such that

$$\sum_{k \geq K_\epsilon} \sum_{j} kP(j,k) + \sum_{j \geq K_\epsilon} \sum_{k} jP(j,k) < \epsilon/2,$$

which implies

$$\sum_{j \wedge k \geq K_\epsilon} kP(j,k) < \epsilon/2.$$

We also have by Lemma 9

$$f_{j,k}(\tau) = P(j,k)\left[\alpha + (1-\alpha)\mathbb{P}(\mathrm{Bin}(j,1-y) \geq \Omega)\right] \leq P(j,k).$$

Let $N^{(n)}(j,k)$ denote the number of vertices with in-degree j and out-degree k at time 0. Again, by Condition 1,

$$\sum_{j,k} kN^{(n)}(j,k)/n = \sum_{j,k} jN^{(n)}(j,k)/n \to \lambda \in (0,\infty), \quad \text{as } n \to \infty.$$

Therefore, for n large enough,

$$\sum_{j\wedge k \geq K_\epsilon} kN^{(n)}(j,k)/n < \epsilon/2,$$

and then

$$\begin{aligned}\sum_{j\wedge k\geq K_\epsilon} k\left|F^{(n)}_{j,k}(t)/n - f_{j,k}(t/n)\right| &\leq \sum_{j\wedge k\geq K_\epsilon} k\left(F^{(n)}_{j,k}(t)/n + f_{j,k}(t/n)\right)\\ &\leq \sum_{j\wedge k\geq K_\epsilon} k\left(N^{(n)}(j,k)/n + P(j,k)\right) < \epsilon. \end{aligned} \tag{13}$$

Let us define

$$f_{out}(\tau) := \sum_{k,j} kf_{j,k}(\tau) - \tau, \quad \text{and} \tag{14}$$

$$f(\tau) = \sum_{k,j} kf_{j,k}(\tau). \tag{15}$$

Then by Lemma 9 we have

$$\begin{aligned} f_{out}(\tau) &= \sum_{k,j} kP(j,k)\left[\alpha + (1-\alpha)\mathbb{P}(\text{Bin}(j,1-y)\geq \Omega)\right] - \tau\\ &= \lambda\alpha + \sum_{k,j} kP(j,k)(1-\alpha)\mathbb{P}(\text{Bin}(j,1-y)\geq\Omega) - \tau\\ &= \lambda y - \lambda(1-\alpha) + (1-\alpha)\\ &\quad \mathbb{E}\left[D_{out}\mathbb{1}\left(\text{Bin}(D_{in},1-y)\geq\Omega\right)\right]\\ &= f_\alpha(y), \end{aligned}$$

where $y = (1-\tau/\lambda)$.

For $\epsilon > 0$, we define $b(\epsilon) := K_\epsilon^2(\Omega+1)$, and the domain $D(\epsilon)$ as

$$\begin{aligned} D(\epsilon) = \Bigg\{&\left(\tau, \{n_{j,k,\theta}, f_{j,k}\}_{\theta<\Omega, 1\leq j,k\leq K_\epsilon}\right) \in \mathbb{R}^{b(\epsilon)+1} : -\epsilon < n_{j,k,\theta} < 1,\ -\epsilon < f_{j,k} < 1,\\ &-\epsilon < \tau < \lambda - \epsilon, \quad \sum_{j\wedge k\leq K_\epsilon} kf_{j,k} - \tau > 0\Bigg\}. \end{aligned}$$

Let $T^{(n)}_D$ be the stopping time for D which is the first time t when

$$\left(t/n, \{N^{(n)}_{j,k,\theta}(t/n)\}, \{F^{(n)}_{j,k}(t/n)\}\right) \notin D.$$

We will use Theorem 7. The domain $D(\epsilon)$ is a bounded open set which contains all initial values of variables which may happen with positive probability. Each variable is bounded by a constant times n. By the definition of our process, the Boundedness Hypothesis is satisfied with $\beta(n) = 1$. Trend Hypothesis is satisfied by some $\lambda_1(n) = O(1/n)$. Finally the third condition (Lipschitz Hypothesis) of the theorem is also satisfied since $\lambda - \tau$ is bounded away from zero. Note that for $0 < \theta < \Omega$; we have $N^{(n)}_{j,k,\theta}(0)/n = 0$, and by Condition 1 and by definition:

$$N^{(n)}_{j,k,0}(0)/n \xrightarrow{p} (1-\alpha)P(j,k), \qquad F^{(n)}_{j,k}(0)/n \xrightarrow{p} \alpha P(j,k).$$

Then we set $\lambda = O(n^{-1/4}) > \lambda_1$. The conclusion of Theorem 7 now gives

$$N^{(n)}_{j,k,\theta}(t)/n = n_{j,k,\theta}(t/n) + O(n^{3/4}), \tag{16}$$

$$F^{(n)}_{j,k}(t)/n = f_{j,k}(t/n) + O(n^{3/4}), \tag{17}$$

with probability $1 - O(n^{7/4}\exp(-n^{1/4}))$ uniformly for all $t \le n\sigma$, where $\sigma = \sigma(n)$ is the supremum of those τ for which the solution of the differential equations (DE) can be extended before reaching within l^∞-distance $Cn^{-1/4}$ of the boundary of $D(\epsilon)$.

Then we have by (13) and (17)

$$\begin{aligned}\sup_{t\le n\sigma}\left|F^{(n)}_{out}(t)/n - f_{out}(t/n)\right| &\le \sup_{t\le n\sigma}\sum_{j,k} k\left|F^{(n)}_{j,k}(t)/n - f_{j,k}(t/n)\right| \\ &\le \epsilon + \sup_{t\le n\sigma}\sum_{j\wedge k\le K_\epsilon} k\left|F^{(n)}_{j,k}(t)/n - f_{j,k}(t/n)\right| = \epsilon + o_p(1),\end{aligned}$$

and by the same argument

$$\sup_{t\le n\sigma}\left|F^{(n)}(t)/n - f(t/n)\right| \le \sup_{t\le n\sigma}\sum_{j,k} k\left|F^{(n)}_{j,k}(t)/n - f_{j,k}(t/n)\right| \le \epsilon + o_p(1).$$

To analyze σ, we need to determine which constraint is violated when the solution reaches the boundary of $D(\epsilon)$. It cannot be the first two constraints, because (17) must give asymptotically feasible values of $N^{(n)}_{j,k,\theta}$ and $F^{(n)}_{j,k}$ up until the boundary is approached. It remains to determine which of the last two constraints is violated when $\tau = \sigma$.

First assume $f_\alpha(y) > 0$ for all $y \in (0,1]$, i.e., $y^* = 0$. Then we have $f_{out}(\tau) > 0$ for all $\tau \in [0,\lambda)$. Now note that if $\sum_{j\wedge k\le K_\epsilon} kf_{j,k}(\tau) - \tau$ becomes zero, by definition of K_ϵ, we will have $f_{out}(\tau) < \epsilon$. Then by choosing ϵ small enough, we conclude that in this case for any $\epsilon' > 0$, and for n large enough, we will have w.h.p. $T^{(n)}_f > n(\lambda - \epsilon')$, which implies $\Phi^{(n)}(\alpha) = 1 - o_p(1)$.

Consider now $y^* > 0$, and suppose further that y^* is not a local minimum point of $f_\alpha(y)$. This means $f_\alpha(y) < 0$ for some interval $(y^* - a, y^*)$. We infer that the first constraint is violated at time $\hat{\tau} \sim \lambda(1 - y^*)$. We apply Corollary 8 with $\hat{D}$ the domain $D(\epsilon)$ defined above, and the domain D replaced by $D'(\epsilon)$, which is the same as D except that the last constraint is omitted:

$$\begin{aligned}D'(\epsilon) = \Big\{\Big(\tau, \{n_{j,k,\theta}, f_{j,k}\}_{\theta<\Omega, 1\le j,k\le K_\epsilon}\Big) \in \mathbb{R}^{b(\epsilon)+1} : -\epsilon < n_{j,k,\theta} < 1,\ -\epsilon < f_{j,k} < 1, \\ -\epsilon < \tau < \lambda - \epsilon\Big\}.\end{aligned}$$

This gives us the convergence up to the point where the solution leaves $D'(\epsilon)$ or when $\sum_{j\wedge k<K_\epsilon} kF_{j,k}^{(n)} - t > 0$ is violated. Since $f_{out}(\tau)$ begins to go negative after $\hat{\tau}$, it follows that $\sum_{j\wedge k<K_\epsilon} kF_{j,k}^{(n)} - t > 0$ must be violated almost asymptotic surely. Then it is easy to conclude (by choosing ϵ small enough) that in this case for any $\epsilon' > 0$, and for n large enough, we will have w.h.p. $T_f^{(n)}/n \in (\hat{\tau}-\epsilon', \hat{\tau}+\epsilon')$, which gives $T_f^{(n)}/n \xrightarrow{p} \hat{\tau}$. We conclude

$$\begin{aligned} F^{(n)}(T_f^{(n)}) &= nf(\hat{\tau}) + o_p(n) \\ &= n\left(1-(1-\alpha)\mathbb{E}\left[\mathbb{1}\left(\mathrm{Bin}(D_{in}, 1-y^*) < \Omega\right)\right]\right) + o_p(n), \end{aligned}$$

which completes the proof.

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