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SEPARATION CUTOFF FOR UPWARD SKIP-FREE CHAINS

Y. H. MAO,* *Beijing Normal University*
C. ZHANG,** *Ocean University of China*
Y. H. ZHANG,* *Beijing Normal University*

Abstract

A computable necessary and sufficient condition of separation cutoff is obtained for a sequence of continuous-time upward skip-free chains with the stochastically monotone time-reversals.

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1. Introduction

Cutoff refers to a family of ergodic Markov chains showing a sharp transition when converging to their stationary distributions. In this paper we will consider the separation cutoff. For two probability measures μ and ν, the separation is defined as

$$\operatorname{sep}(\mu, \nu) = \max_i \left(1 - \frac{\mu_i}{\nu_i}\right).$$

For each $n = 0, 1, \ldots$, let $P^{(n)}(t)$ be the distribution of a finite ergodic Markov chain $X_t^{(n)}$ at time t, whose stationary distribution is $\pi^{(n)}$. Then for any fixed n,

$$\lim_{t\to\infty} \operatorname{sep}(P^{(n)}(t), \pi^{(n)}) = 0.$$

However, involving n, it may happen that

$$\lim_{n\to\infty} \operatorname{sep}(P^{(n)}(ct_n), \pi^{(n)}) = \begin{cases} 0 & \text{for } c > 1, \\ 1 & \text{for } c < 1. \end{cases} \tag{1.1}$$

This is called the (separation) cutoff phenomenon proposed by Persi Diaconis [4]. The separation may be replaced by total variation distance [6] or max-L^2 distance [2], for example.

The concept of separation was introduced in [1] and has been intensively studied since then. Strictly speaking, separation is not a distance (it is not symmetric in μ and ν). However, separation is easily handled and powerful in the following sense. For a finite Markov chain,

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* Postal address: School of Mathematical Sciences, Beijing Normal University, Laboratory of Mathematics and Complex Systems, Ministry of Education, Beijing, 100875, China.
** Postal address: College of Mathematical Sciences, College of information Science and engineering, Ocean University of China, Qingdao, 266100, China. Email address: zhangchi@ouc.edu.cn

let $P(t)$ be its distribution at time t. Then there exists a *fastest strong stationary time* (FSST) τ such that

$$\operatorname{sep}(P(t),\pi)=\mathbb{P}[\tau>t]\quad \text{for all } t\geq 0, \tag{1.2}$$

See [1] for the definitions and properties of FSST, and [7] for the existence of FSST in (1.2).

We have obtained the explicit criteria for separation cutoff of the birth and death processes in [9], while in this paper we will give those of the upward skip-free chains. Let us first recall some basics for the upward skip-free chains.

On finite state space $\{0,1,\dots,N\}$, let $Q=(q_{ij})$ be the generator of an irreducible and conservative upward skip-free chain. That is, for $0\leq i<N$ and $j>i+1$, $q_{i,i+1}>0, q_{ij}=0$; and for $0\leq i\leq N, q_i:=-q_{ii}=\sum_{j\neq i}q_{ij}<\infty$. For $0\leq k<i\leq N$, define $q_i^{(k)}=\sum_{j=0}^{k}q_{ij}$, and

$$F_i^{(i)}=1,\qquad F_i^{(k)}=\sum_{j=k+1}^{i}\frac{F_i^{(j)}q_j^{(k)}}{q_{j,j+1}}. \tag{1.3}$$

Then define

$$m_i=\sum_{k=0}^{i}\frac{F_i^{(k)}}{q_{k,k+1}},\qquad 0\leq i\leq N. \tag{1.4}$$

Here, in (1.3) and (1.4), we set $q_{N,N+1}=1$ for convenience. By [10], the stationary distribution is

$$\pi_i=\frac{F_N^{(i)}}{q_{i,i+1}m_N},\qquad 0\leq i\leq N. \tag{1.5}$$

Define

$$T=\sum_{i=0}^{N}\pi_i\sum_{j=0}^{i-1}m_j,\qquad S=\sum_{i=0}^{N}\pi_i\sum_{j=0}^{i-1}\sum_{k=0}^{j}\frac{F_j^{(k)}}{q_{k,k+1}}\sum_{\ell=0}^{k-1}m_\ell. \tag{1.6}$$

Now we can state the main results in this paper.

Theorem 1.1. *For each n, assume that $X_t^{(n)}$ is an upward skip-free chain on $\{0,1,\dots,N_n\}$, started at 0 and with the stochastically monotone time-reversal. Define $T^{(n)}$ and $S^{(n)}$ as in (1.6) (with N replaced by N_n). Then there exists the separation cutoff in (1.1) with $t_n=T^{(n)}$ if and only if*

$$\lim_{n\to\infty}\frac{S^{(n)}}{[T^{(n)}]^2}=\frac{1}{2}.$$

The following corollary gives a useful and sufficient condition for separation cutoff.

Corollary 1.1. *For each n, let $Q^{(n)}=(q_{ij}^{(n)})$ be the generator of a skip-free chain started at 0 on $\{0,1,\dots,N_n\}$, where $q_{i,i+1}^{(n)}=1$ for $1\leq i<N_n$ and $q_{ki}^{(n)}\leq q_{k,i+1}^{(n)}$ for $k>i+1$. If there is $C>0$ and $\beta>1$ such that $F_i^{(j)}\sim C\beta^{i-j}$ as $i-j\to\infty$, then the separation cutoff occurs.*

Next we would like to present some examples. We will focus on the restricted chains of an upward skip-free chain X_t with generator $Q=(q_{ij})$ on $E=\{0,1,2,\dots\}$. For an increasing sequence $\{N_n\}$ with limit ∞ as $n\to\infty$, we define a sequence of ergodic chains $\{X_t^{(n)}\}$ as follows. For each $X_t^{(n)}$, let $Q^{(n)}=(q_{ij}^{(n)})$ be its generator satisfying $q_{ij}^{(n)}=q_{ij}$ $(1\leq i\leq N_n, 1\leq j<N_n)$ and $q_{N_n,N_n}^{(n)}=-\sum_{j=0}^{N_n-1}q_{N_n,j}$. Then $X_t^{(n)}$ is a restricted chain of X_t on $\{0,1,\dots,N_n\}$. We say that X_t exhibits the separation cutoff if it occurs for the family

of restricted chains $\{X_t^{(n)}\}$. Obviously, the choice of the increasing sequence $\{N_n\}$ going to ∞ has no impact on the occurrence of the separation cutoff for X_t.

Example 1.1. *Let $q_{01} = q_{10} = q_{12} = 1$ and $q_{i,i+1} = q_{i,i-1} = q_{i,i-2} = 1$, $q_{ii} = -3$ $(i \geq 2)$. Then the skip-free chain exhibits the separation cutoff.*

Proof. By (1.3), we have

$$F_i^{(i)} = 1,\ F_i^{(i-1)} = 2, \qquad F_i^{(j)} = 2F_i^{(j-1)} + F_i^{(j-2)} \quad (i-2 \geq j \geq 0).$$

It follows from Corollary 2.1 that the time-reversal chain is stochastically monotone.

Define a generalized Fibonacci sequence $f_0 = 1$, $f_1 = 2$, and $f_i = 2f_{i-1} + f_{i-2}$ $(i \geq 2)$. It is known that $f_i \sim C(\sqrt{2}+1)^i$ for some $C > 0$. Then $F_i^{(j)} = f_{i-j} \sim C(\sqrt{2}+1)^{i-j}$ $(i \geq j \geq 0)$. This implies the separation cutoff by Corollary 1.1. □

Example 1.2. *Let $q_{i,i+1} = 1$ $(i \geq 0)$ and $q_{ij} = 1/i$ $(0 \leq j < i)$. Then the chain exhibits the separation cutoff.*

Proof. We split the proof into two parts.

(a) Since for $j < i$,

$$F_i^{(j)} = (j+1)\sum_{k=j+1}^{i} \frac{F_i^{(k)}}{k} \geq F_i^{(j+1)},$$

it is easy to check that the time-reversal is stochastically monotone by Corollary 2.1.

(b) We claim that

$$F_i^{(j)} = 2^{i-j-1} + O(2^{i-j-2}) \quad \text{as } i-j \to \infty,$$

which implies the separation cutoff by Corollary 1.1.

In fact, inductively, we have

$$\begin{aligned} F_i^{(j)} &= \sum_{k=j+1}^{i} F_i^{(k)} - (j+1)\sum_{k=j+1}^{i} \frac{k-j-1}{k} F_i^{(k)} \\ &\sim 2^{i-j-1} + O(2^{i-j-2}) - \sum_{k=j+2}^{i} \frac{k-j-1}{k}[2^{i-k-1} + O(2^{i-k-2})] \\ &\sim 2^{i-j-1} + O(2^{i-j-2}). \end{aligned}$$

□

Example 1.3. *Let $q_{i,i+1} = 1$, $q_{i0} = p^i$ $(i \geq 0)$, and $q_{ij} = (1-p)p^{i-j-1}$ $(1 \leq j < i)$. Then the chain exhibits the separation cutoff if $0 < p \leq (\sqrt{5}-1)/2$.*

Proof. We split the proof into three parts.

(a) We first prove that

$$F_i^{(j)} = (1+p)^{i-j-1} \quad \text{for } i-j \geq 1. \tag{1.7}$$

Inductively, assume that (1.7) holds for $j = i-1, \ldots, i-k$. Since $F_i^{(i)} = 1$, we have

$$F_i^{(i-k-1)} = \sum_{\ell=i-k}^{i} F_i^{(\ell)} p^{\ell-i+k} = p^k + \sum_{\ell=i-k}^{i-1} (1+p)^{i-\ell-1} p^{\ell-i+k} = (1+p)^k.$$

(b) Next we prove that when $0 \le p \le (\sqrt{5}-1)/2$ the time-reversal chain is stochastically monotone. Indeed, since $q_{ki} \le q_{k,i+1}$ for $2 \le i+1 < k$, it is easy to see that (2.1) holds for $i \ge 1$. For $i = 0$, (2.1) becomes

$$\sum_{k\ge j}(1+p)^{N-k-1}p^k \le (1+p)\sum_{k\ge j}(1+p)^{N-k-1}(1-p)p^{k-1} \quad \text{for } j \ge 1,$$

which is equivalent to $0 \le p \le (\sqrt{5}-1)/2$.

(c) If $0 \le p \le (\sqrt{5}-1)/2$, then the separation cutoff occurs by Corollary 1.1. If $p = 0$, then the birth and death process has the uniform stationary distribution, which was proved in [5], [9] that there is no separation cutoff.

This completes the proof. □

The rest of the paper is organized as follows. In Section 2 we give some properties for the upward skip-free chain. And in Section 3 we present a criterion for the separation cutoff of general Markov chains. Then in Section 4 we show the proofs for Theorem 1.1 and Corollary 1.1.

2. Finite upward skip-free chains

Define the time-reversal $\tilde{Q} = (\tilde{q}_{ij})$ of Q as

$$\tilde{q}_{ij} = \frac{\pi_j}{\pi_i} q_{ji}.$$

It is clear that the process corresponding to $\tilde{Q}$ is a downward skip-free chain. And by [3, Theorem 5.47], we can easily determine its equivalent condition to be stochastically monotone in the following.

Proposition 2.1. *The time-reversal chain of Q is stochastically monotone if and only if*

$$\sum_{k\ge j}\frac{F_N^{(k)}q_{ki}}{q_{k,k+1}} \le \frac{q_{i+1,i+2}F_N^{(i)}}{q_{i,i+1}F_N^{(i+1)}}\sum_{k\ge j}\frac{F_N^{(k)}q_{k,i+1}}{q_{k,k+1}} \quad \textit{for } i+1 < j \le N. \tag{2.1}$$

The following is a simple and practical condition for the time-reversal chain to be stochastically monotone.

Corollary 2.1. *Assume that $q_{i,i+1} \equiv \mathbf{1}_{\{i\ge 0\}}$. If $F_N^{(i)} \ge F_N^{(i+1)}$ for all $0 \le i < N-1$, and $q_{ki} \le q_{k,i+1}$ for all $k > i+1$, then the time-reversal chain is stochastically monotone.*

Under the assumption that the time-reversal chain is stochastically monotone, Fill obtained the following theorem in [8].

Theorem 2.1. *For an ergodic continuous-time upward skip-free chain on the state space $\{0,\ldots,N\}$ started at 0 and with stochastically monotone time-reversal, let Q be its generator. Then the FSST τ has the distribution with the following moment generating function:*

$$\mathbb{E}e^{-\lambda\tau} = \prod_{\nu=1}^{N}\frac{\lambda}{\lambda+\lambda_\nu}, \qquad \lambda > 0,$$

where $\lambda_1,\ldots,\lambda_N$ are the nonzero eigenvalues of $-Q$ and $\mathbb{E}$ is the expected value.

The following boundary theory will be useful for determining the distribution of the FSST. Recall that the hitting time of state k is defined as $\tau_k = \inf\{t \geq 0 \colon X_t = k\}$.

Lemma 2.1. *For the ergodic continuous-time upward skip-free chain X_t on $\{0, 1, \ldots, N\}$, let*

$$\phi_{iN}(\lambda) = 0, \qquad \phi_{ij}(\lambda) = \int_0^\infty \mathrm{e}^{-\lambda t} \mathbb{P}_i[X_t = j,\ t < \tau_N]\,\mathrm{d}t \quad \textit{for } 0 \leq i,\ j < N$$

and

$$\psi_{ij}(\lambda) = \int_0^\infty \mathrm{e}^{-\lambda t} \mathbb{P}_i[X_t = j]\,\mathrm{d}t \quad \textit{for } 0 \leq i,\ j \leq N.$$

It holds that

$$\psi_{ij}(\lambda) = \phi_{ij}(\lambda) + \frac{\xi_i(\lambda)\eta_j(\lambda)}{\lambda \sum_{j=0}^N \eta_j(\lambda)} \quad \textit{for } 0 \leq i,\ j \leq N,$$

where $\xi_i(\lambda) = 1 - \lambda \sum_{k=0}^{N-1} \phi_{ik}(\lambda)$, $\eta_j(\lambda) = \pi_j - \lambda \sum_{k=0}^{N-1} \pi_k \phi_{kj}(\lambda)$.

Proof. Since $(\phi_{ij}(\lambda))$ is the Laplace transform of the transition function for the process before X_t hitting N, it has the generator $\hat{Q} = (q_{ij}, 0 \leq i, j \leq N-1)$. Then we have the following Kolmogorov backward and forward equations:

$$\lambda \phi_{ij}(\lambda) - \sum_{k=0}^{N-1} q_{ik} \phi_{kj}(\lambda) = \delta_{ij}, \qquad 0 \leq i,\ j \leq N-1,$$

$$\lambda \phi_{ij}(\lambda) - \sum_{k=0}^{N-1} \phi_{ik}(\lambda) q_{kj} = \delta_{ij}, \qquad 0 \leq i,\ j \leq N-1.$$

It is straightforward to prove that $(\psi_{ij}(\lambda))$ satisfies the Kolmogorov equations associated to Q and the details are omitted here. □

3. A general condition for separation cutoff

In order to use Theorem 2.1 to derive the criterion, we need the following result. This result was originated in [5] and completed recently in [9].

Proposition 3.1. *For each n, let $\tau^{(n)}$ be a FSST of the ergodic Markov chain $X_t^{(n)}$. Assume that there is $C < \infty$ such that*

$$\mathbb{E}(\tau^{(n)})^3 \leq C(\mathbb{E}\tau^{(n)})^3 \quad \textit{for all } n \geq 1. \tag{3.1}$$

Then there exists the separation cutoff in (1.1) with $t_n = \mathbb{E}\tau^{(n)}$ if and only if

$$\frac{(\mathbb{E}\tau^{(n)})^2}{\operatorname{var}(\tau^{(n)})} \to \infty \quad \textit{or, equivalently,} \quad \frac{(\mathbb{E}\tau^{(n)})^2}{\mathbb{E}(\tau^{(n)})^2} \to 1 \quad \textit{as } n \to \infty. \tag{3.2}$$

Proof. Set

$$\xi^{(n)} = \frac{\tau^{(n)}}{\mathbb{E}\tau^{(n)}}.$$

By (1.1) and (1.2), the separation cutoff in (1.1) with $t_n = \mathbb{E}\tau^{(n)}$ is equivalent to $\xi^{(n)}$ converging to 1 in probability as $n \to \infty$. On the other hand, since

$$\mathbb{E}(\xi^{(n)} - 1)^2 = \frac{\mathbb{E}(\tau^{(n)})^2}{(\mathbb{E}\tau^{(n)})^2} - 1,$$

(3.2) means that $\xi^{(n)}$ converges to 1 in $L^2(\mathbb{P})$. If (3.1) holds, then $\{\xi^{(n)}\}$ is uniformly integrable, which implies that the separation cutoff is equivalent to (3.2). □

We remark that the integrability condition (3.1) is natural for Markov chains. For example, if $X_t^{(n)}$ is a family of upward skip-free chains started at 0 and with stochastically monotone time-reversals, then, from Theorem 2.1, we can easily obtain

$$\mathbb{E}(\tau^{(n)})^k \le k!\,(\mathbb{E}\tau^{(n)})^k, \qquad k = 1, 2, \dots .$$

4. Explicit criterion

In this section we will obtain the explicit criterion for the separation cutoff of upward skip-free chains by deriving the explicit expressions of $\mathbb{E}\tau^{(n)}$ and $\mathbb{E}(\tau^{(n)})^2$ in Proposition 3.1. In the following theorem, we first study the distribution of the FSST.

Theorem 4.1. *Assume that X_t is an ergodic upward skip-free chain on $\{0, 1, \dots, N\}$, started at 0 and with the stochastically monotone time-reversal. Let τ be a FSST and $P_i(t) = \mathbb{P}_0[X_t = i]$ for $0 \le i \le N$. Then*

(i) $\mathbb{P}[\tau > t] = 1 - P_N(t)/\pi_N$;

(ii) *it holds that*

$$\mathbb{E}\mathrm{e}^{-\lambda\tau} = \frac{\lambda}{\pi_N}\int_0^\infty \mathrm{e}^{-\lambda t} P_N(t)\,\mathrm{d}t, \qquad \lambda \ge 0. \tag{4.1}$$

Proof of Theorem 4.1(i). Let $p_{ij}(t) = \mathbb{P}_i[X_t = j]$ and X_t^* be the time-reversal chain of X_t. Then

$$p^*_{ij}(t) := \mathbb{P}_i[X_t^* = j] = \frac{\pi_j p_{ji}(t)}{\pi_i}.$$

Since X_t^* is stochastically monotone, we have

$$\frac{p_{0N}(t)}{\pi_N} = \frac{p^*_{N0}(t)}{\pi_0} = \frac{\min_i p^*_{i0}(t)}{\pi_0} = \frac{\min_i p_{0i}(t)}{\pi_i}.$$

Thus, by (1.2),

$$\frac{1 - P_N(t)}{\pi_N} = \max_i\left(1 - \frac{p_{0i}(t)}{\pi_i}\right) = \mathbb{P}[\tau > t]. \qquad \square$$

Proof of Theorem 4.1(ii). For $\lambda \ge 0$, the integration by parts gives that

$$\mathbb{E}\mathrm{e}^{-\lambda\tau} = \lambda\int_0^\infty \mathrm{e}^{-\lambda t}\mathbb{P}[\tau \le t]\,\mathrm{d}t.$$

Then (4.1) follows from Theorem 4.1(i). □

To derive the explicit formulae for the moments of the FSST, we need the boundary theory below, which establishes a relationship between the FSST and the hitting times.

Theorem 4.2. *For the chain X_t defined in Theorem 4.1, the Laplace transform of the FSST can be expressed as*

$$\mathbb{E}\mathrm{e}^{-\lambda\tau} = \left(\pi_0 + \sum_{k=1}^N \pi_k(\mathbb{E}_0\mathrm{e}^{-\lambda\tau_k})^{-1}\right)^{-1}, \qquad \lambda \ge 0. \tag{4.2}$$

Proof. By Lemma 2.1 and the integration by parts formula, we have

$$\xi_k(\lambda) = \lambda \int_0^\infty e^{-\lambda t} \mathbb{P}_k[\tau_N \le t]\, dt = \int_0^\infty e^{-\lambda t}\, d(\mathbb{P}_k[\tau_N \le t]) = \mathbb{E}_k e^{-\lambda \tau_N} \quad \text{for } 0 \le k \le N.$$

Using the skip-free property and the strong Markov property, we obtain

$$\xi_0(\lambda) = \mathbb{E}_0 e^{-\lambda \tau_N} = \mathbb{E}_0 e^{-\lambda \tau_k} \mathbb{E}_k e^{-\lambda \tau_N} = \mathbb{E}_0 e^{-\lambda \tau_k} \xi_k(\lambda).$$

As $\phi_{0N}(\lambda) = 0$, $\eta_N(\lambda) = \pi_N$, and $\sum_{j=0}^N \eta_j(\lambda) = \sum_{k=0}^N \pi_k \xi_k(\lambda)$, we have

$$\psi_{0N}(\lambda) = \frac{\xi_0(\lambda)\pi_N}{\lambda \sum_{k=0}^N \pi_k \xi_k(\lambda)} = \frac{\pi_N}{\lambda \sum_{k=0}^N \pi_k (\mathbb{E}_0 e^{-\lambda \tau_k})^{-1}}.$$

Then by Theorem 4.1, we have

$$\mathbb{E} e^{-\lambda \tau} = \frac{\lambda}{\pi_N} \psi_{0N}(\lambda) = \left[\pi_0 + \sum_{k=1}^N \pi_k (\mathbb{E}_0 e^{-\lambda \tau_k})^{-1}\right]^{-1}. \qquad \square$$

Now we can deduce the explicit criteria of the separation cutoff in Theorem 1.1 and Corollary 1.1.

Proof of Theorem 1.1. For the chain X_t in Theorem 4.1, we can obtain by (4.2) the explicit expressions for the moments of the FSST τ from those of the hitting times $\{\tau_k\}$. In fact, by taking derivatives in (4.2) twice, we obtain

$$\mathbb{E}\tau = \sum_{i=0}^N \pi_i \mathbb{E}_0 \tau_i, \qquad \mathbb{E}\tau^2 = 2(\mathbb{E}\tau)^2 + \sum_{i=0}^N \pi_i \mathbb{E}_0 \tau_i^2 - 2\sum_{i=0}^N \pi_i (\mathbb{E}_0 \tau_i)^2,$$

while by [10],

$$\mathbb{E}_0 \tau_i = \sum_{k=0}^{i-1} m_k, \qquad \mathbb{E}_0 \tau_i^2 = 2(\mathbb{E}_0 \tau_i)^2 - 2\sum_{k=0}^{i-1} \sum_{\ell=0}^{k} \frac{F_k^{(\ell)}}{q_{\ell,\ell+1}} \mathbb{E}_0 \tau_\ell,$$

from which we can easily obtain

$$\mathbb{E}\tau^2 = 2(\mathbb{E}\tau)^2 - 2\sum_{i=0}^N \pi_i \sum_{j=0}^{i-1} \sum_{k=0}^{j} \frac{F_j^{(k)}}{q_{k,k+1}} \mathbb{E}_0 \tau_k.$$

Let S, T be as in (1.6). Then, we have

$$\frac{\mathbb{E}\tau^2}{(\mathbb{E}\tau)^2} = 2\left(1 - \frac{S}{T^2}\right).$$

Thus, Theorem 1.1 follows from Proposition 3.1. $\square$

Proof of Corollary 1.1. For simplicity, we omit the superscript (n) in the proof below. By (1.4) and (1.5), we have

$$m_i \sim \frac{\beta^{i+1}}{(\beta - 1)}, \qquad \pi_i = \frac{F_N^{(i)}}{m_N} \sim (\beta - 1)\beta^{-i-1}.$$

Thus,

$$T = \sum_{i=0}^{N} \pi_i \sum_{j=0}^{i-1} m_j \sim \sum_{i=0}^{N} \beta^{-i-1} \sum_{j=0}^{i-1} \beta^{j+1} \sim \frac{N}{\beta - 1}$$

and

$$\begin{aligned} S &= \sum_{i=0}^{N} \pi_i \sum_{j=0}^{i-1} \sum_{k=0}^{j} F_j^{(k)} \sum_{l=0}^{k-1} m_l \\ &\sim \sum_{i=0}^{N} \pi_i \sum_{j=0}^{i-1} \frac{j\beta^{j+1}}{(\beta - 1)^2} \\ &\sim \sum_{i=0}^{N} \pi_i \frac{i\beta^{i+1}}{(\beta - 1)^3} \\ &\sim \frac{1}{(\beta - 1)^2} \sum_{i=0}^{N} i \\ &\sim \frac{N^2}{2(\beta - 1)^2}. \end{aligned}$$

Therefore, $S/T^2 \sim \frac{1}{2}$, which implies the separation cutoff by Theorem 1.1. □

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