

The number of distinct adjacent pairs in geometrically distributed words: a probabilistic and combinatorial analysis

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Abstract

The analysis of strings of n random variables with geometric distribution has recently attracted renewed interest: Archibald et al. consider the number of distinct adjacent pairs in geometrically distributed words. They obtain the asymptotic ($n \rightarrow \infty$) mean of this number in the cases of different and identical pairs. In this paper we are interested in all asymptotic moments in the identical case, in the asymptotic variance in the different case and in the asymptotic distribution in both cases. We use two approaches: the first one, the probabilistic approach, leads to variances in both cases and to some conjectures on all moments in the identical case and on the distribution in both cases. The second approach, the combinatorial one, relies on multivariate pattern matching techniques, yielding exact formulas for first and second moments. We use such tools as Mellin transforms, Analytic Combinatorics, Markov Chains.

Keywords: Geometrically distributed words, Number of distinct adjacent pairs, Equal pairs, Distinct pairs, Moments, Asymptotic distribution

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1 Introduction

We follow the notation and setup of Archibald et al. [1]. Let us consider a string of n random variables Z_1, Z_2, \dots, Z_n , with geometric distribution $\mathbb{P}(Z_k = i) = P_i := pq^{i-1}$ for $i \geq 1$. In the sequel, all asymptotics will be related to $n \rightarrow \infty$. We will use the following notations. Many of the results are obtained by studying the precise distribution of the number of times that (i, j) appears as a consecutive pair or couple in Z_1, Z_2, \dots, Z_n , i.e., the number of k 's such that $X_k = i$ and $X_{k+1} = j$. We define

$$\begin{aligned} X_{i,j}^{(n)}(m) &:= \llbracket \text{couple } (i, j) \text{ appears } m \text{ times in the string of size } n \rrbracket, \\ X_{i,j}^{(n)} &:= 1 - X_{i,j}^{(n)}(0) := \llbracket \text{couple } (i, j) \text{ appears at least once in the string of size } n \rrbracket, \\ X_1^{(n)} &:= \sum_{i \geq 1} X_{i,i}^{(n)}, \\ X_2^{(n)} &:= \sum_{i,j \geq 1} X_{i,j}^{(n)}, \\ X_3^{(n)} &:= \sum_{i \neq j} X_{i,j}^{(n)}. \end{aligned}$$

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Asymptotic expressions for the moments are obtained by Mellin transforms applied to Harmonic sums (see for instance, Flajolet, Gourdon, Dumas [3] for a nice exposition). We can derive the dominant part of moments as well as the (tiny) periodic part in the form of a Fourier series.

The paper is organized as follows: In Section 2 we present our main results, that is, asymptotic expressions for the variances of $X_k^{(n)}$, $1 \leq k \leq 3$, and a result concerning asymptotic independence of $X_{i,i}^{(n)}$, $i \in \mathbb{N}$. In Section 3 we conjecture some stronger forms of asymptotic independence, based on which we are able to derive the limiting distribution and asymptotics of higher moments of $X_1^{(n)}$. Section 4 is devoted to the proofs of these results, and to some considerations in support of a conjectured Gaussian limiting distribution of $X_3^{(n)}$. In Section 5 we use a combinatorial approach to derive exact expressions for first and second moments of $X_k^{(n)}$, $1 \leq k \leq 3$. In an Appendix we collect our results pertaining to Mellin transforms.

2 Main results

In a private communication, B. Pittel observed that the asymptotic distribution of $X_{i,j}^{(n)}(m)$ is Poisson,

$$\mathbb{P}[X_{i,j}^{(n)}(m) = 1] \sim e^{-\lambda} \frac{\lambda^m}{m!}, \text{ where } \lambda = nP_i P_j.$$

Asymptotics of $\mathbb{E}X_1^{(n)}$, $\mathbb{E}X_2^{(n)}$ and $\mathbb{E}X_3^{(n)}$ have also recently been obtained by [1], using generating functions of the sequences of expectations. One of our main results deals with asymptotics of $\text{Var} X_i^{(n)}$, $1 \leq i \leq 3$, as $n \rightarrow \infty$. Our approach simply consists in using $\text{Var} X_1^{(n)} = \sum_{i \geq 1} \text{Var} X_{i,i}^{(n)} + \sum_{i \neq j} \text{Cov}(X_{i,i}^{(n)}, X_{j,j}^{(n)})$, and similarly for $\text{Var} X_2^{(n)}$ and $\text{Var} X_3^{(n)}$. This necessitates thorough investigation of the involved covariances. As it turns out, the main term of $\text{Var} X_1^{(n)}$ is given by a term $S_1^{(n)} \sim \sum_{i \geq 1} \text{Var} X_{i,i}^{(n)}$, the double sum of covariances only contributing $\mathcal{O}(\frac{1}{n})$. This is different for $\text{Var} X_2^{(n)}$, whose main term is a sum of $S_2^{(n)} \sim \sum_{i,j \geq 1} \text{Var} X_{i,j}^{(n)}$ and another contribution $T_2^{(n)}$, stemming from the quadruple sum of covariances of different pairs, of order $\Theta(1)$. All of $S_1^{(n)}$, $S_2^{(n)}$, and $T_2^{(n)}$ are expressed in terms of Fourier series in $\ln(np^2)$. A plot of the constant term of $T_2^{(n)}$ is provided in Figure 1.

Theorem 2.1 *Let $L := \ln(1/q)$ and $\chi := 2\pi\mathbf{i}/L$, where \mathbf{i} denotes the imaginary unit. We also define*

$$S_1^{(n)} := \frac{\ln 2}{2L} + \frac{1}{2L} \sum_{\ell \neq 0} \Gamma\left(\frac{\ell\chi}{2}\right) (np^2)^{-\frac{\ell\chi}{2}} \left(1 - 2^{-\frac{\ell\chi}{2}}\right), \quad (1)$$

$$S_2^{(n)} := \frac{\ln 2}{L^2} \ln(np^2) + \frac{\ln 2}{2L^2} (2\gamma + \ln 2 + 2L) + \frac{\ln(np^2)}{L^2} \sum_{\ell \neq 0} \Gamma(\ell\chi) (np^2)^{-\ell\chi} (1 - 2^{-\ell\chi}) \quad (2)$$

$$- \frac{1}{L^2} \sum_{\ell \neq 0} \Gamma(\ell\chi) (np^2)^{-\ell\chi} \left[(1 - 2^{-\ell\chi}) \left(\frac{\Gamma'(\ell\chi)}{\Gamma(\ell\chi)} - L \right) + 2^{-\ell\chi} \ln 2 \right]$$

$$T_2^{(n)} := \frac{2}{L} F_1'(0) + \frac{2}{L} \sum_{\ell \neq 0} \Gamma(\ell\chi) F_1(\ell\chi) (np^2)^{-\ell\chi}, \quad (3)$$

where $F_1(s) = \sum_{i,k \geq 1} [(q^i + q^k - pq^{i+k-1})^{-s} - (q^i + q^k)^{-s}]$, and the constant term of $T_2^{(n)}$ simplifies to

$$\frac{2}{L} F_1'(0) = -\frac{2}{L} \ln \left(\prod_{i,j \geq 1} \left(1 - \frac{p}{q} \frac{q^{i+j}}{q^i + q^j} \right) \right).$$

Then, as $n \rightarrow \infty$, the variances of $X_i^{(n)}$, $1 \leq i \leq 3$, satisfy

$$\text{Var } X_1^{(n)} = S_1^{(n)} + \mathcal{O}\left(\frac{1}{\sqrt{n}}\right), \quad (4)$$

$$\text{Var } X_2^{(n)} = S_2^{(n)} + T_2^{(n)} + \mathcal{O}\left(\frac{\ln n}{\sqrt{n}}\right), \quad (5)$$

$$\text{Var } X_3^{(n)} = S_2^{(n)} - S_1^{(n)} + T_2^{(n)} + \mathcal{O}\left(\frac{\ln n}{\sqrt{n}}\right). \quad (6)$$

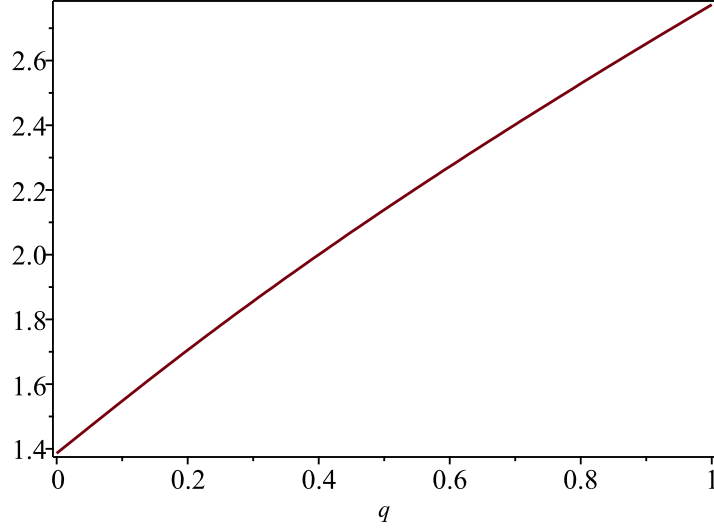


Figure 1: Plot of $2(1-q)F'_1(0)$, showing the dependence of the constant term $\frac{2}{L}F'_1(0)$ on q . We leave it as an exercise to show that, for $q \rightarrow 0$ (resp. $q \rightarrow 1$), the limit is $2 \ln 2$ (resp. $4 \ln 2$).

A question triggered by the observation that $\sum_{i \neq j} \text{Cov}(X_{i,i}^{(n)}, X_{j,j}^{(n)}) = \mathcal{O}\left(\frac{1}{n}\right)$ is: How “close to being independent” are $(X_{i,i}^{(n)})_{i \in \mathbb{N}}$? The following theorem provides a partial answer in that regard.

Theorem 2.2 *The random variables $X_{i,i}^{(n)}$, $i \in \mathbb{N}$ are asymptotically independent, in the sense that, for any $k \in \mathbb{N}$, any subset $I \subseteq \mathbb{N}$ of size k , and any $(x_i)_{i \in I} \in \{0, 1\}^k$ we have*

$$\mathbb{P}(X_{i,i}^{(n)} = x_i, i \in I) - \prod_{i \in I} \mathbb{P}(X_{i,i}^{(n)} = x_i) = \mathcal{O}\left(\frac{1}{n}\right), \quad (7)$$

with implied constant depending on I only via k .

Conjecture 2.3 *The same kind of asymptotic independence as in Theorem 2.2 holds for $(X_{k_i, m_i}^{(n)})_{i \geq 1}$, when the sets $\{k_i, m_i\}$ are pairwise disjoint.*

Remark 2.4 *The random variables $(X_{i,i}^{(n)})_{i \geq 1}$ are negatively correlated: For finite $I \subseteq \mathbb{N}$ we have*

$$\mathbb{P}(X_{i,i}^{(n)} = 1, i \in I) \leq \prod_{i \in I} \mathbb{P}(X_{i,i}^{(n)} = 1),$$

as can easily be deduced from the theorem in [8]. Cases like the following for $n = 5$ and $i \neq j$,

$$\begin{aligned} & \mathbb{P}(X_{i,i}^{(5)} = 1) \mathbb{P}(X_{j,j}^{(5)} = 1) - \mathbb{P}(X_{i,i}^{(5)} = X_{j,j}^{(5)} = 1) \\ &= P_i^2(4 - 2P_i - 2P_i^2 + P_i^3)P_j^2(4 - 2P_j - 2P_j^2 + P_j^3) - P_i^2P_j^2(6 - 2P_i - 2P_j) \\ &= P_i^2P_j^2 [(1 - P_i - P_j)(10 + 4P_i(1 - P_i) + 4P_j(1 - P_j)) + P_iP_j(12 + P_i(2 - P_i)P_j(2 - P_j) - 2P_i^2 - 2P_j^2)] > 0 \end{aligned}$$

suggest that the inequality may be strict for $|I| \geq 2$. This is different for the array $(X_{i,j}^{(n)})_{i,j \geq 1}$, where both strictly positive and strictly negative correlations can be observed: For $n = 3$ and $i \neq j$,

$$\mathbb{P}(X_{i,j}^{(3)} = X_{j,i}^{(3)} = 1) - \mathbb{P}(X_{i,j}^{(3)} = 1)\mathbb{P}(X_{j,i}^{(3)} = 1) = P_i P_j (P_i + P_j) - (2P_i P_j)^2 = P_i P_j (P_i + P_j - 4P_i P_j) > 0$$

holds for P_i, P_j small enough, and for different pairs $((k_i, m_i))_{i \in I}$, with $|I| \geq n$, we clearly have

$$\mathbb{P}(X_{k_i, m_i}^{(n)} = 1, i \in I) = 0 < \prod_{i \in I} \mathbb{P}(X_{k_i, m_i}^{(n)} = 1).$$

3 Further conjectures and results for pairs of identical letters

3.1 Higher moments

The proof of Theorem 2.1 (see Lemma 4.8) shows that $\lim_{n \rightarrow \infty} (\text{Var } X_1^{(n)} - \text{Var } \xi^{(n)}) = 0$, where $\xi^{(n)} := \sum_{i \geq 1} \mathbb{1}[\xi_i^{(n)} \geq 1]$ is a sum of independent random variables, with $\xi_i^{(n)}$ distributed as $\text{Poisson}(nP_i^2)$. Note that $\mathbb{P}[X_{i,i}^{(n)} = 0] \sim \mathbb{P}[\xi_i^{(n)} = 0]$ and $\mathbb{P}[X_{i,i}^{(n)} = 1] \sim \mathbb{P}[\xi_i^{(n)} \geq 1]$. This leads us to the following conjecture.

Conjecture 3.1 For any $k \in \mathbb{N}$ we have $\lim_{n \rightarrow \infty} (\mathbb{E}|X_1^{(n)} - \mathbb{E}X_1^{(n)}|^k - \mathbb{E}|\xi^{(n)} - \mathbb{E}\xi^{(n)}|^k) = 0$.

Theorem 3.2 If Conjecture 3.1 holds, the asymptotics of cumulants $\kappa_m^{(n)}$ of $X_1^{(n)}$ are given by (9), where $V_j^{(n)}$, $j \geq 1$, are given by (8).

We proceed as in Hitczenko and Louchard [5] and Louchard and Prodinger [6].

Let $S_n(\theta) := \ln(\mathbb{E}(e^{\theta \xi^{(n)}})) = \sum_{m=1}^{\infty} \kappa_m^{(n)} \frac{\theta^m}{m!}$ be the cumulant generating function of $\xi^{(n)}$. Furthermore let $n_2 := np^2/q^2$, and observe $\mathbb{E}e^{\theta \mathbb{1}[\xi_i^{(n)} \geq 1]} = 1 + (e^\theta - 1)(1 - e^{-n_2 q^{2i}})$. By independence of $(\xi_i^{(n)})_{i \geq 1}$, we get

$$\begin{aligned} S_n(\theta) &= \sum_{i=1}^{\infty} \ln \left[1 + (e^\theta - 1) (1 - e^{-n_2 q^{2i}}) \right] \\ &= \sum_{j=1}^{\infty} \frac{(-1)^{j+1}}{j} (e^\theta - 1)^j \left[\sum_{i=1}^{\infty} (1 - e^{-n_2 q^{2i}})^j \right]. \end{aligned}$$

Now let

$$\begin{aligned} V_j^{(n)} &:= \sum_{i=1}^{\infty} (1 - e^{-n_2 q^{2i}})^j = \sum_{i=1}^{\infty} \left[\sum_{k=0}^j (-1)^k \binom{j}{k} e^{-kn_2 q^{2i}} \right] \\ &= \sum_{i=1}^{\infty} \left[\sum_{k=0}^j (-1)^k \binom{j}{k} e^{-kn_2 q^{2i}} - \sum_{k=0}^j (-1)^k \binom{j}{k} \right] = \sum_{i=1}^{\infty} \left[\sum_{k=1}^j (-1)^{k+1} \binom{j}{k} (1 - e^{-kn_2 q^{2i}}) \right] \\ &= \sum_{k=1}^j (-1)^{k+1} \binom{j}{k} \sum_{i=1}^{\infty} (1 - e^{-kn_2 q^{2i}}), \end{aligned}$$

where the asymptotics of the inner sum can be obtained using $G(knp^2)$ from Appendix A.1. Setting again $L := \ln(1/q)$, this leads to

$$\begin{aligned} V_j^{(n)} &\sim \frac{\ln(np^2)}{2L} + \frac{\gamma}{2L} + \frac{1}{2} + \frac{1}{2L} \sum_{k=2}^j (-1)^{k+1} \binom{j}{k} \ln k \\ &\quad + \frac{1}{2L} \sum_{\ell \neq 0} \left(\sum_{k=1}^j (-1)^k \binom{j}{k} k^{-\frac{\ell \chi}{2}} \right) \Gamma\left(\frac{\ell \chi}{2}\right) (np^2)^{-\frac{\ell \chi}{2}}, \end{aligned} \tag{8}$$

Finally the cumulants are given by finite linear combinations of the $(V_j^{(n)})_{j \geq 1}$,

$$\kappa_m^{(n)} = [\theta^m] m! \sum_{j=1}^{\infty} \frac{(-1)^{j+1}}{j} (e^\theta - 1)^j V_j^{(n)} = m! \sum_{j=1}^m V_j^{(n)} \frac{(-1)^{j+1}}{j} [\theta^m] (e^\theta - 1)^j, \quad (9)$$

explicit expressions for small m being

$$\kappa_1^{(n)} = V_1^{(n)}, \quad \kappa_2^{(n)} = V_1^{(n)} - V_2^{(n)}, \quad \kappa_3^{(n)} = V_1^{(n)} - 3V_2^{(n)} + 2V_3^{(n)}, \quad \kappa_4^{(n)} = V_1^{(n)} - 7V_2^{(n)} + 12V_3^{(n)} - 6V_4^{(n)}.$$

The sequence of (absolute values of) the coefficients, $(1, 1, 1, 1, 3, 2, 1, 7, 12, 6, \dots)$, seems to coincide with sequence A028246 in the OEIS [14].

The cumulants now allow for computation of moments: The mean of $X_1^{(n)}$ is given by

$$\mathbb{E}X_1^{(n)} \sim V_1^{(n)}.$$

This is identical to Archibald et al. [1, Thm.2], see also (11). Our approach here is simple and general. Note that the mean does not rely on the state of Conjecture 3.1: the mean computation actually depends only on Lemma 4.3. Similarly, the variance of $X_1^{(n)}$ is given by

$$\text{Var } X_1^{(n)} \sim V_1^{(n)} - V_2^{(n)}.$$

After some algebra, we verify that this is identical to Thm 2.1 .

3.2 Limiting distribution

A conjecture weaker than Conjecture 3.1 is

Conjecture 3.3 *For any $t \in \mathbb{R}$ we have $\lim_{n \rightarrow \infty} [\mathbb{P}(X_1^{(n)} \leq t) - \mathbb{P}(\xi^{(n)} \leq t)] = 0$.*

Theorem 3.4 *If Conjecture 3.3 holds, the asymptotic distribution $f(\eta)$ of $X_1^{(n)}$ is given by (10).*

Set again $L = \ln(1/q)$ and $n_2 = np^2/q^2$, set $i^* = \ln(n_2)/(2L)$ (implying $q^{2i^*} = 1/n_2$), define $\eta := i - i^*$, and use $\mathbb{P}(\xi_i^{(n)} = 0) = e^{-n_2 q^{2i}} = \exp(-e^{-2L\eta})$. This leads to

$$\mathbb{P}(\xi_k^{(n)} = 0, k > i) = \exp(-\alpha e^{-2L\eta}), \text{ where } \alpha := \frac{q^2}{1 - q^2}.$$

As in Hitczenko and Louchard [5] and Louchard, Prodinger and Ward [7], we proceed by defining

$$\Psi(\eta) := e^{-e^{-2L\eta}} \prod_{i=1}^{\infty} \left[1 - e^{-e^{-2L(\eta-i)}} \right],$$

and observing that, as $n \rightarrow \infty$, we have

$$\begin{aligned} \mathbb{P}(X_1^{(n)} = i^* + \eta) &\sim f(\eta) := \sum_{v=0}^{\infty} \Psi(\eta - v + 1) e^{-\alpha e^{-2L(\eta+1-v)}} \sum_{\substack{r_1 < \dots < r_v \\ r_j \geq 2-v}} \prod_{i=1}^v \frac{1 - e^{-e^{-2L(\eta+r_i)}}}{e^{-e^{-2L(\eta+r_i)}}}, \quad (10) \\ \mathbb{P}(X_1^{(n)} \leq i^* + \eta) &\sim F(\eta) := \sum_{i=0}^{\infty} f(\eta - i). \end{aligned}$$

$f(\eta)$ depends only on p .

A simulation with $p = 1/4$ and 50000 simulated words for each $n \in \{10000, 11547, 13333, 15396\}$ is given in Figure 2. The fit is excellent. A corresponding table of observed and theoretical non-periodic mean and variance in the equal pairs case (as well as another table for the unequal pairs

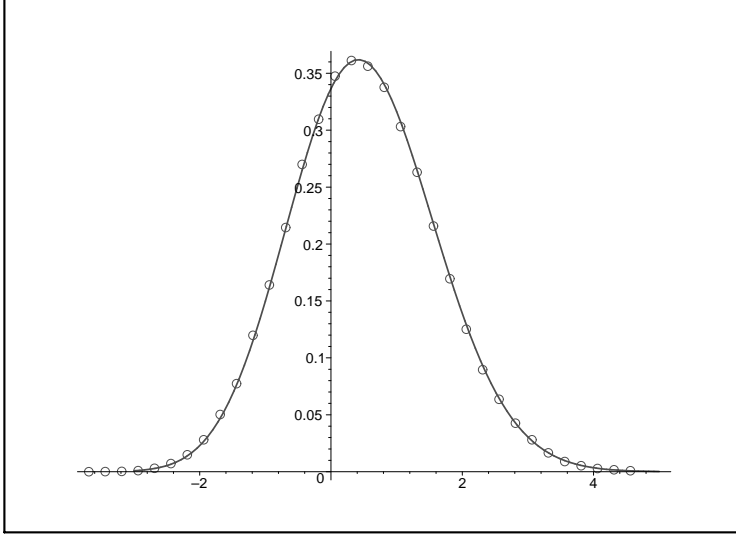


Figure 2: Comparison between $f(\eta)$ (line) and the simulation of $X_1^{(n)}$ (circles), $p = 1/4$, number of simulated words = 50000 for each $n \in \{10000, 11547, 13333, 15396\}$.

case) is given below, all results rounded to 3 decimal places. We define $\bar{X}_j^{(n)} := \frac{1}{N} \sum_{i=1}^N X_j^{(n),i}$ and $s_j^2(n) := \frac{1}{N-1} \sum_{i=1}^N (X_j^{(n),i} - \bar{X}_j^{(n)})^2$ the sample mean and unbiased sample variance of a sample $(X_j^{(n),i})_{i=1}^N$. See Theorem 3.6 for asymptotics of $\mathbb{E}X_1^{(n)}$ and $\mathbb{E}X_3^{(n)}$. Both simulations use $p = 1/4$. The sample size N for each row in the left table is 50000, and in the right table it is 200000, see also Figure 3.

n	$\mathbb{E}X_1^{(n)}$	$\bar{X}_1^{(n)}$	$\text{Var } X_1^{(n)}$	$s_1^2(n)$
10000	12.692	12.676	1.205	1.214
11547	12.942	12.927	1.205	1.206
13333	13.192	13.175	1.205	1.213
15396	13.442	13.427	1.205	1.211

n	$\mathbb{E}X_3^{(n)}$	$\bar{X}_3^{(n)}$	$\text{Var } X_3^{(n)}$	$s_3^2(n)$
500000	750.195	750.198	129.889	130.053

Remark 3.5 Here we briefly sketch, how we obtained the graph of f in Figure 2, where $p = 1/4$. As before, we use random variables $\xi_i^{(n)}$ distributed $\text{Poisson}(np^2q^{2(i-1)})$, but now there is such a random variable for each $i \in \mathbb{Z}$ and each real $n > 0$. For fixed such n the random variables $(\xi_i^{(n)})_{i \in \mathbb{Z}}$ are assumed independent, and also the definition $\xi^{(n)} := \sum_{i \geq 1} \xi_i^{(n)}$ is used for real $n > 0$. We use $i^* = i^*(n) = \ln(np^2/q^2)/(2L)$ again. For any n satisfying $i^* + \eta \in \mathbb{Z}$, we have

$$\begin{aligned}
 f(\eta) &= \lim_{k \rightarrow \infty} \mathbb{P}\left(\xi^{(nq^{-2k})} - k = i^* + \eta\right) = \mathbb{P}\left(\sum_{i \geq 1} \mathbb{I}[\xi_i^{(n)} \geq 1] + \sum_{j \geq 0} (\mathbb{I}[\xi_{-j}^{(n)} \geq 1] - 1) = i^* + \eta\right) \\
 &= \mathbb{P}\left(\sum_{i \geq 1} \mathbb{I}[\xi_i^{(\nu)} \geq 1] + \sum_{j \geq 0} (\mathbb{I}[\xi_{-j}^{(\nu)} \geq 1] - 1) = 0\right),
 \end{aligned}$$

where for $n = \nu = \nu(\eta) := q^{2(1-\eta)}/p^2$ we have $i^* + \eta = 0$, and $\xi_i^{(\nu)} \sim \text{Poisson}(q^{2(i-\eta)})$. We want a good approximation of $f(\eta)$ only for $\eta \in [-3, 5]$. For such η we have

$$\mathbb{P}\left(\sum_{i > 30} \mathbb{I}[\xi_i^{(\nu)} \geq 1] > 0\right) = 1 - \prod_{i > 30} e^{-q^{2i-2\eta}} \leq 1 - \prod_{i > 30} e^{-q^{2i-10}} = 1 - \exp\left(-\frac{q^{52}}{1-q^2}\right) \approx 7.28 \cdot 10^{-7}.$$

and

$$\mathbb{P}\left(\sum_{j>7}(\llbracket \xi_{-j}^{(\nu)} \geq 1 \rrbracket - 1) < 0\right) = 1 - \prod_{j>7} (1 - e^{-q^{-2j-2\eta}}) \leq \sum_{j>7} e^{-q^{6-2j}} \approx e^{-q^{-10}} \approx 1.94 \cdot 10^{-8}.$$

So, up to an error smaller than 10^{-6} , $f(\eta)$ is given by

$$\mathbb{P}\left(\sum_{i=1}^{30} \llbracket \xi_i^{(\nu)} \geq 1 \rrbracket + \sum_{j=0}^7 (\llbracket \xi_{-j}^{(\nu)} \geq 1 \rrbracket - 1) = 0\right) = \mathbb{P}\left(\sum_{i=-7}^{30} \llbracket \xi_i^{(\nu)} \geq 1 \rrbracket = 8\right) = [z^8] \prod_{i=-7}^{30} \left(1 + (z-1)(1 - e^{-q^{2i-2\eta}})\right),$$

where, for each fixed η , the latter coefficient can easily be computed using Maple.

Theorem 3.6 (see [1, Thm. 2, Thm. 3]) *Let $L := \ln(1/q)$ and $\chi := 2\pi i/L$. Then, as $n \rightarrow \infty$, the expectations of $X_i^{(n)}$, $i \in \{1, 3\}$, satisfy*

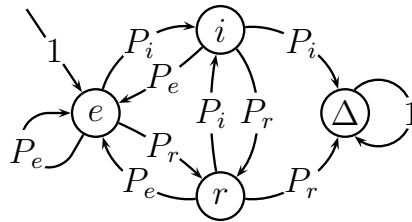
$$\mathbb{E}X_1^{(n)} \sim \frac{\ln(np^2)}{2L} + \frac{1}{2} + \frac{\gamma}{2L} - \frac{1}{2L} \sum_{\ell \neq 0} \Gamma\left(\frac{\ell\chi}{2}\right) (np^2)^{-\ell\chi/2}, \quad (11)$$

$$\begin{aligned} \mathbb{E}X_3^{(n)} \sim & \frac{\ln^2(np^2)}{2L^2} + \left[\frac{\gamma}{L^2} + \frac{1}{2L}\right] \ln(np^2) + \frac{\pi^2 + 6\gamma^2}{12L^2} + \frac{\gamma}{2L} - \frac{1}{12} \\ & - \frac{\ln(np^2)}{L^2} \sum_{\ell \neq 0} \Gamma(\ell\chi) (np^2)^{-\ell\chi} \\ & + \frac{1}{L^2} \sum_{\ell \neq 0} \Gamma'(\ell\chi) (np^2)^{-\ell\chi} - \frac{1}{2L} \sum_{\ell \neq 0} (-1)^\ell \Gamma\left(\frac{\ell\chi}{2}\right) (np^2)^{-\ell\chi/2}. \end{aligned} \quad (12)$$

4 The probability of avoiding certain pairs via Markov chains.

4.1 Two pairs (i, i) and (r, r) of identical letters

The proofs of the theorems rest upon calculation of probabilities of avoiding certain pairs, which we will be doing by employing Markov chains. To illustrate that approach, we consider in greater detail the case of avoiding two fixed pairs (i, i) and (r, r) , where $i \neq r$, in a sequence of length n . No distinction of letters different from i, r is necessary, so for our Markov chain we can use a finite state space $S := \{e, i, r, \Delta\}$, where $e := \mathbb{N} \setminus \{i, r\}$ stands for “everything else”, i.e., the set $\mathbb{N} \setminus \{i, r\}$ is lumped together, and Δ denotes an additional cemetery state. The corresponding state diagram is



From any realization $(z_k)_{k \geq 1}$ of the i.i.d. sequence $(Z_k)_{k \geq 1}$ we obtain a trajectory $(y_k)_{k \geq 0}$ of this finite state Markov chain via

$$(y_0, y_1, y_2, \dots) = (e, \phi(z_1), \phi(z_2), \phi(z_3), \dots),$$

where $\phi(z_k) := \Delta$ if for some $j < k$ we have $(z_j, z_{j+1}) \in \{(i, i), (r, r)\}$, and otherwise

$$\phi(z_k) = \begin{cases} z_k, & z_k \in \{i, r\} \\ e, & \text{else.} \end{cases}$$

Example: If $n = 8, i = 1, j = 2$ then the sequences $(1, 2, 3, 1, 2, 3, 4, 5)$ and $(3, 2, 1, 1, 4, 3, 2, 2)$ yield trajectories $(e, 1, 2, e, 1, 2, e, e, e)$ and $(e, e, 2, 1, \Delta, \Delta, \Delta, \Delta, \Delta)$.

Those trajectories $(y_k)_{k=0}^n$ satisfying $y_n \neq \Delta$ are in correspondence to sequences $(z_k)_{k=1}^n$ that avoid the pairs (i, i) and (r, r) . Using the transition matrix

$$\Pi := \begin{bmatrix} P_e & P_i & P_r & 0 \\ P_e & 0 & P_r & P_i \\ P_e & P_i & 0 & P_r \\ 0 & 0 & 0 & 1 \end{bmatrix},$$

where $P_e := 1 - P_i - P_r$, the sought probability is $[1, 0, 0, 0] \Pi^n [1, 1, 1, 0]^t$, respectively, using the restriction $\bar{\Pi}$ of Π to $\{e, i, r\}$, i.e.,

$$\bar{\Pi} := \begin{bmatrix} P_e & P_i & P_r \\ P_e & 0 & P_r \\ P_e & P_i & 0 \end{bmatrix},$$

and initial probability $\pi(\cdot) := [1, 0, 0]$ and column vector of all ones $\mathbf{1}$, that probability is

$$\mathbb{P}(X_{i,i}^{(n)} = X_{r,r}^{(n)} = 0) = \pi \bar{\Pi}^n \mathbf{1}.$$

A bound on such probability will now be derived in the following more general context. We fix a finite non-empty set of forbidden pairs

$$\mathcal{I} := \{(k_i, m_i) : i \in I\}$$

of size $|I|$, and let

$$J := \bigcup_{i \in I} \{k_i, m_i\} = \{j_1, \dots, j_{|J|}\},$$

where $j_1 < \dots < j_{|J|}$. Moreover we fix $0 < \delta \leq 1/2$ and let

$$\mathcal{D}_\delta^J := \{\mathbf{x} \in \mathbb{R}^{|J|} : x_j \geq 0 \text{ for } j \in J, \sum_{j \in J} x_j \leq 1 - \delta\}.$$

Lemma 4.1 *Let $\varepsilon := \sum_{i \in I} P_{k_i} P_{m_i}$. Then*

$$\mathbb{P}(X_{k_i, m_i}^{(n)} = 0, i \in I) \leq \delta^{-1/2} e^{-\varepsilon n/2} \quad (13)$$

holds for $(P_j)_{j \in J} \in \mathcal{D}_\delta^J$. Furthermore, there are functions λ_1, C_1 and $\Phi_n, n \geq 1$, depending on $P_j, j \in J$, that are C^∞ and positive on an open set \mathcal{F} satisfying $\mathcal{D}_\delta^J \subseteq \mathcal{F}$, such that

$$\mathbb{P}(X_{k_i, m_i}^{(n)} = 0, i \in I) = C_1 \lambda_1^n \Phi_n. \quad (14)$$

Remark 4.2 *At several places we take the liberty to regard $(P_j)_{j \geq 1}$ as variables (which is slight abuse of notation), to the effect, that several results in this section hold more generally also for strings of random variables with a distribution different from the geometric. The reader must be prepared to see expressions involving $\lim_{P_j \rightarrow 0}, \frac{\partial}{\partial P_j}$, and functions of $(P_j)_{j \in J}$ being C^∞ in some domain, etc. all the time.*

Proof of Lemma 4.1. Assume $P_j > 0$ for $j \in J$, as well as $P_e := 1 - \sum_{j \in J} P_j \geq \delta$. Note that $\varepsilon \leq \sum_{j, \ell \in J} P_j P_\ell = (1 - P_e)^2 \leq (1 - \delta)^2 < 1 - \delta$. Define the matrix $\bar{\Pi}$ with rows and columns indexed by the set $J \cup \{e\}$ (which we assume ordered, starting with e and followed by the elements of J in ascending order) via

$$\bar{\Pi}_{k,m} := \begin{cases} 0, & (k, m) \in \mathcal{I}, \\ P_m, & \text{else.} \end{cases}$$

We define a row vector $\mathbf{w} := [\sqrt{P_e}, \sqrt{P_{j_1}}, \dots, \sqrt{P_{j_{|J|}}}]$, satisfying $\|\mathbf{w}\|_2 = 1$, and a diagonal matrix $S := \text{Diag}(\mathbf{w})$, and the matrix

$$\hat{\Pi} := S\bar{\Pi}S^{-1} = S \left[\mathbf{1}\mathbf{1}^t - \sum_{i \in I} \mathbf{e}_{k_i} \mathbf{e}_{m_i}^t \right] S,$$

where the column vectors $\mathbf{e}_j, j \in J \cup \{e\}$, denote the standard unit vectors in $\mathbb{R}^{|J|+1}$, and observe, using the Frobenius norm $\|\hat{\Pi}\|_F = \sqrt{\sum_{k,m \in J \cup \{e\}} \hat{\Pi}_{k,m}^2} = \sqrt{1 - \sum_{i \in I} P_{k_i} P_{m_i}}$, and $\pi = (\mathbf{e}_e)^t$,

$$\begin{aligned} \mathbb{P}(X_{k_i, m_i}^{(n)} = 0, i \in I) &= \pi \bar{\Pi}^n \mathbf{1} = \mathbf{w} \hat{\Pi}^{n-1} \mathbf{w}^t \\ &\leq \|\mathbf{w}\|_2^2 \|\hat{\Pi}\|_2^{n-1} \leq \|\hat{\Pi}\|_F^{n-1} = (1 - \varepsilon)^{(n-1)/2} \leq \delta^{-1/2} (1 - \varepsilon)^{n/2} \leq \delta^{-1/2} e^{-\varepsilon n/2}. \end{aligned}$$

Observe that $\bar{\Pi}$ is non-negative and primitive, therefore, by the Perron-Frobenius Theorem (see [13]), there is a unique positive eigenvalue λ_1 , that is strictly larger in modulus than any other eigenvalue, and corresponding strictly positive left and right eigenvectors \mathbf{u} and \mathbf{v} , such that $\bar{\Pi}^n = \frac{\lambda_1^n}{\mathbf{u}\mathbf{v}} \mathbf{v}\mathbf{u} + \mathcal{O}(n^{|J|} |\lambda_2|^n)$ element-wise, where λ_2 is an eigenvalue of second largest modulus. This leads to

$$\mathbb{P}(X_{k_i, m_i}^{(n)} = 0, i \in I) = \frac{(\pi \mathbf{v})(\mathbf{u}\mathbf{1})}{\mathbf{u}\mathbf{v}} \lambda_1^n + \mathcal{O}(n^{|J|} |\lambda_2|^n).$$

By setting one or more of $(P_j)_{j \in J}$ to zero, one or more of the non-dominant eigenvalues $(\lambda_k)_{k \geq 2}$ become zero, but there is a non-negative primitive submatrix constructed from the non-zero columns (and corresponding rows) of $\bar{\Pi}$, guaranteeing a unique positive eigenvalue larger in modulus than all other eigenvalues. As the row and column corresponding to state e will always be part of that submatrix, the first components u_e and v_e of \mathbf{u} and of \mathbf{v} will be positive. By continuity, these properties also hold in a neighbourhood of such $(P_j)_{j \in J}$, which yields λ_1 being C^∞ in some superset \mathcal{F} of \mathcal{D}_δ^J , by the implicit function theorem, using the facts that the characteristic polynomial $p(\lambda)$ of $\bar{\Pi}$, considered as a function of $(\lambda, (P_j)_{j \in J})$, is C^∞ , and the derivative of $p(\lambda)$ evaluated in a simple zero λ_1 is non-zero. On the set \mathcal{F} , the components of $\frac{1}{u_e} \mathbf{u}$ and $\frac{1}{v_e} \mathbf{v}$ are C^∞ functions of $(P_j)_{j \in J}$ as well.

We let $C_1 := \frac{(\pi \mathbf{v})(\mathbf{u}\mathbf{1})}{\mathbf{u}\mathbf{v}}$ and $\Phi_n := \frac{1}{C_1} \lambda_1^{-n} \mathbb{P}(X_{k_i, m_i}^{(n)} = 0, i \in I)$. Those are positive C^∞ functions of $(P_j)_{j \in J}$ in a probably smaller superset of \mathcal{D}_δ^J , that we still denote \mathcal{F} . Note that primitivity of $\bar{\Pi}$ may cease to hold when $P_e = 0$. Moreover note that $|\lambda_2|$ is continuous on \mathcal{D}_δ^J , but need not be differentiable on that set. ■

The bound (13) fits our needs when ε is large. Equation (14) is useful in the case of small ε , if asymptotics of λ_1, C_1 and Φ_n are known. In order to derive such asymptotics, we let $\bar{\bar{\Pi}}$ be the matrix obtained from $\bar{\Pi}$ by deleting row and column corresponding to state e . Left and right eigenvectors $\mathbf{u} = [1, \beta]$ and $\mathbf{v} = [1/P_e, \mu^t]^t$, with row vector $\beta = (\beta_j)_{j \in J}$ and column vector $\mu = (\mu_j)_{j \in J}$, corresponding to the dominant eigenvalue λ_1 of $\bar{\bar{\Pi}}$, lead to equations

$$\lambda_1 = P_e (1 + \sum_{j \in J} \beta_j) = P_e (1 + \sum_{j \in J} P_j \mu_j), \quad (15)$$

$$\beta = \frac{1}{\lambda_1} [\beta \bar{\bar{\Pi}} + \bar{\mathbf{p}}], \quad (16)$$

$$\mu = \frac{1}{\lambda_1} [\bar{\bar{\Pi}} \mu + \mathbf{1}], \quad (17)$$

with row vector $\bar{\mathbf{p}} = (P_j)_{j \in J}$, and with ascending order of indices in $\beta, \mu, \bar{\mathbf{p}}$. We keep denoting the column vector of all ones of appropriate dimension by $\mathbf{1}$, and express C_1 in terms of β and μ as follows:

$$C_1 = \frac{(\pi \mathbf{v})(\mathbf{u}\mathbf{1})}{\mathbf{u}\mathbf{v}} = \frac{\frac{1}{P_e} (1 + \sum_{j \in J} \beta_j)}{\frac{1}{P_e} + \sum_{j \in J} \beta_j \mu_j} = \frac{1 + \beta \mathbf{1}}{1 + P_e \beta \mu}. \quad (18)$$

Asymptotics up to any fixed order K of λ_1, β, μ are conveniently computed via fixed point iteration as described by the following algorithm:

Algorithm 1 Calculate asymptotics of λ_1, β, μ up to fixed order.

Require: $K \geq 0, k = 0, \bar{\Pi}, \bar{\mathbf{p}}, \lambda = 1, \bar{\beta} = [0, \dots, 0], \bar{\mu} = [1, \dots, 1]^t$

while $k < K$ **do**

$$\bar{\beta} \leftarrow \frac{1}{\lambda} [\bar{\beta} \bar{\Pi} + \bar{\mathbf{p}}]$$

$$\bar{\mu} \leftarrow \frac{1}{\lambda} [\bar{\Pi} \bar{\mu} + \mathbf{1}]$$

$$\lambda \leftarrow P_e [1 + \bar{\beta} \mathbf{1}]$$

$$k \leftarrow k + 1$$

end while

return $\lambda, \bar{\beta}, \bar{\mu}$

The output $\lambda, \bar{\beta}, \bar{\mu}$ of the algorithm then satisfies $\lambda_1 = \lambda + \mathcal{O}_{K+1}^*$, $\beta = \bar{\beta} + \mathcal{O}_{K+1}^*$, $\mu = \bar{\mu} + \mathcal{O}_{K+1}^*$. Here and in the following the notation \mathcal{O}_k^* always refers to the variables $(P_j)_{j \in J}$, but not to P_e . So, for instance, \mathcal{O}_4^* is the same as $\mathcal{O}(\gamma^4)$, where $\gamma = \sum_{j \in J} P_j$.

The next lemma provides asymptotics of probabilities in the case of a single avoided pair.

Lemma 4.3 *The probabilities of avoiding the pair (i, i) , resp. (i, r) for $i \neq r$, in a sequence of length n satisfy*

$$\mathbb{P}(X_{i,i}^{(n)} = 0) = e^{-nP_i^2} + \mathcal{O}(\sqrt{n}P_i^2 e^{-\frac{2-\delta}{4}nP_i^2}), \quad (19)$$

$$\mathbb{P}(X_{i,r}^{(n)} = 0) = e^{-nP_i P_r} + \mathcal{O}(P_i P_r e^{-\frac{2-\delta}{4}nP_i P_r}), \quad (20)$$

as $n \rightarrow \infty$, uniformly for $P_i \in \mathcal{D}_\delta^{\{i\}}$, resp. for $(P_i, P_r) \in \mathcal{D}_\delta^{\{i,r\}}$.

Proof. We first consider the forbidden pair (i, i) . The matrix $\bar{\Pi}$, its characteristic polynomial p , and asymptotics of λ_1 and C_1 are given by

$$\bar{\Pi} = \begin{bmatrix} P_e & P_i \\ P_e & 0 \end{bmatrix}, \quad \begin{aligned} p(\lambda) &= \lambda^2 - (1 - P_i)\lambda - P_i P_e, \\ \lambda_1 &= 1 - P_i^2 + P_i^3 - 2P_i^4 + \mathcal{O}_5^*, \\ C_1 &= 1 + P_i^2 - 2P_i^3 + 6P_i^4 + \mathcal{O}_5^*, \end{aligned}$$

where we used Algorithm 1 (with $K = 4$) and (18).

Following a suggestion by B.Salvy [12], we can easily derive λ_1 from $p(\lambda)$, after replacing P_e by $1 - P_i$. We add an extra variable v , carrying the weight of the P_i : $\tilde{P}_i := vP_i$. We have the local expansion of the solution at 0 by using the Maple package gfun (see [11]):

$$sol := \text{gfun}[\text{algeqtoseries}](p(\lambda), v, \lambda, pr),$$

where pr denotes the precision of the expansion into v . We obtain the solutions as $sol[1], sol[2]$ and we keep the solution close to 1.

Denoting $\pi \bar{\Pi}^n \mathbf{1} = C_1 \lambda_1^n + C_2 \lambda_2^n$, with λ_2 the non-dominant eigenvalue of $\bar{\Pi}$, we have $C_1 \lambda_1^0 + C_2 \lambda_2^0 = 1$, and therefore $C_2 = -P_i^2 + 2P_i^3 - 6P_i^4 + \mathcal{O}_5^*$, which leads to $\Phi_n = 1 + \frac{C_2}{C_1} \left(\frac{\lambda_2}{\lambda_1}\right)^n = 1 + \mathcal{O}(P_i^2)$, uniformly in n . This is used in (14), together with $C_1 = 1 + \mathcal{O}(P_i^2)$ and

$$\lambda_1^n = e^{n \ln \lambda_1} = e^{n(-P_i^2 + P_i^3 + \mathcal{O}(P_i^4))} = e^{-nP_i^2} (1 + \mathcal{O}(nP_i^3))$$

leading to $\mathbb{P}(X_{i,i}^{(n)} = 0) = [1 + \mathcal{O}(P_i^2) + \mathcal{O}(nP_i^3)] e^{-nP_i^2}$, for $nP_i^3 = \mathcal{O}(1)$, resp. for $nP_i^2 = \mathcal{O}(n^{1/3})$. Note that for fixed $\alpha, \beta > 0$ the function $x^\alpha e^{-\beta x}$ is bounded for $x > 0$, implying

$$nP_i^3 e^{-nP_i^2} = \sqrt{n}P_i^2 (nP_i^2)^{1/2} e^{-\frac{2+\delta}{4}nP_i^2} e^{-\frac{2-\delta}{4}nP_i^2} = \mathcal{O}\left(\sqrt{n}P_i^2 e^{-\frac{2-\delta}{4}nP_i^2}\right).$$

Moreover also $P_i^2 e^{-nP_i^2} = \mathcal{O}\left(\sqrt{n}P_i^2 e^{-\frac{2-\delta}{4}nP_i^2}\right)$ holds, and (13) can be built in by observing that $nP_i^2 = \Omega(n^{1/3})$ implies $\delta^{-1/2}e^{-\frac{n}{2}P_i^2} = \mathcal{O}\left(\sqrt{n}P_i^2 e^{-\frac{2-\delta}{4}nP_i^2}\right)$. We have thus obtained (19).

We now consider the forbidden pair (i, r) with $i \neq r$. The matrix $\bar{\Pi}$, its characteristic polynomial p , and asymptotics of λ_1 and C_1 are given by

$$\bar{\Pi} = \begin{bmatrix} P_e & P_i & P_r \\ P_e & P_i & 0 \\ P_e & P_i & P_r \end{bmatrix}, \quad \begin{aligned} p(\lambda) &= \lambda^3 - \lambda^2 + P_i P_r \lambda, \\ \lambda_1 &= 1 - P_i P_r - P_i^2 P_r^2 - 2P_i^3 P_r^3 + \mathcal{O}_8^*, \\ C_1 &= 1 + P_i P_r + 3P_i^2 P_r^2 + 10P_i^3 P_r^3 + \mathcal{O}_8^*. \end{aligned}$$

Clearly, λ_1 , and therefore also C_1 and Φ_n , are C^∞ functions of the coefficient $P_i P_r$ of the characteristic polynomial p , meaning that the error term \mathcal{O}_8^* is in fact $\mathcal{O}(P_i^4 P_r^4)$. Sufficiently accurate for our purposes are the asymptotics $\lambda_1 = 1 - P_i P_r + \mathcal{O}(P_i^2 P_r^2)$ and $C_1 = 1 + \mathcal{O}(P_i P_r)$.

One of the eigenvalues is 0, therefore a representation $\pi \bar{\Pi}^n \mathbf{1} = C_1 \lambda_1^n + C_2 \lambda_2^n$ as before also holds in this case, with $C_2 = \mathcal{O}(P_i P_r)$, and $\Phi_n = 1 + \frac{C_2}{C_1} \left(\frac{\lambda_2}{\lambda_1}\right)^n = 1 + \mathcal{O}(P_i P_r)$, uniformly in n . All this, together with $\lambda_1^n = e^{-nP_i P_r} (1 + \mathcal{O}(nP_i^2 P_r^2))$, leads to (20) via (14), taking care of error terms as above. \blacksquare

The next corollary follows easily from equations (13), (19) and (20).

Corollary 4.4 *The variances of $X_{i,i}^{(n)}$ and $X_{i,r}^{(n)}$ for $i \neq r$ satisfy*

$$\text{Var } X_{i,i}^{(n)} = e^{-nP_i^2} - e^{-2nP_i^2} + \mathcal{O}\left(\sqrt{n}P_i^2 e^{-\frac{2-\delta}{4}nP_i^2}\right), \quad (21)$$

$$\text{Var } X_{i,r}^{(n)} = e^{-nP_i P_r} - e^{-2nP_i P_r} + \mathcal{O}\left(P_i P_r e^{-\frac{2-\delta}{4}nP_i P_r}\right), \quad (22)$$

as $n \rightarrow \infty$, uniformly for $P_i \in \mathcal{D}_\delta^{\{i\}}$, resp. for $(P_i, P_r) \in \mathcal{D}_\delta^{\{i,r\}}$.

Next we obtain asymptotics for the covariance

$$\text{Cov}(X_{i,i}^{(n)}, X_{r,r}^{(n)}) = \mathbb{P}(X_{i,i}^{(n)} = X_{r,r}^{(n)} = 1) - \mathbb{P}(X_{i,i}^{(n)} = 1)\mathbb{P}(X_{r,r}^{(n)} = 1) = \mathbb{P}(X_{i,i}^{(n)} = X_{r,r}^{(n)} = 0) - \mathbb{P}(X_{i,i}^{(n)} = 0)\mathbb{P}(X_{r,r}^{(n)} = 0).$$

Lemma 4.5 *For $i \neq r$ and $(P_i, P_r) \in \mathcal{D}_\delta^{\{i,r\}}$ we have, for $nP_i P_r (P_i + P_r)^2 = \mathcal{O}(1)$,*

$$\text{Cov}(X_{i,i}^{(n)}, X_{r,r}^{(n)}) = \mathcal{O}\left(P_i P_r + nP_i P_r (P_i + P_r)^2\right) \mathbb{P}(X_{i,i}^{(n)} = 0) \mathbb{P}(X_{r,r}^{(n)} = 0). \quad (23)$$

From (13) we derive $\text{Cov}(X_{i,i}^{(n)}, X_{r,r}^{(n)}) = \mathcal{O}\left(e^{-\frac{n}{2}(P_i^2 + P_r^2)}\right)$, that together with (23), where we use

$$nP_i P_r (P_i + P_r)^2 \mathbb{P}(X_{i,i}^{(n)} = 0) \mathbb{P}(X_{r,r}^{(n)} = 0) = \mathcal{O}\left(P_i P_r (nP_i^2 + nP_r^2) e^{-\frac{n}{2}(P_i^2 + P_r^2)}\right) = \mathcal{O}\left(P_i P_r e^{-\frac{2-\delta}{4}n(P_i^2 + P_r^2)}\right),$$

implies the next corollary, since $e^{-\frac{n}{2}(P_i^2 + P_r^2)} = \mathcal{O}\left(P_i P_r e^{-\frac{2-\delta}{4}n(P_i^2 + P_r^2)}\right)$, for $nP_i P_r (P_i + P_r)^2 = \Omega(1)$.

Corollary 4.6 *For $i \neq r$, the covariance of $X_{i,i}^{(n)}$ and $X_{r,r}^{(n)}$ satisfies*

$$\text{Cov}(X_{i,i}^{(n)}, X_{r,r}^{(n)}) = \mathcal{O}\left(P_i P_r e^{-\frac{2-\delta}{4}n(P_i^2 + P_r^2)}\right), \quad (24)$$

as $n \rightarrow \infty$, uniformly for $(P_i, P_r) \in \mathcal{D}_\delta^{\{i,r\}}$.

Proof of Lemma 4.5. We first find asymptotics of λ_1 and C_1 from $\mathbb{P}(X_{i,i}^{(n)} = X_{r,r}^{(n)} = 0) = C_1 \lambda_1^n \Phi_n$, proceeding as in the previous lemma. The matrix $\bar{\Pi}$, its characteristic polynomial p , and asymptotics of λ_1 and C_1 are given by

$$\bar{\Pi} = \begin{bmatrix} P_e & P_i & P_r \\ P_e & 0 & P_r \\ P_e & P_i & 0 \end{bmatrix}, \quad \begin{aligned} p(\lambda) &= \lambda^3 - P_e \lambda^2 - [P_e(P_i + P_r) + P_i P_r] \lambda - P_i P_r P_e, \\ \lambda_1 &= 1 - P_i^2 - P_r^2 + P_i^3 + P_r^3 + \mathcal{O}_4^*, \\ C_1 &= 1 - P_i^2 - P_r^2 + 2P_i^3 + 2P_r^3 + \mathcal{O}_4^*. \end{aligned}$$

Again, we can also replace P_e by $1 - P_i - P_r$ and use gfun. From Lemma 4.1 we know that λ_1, C_1 and Φ_n are C^∞ functions of P_i, P_r in some open superset \mathcal{F} of $\mathcal{D}_\delta^{\{i,r\}}$, such that

$$\mathbb{P}(X_{i,i}^{(n)} = X_{r,r}^{(n)} = 0) = C_1(P_i, P_r)[\lambda_1(P_i, P_r)]^n \Phi_n(P_i, P_r) \quad (25)$$

holds for $(P_i, P_r) \in \mathcal{D}_\delta^{\{i,r\}}$. In fact, we will only need that those functions are C^2 in the following.

Note that $\mathbb{P}(X_{i,i}^{(n)} = 0)$ can be obtained from (25) as the limiting case $P_r \rightarrow 0$. Observe that we have $\lim_{P_i \rightarrow 0} \frac{C_1(P_i, P_r)}{C_1(0, P_r)C_1(P_i, 0)} = \lim_{P_r \rightarrow 0} \frac{C_1(P_i, P_r)}{C_1(0, P_r)C_1(P_i, 0)} = \lim_{P_i \rightarrow 0} \frac{\Phi_n(P_i, P_r)}{\Phi_n(0, P_r)\Phi_n(P_i, 0)} = \lim_{P_r \rightarrow 0} \frac{\Phi_n(P_i, P_r)}{\Phi_n(0, P_r)\Phi_n(P_i, 0)} = 1$, and therefore $\frac{C_1(P_i, P_r)}{C_1(0, P_r)C_1(P_i, 0)} = 1 + \mathcal{O}(P_i P_r)$ and $\frac{\Phi_n(P_i, P_r)}{\Phi_n(0, P_r)\Phi_n(P_i, 0)} = 1 + \mathcal{O}(P_i P_r)$.

To see that the latter holds uniformly in n and $(P_i, P_r) \in \mathcal{D}_\delta^{\{i,r\}}$, we start defining $\check{\Pi} := \bar{\Pi} - \frac{\lambda_1}{\mathbf{uv}} \mathbf{vu}$, so that $\bar{\Pi} = \frac{\lambda_1}{\mathbf{uv}} \mathbf{vu} + \check{\Pi}$, and

$$\pi \bar{\Pi}^n \mathbf{1} = C_1 \lambda_1^n + \pi \check{\Pi}^n \mathbf{1}, \quad (26)$$

where we used that \mathbf{u} and \mathbf{v} are in the left resp. right kernel of the matrix $\check{\Pi}$.

Denoting the spectral radius of a square matrix A by $\rho(A)$, we clearly have $\rho(\check{\Pi}) = |\lambda_2|$, and since $\mathcal{D}_\delta^{\{i,r\}}$ is compact, we have $\max_{(P_i, P_r) \in \mathcal{D}_\delta^{\{i,r\}}} \frac{|\lambda_2|}{\lambda_1} =: \kappa < 1$. All components of $\frac{1}{\lambda_1 \kappa} \check{\Pi}$ are continuous, so there is a constant C' such that $\|\frac{1}{\lambda_1 \kappa} \check{\Pi}\|_F \leq C'$ on $\mathcal{D}_\delta^{\{i,r\}}$. By applying Lemma 4.7 below to the matrix $\frac{1}{\lambda_1 \kappa} \check{\Pi}$, we obtain

$$\Phi_n - 1 = \frac{\pi \check{\Pi}^n \mathbf{1}}{C_1 \lambda_1^n} = \mathcal{O}(n^2 \kappa^n) = \mathcal{O}(\bar{\kappa}^n),$$

for some $\kappa < \bar{\kappa} < 1$, uniformly on $\mathcal{D}_\delta^{\{i,r\}}$. Similarly, we obtain $\frac{\partial \Phi_n}{\partial P_i} = \mathcal{O}(\bar{\kappa}^n)$, $\frac{\partial \Phi_n}{\partial P_r} = \mathcal{O}(\bar{\kappa}^n)$, and $\frac{\partial^2 \Phi_n}{\partial P_i \partial P_r} = \mathcal{O}(\bar{\kappa}^n)$, uniformly on $\mathcal{D}_\delta^{\{i,r\}}$, using, e. g., $\frac{\partial \pi \check{\Pi}^n \mathbf{1}}{\partial P_i} = \sum_{0 \leq j < n} \pi \check{\Pi}^j \frac{\partial \check{\Pi}}{\partial P_i} \check{\Pi}^{n-1-j} \mathbf{1}$, and again Lemma 4.7.

Define $\Psi_n(P_i, P_r) := \frac{\Phi_n(P_i, P_r)}{\Phi_n(0, P_r)\Phi_n(P_i, 0)} - 1$ and observe that $\lim_{n \rightarrow \infty} \frac{\partial^2}{\partial P_i \partial P_r} \Psi_n = 0$ holds uniformly on $\mathcal{D}_\delta^{\{i,r\}}$. Note that we have $\Psi_n(P_i, 0) = \Psi_n(0, P_r) = 0$ for $0 \leq P_i, P_r \leq 1 - \delta$, yielding

$$\Psi_n(P_i, P_r) = \Psi_n(P_i, P_r) - \Psi_n(P_i, 0) - \Psi_n(0, P_r) + \Psi_n(0, 0) = P_i P_r \frac{\partial^2 \Psi_n}{\partial P_i \partial P_r}(p_i, p_r)$$

by the (bivariate) Mean Value Theorem, where $0 \leq p_i \leq P_i$ and $0 \leq p_r \leq P_r$, see [10, Thm. 9.40].

Defining $\bar{C} := \max_{n \geq 1} \max_{(p_i, p_r) \in \mathcal{D}_\delta^{\{i,r\}}} \left| \frac{\partial^2 \Psi_n}{\partial P_i \partial P_r}(p_i, p_r) \right|$, we finally conclude $|\Psi_n(P_i, P_r)| \leq \bar{C} P_i P_r$ for all $n \geq 1$ and $(P_i, P_r) \in \mathcal{D}_\delta^{\{i,r\}}$, establishing the uniformity claim. By our asymptotics for λ_1 , we similarly obtain

$$\ln \lambda_1(P_i, P_r) - \ln \lambda_1(P_i, 0) - \ln \lambda_1(0, P_r) + \ln \lambda_1(0, 0) = P_i P_r \frac{\partial^2 \ln \lambda_1}{\partial P_i \partial P_r}(p_i, p_r) = \mathcal{O}(P_i P_r (P_i + P_r)^2),$$

leading to

$$\frac{\lambda_1(P_i, P_r)}{\lambda_1(P_i, 0)\lambda_1(0, P_r)} = 1 + \mathcal{O}(P_i P_r (P_i + P_r)^2).$$

We summarize

$$\frac{\mathbb{P}(X_{i,i}^{(n)} = X_{r,r}^{(n)} = 0)}{\mathbb{P}(X_{i,i}^{(n)} = 0)\mathbb{P}(X_{r,r}^{(n)} = 0)} = 1 + \mathcal{O}(P_i P_r + n P_i P_r (P_i + P_r)^2),$$

finally arriving at (23). ■

Lemma 4.7 *Let $A \in \mathbb{R}^{k \times k}$, with $k \geq 2$, have spectral radius $\rho(A) \leq 1$ and Frobenius norm $\|A\|_F = C'$. Then, with $C := \max(C', k)$ and $C'' := 2C^{k-1}$, we have*

$$\|A^n\|_F \leq C'' n^{k-1}.$$

Proof. There is an orthogonal matrix Q such that $\bar{A} := QAQ^{-1}$ is upper triangular and satisfies $\rho(\bar{A}) = \rho(A)$ and $\|\bar{A}\|_F = \|A\|_F$. Then

$$\|A^n\|_F = \|Q^{-1}\bar{A}^n Q\|_F = \|\bar{A}^n\|_F.$$

Since $C \geq k$ ensures that $((C/\sqrt{\ell})^\ell)_{1 \leq \ell < k}$ is increasing, we can show $|(\bar{A}^n)_{i,i}| \leq 1$, $|(\bar{A}^n)_{i,i+1}| \leq nC$,

$$\begin{aligned} |(\bar{A}^n)_{i,i+2}| &\leq nC + \binom{n}{2} \left(\frac{C}{\sqrt{2}}\right)^2 \leq \binom{n+1}{2} \left(\frac{C}{\sqrt{2}}\right)^2, \\ |(\bar{A}^n)_{i,i+3}| &\leq nC + \binom{2}{1} \binom{n}{2} \left(\frac{C}{\sqrt{2}}\right)^2 + \binom{n}{3} \left(\frac{C}{\sqrt{3}}\right)^3 \leq \binom{n+2}{3} \left(\frac{C}{\sqrt{3}}\right)^3. \end{aligned}$$

Note that $(\bar{A}^n)_{i,i+3}$ is a sum of terms $\bar{a}_{i_0,i_1} \bar{a}_{i_1,i_2} \cdots \bar{a}_{i_{n-1},i_n}$, where $(i_k)_{k=0}^n$ is an increasing sequence with $i_0 = i$ and $i_n = i+3$. There is $1 = \binom{2}{0}$ way to have a single jump (of size 3) in this sequence, and it can happen at $\binom{n}{1}$ places. We have $|\bar{a}_{i,i}^\ell \cdot \bar{a}_{i,i+3} \cdot \bar{a}_{i+3,i+3}^{n-1-\ell}| \leq C$, because $|\bar{a}_{k,k}| \leq 1$ for any k , and $|\bar{a}_{i,i+3}| \leq \|\bar{A}\|_F \leq C$. There are $\binom{2}{1}$ ways to have two jumps (two orderings of sizes 1 and 2) in this sequence, and there are $\binom{n}{2}$ ways to place each of them. We have $|\bar{a}_{i,i}^\ell \cdot \bar{a}_{i,i+1} \cdot \bar{a}_{i+1,i+1}^m \cdot \bar{a}_{i+1,i+3} \cdot \bar{a}_{i+3,i+3}^{n-2-\ell-m}| \leq \frac{C^2}{2}$, because $\bar{a}_{i,i+1}^2 + \bar{a}_{i+1,i+3}^2 \leq \|\bar{A}\|_F^2 \leq C^2$, and the product of those terms is maximized when they are both equal. There is $1 = \binom{2}{2}$ way to have three jumps (all of size 1) in this sequence, and there are $\binom{n}{3}$ ways to place them. We have $|\bar{a}_{i,i+1} \cdot \bar{a}_{i+1,i+2} \cdot \bar{a}_{i+2,i+3}| \leq (C/\sqrt{3})^3$, because $\bar{a}_{i,i+1}^2 + \bar{a}_{i+1,i+2}^2 + \bar{a}_{i+2,i+3}^2 \leq \|\bar{A}\|_F^2 \leq C^2$, and the product of those terms is maximized when they are all equal. More generally we have $|(\bar{A}^n)_{i,i+\ell}| \leq \binom{n+\ell-1}{\ell} (C/\sqrt{\ell})^\ell \leq \binom{n+k-2}{k-1} (C/\sqrt{k-1})^{k-1}$ for $1 \leq i < i+\ell \leq k$. We obtain

$$\|\bar{A}^n\|_F \leq k \binom{n+k-2}{k-1} \left(\frac{C}{\sqrt{k-1}}\right)^{k-1} \leq 2C^{k-1} n^{k-1},$$

because of $\binom{n+k-2}{k-1} \leq n^{k-1}$ for $k \geq 2$ and $n \geq 1$, and because of $\max_{k \geq 2} \frac{k}{(k-1)^{(k-1)/2}} = 2$, which completes the proof. \blacksquare

4.2 The variance of $X_1^{(n)}$

In this subsection we use the results on variances and covariances in the case of avoided pairs of identical letters, that we have derived so far, to furnish a proof of equation (4) of Theorem 2.1.

Lemma 4.8 *The variance of $X_1^{(n)}$ is asymptotically given by*

$$\text{Var} X_1^{(n)} = \sum_{i \geq 1} \text{Var} X_{i,i}^{(n)} + \mathcal{O}\left(\frac{1}{n}\right) = S_1^{(n)} + \mathcal{O}\left(\frac{1}{\sqrt{n}}\right),$$

with $S_1^{(n)}$ given in (1). In particular the contribution of covariances is negligible.

Proof. Dealing with covariances first, note that (24) guarantees that the double sum of covariances $\sum_{i \neq r} \text{Cov}(X_{i,i}^{(n)}, X_{r,r}^{(n)})$ makes a negligible contribution to the variance of $X_1^{(n)}$: We will use that

$$\sum_{k \geq 1} [nP_k^\beta]^\alpha e^{-nP_k^\beta} = \mathcal{O}(1) \text{ holds for } \alpha, \beta > 0. \quad (27)$$

With the help of (27), which will be proved in Appendix B, we find

$$\sum_{i \geq 1} \sum_{r \geq 1} P_i P_r e^{-\frac{2-\delta}{4} n(P_i^2 + P_r^2)} = \frac{1}{n} \sum_{i \geq 1} (nP_i^2)^{1/2} e^{-\frac{2-\delta}{4} nP_i^2} \sum_{r \geq 1} (nP_r^2)^{1/2} e^{-\frac{2-\delta}{4} nP_r^2} = \mathcal{O}\left(\frac{1}{n}\right).$$

This leads to $\sum_{i \neq r} \text{Cov}(X_{i,i}^{(n)}, X_{r,r}^{(n)}) = \mathcal{O}\left(\frac{1}{n}\right)$.

We now turn to $\sum_{i \geq 1} \text{Var} X_{i,i}^{(n)}$. Observe that the sum of error terms from (21) satisfies

$$\sum_{i \geq 1} \sqrt{n} P_i^2 e^{-\frac{2-\delta}{4} nP_i^2} = \mathcal{O}\left(\frac{1}{\sqrt{n}}\right),$$

by (27). Therefore, up to an error term $\mathcal{O}\left(\frac{1}{\sqrt{n}}\right)$, the variance $\text{Var} X_1^{(n)}$ equals

$$\sum_{i \geq 1} \left[e^{-nP_i^2} - e^{-2nP_i^2} \right] = \sum_{i \geq 1} \left[1 - e^{-2nP_i^2} \right] - \sum_{i \geq 1} \left[1 - e^{-nP_i^2} \right] = G(2np^2) - G(np^2),$$

which can be evaluated using G from Appendix A.1, directly leading to $S_1^{(n)}$ from (1). ■

4.3 Contribution of covariances to the variance of $X_2^{(n)}$

In this subsection we will prove the following lemma, which will also imply equations (5) and (6) of Theorem 2.1.

Lemma 4.9 *The variance of $X_2^{(n)}$ is asymptotically given by*

$$\text{Var} X_2^{(n)} = \sum_{i,j \geq 1} \text{Var} X_{i,j}^{(n)} + 2 \sum_{i,j,k \geq 1} H(i,j,k) + \mathcal{O}\left(\frac{\ln n}{\sqrt{n}}\right) = S_2^{(n)} + T_2^{(n)} + \mathcal{O}\left(\frac{\ln n}{\sqrt{n}}\right), \quad (28)$$

where $H(i,j,k) = (e^{nP_i P_j P_k} - 1)e^{-nP_i P_j - nP_j P_k}$, and $S_2^{(n)}, T_2^{(n)}$ are given in (2) and (3). Only covariances $\text{Cov}(X_{i,j}^{(n)}, X_{j,k}^{(n)})$, resp. $\text{Cov}(X_{j,i}^{(n)}, X_{k,j}^{(n)})$, with i, j, k all different, and $\text{Cov}(X_{i,i}^{(n)}, X_{j,i}^{(n)})$ with i, j different, contribute significantly to $\text{Var} X_2^{(n)}$.

Proof. We start considering distinct forbidden pairs $(i_1, j_1), (i_2, j_2)$, where we allow $i_1 \neq j_1$ or $i_2 \neq j_2$ or both, and are again interested in negligibility of covariance contributions.

Let $J := \{i_1, j_1, i_2, j_2\}$, and assume $P_i > 0$ for $i \in J$, as well as $P_e := 1 - \sum_{i \in J} P_i \geq \delta$. Define the matrix $\bar{\Pi}$ with rows and columns indexed by the set $J \cup \{e\}$ (which we assume ordered, starting with e and followed by the elements of J in ascending order) via

$$\bar{\Pi}_{i,j} := \begin{cases} 0, & (i,j) \in \{(i_1, j_1), (i_2, j_2)\}, \\ P_j, & \text{else,} \end{cases}$$

We will have to distinguish several cases, which however share some common features: The sought probability can be expressed as

$$\mathbb{P}(X_{i_1, j_1}^{(n)} = X_{i_2, j_2}^{(n)} = 0) = \pi \bar{\Pi}^n \mathbf{1} = C_1 \lambda_1^n \Phi_n,$$

where, as previously observed, λ_1, C_1 and Φ_n for $n \geq 1$ are C^∞ functions on an open superset of \mathcal{D}_δ^J . Limits $\lim_{n \rightarrow \infty} \Phi_n = 1$, $\lim_{n \rightarrow \infty} \frac{\partial \Phi_n}{\partial P_{i_1}} = 0$, etc., will again be uniform for $(P_i)_{i \in J} \in \mathcal{D}_\delta^J$. Denoting

$$\mathbb{P}(X_{i_1, j_1}^{(n)} = 0) = C_* \lambda_*^n \Phi_n^*, \quad \mathbb{P}(X_{i_2, j_2}^{(n)} = 0) = C_\circ \lambda_\circ^n \Phi_n^\circ,$$

we observe

$$\lim_{P_i \rightarrow 0} \frac{\lambda_1}{\lambda_* \lambda_\circ} = \lim_{P_i \rightarrow 0} \frac{C_1}{C_* C_\circ} = \lim_{P_i \rightarrow 0} \frac{\Phi_n}{\Phi_n^* \Phi_n^\circ} = 1, \quad \text{for } i \in J,$$

leading to $\frac{\lambda_1}{\lambda_* \lambda_\circ} = 1 + \mathcal{O}(\prod_{i \in J} P_i)$, $\frac{C_1}{C_* C_\circ} = 1 + \mathcal{O}(\prod_{i \in J} P_i)$, and $\frac{\Phi_n}{\Phi_n^* \Phi_n^\circ} = 1 + \mathcal{O}(\prod_{i \in J} P_i)$, with implied constant independent of n . (This independence can be shown as in the proof of Lemma 4.5.) As we will see, more accurate representations for λ_1 , complementing those obtained by Algorithm 1, can always be found in the form

$$\lambda_1 = 1 - P_{i_1} P_{j_1} - P_{i_2} P_{j_2} + Q + \mathcal{O}_4^*,$$

where $Q = \mathcal{O}_3^*$ and $Q \geq 0$. We will observe, that in each of the cases

$$Q = \sum_{i,r,t:(i,r),(r,t) \in \{(i_1,j_1),(i_2,j_2)\}} P_i P_r P_t \quad (29)$$

holds. Using $\lambda_* = 1 - P_{i_1} P_{j_1} + Q_* + \mathcal{O}(P_{i_1}^2 P_{j_1}^2)$ and $\lambda_\circ = 1 - P_{i_2} P_{j_2} + Q_\circ + \mathcal{O}(P_{i_2}^2 P_{j_2}^2)$ (depending on whether $(i_1, j_1) = (i, i)$ or (i, r) , we have $Q_* = P_i^3$ or $Q_* = 0$, and similarly for Q_\circ , see the proof of Lemma 4.3), we will obtain in most of the cases

$$\ln \frac{\lambda_1}{\lambda_* \lambda_\circ} = Q - Q_* - Q_\circ + \mathcal{O}(P_{i_1} P_{j_1} P_{i_2} P_{j_2}), \quad (30)$$

where the error term needs justification in each of these cases. In some cases this is done by employing the MVT, as in the proof of Lemma 4.5. This results in the following expression for a quotient of probabilities, that directly leads to an expression for the covariance, where we denote $\bar{Q} := Q - Q_* - Q_\circ$,

$$\frac{\mathbb{P}(X_{i_1,j_1}^{(n)} = X_{i_2,j_2}^{(n)} = 0)}{\mathbb{P}(X_{i_1,j_1}^{(n)} = 0)\mathbb{P}(X_{i_2,j_2}^{(n)} = 0)} = \left(\frac{\lambda_1}{\lambda_* \lambda_\circ} \right)^n \frac{C_1}{C_* C_\circ} \frac{\Phi_n}{\Phi_n^* \Phi_n^\circ} = e^{n(\bar{Q} + \mathcal{O}(P_{i_1} P_{j_1} P_{i_2} P_{j_2}))} \left(1 + \mathcal{O}\left(\prod_{i \in J} P_i\right) \right),$$

$$\text{Cov}(X_{i_1,j_1}^{(n)}, X_{i_2,j_2}^{(n)}) = \left[(e^{n\bar{Q}} - 1) + \mathcal{O}\left(n P_{i_1} P_{j_1} P_{i_2} P_{j_2} + \prod_{i \in J} P_i\right) e^{n\bar{Q}} \right] \mathbb{P}(X_{i_1,j_1}^{(n)} = 0) \mathbb{P}(X_{i_2,j_2}^{(n)} = 0),$$

valid for $n P_{i_1} P_{j_1} P_{i_2} P_{j_2} = \mathcal{O}(1)$. It will turn out that in some of the cases we have $\bar{Q} = 0$. In cases where $\bar{Q} > 0$ we always have $\bar{Q} = \mathcal{O}(\prod_{i \in J} P_i)$ and $\bar{Q} \leq \frac{1-\delta}{2} \varepsilon$, with $\varepsilon := P_{i_1} P_{j_1} + P_{i_2} P_{j_2}$. Using the latter, and (13), as well as $e^{n\bar{Q}} - 1 \leq n\bar{Q} e^{n\bar{Q}}$, we obtain

$$e^{n\bar{Q}} \mathbb{P}(X_{i_1,j_1}^{(n)} = 0) \mathbb{P}(X_{i_2,j_2}^{(n)} = 0) = \mathcal{O}\left(e^{-\frac{\delta}{2} n \varepsilon}\right),$$

$$(e^{n\bar{Q}} - 1) \left[\mathbb{P}(X_{i_1,j_1}^{(n)} = 0) \mathbb{P}(X_{i_2,j_2}^{(n)} = 0) - e^{-n\varepsilon} \right] = \mathcal{O}\left(n\bar{Q} \sqrt{n} \varepsilon e^{-\frac{\delta}{2} n \varepsilon}\right) = \mathcal{O}\left(\sqrt{n} \bar{Q} e^{-\frac{\delta}{4} n \varepsilon}\right).$$

In case of $n P_{i_1} P_{j_1} P_{i_2} P_{j_2} = \Omega(1)$ we use (13) to obtain

$$\text{Cov}(X_{i_1,j_1}^{(n)}, X_{i_2,j_2}^{(n)}) = \mathcal{O}\left(e^{-\frac{n}{2} \varepsilon}\right) = \mathcal{O}\left(n P_{i_1} P_{j_1} P_{i_2} P_{j_2} e^{-\frac{\delta}{4} n \varepsilon}\right),$$

and all this results in

$$\text{Cov}(X_{i_1,j_1}^{(n)}, X_{i_2,j_2}^{(n)}) = (e^{n\bar{Q}} - 1) e^{-n(P_{i_1} P_{j_1} + P_{i_2} P_{j_2})} + \mathcal{O}\left((n P_{i_1} P_{j_1} P_{i_2} P_{j_2} + \sqrt{n} \prod_{i \in J} P_i) e^{-\frac{\delta}{4} n (P_{i_1} P_{j_1} + P_{i_2} P_{j_2})}\right).$$

We distinguish the following cases, only Cases 1, 5 and 6 involving $\bar{Q} \neq 0$, and Case 6 slightly deviating from the general pattern outlined above.

Case 1: Pairs (i, r) , (r, t) with i, r, t all different.

The matrix $\bar{\Pi}$ and its characteristic polynomial p are given by

$$\bar{\Pi} = \begin{bmatrix} P_e & P_i & P_r & P_t \\ P_e & P_i & 0 & P_t \\ P_e & P_i & P_r & 0 \\ P_e & P_i & P_r & P_t \end{bmatrix}, \quad p(\lambda) = \lambda^4 - \lambda^3 + P_r(P_i + P_t)\lambda^2 - P_i P_r P_t \lambda.$$

Using Algorithm 1 and (18), we obtain

$$\begin{aligned}\lambda_1 &= 1 - P_i P_r - P_r P_t + P_i P_r P_t + \mathcal{O}_4^*, \\ C_1 &= 1 + P_i P_r + P_r P_t - 2P_i P_r P_t + \mathcal{O}_4^*.\end{aligned}$$

We can see that $\lambda_1 = 1 - P_i P_r - P_r P_t + P_r P_i P_t + P_r^2 \mathcal{O}_2^*$ holds, by noting that λ_1 is a C^∞ function of the coefficients $P_r(P_i + P_t)$ and $-P_i P_r P_t$ of the polynomial p , and terms of order 2 or higher contribute $P_r^2 \mathcal{O}_2^*$. Thus, by the MVT, for some $0 < p_i < P_i, 0 < p_t < P_t$,

$$\ln \frac{\lambda_1}{\lambda_* \lambda_\circ} = P_i P_t \frac{\partial^2 \ln \lambda_1}{\partial P_i \partial P_t}(p_i, p_t) = P_i P_t P_r (1 + \mathcal{O}(P_r)).$$

So (30) is established with $\bar{Q} = P_i P_r P_t$, which indeed satisfies $\bar{Q} \leq \frac{1}{4} P_r (P_i + P_t) \leq \frac{1-\delta}{2} \varepsilon$, since $\delta \leq 1/2$.

Case 2a: Pairs $(i, r), (i, t)$ with i, r, t all different.

The matrix $\bar{\Pi}$, its characteristic polynomial p , and asymptotics of λ_1 and C_1 are given by

$$\bar{\Pi} = \begin{bmatrix} P_e & P_i & P_r & P_t \\ P_e & P_i & 0 & 0 \\ P_e & P_i & P_r & P_t \\ P_e & P_i & P_r & P_t \end{bmatrix}, \quad \begin{aligned} p(\lambda) &= \lambda^4 - \lambda^3 + P_i(P_r + P_t)\lambda^2, \\ \lambda_1 &= 1 - P_i P_r - P_i P_t + \mathcal{O}_4^*, \\ C_1 &= 1 + P_i P_r + P_i P_t + \mathcal{O}_4^*. \end{aligned}$$

Again, λ_1 is a C^∞ function of the coefficient $P_i(P_r + P_t)$, leading to $\lambda_1 = 1 - P_i P_r - P_i P_t + P_i^2 \mathcal{O}_2^*$, which we use to derive $\ln(\frac{\lambda_1}{\lambda_* \lambda_\circ}) = P_r P_t \frac{\partial^2 \ln \lambda_1}{\partial P_r \partial P_t}(p_r, p_t) = \mathcal{O}(P_r P_t P_i^2)$, yielding (30) with $\bar{Q} = 0$.

Case 2b: Pairs $(r, i), (t, i)$ with i, r, t all different.

Here the matrix (call it $\bar{\Pi}_b$) can be seen to be a similarity transformation involving diagonal matrices of the transposed matrix (call it $\bar{\Pi}_a$) in Case 2a, more precisely, with $\mathbf{p} := \pi \bar{\Pi} = [P_e, (P_i)_{i \in I}]$, we have $\bar{\Pi}_b = \text{Diag}(\mathbf{p})^{-1} \bar{\Pi}_a^t \text{Diag}(\mathbf{p})$, leading to $\mathbf{p} \bar{\Pi}_b^{n-1} \mathbf{1} = \mathbf{p} \bar{\Pi}_a^{n-1} \mathbf{1}$, and implying that $p(\lambda), \lambda_1, C_1$, and also the covariance, are the same as in Case 2a.

Case 3: Pairs $(i, i), (r, t)$ with i, r, t all different.

The matrix $\bar{\Pi}$, its characteristic polynomial p , and asymptotics of λ_1 and C_1 are given by

$$\bar{\Pi} = \begin{bmatrix} P_e & P_i & P_r & P_t \\ P_e & 0 & P_r & P_t \\ P_e & P_i & P_r & 0 \\ P_e & P_i & P_r & P_t \end{bmatrix}, \quad \begin{aligned} p(\lambda) &= \lambda^4 - (1 - P_i)\lambda^3 - (P_i - P_i^2 - P_r P_t)\lambda^2 + P_i P_r P_t \lambda, \\ \lambda_1 &= 1 - P_i^2 - P_r P_t + P_i^3 + \mathcal{O}_4^*, \\ C_1 &= 1 + P_i^2 + P_r P_t - 2P_i^3 + \mathcal{O}_4^*. \end{aligned}$$

Denoting by $\lambda_\circ = \lim_{P_i \rightarrow 0} \lambda_1$ the largest zero of $\lambda^2 - \lambda + P_r P_t$, and $r(\lambda) = \frac{p(\lambda)}{\lambda}$, we compute

$$r(\lambda_\circ + P_i^2 \mu) = P_i^2 \lambda_\circ + P_i^2 (P_i^2 + 2P_i \lambda_\circ + 2\lambda_\circ^2 - P_i - \lambda_\circ) \mu + P_i^4 (P_i + 3\lambda_\circ - 1) \mu^2 + P_i^6 \mu^3 = 0,$$

and conclude by the implicit function theorem, using $\lambda_\circ = 1 + \mathcal{O}_2^*$, that there is a unique C^∞ function μ of P_i, P_r, P_t near the origin, satisfying $\mu(0, 0, 0) = -1$, such that $\lambda_1 = \lambda_\circ + P_i^2 \mu$. This leads to $\frac{\partial^2 \lambda_1}{\partial P_i \partial P_r} = \mathcal{O}(P_i)$, and similarly $\frac{\partial^2 \lambda_1}{\partial P_i \partial P_t} = \mathcal{O}(P_i)$, resulting in $\ln(\frac{\lambda_1}{\lambda_* \lambda_\circ}) = \mathcal{O}(P_r P_t P_i^2)$, yielding (30).

Case 4: Pairs $(i, j), (r, t)$ with i, j, r, t all different.

The matrix $\bar{\Pi}$, its characteristic polynomial p , and asymptotics of λ_1 and C_1 are given by

$$\bar{\Pi} = \begin{bmatrix} P_e & P_i & P_j & P_r & P_t \\ P_e & P_i & 0 & P_r & P_t \\ P_e & P_i & P_j & P_r & P_t \\ P_e & P_i & P_j & P_r & 0 \\ P_e & P_i & P_j & P_r & P_t \end{bmatrix}, \quad \begin{aligned} p(\lambda) &= \lambda^5 - \lambda^4 + (P_i P_j + P_r P_t) \lambda^3, \\ \lambda_1 &= 1 - P_i P_j - P_r P_t + \mathcal{O}_4^*, \\ C_1 &= 1 + P_i P_j + P_r P_t + \mathcal{O}_4^*. \end{aligned}$$

Observe that $\frac{\partial^2 \ln \lambda_1}{\partial P_i \partial P_r} = \mathcal{O}_2^*$ and $\frac{\partial^2 \ln \lambda_1}{\partial P_i \partial P_i} = \mathcal{O}_2^*$ lead to $\ln(\frac{\lambda_1}{\lambda_* \lambda_o}) = \mathcal{O}(P_i P_j P_r P_t)$, yielding (30).

Case 5: Pairs $(i, r), (r, i)$ with i, r different.

The matrix $\bar{\Pi}$, its characteristic polynomial p , and asymptotics of λ_1 and C_1 are given by

$$\bar{\Pi} = \begin{bmatrix} P_e & P_i & P_r \\ P_e & P_i & 0 \\ P_e & 0 & P_r \end{bmatrix}, \quad \begin{aligned} p(\lambda) &= \lambda^3 - \lambda^2 + P_i P_r \lambda + P_e P_i P_r, \\ \lambda_1 &= 1 - 2P_i P_r + P_i^2 P_r + P_i P_r^2 + \mathcal{O}_4^*, \\ C_1 &= 1 + 2P_i P_r - 2P_i^2 P_r - 2P_i P_r^2 + \mathcal{O}_4^*. \end{aligned}$$

Note that λ_1 is a C^∞ function of the coefficients $P_i P_r$ and $P_i P_r (1 - P_i - P_r)$, leading to

$$\lambda_1 = 1 - 2P_i P_r + P_i P_r (P_i + P_r) + \mathcal{O}(P_i^2 P_r^2),$$

which, together with $\lambda_* = \lambda_o = 1 - P_i P_r + \mathcal{O}(P_i^2 P_r^2)$, we use to derive

$$\frac{\lambda_1}{\lambda_* \lambda_o} = 1 + P_i^2 P_r + P_i P_r^2 + \mathcal{O}(P_i^2 P_r^2).$$

This is in accordance with (30), with $\bar{Q} = P_i^2 P_r + P_i P_r^2 = P_i P_r (P_i + P_r) \leq P_i P_r (1 - \delta) = \frac{1-\delta}{2} \varepsilon$.

Case 6a: Pairs $(i, i), (i, r)$ with i, r different.

The matrix $\bar{\Pi}$, its characteristic polynomial p , and asymptotics of λ_1 and C_1 are given by

$$\bar{\Pi} = \begin{bmatrix} P_e & P_i & P_r \\ P_e & 0 & 0 \\ P_e & P_i & P_r \end{bmatrix}, \quad \begin{aligned} p(\lambda) &= \lambda^3 - (1 - P_i) \lambda^2 - P_i P_e \lambda, \\ \lambda_1 &= 1 - P_i^2 - P_i P_r + P_i^2 P_r + P_i^3 + \mathcal{O}_4^*, \\ C_1 &= 1 + P_i^2 + P_i P_r - 2P_i^2 P_r - 2P_i^3 + \mathcal{O}_4^*. \end{aligned}$$

We start deriving the more precise estimate $\lambda_1 = 1 - P_i^2 - P_i P_r + P_i^2 P_r + P_i^3 + P_i^2 \mathcal{O}_2^*$:

Abbreviating $\sigma = P_i + P_r$, $\kappa = P_i - P_i^2$, we use $p(\lambda_1) = 0$ to infer the existence of a function μ that satisfies $\lambda_1 = 1 - \kappa \sigma + P_i^2 \mu$. Indeed, from

$$\begin{aligned} 0 &= \lambda_1^2 - (1 - P_i) \lambda_1 - P_i (1 - \sigma) \\ &= (1 - \kappa \sigma + P_i^2 \mu)^2 - (1 - P_i) (1 - \kappa \sigma + P_i^2 \mu) - P_i (1 - \sigma) \\ &= \kappa^2 \sigma^2 + \sigma (P_i - \kappa - P_i \kappa) + P_i^2 \mu (1 + P_i - 2\kappa \sigma) + P_i^4 \mu^2 \\ &= P_i^2 [(1 - P_i)^2 \sigma^2 + \sigma P_i + (1 + P_i - 2\kappa \sigma) \mu + P_i^2 \mu^2] \end{aligned}$$

we conclude by the implicit function theorem that there is a unique C^∞ function μ of P_i, P_r near the origin, satisfying $\mu = \mathcal{O}_2^*$.

Since $\lim_{P_r \rightarrow 0} \lambda_1 = \lambda_*$ and $\lim_{P_r \rightarrow 0} \lambda_o = 1$, we have $\frac{\lambda_1}{\lambda_* \lambda_o} = 1 + \mathcal{O}(P_r)$. This estimate will now be refined. From $\lambda_* = 1 - P_i^2 + P_i^3 + \mathcal{O}(P_i^4)$ and $\lambda_o = 1 - P_i P_r + \mathcal{O}(P_i^2 P_r^2)$ we deduce $\lambda_* \lambda_o = 1 - P_i^2 - P_i P_r + P_i^3 + P_i^2 \mathcal{O}_2^*$ and

$$\frac{\lambda_1}{\lambda_* \lambda_o} = \frac{\lambda_* \lambda_o + P_i^2 P_r + P_i^2 \mathcal{O}_2^*}{\lambda_* \lambda_o} = 1 + P_i^2 P_r + P_i^2 \mathcal{O}_2^* = 1 + P_i^2 P_r + P_i^2 P_r \mathcal{O}_1^* = 1 + P_i^2 P_r + \mathcal{O}(P_i^2 P_r).$$

This is not quite (30), but $\bar{Q} = P_i^2 P_r = \frac{P_r}{2} P_i^2 + \frac{P_i}{2} P_i P_r \leq \frac{1-\delta}{2} \varepsilon$ is satisfied, and $\mathcal{O}(P_i^2 P_r)$ turns out to be a sufficiently good substitute for $\mathcal{O}(P_{i_1} P_{j_1} P_{i_2} P_{j_2})$.

Case 6b: Pairs $(i, i), (r, i)$ with i, r different.

Here the matrix $\bar{\Pi}$ can be seen to be a similarity transformation of the transposed matrix in Case 6a, implying that $p(\lambda), \lambda_1, C_1$, and also the covariance, are the same as in Case 6a.

We summarize the covariances $\text{Cov}(X_{i_1, j_1}^{(n)}, X_{i_2, j_2}^{(n)})$, asymptotics valid for $(P_j)_{j \in J} \in \mathcal{D}_\delta^J$,

$$\text{Cov}(X_{i,r}^{(n)}, X_{r,t}^{(n)}) = (e^{nP_i P_r P_t} - 1) e^{-n(P_i P_r + P_r P_t)} + \mathcal{O}(nP_i P_r^2 P_t + \sqrt{n} P_i P_r P_t) e^{-\frac{\delta}{4} n(P_i P_r + P_r P_t)} \quad (\text{Case 1})$$

$$\text{Cov}(X_{i,r}^{(n)}, X_{i,t}^{(n)}) = \text{Cov}(X_{r,i}^{(n)}, X_{t,i}^{(n)}) = \mathcal{O}(nP_i^2 P_r P_t + P_i P_r P_t) e^{-\frac{\delta}{4}n(P_i P_r + P_i P_t)} \quad (\text{Cases 2})$$

$$\text{Cov}(X_{i,i}^{(n)}, X_{r,t}^{(n)}) = \mathcal{O}(nP_i^2 P_r P_t + P_i P_r P_t) e^{-\frac{\delta}{4}n(P_i^2 + P_r P_t)} \quad (\text{Case 3})$$

$$\text{Cov}(X_{i,j}^{(n)}, X_{r,t}^{(n)}) = \mathcal{O}(nP_i P_j P_r P_t) e^{-\frac{\delta}{4}n(P_i P_j + P_r P_t)} \quad (\text{Case 4})$$

$$\text{Cov}(X_{i,r}^{(n)}, X_{r,i}^{(n)}) = (e^{nP_i P_r (P_i + P_r)} - 1) e^{-2nP_i P_r} + \mathcal{O}(nP_i^2 P_r^2 + \sqrt{n} P_i P_r) e^{-\frac{\delta}{2}nP_i P_r} \quad (\text{Case 5})$$

$$\text{Cov}(X_{i,i}^{(n)}, X_{i,r}^{(n)}) = \text{Cov}(X_{i,i}^{(n)}, X_{r,i}^{(n)}) = \mathcal{O}(nP_i^2 P_r + P_i P_r) e^{-\frac{\delta}{4}n(P_i^2 + P_i P_r)} \quad (\text{Cases 6})$$

We continue showing that the multiple sums of error terms arising in (22) and Cases 1–6 are negligible. In addition to (27) we will also use that

$$\sum_{i,k \geq 1} (nP_i P_k)^\alpha e^{-nP_i P_k} = \mathcal{O}(\ln n) \quad \text{holds for } \alpha > 0. \quad (31)$$

Note that (31), proven in Appendix B, yields $\sum_{i,r \geq 1} P_i P_r e^{-\frac{\delta}{4}nP_i P_r} = \mathcal{O}\left(\frac{\ln n}{n}\right)$, which settles (22), and also Case 5, where the double sum is $\mathcal{O}\left(\frac{\ln n}{\sqrt{n}}\right)$, and Case 4, with quadruple sum of order $\mathcal{O}\left(\frac{\ln^2 n}{n}\right)$. Using $P_i P_t \leq \sqrt{P_i P_t}$, Case 1 can be reduced to bounding the sum

$$\frac{1}{\sqrt{n}} \sum_{i,r,t \geq 1} \sqrt{n P_i P_r} \sqrt{n P_r P_t} e^{-\frac{\delta}{4}n(P_i P_r + P_r P_t)} \leq \frac{1}{\sqrt{n}} \sum_{i,r \geq 1} \sqrt{n P_i P_r} e^{-\frac{\delta}{4}nP_i P_r} = \mathcal{O}\left(\frac{\ln n}{\sqrt{n}}\right),$$

where for the inner sum (w.r.t. t) we used (27). Similarly Cases 2 give rise to triple sums of order $\mathcal{O}\left(\frac{\ln n}{n}\right)$. The same is true for Case 3, which is seen by upper bounding the triple sums by

$$\frac{1}{n} \sum_{i,r,t \geq 1} (nP_i^2)^\alpha (nP_r P_t)^\alpha e^{-\frac{\delta}{4}n(P_i^2 + P_r P_t)} = \frac{1}{n} \sum_{i \geq 1} (nP_i^2)^\alpha e^{-\frac{\delta}{4}nP_i^2} \sum_{r,t \geq 1} (nP_r P_t)^\alpha e^{-\frac{\delta}{4}nP_r P_t} = \mathcal{O}\left(\frac{\ln n}{n}\right),$$

where $\alpha \in \{1/2, 1\}$. Finally, the following estimates

$$\sum_{i,r \geq 1} nP_i^2 P_r e^{-\frac{\delta}{4}n(P_i^2 + P_i P_r)} = \frac{1}{\sqrt{n}} \sum_{i \geq 1} (nP_i^2)^{1/2} e^{-\frac{\delta}{4}nP_i^2} \sum_{r \geq 1} nP_i P_r e^{-\frac{\delta}{4}nP_i P_r} = \mathcal{O}\left(\frac{\ln n}{\sqrt{n}}\right), \quad (32)$$

$$\sum_{i,r \geq 1} P_i P_r e^{-\frac{\delta}{4}n(P_i^2 + P_i P_r)} \leq \frac{1}{n^{\frac{3}{4}}} \sum_{i \geq 1} (nP_i^2)^{1/4} e^{-\frac{\delta}{4}nP_i^2} \sum_{r \geq 1} (nP_i P_r)^{1/2} e^{-\frac{\delta}{4}nP_i P_r} = \mathcal{O}\left(\frac{\ln n}{n^{\frac{3}{4}}}\right),$$

deal with Cases 6. The total contribution of error terms is therefore of order $\mathcal{O}\left(\frac{\ln n}{\sqrt{n}}\right)$.

We are left with dealing with the sums of the main terms of Cases 1 and 5, and (22). Note that Case 1 has a twin case, $\text{Cov}(X_{i,r}^{(n)}, X_{r,t}^{(n)}) = \text{Cov}(X_{r,i}^{(n)}, X_{t,r}^{(n)})$.

Denote $H(i, j, k) = (e^{nP_i P_j P_k} - 1) e^{-nP_i P_j - nP_j P_k}$ and $H^\circ(i, j) = (e^{nP_i P_j (P_i + P_j)} - 1) e^{-2nP_i P_j}$. Observe that

$$\begin{aligned} \sum_{i \neq j} (e^{nP_i^2 P_j} - 1) (e^{nP_i P_j^2} - 1) e^{-2nP_i P_j} &\leq \sum_{i,j} nP_i^2 P_j e^{nP_i^2 P_j} nP_i P_j^2 e^{nP_i P_j^2} e^{-2nP_i P_j} \\ &\leq \sum_{i,j} n^2 P_i^3 P_j^3 e^{-2\delta n P_i P_j} = \mathcal{O}\left(\frac{\ln n}{n}\right) \end{aligned}$$

and $(e^{a+b} - 1) = (e^a - 1) + (e^b - 1) + (e^a - 1)(e^b - 1)$ imply $\sum_{i \neq j} H^\circ(i, j) = 2 \sum_{i \neq j} H(i, j, i) + \mathcal{O}\left(\frac{\ln n}{n}\right)$. Therefore we have

$$2 \sum_{\substack{i,j,k \geq 1 \\ |\{i,j,k\}|=3}} H(i, j, k) + \sum_{\substack{i,j \geq 1 \\ |\{i,j\}|=2}} H^\circ(i, j) \sim 2 \sum_{\substack{i,j,k \geq 1 \\ j \notin \{i,k\}}} H(i, j, k)$$

$$= 2 \sum_{i,j,k \geq 1} H(i,j,k) - 4 \sum_{i,j \geq 1} \overbrace{H(i,i,j)}^{\mathcal{O}\left(\frac{\ln n}{\sqrt{n}}\right)} + 2 \sum_{i \geq 1} \overbrace{H(i,i,i)}^{\mathcal{O}\left(\frac{1}{\sqrt{n}}\right)},$$

where we have estimated two of the sums using (27) and (32). Asymptotics of the sum $\sum_{i,j,k \geq 1} H(i,j,k)$ are computed in Appendix A.4, confirming $T_2^{(n)}$ as given in (3). The sum

$$\sum_{i,r \geq 1} [e^{-nP_i P_r} - e^{-2nP_i P_r}] = \sum_{i,r \geq 1} [1 - e^{-2nP_i P_r}] - \sum_{i,r \geq 1} [1 - e^{-nP_i P_r}] = \tilde{G}(2np^2) - \tilde{G}(np^2),$$

which, as we have seen, is an asymptotic equivalent of $\sum_{i,r \geq 1} \text{Var } X_{i,r}^{(n)}$, is evaluated in Appendix A.3, confirming $S_2^{(n)}$ as given in (2). This completes the proof of the lemma, and also proves (6), as we have seen, that multiple sums of covariances $\text{Cov}(X_{i_1, j_1}^{(n)}, X_{i_2, j_2}^{(n)})$ with $i_1 = j_1$, but $i_2 \neq j_2$, are negligible. \blacksquare

Remark 4.10 *Along the lines of the two preceding proofs an independent proof of Theorem 3.6 could easily be furnished. We would use (13), (19), (20) to identify $\sum_{i \geq 1} (1 - e^{-nP_i^2})$ and $\sum_{i \neq j} (1 - e^{-nP_i P_j})$ as asymptotic equivalents of $\mathbb{E}X_1^{(n)}$ and $\mathbb{E}X_3^{(n)}$, leading to $\mathbb{E}X_1^{(n)} \sim G(np^2)$ and $\mathbb{E}X_3^{(n)} \sim \tilde{G}(np^2) - G(np^2)$, with G, \tilde{G} from Appendices A.1 and A.3.*

4.4 More than two pairs of identical letters

We now turn to the case of k pairs $(i_1, i_1), \dots, (i_k, i_k)$, allowing for $k > 2$.

Lemma 4.11 *Fix a set $I := \{i_1, i_2, \dots, i_k\}$ of size k , assuming $i_k < \dots < i_1$, and thus $P_{i_1} < \dots < P_{i_k}$. Let $\varepsilon := \sum_{i \in I} P_i^2$. Then we have*

$$\mathbb{P}(X_{i,i}^{(n)} = 0, i \in I) = \sum_{j=1}^{k+1} C_j \lambda_j^n = \begin{cases} \mathcal{O}\left(\frac{1}{n}\right), & \text{for } \varepsilon \geq \frac{3 \ln n}{n}, \\ C_1 \lambda_1^n + \mathcal{O}\left(\frac{1}{n}\right), & \text{for } \varepsilon \leq 1/4, \end{cases} \quad (33)$$

with all λ_i different, and error terms holding uniformly in k . More precisely, we have $\lambda_1 > |\lambda_j| > 0$ for $2 \leq j \leq k+1$, and $-P_{i_k} < \lambda_{k+1} < -P_{i_{k-1}} < \lambda_k < \dots < -P_{i_1} < \lambda_2 < 0$. Moreover,

$$\lambda_1 = 1 - \sum_{i \in I} P_i^2 + \sum_{i \in I} P_i^3 + \mathcal{O}(\varepsilon^2), \quad (34)$$

$$C_1 = 1 + \mathcal{O}(\varepsilon), \quad (35)$$

again with error terms holding uniformly in k .

Proof. As before, we let $e := \mathbb{N} \setminus I$ and $P_e := 1 - \sum_{i \in I} P_i$, and introduce the matrix

$$\bar{\Pi} = \begin{bmatrix} P_e & P_{i_1} & P_{i_2} & \cdots & P_{i_k} \\ P_e & 0 & P_{i_2} & \cdots & P_{i_k} \\ P_e & P_{i_1} & 0 & \cdots & P_{i_k} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ P_e & P_{i_1} & P_{i_2} & \cdots & 0 \end{bmatrix}.$$

In order to find eigenvalues and corresponding left and right eigenvectors of $\bar{\Pi}$, we have to solve the following systems,

$$\begin{aligned} \lambda &= P_e \left(1 + \sum_{j \in I} \beta_j\right) & \lambda &= P_e \left(1 + \sum_{j \in I} P_j \mu_j\right) \\ \lambda \beta_i &= P_i \left(1 + \sum_{j \in I \setminus \{i\}} \beta_j\right), \quad i \in I & \lambda \mu_i &= 1 + \sum_{j \in I \setminus \{i\}} P_j \mu_j, \quad i \in I \end{aligned} \quad (36)$$

Note that $(\mu_i)_{i \in I}$ solves the right system if and only if $(\beta_i)_{i \in I} = (P_i \mu_i)_{i \in I}$ solves the left system. From the left system we easily obtain

$$\beta_i = \frac{\lambda P_i}{P_e(\lambda + P_i)}, \text{ for } i \in I, \quad (37)$$

and, upon inserting into the first equation of the left system,

$$\lambda = P_e + \sum_{i \in I} \frac{\lambda P_i}{\lambda + P_i} = P_e + \sum_{i \in I} P_i - \sum_{i \in I} \frac{P_i^2}{\lambda + P_i} = 1 - \sum_{i \in I} \frac{P_i^2}{\lambda + P_i}. \quad (38)$$

There are at most $k + 1$ different solutions to (38), those being exactly the eigenvalues of $\tilde{\Pi}$. Defining $f(\lambda) := \lambda - 1 + \sum_{i \in I} \frac{P_i^2}{\lambda + P_i}$, we observe the following $k + 1$ sign changes on the interval $[-P_i, 1]$,

$$\sum_{i \in I} \frac{P_i^2}{1 + P_i} = f(1) > 0 > f(0) = -P_e, \quad \lim_{\lambda \nearrow -P_i} f(\lambda) = -\infty, \quad \lim_{\lambda \searrow -P_i} f(\lambda) = \infty, \text{ for } i \in I,$$

from which we obtain the result regarding the locations of the eigenvalues.

We continue with the proof of (33). The first estimate, $\mathcal{O}(\frac{1}{n})$, directly follows from (13). For the second, note that $\varepsilon \leq 1/4$ implies $P_{i_k} \leq 1/2$. We then use (26) and S and \mathbf{w} as defined in the proof of Lemma 4.1. Then for some orthogonal matrix Q the matrix $\tilde{\Pi} := QS\tilde{\Pi}S^{-1}Q^{-1}$ is diagonal and satisfies $\rho(\tilde{\Pi}) = |\lambda_{k+1}| < P_{i_k} \leq 1/2$, and $|\lambda_{k+1-j}| < P_{i_{k-j}} \leq \frac{q^j}{2}$ for $j \geq 1$, implying $\|\tilde{\Pi}^n\|_F \leq \frac{1}{1-q} 2^{-n}$. This leads to

$$\pi \tilde{\Pi}^n \mathbf{1} = \mathbf{w}(S\tilde{\Pi}S^{-1})^{n-1} \mathbf{w}^t = \mathbf{w}Q^{-1}\tilde{\Pi}^{n-1}Q\mathbf{w}^t \leq \|\tilde{\Pi}^{n-1}\|_2 \leq \|\tilde{\Pi}^{n-1}\|_F \leq \frac{2}{1-q} 2^{-n} = \mathcal{O}\left(\frac{1}{n}\right).$$

Turning now to asymptotic expansions of λ_1 and C_1 , we first provide a convenient representation of the latter in the spirit of (38), starting from (18),

$$C_1 = \frac{1 + \sum_{i \in I} \beta_i}{1 + P_e \sum_{i \in I} \frac{\beta_i^2}{P_i}} = \frac{\lambda_1}{P_e + \sum_{i \in I} \frac{\lambda_1^2 P_i}{(\lambda_1 + P_i)^2}} = \frac{\lambda_1}{\lambda_1 - \sum_{i \in I} P_i \left[\frac{\lambda_1}{\lambda_1 + P_i} - \frac{\lambda_1^2}{(\lambda_1 + P_i)^2} \right]} = \frac{1}{1 - \sum_{i \in I} \frac{P_i^2}{(\lambda_1 + P_i)^2}}. \quad (39)$$

Note that asymptotic estimates of higher order than those given in (34) and (35) could easily be obtained by Algorithm 1, but as we need error terms uniformly in k , we choose another route. We assume $\varepsilon \leq 1/9$ and observe $f(1 - \frac{3}{2}\varepsilon) = -\frac{3}{2}\varepsilon + \sum_{i \in I} \frac{P_i^2}{1 - \frac{3}{2}\varepsilon + P_i} < -\frac{3}{2}\varepsilon + \sum_{i \in I} \frac{P_i^2}{1 - \frac{3}{2}\varepsilon} \leq -\frac{3}{2}\varepsilon + \frac{6}{5}\varepsilon \leq 0$, which implies $\lambda_1 > 1 - \frac{3}{2}\varepsilon$. Using $\lambda_1 + P_i \leq 1 + 1/3 = 4/3$ in equation (38), we obtain

$$\lambda_1 = 1 - \sum_{i \in I} \frac{P_i^2}{\lambda_1 + P_i} \leq 1 - \frac{3}{4} \sum_{i \in I} P_i^2 = 1 - \frac{3}{4}\varepsilon.$$

Next we employ $1 - x \leq \frac{1}{1+x} \leq 1 - x + 2x^2$, holding for $x \in [-1/2, 1]$, in

$$\begin{aligned} \lambda_1 &\leq 1 - \sum_{i \in I} \frac{P_i^2}{1 - \frac{3}{4}\varepsilon + P_i} \leq 1 - \sum_{i \in I} P_i^2 + \sum_{i \in I} P_i^3 - \frac{3}{4}\varepsilon^2, \\ \lambda_1 &\geq 1 - \sum_{i \in I} \frac{P_i^2}{1 - \frac{3}{2}\varepsilon + P_i} \geq 1 - \sum_{i \in I} P_i^2 + \sum_{i \in I} P_i^3 - \frac{3}{2}\varepsilon^2 - 2 \sum_{i \in I} P_i^4 + 6\varepsilon \sum_{i \in I} P_i^3 - \frac{9}{2}\varepsilon^3 \\ &\geq 1 - \sum_{i \in I} P_i^2 + \sum_{i \in I} P_i^3 - 4\varepsilon^2, \end{aligned}$$

proving (34). Similarly, (35) follows from (39), using $\lambda_1 + P_i \geq 1 - \frac{3}{2}\varepsilon \geq 5/6$:

$$1 \leq C_1 = \left[1 - \sum_{i \in I} \frac{P_i^2}{(\lambda_1 + P_i)^2} \right]^{-1} \leq \left[1 - \frac{36}{25} \sum_{i \in I} P_i^2 \right]^{-1} \leq 1 + 2\varepsilon.$$

This completes the proof of the lemma. ■

Proof of Theorem 2.2: We first consider $x_i = 0$ for all $i \in I$. Letting $\varepsilon := \sum_{i \in I} P_i^2$ again, by the previous lemma we have

$$\mathbb{P}(X_{i,i}^{(n)} = 0, i \in I) = C_1 \lambda_1^n + \sum_{j=2}^{k+1} C_j \lambda_j^n = \prod_{i \in I} e^{-n(P_i^2 - P_i^3)} \left(1 + \mathcal{O}(\varepsilon) + n\mathcal{O}(\varepsilon^2)\right) + \mathcal{O}\left(\frac{1}{n}\right).$$

By letting $P_j \rightarrow 0$ for $j \in I \setminus \{i\}$, we obtain

$$\mathbb{P}(X_{i,i}^{(n)} = 0) = e^{-n(P_i^2 - P_i^3)} \left(1 + \mathcal{O}(P_i^2) + n\mathcal{O}(P_i^4)\right) + \mathcal{O}\left(\frac{1}{n}\right),$$

and finally

$$\mathbb{P}(X_{i,i}^{(n)} = 0, i \in I) - \prod_{i \in I} \mathbb{P}(X_{i,i}^{(n)} = 0) = \left(\prod_{i \in I} e^{-n(P_i^2 - P_i^3)}\right) \left(\mathcal{O}(\varepsilon) + n\mathcal{O}(\varepsilon^2)\right) + \mathcal{O}\left(\frac{1}{n}\right) = \mathcal{O}\left(\frac{1}{n}\right), \quad (40)$$

using $\prod_{i \in I} e^{-n(P_i^2 - P_i^3)} \leq e^{-n\varepsilon(1 - P_1)}$, and the fact that $e^{-x(1 - P_1)}(x + x^2)$ is bounded for $x \geq 0$.

Clearly, equation (40) holds for $I = \{i\}$ and all $x_i \in \{0, 1\}$. Assume that equation (40) has been shown for all I with $|I| = k$. Consider I' with $|I'| = k + 1$. Then, as we have just shown, equation (40) holds for I' when $\sum_{i \in I'} x_i = 0$. It also holds when $\sum_{i \in I'} x_i = 1$: If $x_j = 1$, $x_i = 0$ for $i \in I' \setminus \{j\}$, then

$$\begin{aligned} \mathbb{P}(X_{i,i}^{(n)} = x_i, i \in I') &= \mathbb{P}(X_{i,i}^{(n)} = 0, i \in I' \setminus \{j\}) - \mathbb{P}(X_{i,i}^{(n)} = 0, i \in I'), \\ \prod_{i \in I'} \mathbb{P}(X_{i,i}^{(n)} = x_i) &= \prod_{i \in I' \setminus \{j\}} \mathbb{P}(X_{i,i}^{(n)} = 0) - \prod_{i \in I'} \mathbb{P}(X_{i,i}^{(n)} = 0), \end{aligned}$$

so, by taking the difference of these equations, we have

$$\mathbb{P}(X_{i,i}^{(n)} = x_i, i \in I') - \prod_{i \in I'} \mathbb{P}(X_{i,i}^{(n)} = x_i) = \mathcal{O}\left(\frac{1}{n}\right).$$

Similarly, by induction on $\kappa := \sum_{i \in I'} x_i$, we can prove that (40) holds for all I' with $|I'| = k + 1$ and all $x \in \{0, 1\}^{k+1}$. Clearly the error terms $\mathcal{O}\left(\frac{1}{n}\right)$ may now suffer from dependence on $|I|$, but not on I , as the values $\{P_i\}_{i \in I}$ did not enter the proof. \blacksquare

4.5 Some insights regarding the dependence of λ_1 and C_1 on the matrix $\bar{\bar{\Pi}}$

Fix a finite non-empty set of forbidden pairs $\mathcal{I} := \{(k_i, m_i) : i \in I\}$ and let $J := \bigcup_{i \in I} \{k_i, m_i\}$. We would like to better understand λ_1 and C_1 given in (14), as the examples in the proof of Lemma 4.9 constituted by Cases 1 to 6 suggest that there may be a simple relationship between λ_1 and C_1 . Using $\bar{\bar{\Pi}}$ introduced shortly before Algorithm 1, we define $\tilde{\bar{\Pi}} := \mathbf{1}\bar{\mathbf{p}} - \bar{\bar{\Pi}}$, i.e.,

$$\tilde{\bar{\Pi}}_{k,m} := \begin{cases} P_m, & (k, m) \in \mathcal{I}, \\ 0, & \text{else,} \end{cases}$$

and use it to define $\psi_1 := \bar{\mathbf{p}}\mathbf{1} = \sum_{j \in J} P_j = 1 - P_e$ and

$$\psi_{i+1} := \bar{\mathbf{p}}\tilde{\bar{\Pi}}^i\mathbf{1} = \sum_{k_0, \dots, k_i: (k_0, k_1), \dots, (k_{i-1}, k_i) \in \mathcal{I}} P_{k_0} P_{k_1} \cdots P_{k_i},$$

for $i \geq 1$. Note that $\psi_2 = \varepsilon$, with ε introduced in Lemma 4.1, and ψ_3 is a generalization of Q introduced in (29). Moreover $\psi_i \leq (1 - P_e)^i$ holds for $i \geq 1$. We can express λ_1 and C_1 in terms of $(\psi_i)_{i \geq 2}$ as follows,

$$\lambda_1 = 1 - \psi_2 + \psi_3 - (\psi_2^2 + \psi_4) + (3\psi_2\psi_3 + \psi_5) - (2\psi_2^3 + 4\psi_2\psi_4 + 2\psi_3^2 + \psi_6)$$

$$\begin{aligned}
& + (10\psi_2^2\psi_3 + 5\psi_2\psi_5 + 5\psi_3\psi_4 + \psi_7) \\
& - (5\psi_2^4 + 15\psi_2^2\psi_4 + 15\psi_2\psi_3^2 + 6\psi_2\psi_6 + 6\psi_3\psi_5 + 3\psi_3^2 + \psi_8) \\
& + (35\psi_2^3\psi_3 + 21\psi_2^2\psi_5 + 42\psi_2\psi_3\psi_4 + 7\psi_3^3 + 7\psi_2\psi_7 + 7\psi_3\psi_6 + 7\psi_4\psi_5 + \psi_9) + \mathcal{O}_{10}^*, \\
C_1 = & 1 + \psi_2 - 2\psi_3 + 3(\psi_2^2 + \psi_4) - 4(3\psi_2\psi_3 + \psi_5) + 5(2\psi_2^3 + 4\psi_2\psi_4 + 2\psi_3^2 + \psi_6) + \mathcal{O}_7^*,
\end{aligned}$$

and further terms of λ_1 can be extracted, using gfun, from the equation

$$\lambda = \frac{1 - v\psi_1}{1 - \Psi(\frac{v}{\lambda})}, \quad (41)$$

where $\Psi(z) = -\sum_{i \geq 1} \psi_i(-z)^i$, the solution being a power series in v , starting $\lambda(v) = 1 - \psi_2v^2 + \psi_3v^3 + \dots$, upon substituting $v = 1$. Furthermore an analogous power series for C_1 satisfies

$$C(v) = \lambda(v) - v\lambda'(v). \quad (42)$$

Also the generating function of the probabilities $p_I^{(n)} := \mathbb{P}(X_{k_i, m_i}^{(n)} = 0, i \in I)$ can be expressed in terms of Ψ , and in fact again in terms of $(\psi_i)_{i \geq 2}$:

$$\begin{aligned}
\sum_{n \geq 0} p_I^{(n)} z^n &= \frac{1}{1 - (1 - \psi_1)z - \Psi(z)} \\
&= 1 + z + (1 - \psi_2)z^2 + (1 - 2\psi_2 + \psi_3)z^3 + (1 - 3\psi_2 + 2\psi_3 + \psi_2^2 - \psi_4)z^4 \\
&\quad + (1 - 4\psi_2 + 3\psi_3 - 2\psi_4 + 3\psi_2^2 + \psi_5 - 2\psi_2\psi_3)z^5 + \mathcal{O}(z^6).
\end{aligned} \quad (43)$$

For a proof of (41) we would start with (15) and (16), i.e., $\lambda = P_e(1 + \beta \mathbf{1})$, $\beta = \frac{1}{\lambda} [\beta \bar{\Pi} + \bar{\mathbf{p}}]$, and replace P_j with vP_j for $j \in J$, leading to $\lambda = (1 - v\psi_1)(1 + \beta \mathbf{1})$, $\beta = \frac{v}{\lambda} [\beta \bar{\Pi} + \bar{\mathbf{p}}]$. Iterating the latter yields

$$\beta = \frac{v}{\lambda} \sum_{k \geq 0} \left(\frac{v}{\lambda}\right)^k \bar{\mathbf{p}} \bar{\Pi}^k,$$

and plugging this into the former we obtain

$$\lambda = (1 - v\psi_1) \left[1 + \sum_{k \geq 0} \left(\frac{v}{\lambda}\right)^{k+1} \bar{\mathbf{p}} \bar{\Pi}^k \mathbf{1} \right].$$

Denoting $F(z) := 1 + \sum_{k \geq 0} z^{k+1} \bar{\mathbf{p}} \bar{\Pi}^k \mathbf{1}$ and using

$$\bar{\Pi}^k = (\mathbf{1} \bar{\mathbf{p}} - \bar{\Pi})^k = (-\bar{\Pi})^k + \sum_{\ell=0}^{k-1} (-\bar{\Pi})^{k-1-\ell} \mathbf{1} \bar{\mathbf{p}} \bar{\Pi}^\ell,$$

we derive

$$\begin{aligned}
F(z) &= 1 + \sum_{k \geq 0} z^{k+1} \bar{\mathbf{p}} (-\bar{\Pi})^k \mathbf{1} + \sum_{k \geq 1} z^{k+1} \sum_{\ell=0}^{k-1} \bar{\mathbf{p}} (-\bar{\Pi})^{k-1-\ell} \mathbf{1} \bar{\mathbf{p}} \bar{\Pi}^\ell \mathbf{1} \\
&= 1 + \Psi(z) + \sum_{m \geq 0} z^{m+1} \bar{\mathbf{p}} \bar{\Pi}^\ell \mathbf{1} \sum_{\ell \geq 0} z^{\ell+1} \bar{\mathbf{p}} (-\bar{\Pi})^m \mathbf{1} \\
&= 1 + \Psi(z) + (F(z) - 1)\Psi(z) = 1 + \Psi(z)F(z),
\end{aligned}$$

from which we deduce $F(z) = \frac{1}{1 - \Psi(z)}$. For a proof of (42), which involves $\lambda'(v)$, we use (41), differentiating $\lambda - \lambda\Psi(\frac{v}{\lambda}) - 1 + v\psi_1 = 0$ w.r.t. v , which leads to

$$0 = \lambda' - \lambda' \Psi(\frac{v}{\lambda}) - \lambda \left[\frac{1}{\lambda} - \lambda' \frac{v}{\lambda^2} \right] \Psi'(\frac{v}{\lambda}) + \psi_1 = \lambda' \frac{1 - v\psi_1}{\lambda} - [1 - \lambda' \frac{v}{\lambda}] \Psi'(\frac{v}{\lambda}) + \psi_1$$

$$= \frac{\lambda'}{\lambda} - \left[1 - \lambda' \frac{v}{\lambda}\right] (\Psi'(\frac{v}{\lambda}) - \psi_1),$$

and finally to

$$\Psi' \left(\frac{v}{\lambda} \right) - \psi_1 = \frac{\lambda'}{\lambda - v\lambda'}. \quad (44)$$

Next we iterate $\mu = \frac{1}{\lambda} \left[v\bar{\Pi}\mu + \mathbf{1} \right]$ obtained from (17), which yields $\mu = \frac{1}{\lambda} \sum_{k \geq 0} \left(\frac{v}{\lambda} \right)^k \bar{\Pi}^k \mathbf{1}$. Note that we have

$$\begin{aligned} \beta\mu &= \sum_{k, \ell \geq 0} \left(\frac{v}{\lambda} \right)^{k+1} \bar{\mathbf{p}} \bar{\Pi}^k \frac{1}{\lambda} \left(\frac{v}{\lambda} \right)^\ell \bar{\Pi}^\ell \mathbf{1} = \frac{1}{\lambda} \sum_{k, \ell \geq 0} \left(\frac{v}{\lambda} \right)^{k+\ell+1} \bar{\mathbf{p}} \bar{\Pi}^{k+\ell} \mathbf{1} = \frac{1}{\lambda} \sum_{m \geq 0} (m+1) \left(\frac{v}{\lambda} \right)^{m+1} \bar{\mathbf{p}} \bar{\Pi}^m \mathbf{1} \\ &= \frac{1}{\lambda} \frac{v}{\lambda} F' \left(\frac{v}{\lambda} \right) = \frac{1}{\lambda} \frac{v}{\lambda} \frac{\Psi' \left(\frac{v}{\lambda} \right)}{\left(1 - \Psi \left(\frac{v}{\lambda} \right) \right)^2} = \frac{v \Psi' \left(\frac{v}{\lambda} \right)}{\left(1 - v\psi_1 \right)^2}. \end{aligned}$$

This we plug into (18), thus establishing (42),

$$C(v) = \frac{1 + \beta \mathbf{1}}{1 + (1 - v\psi_1)\beta\mu} = \frac{\lambda}{1 - v\psi_1 + (1 - v\psi_1)^2 \beta\mu} = \frac{\lambda}{1 - v\psi_1 + v \Psi' \left(\frac{v}{\lambda} \right)} = \frac{\lambda}{1 + v \frac{\lambda'}{\lambda - v\lambda'}} = \lambda(v) - v\lambda'(v).$$

The proof of (43) starts with $\mathbb{P}_n(X_{k_i, m_i}^{(n)} = 0, i \in I) = \bar{\mathbf{p}} \bar{\Pi}^{n-1} \mathbf{1}$ for $n \geq 1$, with $\mathbf{p} = [P_e, \bar{\mathbf{p}}]$, uses $\mathbf{p}(\mathbf{1}\mathbf{p} - \bar{\Pi})^{n-1} \mathbf{1} = \bar{\mathbf{p}} \bar{\Pi}^{n-1} \mathbf{1} = \psi_n$, and then uses ideas from the proof of (41).

Let us finally remark that using the function $\tilde{\Psi}(z) := -\sum_{i \geq 2} \psi_i(-z)^i$, equations (41) and (43) can be recast in the following, somewhat simpler forms,

$$\lambda = \frac{1}{1 - \tilde{\Psi} \left(\frac{v}{\lambda} \right)}, \quad \sum_{n \geq 0} p_I^{(n)} z^n = \frac{1}{1 - z - \tilde{\Psi}(z)}.$$

We will meet the latter generating function again in Section 5, where, employing a combinatorial approach, we are able to show that in case of one or two forbidden pairs, the generating function is rational with a denominator of degree at most three, which allows for very explicit expressions for the coefficients.

4.6 Limiting distribution of $X_3^{(n)}$

Conjecture 4.12 *The asymptotic distribution of $X_3^{(n)}$ is Gaussian*

Proof. Heuristic

We assume asymptotic independence of $X_{i,j}$, as the covariance total contribution is $\mathcal{O}(1)$. Let $n_2 q^{u^*} = 1$, $u^* = \ln(n_2)/L$, and $\tilde{u} := \lfloor u^* \rfloor$. The total number of distinct $X_{i,j}$ cells up to diagonal \tilde{u} is given by

$$\sum_1^{\tilde{u}} (v-1) - \left\lfloor \frac{\tilde{u}}{2} \right\rfloor = \frac{\tilde{u}^2}{2} - \frac{\tilde{u}}{2} - \left\lfloor \frac{\tilde{u}}{2} \right\rfloor \sim \frac{\ln(n)^2}{2L^2} + \mathcal{O}(\ln(n))$$

, Now set $\eta := u - u^*$, $\mathbb{P}[X_{i,j}(0) = 1] \sim e^{-e^{-L\eta}}$, $u := i + j$, $\tilde{u} - u^* = \lfloor u^* \rfloor - u^* =: \eta_1$, $-1 \leq \eta_1 \leq 0$, $\tilde{u} + 1 - u^* = \lfloor u^* \rfloor + 1 - u^* = \lceil u^* \rceil - u^* =: \eta_2$, $0 \leq \eta_2 \leq 1$. The number of cells on diagonal u is given by $c(u) = u - 1 - \llbracket \text{even}(u) \rrbracket$. We must now add the contribution of full cells corresponding to diagonal $\tilde{u} + 1$: $\text{Bin}(c(\tilde{u} + 1), 1 - e^{-e^{-L\eta_2}})$, which is asymptotically Gaussian. Similarly for the contributions of $\tilde{u} + i$, $i \geq 2$, we must now subtract the contribution of full cells corresponding to diagonal \tilde{u} : $-\text{Bin}(c(\tilde{u}), e^{-e^{-L\eta_1}})$, which is asymptotically Gaussian. Similarly for the contributions of $\tilde{u} - i$, $i \geq 1$. So the asymptotic total random contribution is Gaussian. ■

The result of a simulation with $p = 1/4$, $n = 500000$, and number of simulated words $N = 200000$ can be seen in Figure 3. The observed mean $\bar{X}_3^{(n)} \approx 750.19$ and observed variance $s_3^2(n) \approx 130.05$ are very close to $\mathbb{E}X_3^{(n)} \approx 750.19$ and $\text{Var} X_3^{(n)} \approx 129.88$. The density of a Gaussian with mean $\mathbb{E}X_3^{(n)}$ and variance $\text{Var} X_3^{(n)}$ is also shown in Figure 3. The fit is excellent.

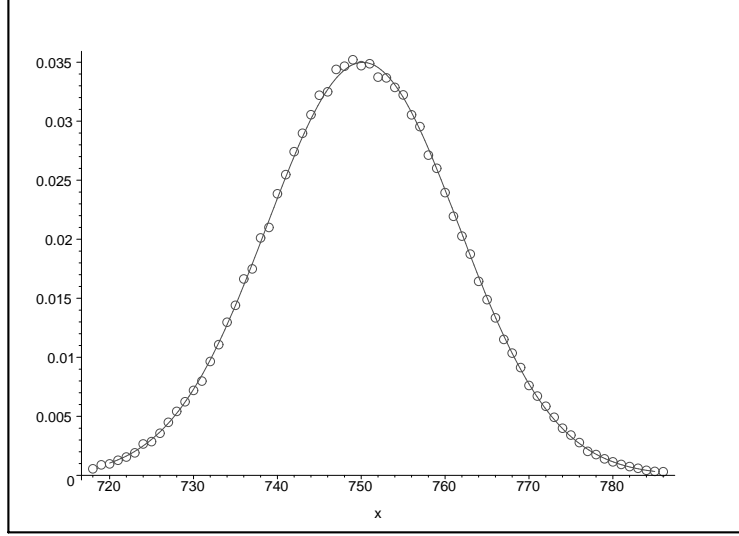


Figure 3: Comparison between Gaussian density $f(x)$ (line) and the simulation of $X_3^{(n)}$ (circles), with $p = 1/4, n = 500000$, and number of simulated words $N = 200000$.

4.7 Another approach to the asymptotic distribution of $X_3^{(n)}$

Let us turn to the couple (i, j) . Let us first assume full independence. We first consider $X_2^{(n)} := \sum_{i,j} X_{i,j}^{(n)}$. The mean is simply given by $M(X_2^{(n)}) = \sum_{i,j} E(X_{i,j}^{(n)})$. The variance $VAR(X_2^{(n)})$ is made of two parts: the first part is related to $\sum_{i,j} VAR(X_{i,j}^{(n)})$, the second part is related to $\sum_{i,j} \sum_{u,v} COV(X_{i,j}^{(n)}, X_{u,v}^{(n)})$ which, as we have seen, is only due to $\sum_{i,j,k} COV(X_{i,j}^{(n)}, X_{j,k}^{(n)})$. So we first proceed as in the (i, i) case. Next we will deal with $X_3^{(n)} := \sum_{i \neq j} X_{i,j}^{(n)}$ i.e. subtract the contribution of the (i, i) couples. Finally, we will deal with the dependence property.

4.7.1 Mean and $\sum_{i,j} VAR(X_{i,j}^{(n)})$ contribution

Set

$$G_{n,2}(\theta) := E\left(e^{\theta X_2^{(n)}}\right), \quad S_{n,2}(\theta) := \ln(G_{n,2}(\theta)).$$

We proceed as in Sec. 3.1.

$$\begin{aligned} \text{Set } Q_2 &:= \frac{1}{q}, L_2 := \ln(Q_2) = -\ln(q), n^* := n_2 k, \log := \log_{Q_2}, L_1 = 2L_2, \\ \mathbb{P}(X_{i,j}(0) = 1) &\sim \bar{P}(i, j) = e^{-n_2 q^{i+j}}, \\ V_v &= \sum_i \sum_j \sum_{k=0}^v (-1)^k \binom{v}{k} \bar{P}(i, j)^k = \sum_i \sum_j \sum_{k=1}^v (-1)^{k+1} \binom{v}{k} \left[1 - \bar{P}(i, j)^k\right], \\ \sum_i \sum_j \left[1 - \bar{P}(i, j)^k\right] &= \sum_{u=2} (u-1) \left[1 - e^{-n^* q^u}\right] = \sum_{u=1} (u-1) \left[1 - e^{-n^* q^u}\right] \\ &= \sum_{u=1} u \left[1 - e^{-n^* q^u}\right] - \sum_{u=1} \left[1 - e^{-n^* q^u}\right] := V_{v,1} - V_{v,2}, \end{aligned}$$

The second summation leads, using the previous results on (i, i) to

$$\sum_{u=1} \left[1 - e^{-n^* q^u} \right] = U_1(Q_2) + \log_{Q_2} k + \beta_k(Q_2),$$

where

$$U_1(Q_2) := \frac{\ln(n_2)}{L_2} - \frac{1}{2} + \frac{\gamma}{L_2}, \beta_k(Q_2) = -\frac{1}{L_2} \sum_{\ell \in \mathbb{Z} \setminus \{0\}} \Gamma\left(\frac{2i\ell\pi}{L_2}\right) e^{-2i\ell\pi \log_{Q_2}(kn_2)},$$

This leads to

$$V_{v,2} = -\sum_{k=1}^v (-1)^{k+1} \binom{v}{k} [U_1(Q_2) + \log_{Q_2} k + \beta_k(Q_2)],$$

omitting the periodic contribution,

$$V_{v,2} = -U_1(Q_2) + C_1(v), C_1(1) = 0, C_1(2) = \log_{Q_2} 2$$

$$V_{1,2} = -U_1(Q_2) - \beta_1(Q_2),$$

$$V_{2,2} = -U_1(Q_2) + \log_{Q_2} 2 - \sum_{k=1}^2 (-1)^{k+1} \binom{2}{k} \beta_k(Q_2).$$

From Appendix A.2, the first summation gives

$$\begin{aligned} V_{v,1} &= \sum_{k=1}^v (-1)^{k+1} \binom{v}{k} \left[\frac{\ln(n_2)^2 + 2 \ln(n_2) \ln(k) + \ln(k)^2}{2L_2^2} + \frac{\gamma(\ln(n_2) + \ln(k))}{L_2^2} \right. \\ &\quad \left. - \left[-\frac{\pi^2/12 + \gamma^2/2}{L_2^2} + \frac{1}{12} \right] \right] + \tilde{\beta}_{v,1}, \\ &= U_2(Q_2) + B_{v,1} + \tilde{\beta}_{v,1}, \end{aligned}$$

where

$$\begin{aligned} U_2(Q_2) &= \frac{\ln(n_2)^2}{2L_2^2} + \frac{\gamma \ln(n_2)}{L_2^2} - \left[-\frac{\pi^2/12 + \gamma^2/2}{L_2^2} + \frac{1}{12} \right] \\ &= \frac{\ln(n)^2}{2L_2^2} + \ln(n) \left[\frac{\gamma + 2 \ln(p) + 2 L_2}{L_2^2} \right] \\ &\quad + 1/12 \frac{\pi^2 + 6 \gamma^2 + 23 L_2^2 + 24 \gamma \ln(p) + 24 \gamma L_2 + 24 (\ln(p))^2 + 48 \ln(p) L_2}{L_2^2}, \end{aligned}$$

Now define

$$B_{v,1} := \sum_{k=2}^v (-1)^{k+1} \binom{v}{k} \left[\frac{2 \ln(n_2) \ln(k) + \ln(k)^2}{2L_2^2} + \frac{\gamma \ln(k)}{L_2^2} \right] = C_2(v) \ln(n) + C_3(v),$$

with, say, $C_2(1) = C_3(1) = 0$, and

$$B_{1,1} = 0,$$

$$B_{2,1} = - \left[\frac{2 \ln(n_2) \ln(2) + \ln(2)^2}{2L_2^2} + \frac{\gamma \ln(2)}{L_2^2} \right],$$

$$\tilde{\beta}_{v,1} = \sum_{k=1}^v (-1)^{k+1} \binom{v}{k} \beta_{k,1}, \tilde{\beta}_{1,1} = \beta_{1,1}, \tilde{\beta}_{2,1} = 2\beta_{1,1} - \beta_{2,1},$$

$$\beta_{k,1} = \frac{1}{L_2} \sum_{\ell \in \mathbb{Z} \setminus \{0\}} \left[-\frac{\ln(n_2 k)}{L_2} \Gamma\left(\frac{2i\ell\pi}{L_2}\right) + \frac{\Gamma'\left(\frac{2i\ell\pi}{L_2}\right)}{L_2} \right] e^{-2i\ell\pi \log(knp^2)},$$

$$\begin{aligned} V_{1,1} &= U_2(Q_2) + \beta_{1,1}, \\ V_{2,1} &= U_2(Q_2) + B_{2,1} + \tilde{\beta}_{2,1}, \end{aligned}$$

Finally, omitting the periodic contribution,

$$\begin{aligned} V_1 &= V_{1,1} + V_{1,2} \sim U_2(Q_2) - U_1(Q_2), \\ V_2 &= V_{2,1} + V_{2,2} \sim U_2(Q_2) - U_1(Q_2) + B_{2,1} + C_1(2), \\ V_v &\sim U_2(Q_2) - U_1(Q_2) + C_2(v) \ln(n) + C_4(v), C_4(v) = C_1(v) + C_3(v), C_4(1) = 0, \end{aligned}$$

We can now compute the mean $M_1(X_2^{(n)})$ and $VAR_1(X_2^{(n)})$ (see (9)). We get

$$\begin{aligned} M_1(X_2^{(n)}) &= V_1 = U_2(Q_2) - U_1(Q_2) + \beta_{1,1} - \beta_1(Q_2), \\ VAR_1(X_2^{(n)}) &= \kappa_2(X_2^{(n)}) = V_1 - V_2 = -B_{2,1} - \log_{Q_2} 2 + \beta_{1,1} - \beta_1(Q_2) - \tilde{\beta}_{2,1} + \sum_{k=1}^2 (-1)^{k+1} \binom{2}{k} \beta_k(Q_2), \\ &= \left[\frac{2 \ln(n_2) \ln(2) + \ln(2)^2}{2L_2^2} + \frac{\gamma \ln(2)}{L_2^2} \right] - \log_{Q_2} 2 - \beta_{1,1} + \beta_{2,1} + \beta_1(Q_2) - \beta_2(Q_2) \end{aligned}$$

4.7.2 Subtraction of the contribution from all couples (i, i)

We obtain for the non-periodic contribution $M_{NP}(X_3^{(n)})$

$$\begin{aligned} M_{NP}(X_3^{(n)}) &:= U_2(Q_2) - U_1(Q_2) - U_1(Q_1) = \frac{\ln(n)^2}{2L_2^2} + \ln(n) \left[1/2 \frac{L_2 + 2\gamma + 4 \ln(p)}{L_2^2} \right] \\ &\quad - 1/12 \frac{-\pi^2 - 6\gamma^2 + L_2^2 - 24\gamma \ln(p) - 6\gamma L_2 - 24(\ln(p))^2 - 12 \ln(p) L_2}{L_2^2}, \end{aligned}$$

Next, for the periodic contribution $M_P(X_3^{(n)})$, we obtain

$$\begin{aligned} M_P(X_3^{(n)}) &= \beta_{1,1} - \beta_1(Q_2) - \beta_1(Q_1) = \frac{1}{L_2} \sum_{\ell \in \mathbb{Z} \setminus \{0\}} \left[-\frac{\ln(n_2)}{L_2} \Gamma\left(\frac{2i\ell\pi}{L_2}\right) + \frac{\Gamma'\left(\frac{2i\ell\pi}{L_2}\right)}{L_2} \right] e^{-2i\ell\pi \log_{Q_2}(np^2)} \\ &\quad + \frac{1}{L_2} \sum_{\ell \in \mathbb{Z} \setminus \{0\}} \left[\Gamma\left(\frac{2i\ell\pi}{L_2}\right) \right] e^{-2i\ell\pi \log_{Q_2}(np^2)} \\ &\quad + \frac{1}{L_1} \sum_{\ell \in \mathbb{Z} \setminus \{0\}} \left[\Gamma\left(\frac{2i\ell\pi}{L_1}\right) \right] e^{-2i\ell\pi \log_{Q_1}(np^2)}. \end{aligned}$$

Similarly, the variance of $X_3^{(n)}$ (without dependence property) is given by

$$\begin{aligned} VAR_2(X_3^{(n)}) &= \left[\frac{2 \ln(n_2) \ln(2) + \ln(2)^2}{2L_2^2} + \frac{\gamma \ln(2)}{L_2^2} \right] - \log_{Q_2} 2 - \beta_{1,1} + \beta_{2,1} + \beta_1(Q_2) - \beta_2(Q_2) \\ &\quad - [\log_{Q_1} 2 + \beta_2(Q_1) - \beta_1(Q_1)]. \end{aligned}$$

After some algebra, we can check that this is identical to Thm 2.1 (except for the term $T_2^{(n)}$, of course). Also the mean is identical with the expression given in Archibald and al. [1], Thm 3. Our approach is simple and general. Note again that the mean does not rely on the dependence property.

4.7.3 The dominant terms, without the periodic components

We have, successively (we keep only dominant terms), and setting

$$\tilde{X}_{i,j}^{(n)} := X_{i,j}^{(n)} - \mathbb{E}(X_{i,j}^{(n)}), \quad \mu_k(X) := \mathbb{E}[(X - \mathbb{E}(X))^k],$$

we have

$$S_{n_2}(\theta) = \sum_{v=1}^{\infty} \frac{(-1)^{v+1}}{v} \left(e^\theta - 1 \right)^v V_v,$$

We first deal without dependence property,

$$\begin{aligned} \kappa_2(X_2^{(n)}) &= \mu_2(X_2^{(n)}) = VAR_1(X_2^{(n)}) = -C_2(2) \ln(n) - C_4(2), \\ \kappa_3(X_2^{(n)}) &= \mu_3(X_2^{(n)}) \\ &= V_1 - 3V_2 + 2V_3 \\ &= [-3C_2(2) + 2C_2(3)] \ln(n) + [-3C_4(2) + 2C_4(3)] \\ &= C_5 \ln(n) + C_6, \text{ say,} \end{aligned}$$

but

$$\kappa_2(X_2^{(n)}) = \mathbb{E} \left[\left(\sum_{i \neq j} \tilde{X}_{i,j}^{(n)} + \sum_i \tilde{X}_{i,i}^{(n)} \right)^2 \right] = \kappa_2(X_3^{(n)}) + \kappa_2(X_1^{(n)}) = \kappa_2(X_3^{(n)}) + C_7, \text{ say,}$$

hence,

$$VAR_2(X_3^{(n)}) = \mu_2(X_3^{(n)}) = \kappa_2(X_3^{(n)}) = -C_2(2) \ln(n) - C_4(2) - C_7 = -C_2(2) \ln(n) + C_8, \text{ say,}$$

Now we calculate

$$\kappa_3(X_2^{(n)}) = \mathbb{E} \left[\left(\sum_{i \neq j} \tilde{X}_{i,j}^{(n)} + \sum_i \tilde{X}_{i,i}^{(n)} \right)^3 \right] = \kappa_3(X_3^{(n)}) + \kappa_3(X_1^{(n)}) = \kappa_3(X_3^{(n)}) + C_9, \text{ say,}$$

hence,

$$\kappa_3(X_3^{(n)}) = \mu_3(X_3^{(n)}) = C_5 \ln(n) + C_6 - C_9 = C_5 \ln(n) + C_{10}, \text{ say.}$$

Now we deal with dependence property,

$$\sigma^2 = VAR(X_3^{(n)}) = \kappa_2(X_3^{(n)}) + T_2^{(n)} = -C_2(2) \ln(n) + C_{11}, \text{ say,}$$

Then $\bar{\kappa}_3(X_3^{(n)})$ is the new third cumulant, including the correlations, and T_3 is the correction, similar to T_2 , so that

$$\bar{\kappa}_3(X_3^{(n)}) = \kappa_3(X_3^{(n)}) + T_3 = C_5 \ln(n) + C_{10} + T_3.$$

A bound such that $|T_3| = \mathcal{O}(1)$ would be enough. We now have

$$\mathbb{E} \left[\exp \left[\theta \frac{X_3^{(n)} - M(X_3^{(n)})}{\sigma} \right] \right] \sim \exp \left[\frac{\theta^2}{2} + \frac{\theta^3}{3!} \frac{C_5 \ln(n) + C_{10} + T_3}{(-C_2(2) \ln(n) + C_{11})^{3/2}} + \dots \right]$$

Let us, for instance, deal with the fourth cumulant. We have, without dependence

$$\kappa_4(X_2^{(n)}) = V_1 - 7V_2 + 12V_3 - 6V_4 = C_{12} \ln(n) + C_{13}, \text{ say,}$$

and

$$\mu_4(X_2^{(n)}) = \kappa_4(X_2^{(n)}) + 3\kappa_2^2(X_2^{(n)}),$$

but

$$\mu_4(X_2^{(n)}) = \mu_4(X_3^{(n)}) + \mu_4(X_1^{(n)}) + 6\mu_2(X_3^{(n)})\mu_2(X_1^{(n)}),$$

hence

$$\mu_4(X_3^{(n)}) = \mu_4(X_2^{(n)}) - [\mu_4(X_1^{(n)}) + 6\mu_2(X_3^{(n)})\mu_2(X_1^{(n)})]$$

and

$$\mu_4(X_3^{(n)}) = \kappa_4(X_2^{(n)}) + 3\kappa_2^2(X_2^{(n)}) - \mu_4(X_1^{(n)}) - 6\mu_2(X_3^{(n)})\mu_2(X_1^{(n)});$$

Now, with dependence,

$$\bar{\mu}_4(X_3^{(n)}) = \mu_4(X_3^{(n)}) + T_4,$$

$$\begin{aligned} \bar{\kappa}_4(X_3^{(n)}) &= \kappa_4(X_2^{(n)}) + 3\mu_2^2(X_2^{(n)}) - \mu_4(X_1^{(n)}) - 6\mu_2(X_3^{(n)})\mu_2(X_1^{(n)}) + T_4 - 3\mu_2^2(X_3^{(n)}) - 6\mu_2(X_3^{(n)})T_2 - 3T_2^2 \\ &= \kappa_4(X_2^{(n)}) + 3\mu_2^2(X_1^{(n)}) - \mu_4(X_1^{(n)}) - 6\mu_2(X_3^{(n)})T_2 + T_4 - 3T_2^2 \\ &= C_{14} \ln(n) + C_{15} + T_4 - 3T_2^2, \text{ say.} \end{aligned}$$

Again a bound such that $|T_4| = \mathcal{O}(1)$ would be enough. We proceed similarly for all cumulants.

Conjecture 4.13

$$|T_i| = \mathcal{O}(1).$$

This leads to the asymptotic Gaussian distribution.

5 Combinatorial Pattern Matching Approach

For a combinatorial approach, we utilize the methodology of the paper [2]. The full strength of this paper is not needed, because (in this case) we are only studying “reduced” sets of patterns, i.e., we are always analyzing patterns of length 2. So we *only* need to understand Sections 4.1 and 4.2 of [2]. We define $X^{(n)}$ as the total number of distinct (adjacent) pairs in a word Z_1, \dots, Z_n , and we have

$$X^{(n)} = \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} X_{i,j}^{(n)}$$

5.1 Lemmas and notation about solving cubic formulas

Lemma 5.1 Consider a, b and $c = 1$. Let $r = \frac{-b + \sqrt{b^2 - 4a}}{2a}$ and $s = \frac{-b - \sqrt{b^2 - 4a}}{2a}$ denote the roots of $az^2 + bz + c$. If these two roots are distinct, then

$$\begin{aligned} \frac{1}{az^2 + bz + c} &= \frac{1}{(1 - z/r)(1 - z/s)} \\ &= \frac{s}{(s - r)(1 - z/r)} + \frac{r}{(r - s)(1 - z/s)}. \end{aligned}$$

The following lemma uses the notation from the “General cubic formula” section of https://en.wikipedia.org/wiki/Cubic_equation

Lemma 5.2 Consider a, b, c and $d = 1$, and define

$$\begin{aligned} \Delta_0 &= b^2 - 3ac \\ \Delta_1 &= 2b^3 - 9abc + 27a^2d \\ C &= \left(\frac{\Delta_1 + \sqrt{\Delta_1^2 - 4\Delta_0^3}}{2} \right)^{1/3} \\ \xi &= \frac{-1 + \sqrt{-3}}{2} \end{aligned}$$

Let $r = -\frac{1}{3a}(b+C+\Delta_0/C)$ and $s = -\frac{1}{3a}(b+\xi C+\Delta_0/(\xi C))$ and $t = -\frac{1}{3a}(b+\xi^2 C+\Delta_0/(\xi^2 C))$ denote the roots of $az^3 + bz^2 + cz + d$. If these three roots r, s, t are distinct, then

$$\begin{aligned} \frac{1}{az^3 + bz^2 + cz + d} &= \frac{1}{(1-z/r)(1-z/s)(1-z/t)} \\ &= \frac{st}{(s-r)(t-r)(1-z/r)} + \frac{rt}{(r-s)(t-s)(1-z/s)} + \frac{rs}{(r-t)(s-t)(1-z/t)}. \end{aligned}$$

In all the instances that we use Lemma 5.2, the three roots r, s, t exist and are distinct, or they exist in the limit, i.e., there is a removable singularity that can be dealt with in a straightforward manner, by using continuity to remedy the removable singularity.

Lemma 5.3 *The roots of the polynomial in the denominators of the generating functions in Table 1 exist and are unique, or there is a removable singularity that can be defined by using continuity.*

Proof. The proof follows directly from Lemma 5.1. To understand the comment about removable singularity, consider (for instance) Table 1A. In the case when $p = q = 1/2$ and $i = j = 1$, we note that the “ r ” and “ s ” from Lemma 5.1 are identical, but nonetheless, the partial fraction decomposition holds in the limit. In this special case, the generating function $1/(1-z+P_i P_j z^2)$ becomes

$$\begin{aligned} \frac{1}{1-z+z^2/4} &= \frac{1}{(1-z/2)^2} = \lim_{p \rightarrow 1/2} \left(\frac{2p^2}{(1-\sqrt{1-4p^2})\sqrt{1-4p^2} \left(1 - \frac{2p^2}{1-\sqrt{1-4p^2}}z\right)} \right. \\ &\quad \left. - \frac{2p^2}{(1+\sqrt{1-4p^2})\sqrt{1-4p^2} \left(1 - \frac{2p^2}{1+\sqrt{1-4p^2}}z\right)} \right) \end{aligned}$$

In other words, the partial fraction decomposition and the coefficients of z^n are valid in the limit in Table 1A, even in this special case. The other cases that have removable singularities are straightforward, and we do not comment on these further. ■

Lemma 5.4 *The roots of the polynomial in the denominators of the generating functions in Table 2 exist and are unique, or there is a removable singularity that can be defined by using continuity.*

Proof. The proof follows directly from Lemma 5.2. Given the values of a, b, c, d , we define the three roots r, s, t as in Lemma 5.2, and everything follows.

To understand the comment about removable singularity, consider (for instance) Table 2E.

In the case when $p = q = 1/2$ and $i = k = 1$, the “ s ” in Lemma 5.2 is undefined, but nonetheless, again Table 2E holds in the limit. In this special case, we have

$$\begin{aligned} \frac{1}{1-z + \frac{P_i^2 z^2}{1+P_i z} + \frac{P_k^2 z^2}{1+P_k z}} &= \frac{2+z}{2-z} \\ &= \lim_{p \rightarrow 1/2} \left((1+pz)(1+pz) \right. \\ &\quad \times \left(\frac{rs}{(r-t)(s-t)(1-z/t)} + \frac{rt}{(r-s)(t-s)(1-z/s)} \right. \\ &\quad \left. \left. + \frac{st}{(s-r)(t-r)(1-z/r)} \right) \right) \end{aligned}$$

In other words, as before, the partial fraction decomposition and the coefficients of z^n are valid in the limit in this special case. Other cases that have removable singularities are similarly easy to handle. ■

A	gen. func.	$\frac{1}{1-z+P_iP_jz^2}$
	par. frac.	$\frac{1-\sqrt{1-4P_iP_j}}{2P_iP_j\sqrt{1-4P_iP_j}} \left(1 - \frac{2P_iP_j}{1-\sqrt{1-4P_iP_j}}z\right)^{-1} - \frac{1+\sqrt{1-4P_iP_j}}{2P_iP_j\sqrt{1-4P_iP_j}} \left(1 - \frac{2P_iP_j}{1+\sqrt{1-4P_iP_j}}z\right)^{-1}$
	coeff. of z^n	$\frac{(2P_iP_j)^{n+1}}{\sqrt{1-4P_iP_j}} \left(\frac{1}{(1-\sqrt{1-4P_iP_j})^{n+1}} - \frac{1}{(1+\sqrt{1-4P_iP_j})^{n+1}} \right)$
B	gen. func.	$\left(1 - z + \frac{P_i^2z^2}{1+P_iz}\right)^{-1} = \frac{1+P_iz}{1-(1-P_i)z-P_i(1-P_i)z^2}$
	par. frac.	$\left(\frac{1}{2} - \frac{1+P_i}{2\sqrt{(1-P_i)(1+3P_i)}}\right) \left(1 - \frac{-2P_i(1-P_i)}{1-P_i+\sqrt{(1-P_i)(1+3P_i)}}z\right)^{-1}$ $- \left(\frac{1}{2} + \frac{1+P_i}{2\sqrt{(1-P_i)(1+3P_i)}}\right) \left(1 - \frac{-2P_i(1-P_i)}{1-P_i-\sqrt{(1-P_i)(1+3P_i)}}z\right)^{-1}$
	coeff. of z^n	$\left(\frac{1}{2} - \frac{1+P_i}{2\sqrt{(1-P_i)(1+3P_i)}}\right) \left(\frac{-2P_i(1-P_i)}{1-P_i+\sqrt{(1-P_i)(1+3P_i)}}\right)^n$ $- \left(\frac{1}{2} + \frac{1+P_i}{2\sqrt{(1-P_i)(1+3P_i)}}\right) \left(\frac{-2P_i(1-P_i)}{1-P_i-\sqrt{(1-P_i)(1+3P_i)}}\right)^n$
C	gen. func.	$\frac{1}{1-z+P_iP_jz^2+P_kP_\ell z^2}$
	par. frac.	$\frac{1+\sqrt{1-4(P_iP_j+P_kP_\ell)}}{2\sqrt{1-4(P_iP_j+P_kP_\ell)}} \left(1 - \frac{2(P_iP_j+P_kP_\ell)}{1-\sqrt{1-4(P_iP_j+P_kP_\ell)}}z\right)^{-1} - \frac{1-\sqrt{1-4(P_iP_j+P_kP_\ell)}}{2\sqrt{1-4(P_iP_j+P_kP_\ell)}} \left(1 - \frac{2(P_iP_j+P_kP_\ell)}{1+\sqrt{1-4(P_iP_j+P_kP_\ell)}}z\right)^{-1}$
	coeff. of z^n	$\frac{(2(P_iP_j+P_kP_\ell))^{n+1}}{\sqrt{1-4(P_iP_j+P_kP_\ell)}} \left(\frac{1}{(1-\sqrt{1-4(P_iP_j+P_kP_\ell)})^{n+1}} - \frac{1}{(1+\sqrt{1-4(P_iP_j+P_kP_\ell)})^{n+1}} \right)$
D	gen. func.	$\left(1 - z + \frac{P_iz(P_iz+P_\ell z)}{1+P_iz}\right)^{-1} = \frac{1+P_iz}{1-(1-P_i)z+(P_i^2+P_\ell P_i-P_i)z^2}$
	par. frac.	$\left(\frac{1}{2} - \frac{1+P_i}{2\sqrt{(1-P_i)(1+3P_i)-4P_iP_\ell}}\right) \left(1 - \frac{-2P_i(1-P_i-P_\ell)}{1-P_i+\sqrt{(1-P_i)(1+3P_i)-4P_iP_\ell}}z\right)^{-1}$ $- \left(\frac{1}{2} + \frac{1+P_i}{2\sqrt{(1-P_i)(1+3P_i)-4P_iP_\ell}}\right) \left(1 - \frac{-2P_i(1-P_i-P_\ell)}{1-P_i-\sqrt{(1-P_i)(1+3P_i)-4P_iP_\ell}}z\right)^{-1}$
	coeff. of z^n	$\left(\frac{1}{2} - \frac{1+P_i}{2\sqrt{(1-P_i)(1+3P_i)-4P_iP_\ell}}\right) \left(\frac{-2P_i(1-P_i-P_\ell)}{1-P_i+\sqrt{(1-P_i)(1+3P_i)-4P_iP_\ell}}\right)^n$ $- \left(\frac{1}{2} + \frac{1+P_i}{2\sqrt{(1-P_i)(1+3P_i)-4P_iP_\ell}}\right) \left(\frac{-2P_i(1-P_i-P_\ell)}{1-P_i-\sqrt{(1-P_i)(1+3P_i)-4P_iP_\ell}}\right)^n$

Table 1: Table of generating functions, partial fraction decompositions, and coefficients of z^n , $n \geq 2$, in each.

Lemma 5.5 For $n \geq 2$, and for $i \neq j$, the probability that ij occurs (at least once) as an adjacent pattern in Z_1, \dots, Z_n is exactly

$$E[X_{i,j}^{(n)}] = 1 - \frac{(2P_iP_j)^{n+1}}{\sqrt{1-4P_iP_j}} \left(\frac{1}{(1-\sqrt{1-4P_iP_j})^{n+1}} - \frac{1}{(1+\sqrt{1-4P_iP_j})^{n+1}} \right).$$

Of course, for $n < 2$, we have $E[X_{i,j}^{(n)}] = 0$.

Proof. The proof of Lemma 5.5 is in subsection 5.3.1. ■

E	<i>gen. func.</i>	$\left(1 - z + \frac{P_i^2 z^2}{1+P_i z} + \frac{P_k^2 z^2}{1+P_k z}\right)^{-1} = \frac{(1+P_i z)(1+P_k z)}{(1-z)(1+P_i z)(1+P_k z) + P_i^2 z^2(1+P_k z) + P_k^2 z^2(1+P_i z)}$
	a, b, c, d	$a = P_i P_k (P_i + P_k - 1), b = P_i^2 + P_i P_k + P_k^2 - P_i - P_k, c = P_k + P_i - 1, d = 1$
	<i>par. frac.</i>	$\frac{(1+P_i z)(1+P_k z)}{az^3+bz^2+cz+d}$ $= (1 + P_i z)(1 + P_k z) \left(\frac{rs}{(r-t)(s-t)(1-z/t)} + \frac{rt}{(r-s)(t-s)(1-z/s)} + \frac{st}{(s-r)(t-r)(1-z/r)} \right)$
	<i>coeff. of z^n</i>	$\frac{(1+P_i t)(1+P_k t)rs}{(r-t)(s-t)t^n} + \frac{(1+P_i s)(1+P_k s)rt}{(r-s)(t-s)s^n} + \frac{(1+P_i r)(1+P_k r)st}{(s-r)(t-r)r^n}$
F	<i>gen. func.</i>	$\left(1 - z + \frac{P_i^2 z^2}{1+P_i z} + P_k P_\ell z^2\right)^{-1} = \frac{1+P_i z}{(1-z)(1+P_i z) + P_i^2 z^2 + P_k P_\ell z^2(1+P_i z)}$
	a, b, c, d	$a = P_i P_k P_\ell, b = P_i P_i + P_k P_\ell - P_i, c = P_i - 1, d = 1$
	<i>par. frac.</i>	$\frac{1+P_i z}{az^3+bz^2+cz+d} = (1 + P_i z) \left(\frac{rs}{(r-t)(s-t)(1-z/t)} + \frac{rt}{(r-s)(t-s)(1-z/s)} + \frac{st}{(s-r)(t-r)(1-z/r)} \right)$
	<i>coeff. of z^n</i>	$\frac{(1+P_i t)rs}{(r-t)(s-t)t^n} + \frac{(1+P_i s)rt}{(r-s)(t-s)s^n} + \frac{(1+P_i r)st}{(s-r)(t-r)r^n}$
G	<i>gen. func.</i>	$\frac{1}{1-z+P_i P_j z^2 + P_j P_\ell z^2 - P_i P_j P_\ell z^3}$
	a, b, c, d	$a = -P_i P_j P_\ell, b = P_i P_j + P_j P_\ell, c = -1, d = 1$
	<i>par. frac.</i>	$\frac{1}{az^3+bz^2+cz+d} = \frac{rs}{(r-t)(s-t)(1-z/t)} + \frac{rt}{(r-s)(t-s)(1-z/s)} + \frac{st}{(s-r)(t-r)(1-z/r)}$
	<i>coeff. of z^n</i>	$\frac{rs}{(r-t)(s-t)t^n} + \frac{rt}{(r-s)(t-s)s^n} + \frac{st}{(s-r)(t-r)r^n}$
H	<i>gen. func.</i>	$\left(1 - z + \frac{2P_i P_j z^2}{1-P_i P_j z^2} - \frac{P_i^2 P_j z^3}{1-P_i P_j z^2} - \frac{P_i P_j^2 z^3}{1-P_i P_j z^2}\right)^{-1} = \frac{1-P_i P_j z^2}{(1-z)(1-P_i P_j z^2) + 2P_i P_j z^2 - P_i^2 P_j z^3 - P_i P_j^2 z^3}$
	a, b, c, d	$a = P_i P_j (1 - P_i - P_j), b = P_i P_j, c = -1, d = 1$
	<i>par. frac.</i>	$\frac{1-P_i P_j z^2}{az^3+bz^2+cz+d} = (1 - P_i P_j z^2) \left(\frac{rs}{(r-t)(s-t)(1-z/t)} + \frac{rt}{(r-s)(t-s)(1-z/s)} + \frac{st}{(s-r)(t-r)(1-z/r)} \right)$
	<i>coeff. of z^n</i>	$\frac{(1-P_i P_j t^2)rs}{(r-t)(s-t)t^n} + \frac{(1-P_i P_j s^2)rt}{(r-s)(t-s)s^n} + \frac{(1-P_i P_j r^2)st}{(s-r)(t-r)r^n}$

Table 2: Table of generating functions, partial fraction decompositions, and coefficients of z^n , $n \geq 2$, in each.

Lemma 5.6 For $n \geq 2$, the probability that ii occurs (at least once) as an adjacent pattern in Z_1, \dots, Z_n is exactly

$$E[X_{i,i}^{(n)}] = 1 - \left(\frac{1}{2} - \frac{1+P_i}{2\sqrt{(1-P_i)(1+3P_i)}} \right) \left(\frac{-2P_i(1-P_i)}{1-P_i + \sqrt{(1-P_i)(1+3P_i)}} \right)^n + \left(\frac{1}{2} + \frac{1+P_i}{2\sqrt{(1-P_i)(1+3P_i)}} \right) \left(\frac{-2P_i(1-P_i)}{1-P_i - \sqrt{(1-P_i)(1+3P_i)}} \right)^n.$$

Again, for $n < 2$, we have $E[X_{i,i}^{(n)}] = 0$.

Proof. The proof of Lemma 5.6 is in subsection 5.3.2. ■

5.2 Main results

By adding the results from Lemmas 5.5 and 5.6, we establish the following theorem:

Theorem 5.1 *For $n \geq 2$, the mean number of distinct (adjacent) pairs in a word Z_1, \dots, Z_n is exactly*

$$E[X^{(n)}] = \sum_{i=1}^{\infty} \sum_{j \neq i} \left[1 - \frac{(2P_i P_j)^{n+1}}{\sqrt{1-4P_i P_j}} \left(\frac{1}{(1-\sqrt{1-4P_i P_j})^{n+1}} - \frac{1}{(1+\sqrt{1-4P_i P_j})^{n+1}} \right) \right] \\ + \sum_{i=1}^{\infty} \left[1 - \left(\frac{1}{2} - \frac{1+P_i}{2\sqrt{(1-P_i)(1+3P_i)}} \right) \left(\frac{-2P_i(1-P_i)}{1-P_i+\sqrt{(1-P_i)(1+3P_i)}} \right)^n \right. \\ \left. + \left(\frac{1}{2} + \frac{1+P_i}{2\sqrt{(1-P_i)(1+3P_i)}} \right) \left(\frac{-2P_i(1-P_i)}{1-P_i-\sqrt{(1-P_i)(1+3P_i)}} \right)^n \right]$$

For $n < 2$, we have $E[X^{(n)}] = 0$.

5.3 Analysis of the average number of distinct (adjacent) pairs

5.3.1 Analysis of distinct (adjacent) two letter patterns ij with $i \neq j$

If we fix $i \neq j$ and we analyze the occurrences of the pattern ij , then the only “cluster” (to use Bassino et al.’s terminology) is ij itself. So the generating function $\xi(z, t)$ of the set of clusters $C = \{ij\}$ becomes only (compare with (6) in Bassino et al.):

$$\xi(z, t) = P_i P_j t z^2.$$

The generating function of the *decorated texts* (with z marking the length of the words, and t marking the number of decorated occurrences of ij , and the coefficients are the associated probabilities) is

$$T(z, t) = \frac{1}{1 - A(z) - \xi(z, t)} = \frac{1}{1 - z - P_i P_j t z^2},$$

where $A(z) = 1$ is the probability generating function of the set \mathcal{A} of all finite-length words.

Now we use $F(z, x)$ to denote the bivariate probability generating function of occurrences of ij (with z marking the length of the words, and x marking the number of occurrences of ij , and the coefficients are the associated probabilities), i.e., we define

$$F(z, x) := \sum_{n=0}^{\infty} \sum_{k=0}^{\infty} P(Z_1, \dots, Z_n \text{ has exactly } k \text{ occurrences of } ij \text{ as a subword}) x^k z^n.$$

We know from inclusion-exclusion (see [4, Chapter 3] or [2]) that $F(z, x) = T(z, x - 1)$, so we obtain

$$F(z, x) = T(z, x - 1) = \frac{1}{1 - z - P_i P_j (x - 1) z^2}.$$

The probability generating function of words with *zero occurrences* of pattern ij can be obtained by considering the case $k = 0$, corresponding to the coefficients of x^0 . To extract those coefficients, we can evaluate $F(z, x)$ at $x = 0$, and we obtain

$$[x^0]F(z, x) = F(z, 0) = \frac{1}{1 - z + P_i P_j z^2},$$

so, finally, the probability generating function of the words with *at least one occurrence* of ij is

$$\sum_{n=0}^{\infty} E[X_{i,j}^{(n)}] z^n = \frac{1}{1 - z} - \frac{1}{1 - z + P_i P_j z^2}$$

and it follows, using Table 1A, that

$$\begin{aligned} \sum_{n=0}^{\infty} E[X_{i,j}^{(n)}]z^n &= \sum_{n=0}^{\infty} z^n + \frac{2P_iP_j}{(1 + \sqrt{1 - 4P_iP_j})\sqrt{1 - 4P_iP_j}} \sum_{n=0}^{\infty} \left(\frac{2P_iP_j}{1 + \sqrt{1 - 4P_iP_j}} \right)^n z^n \\ &\quad - \frac{2P_iP_j}{(1 - \sqrt{1 - 4P_iP_j})\sqrt{1 - 4P_iP_j}} \sum_{n=0}^{\infty} \left(\frac{2P_iP_j}{1 - \sqrt{1 - 4P_iP_j}} \right)^n z^n \end{aligned}$$

and we conclude with the *exact* expression for $E[X_{i,j}^{(n)}]$ in Lemma 5.5.

5.3.2 Analysis of distinct (adjacent) two letter patterns ij with $i = j$

Now we fix i and we analyze the occurrences of the pattern ii . The clusters have the form $ii \cdots i$, i.e., they are all words that consist of 2 or more consecutive occurrences of i . So the generating function $\xi(z, t)$ of the set of clusters $C = \{ii, iii, iiii, iiii, \dots\}$ becomes

$$\xi(z, t) = \frac{P_i^2 tz^2}{1 - P_i tz}.$$

The analysis is similar to the reasoning in subsection 5.3.1, and we get

$$\sum_{n=0}^{\infty} E[X_{i,i}^{(n)}]z^n = \frac{1}{1 - z} - \frac{1}{1 - z + \frac{P_i^2 z^2}{1 + P_i z}}$$

and then, using Table 1B, we have

$$\begin{aligned} \sum_{n=0}^{\infty} E[X_{i,i}^{(n)}]z^n &= \frac{1}{1 - z} - \frac{(1 + P_i z)(-1 + P_i + \sqrt{(1 - P_i)(1 + 3P_i)})}{2\sqrt{(1 - P_i)(1 + 3P_i)} \left(1 - \frac{-2P_i(1 - P_i)}{1 - P_i + \sqrt{(1 - P_i)(1 + 3P_i)}} z\right)} \\ &\quad + \frac{(1 + P_i z)(-1 + P_i - \sqrt{(1 - P_i)(1 + 3P_i)})}{2\sqrt{(1 - P_i)(1 + 3P_i)} \left(1 - \frac{-2P_i(1 - P_i)}{1 - P_i - \sqrt{(1 - P_i)(1 + 3P_i)}} z\right)} \end{aligned}$$

and we conclude with the *exact* expression for $E[X_{i,i}^{(n)}]$ in Lemma (5.6).

5.4 Analysis of the second moment of the number of distinct (adjacent) pairs

Now we study the second moment of $X^{(n)}$, namely, $E[(X^{(n)})^2]$. We have

$$(X^{(n)})^2 = \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} X_{i,j}^{(n)} \sum_{k=1}^{\infty} \sum_{\ell=1}^{\infty} X_{k,\ell}^{(n)}$$

so the second moment is, by linearity of expectation,

$$E[(X^{(n)})^2] = \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} \sum_{k=1}^{\infty} \sum_{\ell=1}^{\infty} E[X_{i,j}^{(n)} X_{k,\ell}^{(n)}].$$

We break the analysis into 4 regimes, namely:

- $i = j$ and $k = \ell$
- $i = j$ and $k \neq \ell$
- $i \neq j$ and $k = \ell$
- $i \neq j$ and $k \neq \ell$

5.4.1 $i = j$ and $k = \ell$

In the case $i = j$ and $k = \ell$, we have two possibilities, namely, either $i = j = k = \ell$ or $i = j \neq k = \ell$.

5.4.1.1 $i = j = k = \ell$ In the case $i = j = k = \ell$, we have $X_{i,j}^{(n)} X_{k,\ell}^{(n)} = X_{i,i}^{(n)}$, so we get $E[X_{i,j}^{(n)} X_{k,\ell}^{(n)}] = E[X_{i,i}^{(n)}]$, which we already handled in Lemma 5.6.

5.4.1.2 $i = j \neq k = \ell$ In the case $i = j \neq k = \ell$, we need to analyze the occurrences of the patterns ii and kk . The clusters each have the form $ii \cdots i$ or $kk \cdots k$, i.e., they are all words that consist of 2 or more consecutive occurrences of i , or consist of 2 or more consecutive occurrences of k . So the generating function $\xi(z, t, u)$ of the set of clusters $C = \{ii, iii, iiii, \dots, kk, kkk, kkkk, \dots\}$ becomes

$$\xi(z, t, u) = \frac{P_i^2 t z^2}{1 - P_i t z} + \frac{P_k^2 u z^2}{1 - P_k u z}$$

(with z marking the length of the words, and t marking the number of decorated occurrences of ii , and u marking the number of decorated occurrences of kk , and the coefficients are the associated probabilities). The methodology now proceeds in a very similar way to the method from Section 5.3.1, but ξ , T , and F all have an additional variable, as compared to that earlier (more simple) analysis. We have

$$T(z, t, u) = \frac{1}{1 - A(z) - \xi(z, t, u)} = \frac{1}{1 - z - \frac{P_i^2 t z^2}{1 - P_i t z} - \frac{P_k^2 u z^2}{1 - P_k u z}},$$

and it follows that the probability generating function of occurrences of ii and kk (with z marking the length of the words, and x marking the number of occurrences of ii , and y marking the number of occurrences of kk , and the coefficients are the associated probabilities) is

$$F(z, x, y) = T(z, x - 1, y - 1) = \frac{1}{1 - z - \frac{P_i^2 (x-1) z^2}{1 - P_i (x-1) z} - \frac{P_k^2 (y-1) z^2}{1 - P_k (y-1) z}}.$$

It follows that the probability generating function of the words with *at least one occurrence of ii* and *at least one occurrence of kk* is

$$\begin{aligned} \sum_{n=0}^{\infty} E[X_{i,j}^{(n)} X_{k,\ell}^{(n)}] z^n &= \sum_{n=0}^{\infty} E[X_{i,i}^{(n)} X_{k,k}^{(n)}] z^n \\ &= \frac{1}{1 - z} - F(z, 0, 1) - F(z, 1, 0) + F(z, 0, 0) \\ &= \frac{1}{1 - z} - \frac{1}{1 - z + \frac{P_i^2 z^2}{1 + P_i z}} - \frac{1}{1 - z + \frac{P_k^2 z^2}{1 + P_k z}} + \frac{1}{1 - z + \frac{P_i^2 z^2}{1 + P_i z} + \frac{P_k^2 z^2}{1 + P_k z}} \end{aligned}$$

The partial fraction decomposition for the second term is given in Table 1B.

The third term is the same as the second term, using k instead of i .

The partial fraction decomposition for the fourth term is given in Table 2E.

5.4.2 $i = j$ and $k \neq \ell$

5.4.2.1 $i = j$ and k and ℓ are distinct The clusters each have the form $ii \cdots i$ or $k\ell$, i.e., they are all words that consist of either 2 or more consecutive occurrences of i , or simply the word $k\ell$. So $\xi(z, t, u)$ of the set of clusters $C = \{ii, iii, iiii, \dots, k\ell\}$ becomes

$$\xi(z, t, u) = \frac{P_i^2 t z^2}{1 - P_i t z} + P_k P_\ell u z^2$$

(with z marking the length of the words, and t marking the number of decorated occurrences of ij , and u marking the number of decorated occurrences of $k\ell$, and the coefficients are the associated probabilities). It follows that

$$T(z, t, u) = \frac{1}{1 - z - \frac{P_i^2 t z^2}{1 - P_i t z} - P_k P_\ell u z^2},$$

and

$$F(z, x, y) = T(z, x - 1, y - 1) = \frac{1}{1 - z - \frac{P_i^2 (x-1) z^2}{1 - P_i (x-1) z} - P_k P_\ell (y - 1) z^2}.$$

It follows that the probability generating function of the words with *at least one occurrence of ij and at least one occurrence of $k\ell$* is

$$\begin{aligned} \sum_{n=0}^{\infty} E[X_{i,j}^{(n)} X_{k,\ell}^{(n)}] z^n &= \frac{1}{1 - z} - F(z, 0, 1) - F(z, 1, 0) + F(z, 0, 0) \\ &= \frac{1}{1 - z} - \frac{1}{1 - z + \frac{P_i^2 z^2}{1 + P_i z}} - \frac{1}{1 - z + P_k P_\ell z^2} + \frac{1}{1 - z + \frac{P_i^2 z^2}{1 + P_i z} + P_k P_\ell z^2} \end{aligned}$$

The partial fraction decomposition for the second term is given in Table 1B.

The partial fraction decomposition for the third term is given in Table 1A, using k and ℓ instead of i and j .

The partial fraction decomposition for the fourth term is given in Table 2F.

5.4.2.2 $i = j = k \neq \ell$ The clusters each have the form $ii \cdots i$ or $ii \cdots i\ell$, i.e., they are all words that consist of 2 or more consecutive occurrences of i , or of 1 or more consecutive occurrences of i followed by ℓ . So $\xi(z, t, u)$ of the set of clusters $C = \{ii, iii, iiii, \dots, i\ell, i\ell, i\ell, i\ell, \dots\}$ becomes

$$\xi(z, t, u) = \frac{P_i^2 t z^2}{1 - P_i t z} + \frac{P_i P_\ell u z^2}{1 - P_i t z} = \frac{P_i z (P_i t z + P_\ell u z)}{1 - P_i t z},$$

and

$$F(z, x, y) = \frac{1}{1 - z - \frac{P_i z (P_i (x-1) z + P_\ell (y-1) z)}{1 - P_i (x-1) z}}.$$

It follows that the probability generating function of the words with *at least one occurrence of ij and at least one occurrence of $k\ell$* is

$$\begin{aligned} \sum_{n=0}^{\infty} E[X_{i,j}^{(n)} X_{k,\ell}^{(n)}] z^n &= \frac{1}{1 - z} - F(z, 0, 1) - F(z, 1, 0) + F(z, 0, 0) \\ &= \frac{1}{1 - z} - \frac{1}{1 - z + \frac{P_i^2 z^2}{1 + P_i z}} - \frac{1}{1 - z + P_i P_\ell z^2} + \frac{1}{1 - z + \frac{P_i z (P_i z + P_\ell z)}{1 + P_i z}} \end{aligned}$$

The partial fraction decomposition for the second term is given in Table 1B.

The partial fraction decomposition for the third term is given in Table 1A, using ℓ instead of j .

The partial fraction decomposition for the fourth term is given in Table 1D.

5.4.2.3 $i = j = \ell \neq k$ The cluster have the form $ki \cdots i$ or $ii \cdots i$, i.e., they are all words that consist of k followed by 1 or more consecutive occurrences of i , or of 2 or more consecutive occurrences of i . So $\xi(z, t, u)$ of the set of clusters $C = \{ki, kii, kiii, kiiii, \dots, ii, iii, iiii, iiiii, \dots\}$ becomes

$$\xi(z, t, u) = \frac{P_i P_k u z^2}{1 - P_i t z} + \frac{P_i^2 t z^2}{1 - P_i t z} = \frac{P_i z (P_k u z + P_i t z)}{1 - P_i t z},$$

and

$$F(z, x, y) = \frac{1}{1 - z - \frac{P_i z (P_k (y-1)z + P_i (x-1)z)}{1 - P_i (x-1)z}}.$$

It follows that the probability generating function of the words with *at least one occurrence of ij and at least one occurrence of kl* is

$$\begin{aligned} \sum_{n=0}^{\infty} E[X_{i,j}^{(n)} X_{k,\ell}^{(n)}] z^n &= \frac{1}{1-z} - F(z, 0, 1) - F(z, 1, 0) + F(z, 0, 0) \\ &= \frac{1}{1-z} - \frac{1}{1-z + \frac{P_i^2 z^2}{1+P_i z}} - \frac{1}{1-z + P_i P_k z^2} + \frac{1}{1-z + \frac{P_i z (P_k z + P_i z)}{1+P_i z}} \end{aligned}$$

The partial fraction decomposition for the second term is given in Table 1B.

The partial fraction decomposition for the third term is given in Table 1A, using k instead of j .

The partial fraction decomposition for the fourth term is given in Table 1D, using k instead of ℓ .

5.4.3 $i \neq j$ and $k = \ell$

5.4.3.1 $k = \ell$ and i and j are distinct Same as section 5.4.2.1 but with i and k exchanged, and with j and ℓ exchanged.

5.4.3.2 $k = \ell = i \neq j$ Same as section 5.4.2.2 but with i and k exchanged, and with j and ℓ exchanged.

5.4.3.3 $k = \ell = j \neq i$ Same as section 5.4.2.3 but with i and k exchanged, and with j and ℓ exchanged.

5.4.4 $i \neq j$ and $k \neq \ell$

5.4.4.1 i and j and k and ℓ are distinct The clusters are ij and kl . So $\xi(z, t, u)$ of the set of clusters $C = \{ij, kl\}$ becomes

$$\xi(z, t, u) = P_i P_j t z^2 + P_k P_\ell u z^2,$$

and

$$F(z, x, y) = \frac{1}{1 - z - P_i P_j (x-1)z^2 - P_k P_\ell (y-1)z^2}.$$

It follows that the probability generating function of the words with *at least one occurrence of ij and at least one occurrence of kl* is

$$\begin{aligned} \sum_{n=0}^{\infty} E[X_{i,j}^{(n)} X_{k,\ell}^{(n)}] z^n &= \frac{1}{1-z} - F(z, 0, 1) - F(z, 1, 0) + F(z, 0, 0) \\ &= \frac{1}{1-z} - \frac{1}{1-z + P_i P_j z^2} - \frac{1}{1-z + P_k P_\ell z^2} \\ &\quad + \frac{1}{1-z + P_i P_j z^2 + P_k P_\ell z^2} \end{aligned}$$

The partial fraction decomposition for the second term is given in Table 1A.

The partial fraction decomposition for the third term is given in Table 1A, using k and ℓ instead of i and j .

The partial fraction decomposition for the fourth term is given in Table 1C.

5.4.4.2 $k = i$ and j and ℓ are distinct The clusters are ij and $i\ell$. So, by the same analysis from section 5.4.4.1, we get

$$\begin{aligned} \sum_{n=0}^{\infty} E[X_{i,j}^{(n)} X_{i,\ell}^{(n)}] z^n &= \frac{1}{1-z} - F(z, 0, 1) - F(z, 1, 0) + F(z, 0, 0) \\ &= \frac{1}{1-z} - \frac{1}{1-z + P_i P_j z^2} - \frac{1}{1-z + P_i P_\ell z^2} \\ &\quad + \frac{1}{1-z + P_i P_j z^2 + P_i P_\ell z^2} \end{aligned}$$

Exactly as in section 5.4.4.1 above:

The partial fraction decomposition for the second term is given in Table 1A.

The partial fraction decomposition for the third term is given in Table 1A, using ℓ instead of j .

The partial fraction decomposition for the fourth term is given in Table 1C, using i instead of k .

5.4.4.3 $k = j$ and i and ℓ are distinct The clusters are ij , $ij\ell$ and $j\ell$. So $\xi(z, t, u)$ of the set of clusters $C = \{ij, ij\ell, j\ell\}$ becomes

$$\xi(z, t, u) = P_i P_j t z^2 + P_j P_\ell u z^2 + P_i P_j P_\ell t u z^3,$$

and

$$F(z, x, y) = \frac{1}{1-z - P_i P_j (x-1) z^2 - P_j P_\ell (y-1) z^2 - P_i P_j P_\ell (x-1)(y-1) z^3}.$$

It follows that the probability generating function of the words with *at least one occurrence of ij and at least one occurrence of $j\ell$* is

$$\begin{aligned} \sum_{n=0}^{\infty} E[X_{i,j}^{(n)} X_{j,\ell}^{(n)}] z^n &= \frac{1}{1-z} - F(z, 0, 1) - F(z, 1, 0) + F(z, 0, 0) \\ &= \frac{1}{1-z} - \frac{1}{1-z + P_i P_j z^2} - \frac{1}{1-z + P_j P_\ell z^2} + \frac{1}{1-z + P_i P_j z^2 + P_j P_\ell z^2 - P_i P_j P_\ell z^3} \end{aligned}$$

The partial fraction decompositions for the second and third terms are given in Table 1A, once using j and ℓ instead of i and j .

The partial fraction decomposition for the fourth term is given in Table 2G.

5.4.4.4 $i = \ell$ and k and j are distinct Same as section 5.4.4.3 but with i and k exchanged, and with j and ℓ exchanged.

5.4.4.5 $\ell = j$ and i and k are distinct The clusters are ij and kj . So, by the same analysis from section 5.4.4.1, we get

$$\begin{aligned} \sum_{n=0}^{\infty} E[X_{i,j}^{(n)} X_{k,j}^{(n)}] z^n &= \frac{1}{1-z} - F(z, 0, 1) - F(z, 1, 0) + F(z, 0, 0) \\ &= \frac{1}{1-z} - \frac{1}{1-z + P_i P_j z^2} - \frac{1}{1-z + P_k P_j z^2} \\ &\quad + \frac{1}{1-z + P_i P_j z^2 + P_k P_j z^2} \end{aligned}$$

Exactly as in section 5.4.4.1 above:

The partial fraction decomposition for the second term is given in Table 1A.

The partial fraction decomposition for the third term is given in Table 1A, using k instead of i .

The partial fraction decomposition for the fourth term is given in Table 1C, using j instead of ℓ .

5.4.4.6 $i = k$ and $j = \ell$ are distinct In this case we have $X_{i,j}^{(n)} X_{k,\ell}^{(n)} = X_{i,j}^{(n)}$, so we get $E[X_{i,j}^{(n)} X_{k,\ell}^{(n)}] = E[X_{i,j}^{(n)}]$, which we already handled in Lemma 5.5.

5.4.4.7 $i = \ell$ and $j = k$ are distinct The clusters each have the form $ijji\dots$ or $jijj\dots$. So $\xi(z, t, u)$ of the set of clusters $C = \{ij, iji, ijij, ijiji\dots, ji, jij, jiji, jijij\dots\}$ becomes

$$\xi(z, t, u) = \frac{P_i P_j t z^2}{1 - P_i P_j t u z^2} + \frac{P_i^2 P_j t u z^3}{1 - P_i P_j t u z^2} + \frac{P_j P_i u z^2}{1 - P_i P_j t u z^2} + \frac{P_i P_j^2 t u z^3}{1 - P_i P_j t u z^2},$$

and $F(z, x, y) = 1/(1 - z - \xi(z, x - 1, y - 1))$. It follows that the probability generating function of the words with *at least one occurrence of ij* and *at least one occurrence of kl* is

$$\begin{aligned} \sum_{n=0}^{\infty} E[X_{i,j}^{(n)} X_{k,\ell}^{(n)}] z^n &= \frac{1}{1 - z} - F(z, 0, 1) - F(z, 1, 0) + F(z, 0, 0) \\ &= \frac{1}{1 - z} - \frac{1}{1 - z + P_i P_j z^2} - \frac{1}{1 - z + P_j P_i z^2} \\ &\quad + \frac{1}{1 - z + \frac{P_i P_j z^2}{1 - P_i P_j z^2} - \frac{P_i^2 P_j z^3}{1 - P_i P_j z^2} + \frac{P_j P_i z^2}{1 - P_i P_j z^2} - \frac{P_i P_j^2 z^3}{1 - P_i P_j z^2}} \end{aligned}$$

The partial fraction decomposition for the second and for the third term is given in Table 1A. The partial fraction decomposition for the fourth term is given in Table 2H.

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References

- [1] M. Archibald, A. Blecher, C. Brennan, A. Knopfmacher, S. Wagner and M.D. Ward. The number of distinct adjacent pairs in geometrically distributed words. *Discrete Mathematics and Theoretical Computer Science*, 22(4), 2021.
- [2] F. Bassino, J. Clément, and P. Nicodème. Counting Occurrences for a Finite Set of Words: Combinatorial Methods. *ACM Transactions on Algorithms*, 8(3), article 31, 2012.
- [3] P. Flajolet, X. Gourdon and P. Dumas. Mellin Transforms and Asymptotics: Harmonic sums. *Theoretical Computer Science*, 144:3–58, 1995.
- [4] P. Flajolet and R. Sedgewick. *Analytic Combinatorics*. Cambridge, 2009.
- [5] P. Hitczenko and G. Louchard. Distinctness of compositions of an integer: a Probabilistic Analysis. *Random Structures and Algorithms*, 19(3,4):407–437, 2001.
- [6] G. Louchard and H. Prodinger. Asymptotics of The Moments of Extreme-value related distribution functions. *Algorithmica*, 46:431–467, 2006.

- [7] G. Louchard, H. Prodinger and M.D. Ward. The number of distinct values of some multiplicity in sequences of geometrically distributed random variables. *Discrete Mathematics and Theoretical Computer Science*, AD:231–256, 2005. 2005 International Conference on Analysis of Algorithms
- [8] C. McDiarmid. On a Correlation Inequality of Farr. *Combinatorics, Probability and Computing*, 1:157–160, 1992.
- [9] B. Pittel. Technical report. Private communication.
- [10] W. Rudin. *Principles of Mathematical Analysis, 3rd ed.* McGraw-Hill, 1976.
- [11] B. Salvy and P. Zimmermann. Gfun: a Maple package for the manipulation of generating and holonomic functions in one variable. *ACM Transactions on Mathematical Software*, 20(2):163–177, 1994.
- [12] B. Salvy. Private communication.
- [13] E. Seneta. *Non-negative Matrices and Markov Chains, 2nd ed.* Springer, 1981.
- [14] N. J. A. Sloane. The On-Line Encyclopedia of Integer Sequences, <http://oeis.org>. Sequence A028246.

Appendix. Some Mellin transforms and some proofs

A Some Mellin transforms

We will use the fundamental correspondence. Let a pole $\xi = \sigma + it$ to the right of the fundamental strip :

$$\frac{1}{(s - \xi)^{k+1}}.$$

This induces an expansion at ∞

$$-\frac{(-1)^k}{k!} \ln(n)^k n^{-\sigma} e^{-it \ln(n)}.$$

We also need the rescaling rule:

$$\mathcal{M} \left[\sum_k \lambda_k f(\mu_k x; s) \right] = \sum_k \frac{\lambda_k}{\mu_k^s} \cdot f^*(s).$$

Recall the notations

$$L := \ln \frac{1}{q} \text{ and } \chi := \frac{2i\pi}{L}.$$

We will use the rapid decrease property: $\Gamma(s)$ decreases exponentially in the direction $i\infty$:

$$|\Gamma(\sigma + it)| \sim \sqrt{2\pi} |t|^{\sigma-1/2} e^{-\pi|t|/2}.$$

Also, this property is true for all other functions we encounter. So inverting the Mellin transforms is easily justified (see [6], Sec.4 for example). All our expressions are given with an error term $n^{-\beta}$, with $\beta > \Re(\chi)$, where χ is the rightmost pole used in our singular expansions.

A.1

Let

$$G(n) := \sum_{i \geq 0} \left(1 - e^{-nq^{2i}}\right).$$

The Mellin transform (MT) of this sum is $F(s) = -\frac{1}{1 - q^{-2s}}\Gamma(s)$, with fundamental strip (FS) $\langle -1, 0 \rangle$, to the right of which we have the singularities

$$F(s) \asymp \frac{1}{2Ls^2} - \left[\frac{\gamma}{2L} + \frac{1}{2}\right] \frac{1}{s}, \quad \text{and } F(s) \asymp \frac{1}{2L} \frac{\Gamma\left(\frac{\ell\chi}{2}\right)}{\left(s - \frac{\ell\chi}{2}\right)}, \quad \text{for } \ell \in \mathbb{Z} \setminus \{0\}.$$

Noting that there are no other singularities to the right of $\langle -1, 0 \rangle$, the error term in the following expansion can be chosen $\mathcal{O}(n^{-\beta})$ with any fixed $\beta > 0$.

$$G(n) \sim \frac{1}{2L} \ln(n) + \left[\frac{\gamma}{2L} + \frac{1}{2}\right] - \frac{1}{2L} \sum_{\ell \in \mathbb{Z} \setminus \{0\}} \Gamma\left(\frac{\ell\chi}{2}\right) n^{-\ell\chi/2}.$$

A.2

Let

$$G := \sum_i i \left(1 - e^{-nq^i}\right).$$

This has the MT, with FS $\langle -1, 0 \rangle$ and $\chi := \frac{2i\pi}{L}$

$$F(s) = -\frac{Q^s}{(1 - Q^s)^2} \Gamma(s) \asymp -\frac{1}{L^2 s^3} + \frac{\gamma}{L^2 s^2} + \left(-\frac{\pi^2/12 + \gamma^2/2}{L^2} + \frac{1}{12}\right) \frac{1}{s} - \frac{\Gamma(\ell\chi)}{L^2} \frac{1}{(s - \ell\chi)^2} - \frac{\Gamma'(\ell\chi)}{L^2(s - \ell\chi)},$$

$$G \sim \frac{\ln(n)^2}{2L^2} + \frac{\gamma}{L^2} \ln(n) + \left[\frac{\pi^2/12 + \gamma^2/2}{L^2} - \frac{1}{12}\right] + \frac{1}{L^2} \sum_{\ell \in \mathbb{Z} \setminus \{0\}} \left[-\Gamma\left(\frac{2i\ell\pi}{L}\right) \ln(n) + \Gamma'\left(\frac{2i\ell\pi}{L}\right)\right] e^{-2i\ell\pi \ln(n)/L}.$$

A.3

Let

$$\tilde{G}(n) := \sum_{i,j \geq 0} \left(1 - e^{-nq^{i+j}}\right) = \sum_{k \geq 0} (k+1) \left(1 - e^{-nq^k}\right).$$

This has the MT $F(s) = -\frac{1}{(1 - q^{-s})^2} \Gamma(s)$, with FS $\langle -1, 0 \rangle$ and singularities to the right of the fundamental strip

$$F(s) \asymp -\frac{1}{L^2 s^3} + \left[\frac{\gamma}{L^2} + \frac{1}{L}\right] \frac{1}{s^2} - \left[\frac{\pi^2 + 6\gamma^2}{12L^2} + \frac{5}{12} + \frac{\gamma}{L}\right] \frac{1}{s},$$

and

$$F(s) \asymp -\frac{\Gamma(\ell\chi)}{L^2(s - \ell\chi)^2} - \frac{\Gamma'(\ell\chi) - L\Gamma(\ell\chi)}{L^2(s - \ell\chi)}, \quad \text{for } \ell \in \mathbb{Z} \setminus \{0\},$$

leading to

$$\tilde{G}(n) \sim \frac{\ln(n)^2}{2L^2} + \left[\frac{\gamma}{L^2} + \frac{1}{L}\right] \ln(n) + \left[\frac{\pi^2 + 6\gamma^2}{12L^2} + \frac{5}{12} + \frac{\gamma}{L}\right] + \frac{1}{L^2} \sum_{\ell \in \mathbb{Z} \setminus \{0\}} [\Gamma'(\ell\chi) - (\ln(n) + L)\Gamma(\ell\chi)] n^{-\ell\chi},$$

again with error term $\mathcal{O}(n^{-\beta})$ with any fixed $\beta > 0$.

A.4

Set

$$G := \sum_{i,j,k} (e^{nP_i P_j P_k} - 1) e^{-nP_i P_j - nP_j P_k}.$$

This leads to the MT, with FS $\langle -1, 0 \rangle$

$$\begin{aligned} F(s) &= \sum_{i,j,k} \int_0^\infty (e^{xP_i P_j P_k} - 1) e^{-xP_i P_j - xP_j P_k} x^{s-1} dx \\ &= \sum_j P_j^{-s} \sum_{i,k} \int_0^\infty [e^{-y(P_i + P_k - P_i P_k)} - e^{-y(P_i + P_k)}] y^{s-1} dy \\ &= \frac{q^s}{p^s(q^s - 1)} \Gamma(s) \sum_{i,k} [(P_i + P_k - P_i P_k)^{-s} - (P_i + P_k)^{-s}] \\ &= \left(\frac{q}{p}\right)^{2s} \frac{\Gamma(s)}{q^s - 1} F_1(s), \end{aligned}$$

where

$$\begin{aligned} F_1(s) &= \sum_{i,k} [(q^i + q^k - pq^{i+k-1})^{-s} - (q^i + q^k)^{-s}] \\ &= \sum_{i \geq 1} q^{-is} \left[(2 - P_i)^{-s} - 2^{-s} + 2 \sum_{j \geq 1} [(1 + q^j - pq^{i+j-1})^{-s} - (1 + q^j)^{-s}] \right]. \end{aligned}$$

Note that $F_1(s)$, being a general Dirichlet series in the variable $-s$, is analytic at least for $\sigma = \Re s < 1$, since, using the MVT, we have

$$|(1 + q^j - pq^{i+j-1})^{-\sigma} - (1 + q^j)^{-\sigma}| \leq |\sigma| \frac{pq^{i+j-1}}{(1 + q^j)^{1+\sigma}},$$

and therefore

$$|F_1(s)| \leq 2|\sigma| \sum_{i \geq 1} q^{i(1-\sigma)} \sum_{j \geq 0} \frac{P_j}{(1 + q^j)^{1+\sigma}} < \infty.$$

Moreover, $F_1(0) = 0$, so to the right of the fundamental strip we have the singularities

$$F(s) \asymp -\frac{F_1'(0)}{Ls}, \quad \text{and } F(s) \asymp -p^{-2\ell\chi} \frac{\Gamma(\ell\chi)}{L} \frac{F_1(\ell\chi)}{s - \ell\chi}, \quad \text{for } \ell \in \mathbb{Z} \setminus \{0\}.$$

This leads to

$$G = \frac{F_1'(0)}{L} + \frac{1}{L} \sum_{\ell \in \mathbb{Z} \setminus \{0\}} \Gamma(\ell\chi) F_1(\ell\chi) (np^2)^{-\ell\chi} + \mathcal{O}(n^{-\beta}),$$

with any fixed $\beta < 1$, where the constant term simplifies to

$$\frac{F_1'(0)}{L} = \frac{1}{L} \ln \left(\prod_{i,k \geq 1} \frac{q^i + q^k}{q^i + q^k - pq^{i+k-1}} \right).$$

B Proofs of equations (27) and (31)

The estimate (27) follows from the following general result: If for some $c < 1$ a set $\mathcal{P} = \{x_i : i \in \mathbb{N}\}$ satisfies $x_i > 0$ and $\frac{x_{i+1}}{x_i} \leq c$ for $i \in \mathbb{N}$, then $\sum_{x \in \mathcal{P}} x^\alpha e^{-x} < \infty$. For a proof observe that there is a constant $C_\alpha > 0$ such that $x^\alpha e^{-x} \leq \min(x^\alpha, C_\alpha x^{-\alpha})$ for $x > 0$. Let $\bar{x} := (C_\alpha)^{1/(2\alpha)}$. Then

$$\sum_{x \in \mathcal{P}} x^\alpha e^{-x} \leq \sum_{x \in \mathcal{P} \cap]0, \bar{x}] } x^\alpha + \sum_{x \in \mathcal{P} \cap [\bar{x}, \infty[} C_\alpha x^{-\alpha} \leq \bar{x}^\alpha \sum_{i \geq 0} c^i + C_\alpha \bar{x}^{-\alpha} \sum_{i \geq 0} c^i = 2 \frac{\sqrt{C_\alpha}}{1-c}.$$

The estimate (31) can be deduced from (27), using $\beta = 1$, observing

$$\sum_{i,k \geq 1} (nP_i P_k)^\alpha e^{-nP_i P_k} = \sum_{\ell \geq 2} (\ell - 1) (n \frac{P}{q} P_\ell)^\alpha e^{-n \frac{P}{q} P_\ell},$$

and furthermore

$$\sum_{\ell \geq 2} \ell (nP_\ell)^\alpha e^{-nP_\ell} = \sum_{\ell \geq 2} \mathcal{O}(\ln n - \ln(nP_\ell)) (nP_\ell)^\alpha e^{-nP_\ell} = \mathcal{O}(\ln n),$$

because of $x^\alpha \ln x = \mathcal{O}(x^{\alpha/2})$.