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Mode and Edgeworth Expansion for the Ewens Distribution and the Stirling Numbers

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Abstract

We provide asymptotic expansions for the Stirling numbers of the first kind and, more generally, the Ewens (or Karamata-Stirling) distribution. Based on these expansions, we obtain some new results on the asymptotic properties of the mode and the maximum of the Stirling numbers and the Ewens distribution. For arbitrary $\theta > 0$ and for all sufficiently large $n \in \mathbb{N}$, the unique maximum of the Ewens probability mass function

$$\mathbb{L}_n(k) = \frac{\theta^k}{\theta(\theta+1)\cdots(\theta+n-1)} \begin{bmatrix} n \\ k \end{bmatrix}, \quad k = 1, \dots, n,$$

is attained at $k = \lfloor a_n \rfloor$ or $\lceil a_n \rceil$, where $a_n = \theta \log n - \theta \Gamma'(\theta)/\Gamma(\theta) - 1/2$. We prove that the mode is the nearest integer to a_n for a set of n's of asymptotic density 1, yet this formula is not true for infinitely many n's.

1 Introduction and statement of results

1.1 Introduction

The (unsigned) *Stirling numbers* of the first kind $\begin{bmatrix} n \\ k \end{bmatrix}$ are defined, for $n \in \mathbb{N}$ and $1 \le k \le n$, by the formula

$$x^{(n)} := x(x+1)\cdots(x+n-1) = \sum_{k=1}^{n} \begin{bmatrix} n \\ k \end{bmatrix} x^k, \quad x \in \mathbb{R}. \tag{1}$$

For $n \in \mathbb{N}$, a random variable $K_n(\theta)$ is said to have the *Ewens distribution* with parameter $\theta > 0$ if its probability mass function is given by the formula

$$\mathbb{P}(K_n(\theta) = k) = \frac{\theta^k}{\theta^{(n)}} \begin{bmatrix} n \\ k \end{bmatrix}, \quad k = 1, \dots, n.$$

Bingham [2] called this distribution the *Karamata-Stirling law*. One can interpret $K_n(\theta)$ as the number of blocks in a random partition of $\{1, \dots, n\}$ distributed according to the Ewens sampling formula, or, equivalently, the number of different alleles in the infinite alleles model, the number of tables in a Chinese restaurant process, or the number of colors in the Hoppe urn. The Ewens sampling formula plays an important role in population genetics [6], [4, Section 1.3]. There is a distributional representation of $K_n(\theta)$ as a sum of independent random variables

$$K_n(\theta) \stackrel{d}{=} \xi_1 + \cdots + \xi_n, \text{ where } \xi_i \sim \mathrm{Bern}(\theta/(\theta+i-1))$$

and $\mathrm{Bern}(p)$ denotes the Bernoulli distribution with parameter p. In the special case $\theta = 1$, classical results going back at least to Feller [7] and Rényi [21] state that the random variable $K_n(1)$ has the same distribution as the number of cycles in a uniformly chosen random permutation of n objects, or the number of records in a sample of n i.i.d. variables from a continuous distribution. It follows easily from Lindeberg's theorem that $K_n(\theta)$ satisfies a central limit theorem of the form

$$\frac{K_n(\theta) - \theta \log n}{\sqrt{\theta \log n}} \xrightarrow[n\to\infty]{d} \mathrm{N}(0,1)$$

known as Goncharov's CLT in the case $\theta = 1$.

Asymptotic expansions, as $n \to \infty$, of the Stirling numbers $\left[{n \atop k}\right]$ in various regions of k were provided in numerous works [12, 13, 18, 20, 23, 24]. Most notably, Hwang [13, Theorem 2] (and Theorem 14 on page 108 of his dissertation [12] for a more general result) gave an asymptotic expansion valid uniformly in the domain $2 \le k \le \eta \log n$, for any fixed $\eta > 0$. Louchard [18, Theorem 2.1] computed three non-trivial terms of the asymptotic expansion in the central regime $k = \log n + O(\sqrt{\log n})$ which is similar to the classical Edgeworth expansion in the central limit theorem.

In this short note we start by deriving a full Edgeworth expansion, as $n \to \infty$, for the sequence of probability mass functions $k \mapsto \mathbb{P}(K_n(\theta) = k)$ which is uniform both in $\theta \in [1/\eta, \eta]$ (where $\eta > 1$) and in $k \in \{1, \dots, n\}$; see Theorem 1. Our result is an application of the general Edgeworth expansion for deterministic or random profiles which the authors [16] recently obtained. Using this asymptotic expansion we derive some new results on the mode and the maximum of the Ewens distribution. In the case $\theta = 1$ the mode can be interpreted as the most probable number of cycles in a random permutation of n objects. It was investigated in the works of Hammersley [10, 11] and Erdős [5]. Our results on the mode and the maximum will be stated in Theorems 5 and 7 below.

1.2 Asymptotic expansion of the Ewens distribution

Before stating our main result we need to recall some notions. The (complete) *Bell polynomials* $B_j(z_1, \dots, z_j)$ are defined by the formal identity

$$\exp\left(\sum_{j=1}^{\infty} \frac{x^j}{j!} z_j\right) = \sum_{j=0}^{\infty} \frac{x^j}{j!} B_j(z_1, \dots, z_j).$$

Therefore $B_0 = 1$ and, for $j \in \mathbb{N}$,

$$B_j(z_1, \dots, z_j) = \sum{}' \frac{j!}{i_1! \cdots i_j!} \left(\frac{z_1}{1!}\right)^{i_1} \cdots \left(\frac{z_j}{j!}\right)^{i_j}, \tag{2}$$

where the sum $\sum'$ is taken over all $i_1, \dots, i_j \in \mathbb{N}_0$ satisfying $1i_1 + 2i_2 + \dots + ji_j = j$. For example, the first three Bell polynomials are given by

$$B_1(z_1) = z_1, \quad B_2(z_1, z_2) = z_1^2 + z_2, \quad B_3(z_1, z_2, z_3) = z_1^3 + 3z_1 z_2 + z_3. \tag{3}$$

Further, we will use the "probabilist" *Hermite polynomials* $\mathrm{He}_n(x)$ defined by

$$\mathrm{He}_n(x) = e^{\frac{1}{2}x^2} \left(-\frac{\mathrm{d}}{\mathrm{d}x}\right)^n e^{-\frac{1}{2}x^2}, \quad n \in \mathbb{N}_0. \tag{4}$$

The first few Hermite polynomials needed for the first three terms of the expansion are

$$\mathrm{He}_0(x) = 1, \quad \mathrm{He}_1(x) = x, \quad \mathrm{He}_2(x) = x^2 - 1, \quad \mathrm{He}_3(x) = x^3 - 3x,$$
$$\mathrm{He}_4(x) = x^4 - 6x^2 + 3, \quad \mathrm{He}_6(x) = x^6 - 15x^4 + 45x^2 - 15.$$

Theorem 1. *Fix $r \in \mathbb{N}_0$ and a compact subset $L \subset (0, \infty)$. Uniformly over $\theta \in L$ we have*

$$\lim_{n\to\infty} (\log n)^{\frac{r+1}{2}} \sup_{k=1,\ldots,n} \left| \mathbb{P}(K_n(\theta) = k) - \frac{e^{-\frac{1}{2}x_n^2(k,\theta)}}{\sqrt{2\pi\theta \log n}} \sum_{j=0}^{r} \frac{H_j(x_n(k,\theta))}{(\theta \log n)^{j/2}} \right| = 0.$$

Here, $x_n(k,\theta) = \frac{k-\theta\log n}{\sqrt{\theta \log n}}$ and $H_j(x)$ is a polynomial of degree $3j$ given by

$$H_j(x) := H_j(x,\theta) = \frac{(-1)^j}{j!} e^{\frac{1}{2}x^2} B_j(\widetilde{D_1}, \ldots, \widetilde{D_j}) e^{-\frac{1}{2}x^2}, \tag{5}$$

where B_j is the j-th Bell polynomial and $\widetilde{D_1}, \widetilde{D_2}, \ldots$ are differential operators given by

$$\widetilde{D_j} := \widetilde{D_j}(\theta) = \frac{1}{(j+1)(j+2)} \left(\frac{\mathrm{d}}{\mathrm{d}x}\right)^{j+2} + \widetilde{\chi}_j(0) \left(\frac{\mathrm{d}}{\mathrm{d}x}\right)^{j} \tag{6}$$

with $\widetilde{\chi}_j(\beta) = -\left(\frac{\mathrm{d}}{\mathrm{d}\beta}\right)^j \log\Gamma(\theta e^\beta)$ and Γ denoting the Euler gamma function.

Remark 2. It follows from (3), (5) and (6) that the first three coefficients of the expansion are

$$H_0(x) = 1,$$
$$H_1(x) = -\frac{\Gamma'(\theta)}{\Gamma(\theta)}\theta x + \frac{1}{6}\mathrm{He}_3(x),$$
$$H_2(x) = \left(\theta^2 \frac{\Gamma'^2(\theta)}{\Gamma^2(\theta)} - \frac{\theta^2\Gamma''(\theta) + \theta\Gamma'(\theta)}{2\Gamma(\theta)}\right)\mathrm{He}_2(x) + \left(\frac{1}{24} - \frac{\Gamma'(\theta)}{6\Gamma(\theta)}\theta\right)\mathrm{He}_4(x) + \frac{1}{72}\mathrm{He}_6(x).$$

An expression for $\widetilde{\chi}_j(0)$ involving polygamma functions and Stirling numbers of the second kind will be given below in (13). The tilde in $\widetilde{D_j}$ and $\widetilde{\chi}_j$ is needed to keep the notation consistent with our more general work [16]. It is easy to check that $H_j(-x) = (-1)^j H_j(x)$ [16, Remark 2.4].

To compute $H_j(x)$ one can proceed as follows. First, express $\frac{1}{j!}B_j(\widetilde{D_1}, \ldots, \widetilde{D_j})$ as a polynomial in $D := \frac{\mathrm{d}}{\mathrm{d}x}$ (and note that only even/odd powers of D are present if j is even/odd). Then replace each occurrence of D^l by $\mathrm{He}_l(x)$; see (4) for justification.

Remark 3. It is possible to choose the value of θ as a function of k. One natural choice is $\theta = 1$ which provides a full version of Louchard's expansion [18, Theorem 2.1] (although he used a slightly different normalization in his analogue of $x_n(k,1)$ and his term $-355x^3/144$ should be replaced by $-47x^3/144$). Another possible choice is $\theta = k/\log n$ (so that $x_n(k,\theta) = 0$), which gives a large-deviation-type expansion valid uniformly in the region $\eta^{-1}\log n < k < \eta \log n$, for fixed $\eta > 1$ and $q \in \mathbb{N}_0$:

$$\frac{(k/\log n)^k}{(k/\log n)^{(n)}} \begin{bmatrix} n \\ k \end{bmatrix} = \frac{1}{\sqrt{2\pi k}} \sum_{s=0}^{q} \frac{H_{2s}(0, k/\log n)}{k^s} + o\left(\frac{1}{(\log n)^{q+1}}\right).$$

Observe that the terms with half-integer powers of k are not present in the sum because $H_{2j+1}(0) = 0$. Using the formula

$$\frac{\Gamma(n+\theta)}{n!} = n^{\theta-1}\left(1 + O\left(\frac{1}{n}\right)\right)$$

yields the expansion

$$\frac{1}{n!}\begin{bmatrix} n \\ k \end{bmatrix} = \frac{1}{\Gamma(\theta)} n^{\theta - \theta\log\theta - 1}\left(\frac{1}{\sqrt{2\pi k}}\sum_{s=0}^{q}\frac{H_{2s}(0,\theta)}{k^s} + o\left(\frac{1}{(\log n)^{q+1}}\right)\right) \tag{7}$$

valid as $n \to \infty$ uniformly over k in the region $\theta = k/\log n \in (\eta^{-1}, \eta)$. In this region, this expansion must be equivalent to Hwang's result [13, Theorem 2]. It is not easy to rigorously verify this equivalence by a direct comparison, but we checked using Mathematica 9 that the first three non-trivial terms coincide. Note a misprint in the formula for the remainder term $Z_\mu(m,n)$ in Hwang [13, Theorem 2]: $(\log n)^m/(m!n)$ should be replaced by $(\log n)/(mn)$. Expansion (7) could be also deduced from the work of Féray et al. [8, Theorem 3.4].

Taking sums over k in Theorem 1 and using the Euler-Maclaurin formula to approximate Riemann sums by integrals, one obtains that

$$\mathbb{P}\left(\frac{K_n(\theta) - \theta\log n}{\sqrt{\theta\log n}} \le x\right) = \Phi(x) + \frac{e^{-x^2/2}}{\sqrt{2\pi\theta\log n}}\left(\frac{1}{2} - \frac{x^2-1}{6} + \theta\frac{\Gamma'(\theta)}{\Gamma(\theta)}\right) + O\left(\frac{1}{\log n}\right),$$

uniformly in $x \in (\theta\log n)^{-1/2}(\mathbb{Z} - \theta\log n)$, where $\Phi(x)$ is the standard normal distribution function. The proof follows Grübel and Kabluchko [9, Proposition 2.5] and is therefore omitted. Yamato [25] recently stated a slightly incorrect version of this expansion missing the term $1/2$ which comes from the Euler-Maclaurin formula. Similarly, one can obtain further terms in the expansion of the distribution function of $(K_n(\theta) - \theta\log n)/\sqrt{\theta\log n}$.

Remark 4. Since the set $L \subseteq (0,\infty)$ in Theorem 1 has to be chosen compact, our results do not yield asymptotic expansions for $\mathbb{P}(K_n(\theta) = k)$ in the regime $k = o(\log n)$ of the same precision as Hwang's [13, Theorems 1 and 2]. Also, they do not extend straightforwardly to the case $k = n - O(n^\alpha)$ for $0 < \alpha < 1$ treated by Louchard [18, Section 3]. A generalization of our approach to cover these regions will be content of future work.

1.3 Mode and maximum of the Ewens distribution

Theorem 1 allows us to deduce various results on the *mode* and the *maximum* of the Ewens distribution. A mode is any value $k \in \{1, \ldots, n\}$ maximizing $\mathbb{P}(K_n(\theta) = k)$, while the maximum $M_n(\theta)$ is defined by

$$M_n(\theta) = \max_{1 \le k \le n} \mathbb{P}(K_n(\theta) = k).$$

Let $u_n(\theta)$ denote the least mode. In this context, it is important to note that, for all $\theta > 0$, the function $k \mapsto \mathbb{P}(K_n(\theta) = k)$ is log-concave by a theorem attributed to Newton [11, 22], and

$$\begin{aligned} \mathbb{P}(K_n(\theta) = 1) < \ldots < \mathbb{P}(K_n(\theta) = u_n(\theta)) \\ \ge \mathbb{P}(K_n(\theta) = u_n(\theta) + 1) > \ldots > \mathbb{P}(K_n(\theta) = n). \end{aligned} \tag{8}$$

In particular, there are at most two modes. For $\theta = 1$, Erdős [5], proving a conjecture of Hammersley [11], showed that the mode is unique for all $n \ge 3$. By (8), uniqueness also holds for irrational θ; however, for rational θ, the mode need not be unique since, for example,

$$\frac{2}{3}\begin{bmatrix}3\\1\end{bmatrix} = \left(\frac{2}{3}\right)^2 \begin{bmatrix}3\\2\end{bmatrix} > \left(\frac{2}{3}\right)^3 \begin{bmatrix}3\\3\end{bmatrix}.$$

Theorem 5. *Fix $\theta > 0$. There exists $N_1 \in \mathbb{N}$ such that for $n \ge N_1$, $u_n(\theta)$ is the unique mode of the Ewens distribution with parameter θ. The mode $u_n(\theta)$ equals one of the numbers $\lfloor u_n^*(\theta) \rfloor$ or $\lceil u_n^*(\theta) \rceil$, where*

$$u_n^*(\theta) = \theta \log n - \frac{\theta \Gamma'(\theta)}{\Gamma(\theta)} - \frac{1}{2}$$

and $\lfloor \cdot \rfloor$, $\lceil \cdot \rceil$ denote the floor and the ceiling functions, respectively. Write $\delta_n(\theta) := \min_{k \in \mathbb{Z}} |u_n^*(\theta) - k|$. For the maximum $M_n(\theta)$, we have

$$\sqrt{2\pi\theta \log n}\; M_n(\theta) = 1 + \frac{\theta (\log \Gamma)'(\theta) + \theta^2 (\log \Gamma)''(\theta) + 1/12 - \delta_n^2(\theta)}{2\theta \log n} + o\left(\frac{1}{\log n}\right).$$

In the case $\theta = 1$, Hammersley [11] and Erdős [5] derived related results for the mode. Cramer [3] discusses statistical applications and Mező [19] provides an overview and generalizations. Theorem 5 states that the mode is one of the numbers $\lfloor \log n + \gamma - \frac{1}{2} \rfloor$ or $\lceil \log n + \gamma - \frac{1}{2} \rceil$, for sufficiently large n. In fact, this holds for all $n \in \mathbb{N}$.

Proposition 6. $u_n(1) \in \{\lfloor \log n + \gamma - \frac{1}{2} \rfloor, \lceil \log n + \gamma - \frac{1}{2} \rceil\}$ *for all $n \in \mathbb{N}$.*

The proof uses the following formula of Hammersley [11]:

$$u_n(1) = \left\lfloor \log n + \gamma + \frac{\zeta(2) - \zeta(3)}{\log n + \gamma - \frac{3}{2}} + \frac{h(n)}{(\log n + \gamma - \frac{3}{2})^2} \right\rfloor, \tag{9}$$

for some $-1.098011 < h(n) < 1.430089$. Hwang [12, Section 5.7.9] gives a more precise expansion. Erdős [5] observed that, for $n > 189$, Hammersley's formula implies that the mode is one of the numbers $\lfloor \log(n-1) + \frac{1}{2} \rfloor$ or $\lfloor \log(n-1) + 1 \rfloor$. Note that his $\Sigma_{n,s}$ equals $\left[{n+1 \atop n+1-s}\right]$ and his $n - f(n)$ is $u_{n+1}(1) - 1$ in our notation.

The next theorem provides more precise information about the behavior of the mode. Recall that a set $A \subset \mathbb{N}$ has *asymptotic density* $\alpha \in [0,1]$ if

$$\lim_{n\to\infty} \frac{\#(A \cap \{1,\dots,n\})}{n} = \alpha.$$

For $x \in \mathbb{R}$, let $\{x\} = x - \lfloor x \rfloor$ denote the fractional part of x. Let $\mathrm{nint}(x)$ be the integer closest to x (if $\{x\} = 1/2$, we agree to take $\mathrm{nint}(x) = \lceil x \rceil$). That is,

$$\mathrm{nint}(x) := \arg\min_{k\in\mathbb{Z}} |x - k| = \left\lfloor x + \frac{1}{2} \right\rfloor.$$

Theorem 7. *Fix $\theta > 0$. The mode $u_n(\theta)$ of the Ewens distribution with parameter θ has the following properties:*

(i) *there exists a constant $C_0 > 0$ such that, for all $n \in \mathbb{N}$ satisfying*

$$\left| \{u_n^*(\theta)\} - \frac{1}{2} \right| > \frac{C_0}{\log n},$$

the mode $u_n(\theta)$ equals

$$\mathrm{nint}(u_n^*(\theta)) = \left\lfloor \theta \log n - \frac{\theta\Gamma'(\theta)}{\Gamma(\theta)} \right\rfloor;$$

(ii) *there are arbitrarily long intervals of consecutive n's for which $u_n(\theta) = \lceil u_n^*(\theta) \rceil$; similarly, there are arbitrarily long intervals of consecutive n's for which $u_n(\theta) = \lfloor u_n^*(\theta) \rfloor$;*

(iii) *the set of $n \in \mathbb{N}$ such that $u_n(\theta) = \mathrm{nint}(u_n^*(\theta))$ has asymptotic density one;*

(iv) *there are infinitely many $n \in \mathbb{N}$ such that $u_n(\theta) \neq \mathrm{nint}(u_n^*(\theta))$.*

The proof of part (iv) uses five terms in the Edgeworth expansion, where the first two terms influence the form of $u_n^*(\theta)$, while the remaining terms are needed for technical reasons. The idea is that the formula $u_n(\theta) = \mathrm{nint}(u_n^*(\theta))$ becomes wrong if the fractional part of $u_n^*(\theta)$ is slightly below $\frac{1}{2}$, so that higher order terms in the Edgeworth expansion decide which of the values $\lfloor u_n^*(\theta) \rfloor$ and $\lceil u_n^*(\theta) \rceil$ is the mode. Using even more terms in the expansion, it is possible to replace $u_n^*(\theta)$ by some more complicated expressions involving higher-order corrections in inverse powers of $\theta \log n$ [12, Section 5.7.9]. However, it seems that there is no formula of the form

$$u_n(1) = \mathrm{nint}\left(\log n + a_0 + \frac{a_1}{\log n} + \cdots + \frac{a_r}{(\log n)^r} \right)$$

which is valid for all sufficiently large n.

Finally, we would like to mention that one can easily obtain counterparts of the above results for the B- and D-analogues of Stirling numbers of the first kind. These are defined as the coefficients of $(x+1)(x+3)\cdots(x+2n-1)$ and $((x+1)(x+3)\cdots(x+2n-3))(x+n-1)$, respectively. They appear, for example, in the study of intrinsic volumes of Weyl chambers [14].

2 Proofs

Proof of Theorem 1. The proof follows from the general Edgeworth expansion for random or deterministic profiles [16, Theorem 2.1]. We consider the sequence of "profiles"

$$\mathbb{L}_n(k) := \mathbb{P}(K_n(\theta) = k) = \frac{\theta^k}{\theta^{(n)}} \begin{bmatrix} n \\ k \end{bmatrix} \mathbb{1}_{\{k \in \{1,\dots,n\}\}},$$

and define

$$w_n := \theta \log n, \quad \varphi(\beta) := e^\beta - 1, \quad (\beta_-, \beta_+) = \mathbb{R}, \quad \mathscr{D} = \{z \in \mathbb{C}\colon |\mathrm{Im}\, z| < \pi\}.$$

In order to apply [16, Theorem 2.1], we need to check Conditions A1–A4 given in the beginning of Section 2 of the cited paper. Note that

$$\begin{aligned} W_n(\beta) &:= e^{-\varphi(\beta) w_n} \sum_{k \in \mathbb{Z}} e^{\beta k} \mathbb{L}_n(k) = n^{-\theta(e^\beta - 1)} \sum_{k=1}^{n} e^{\beta k} \frac{\theta^k}{\theta^{(n)}} \begin{bmatrix} n \\ k \end{bmatrix} \\ &= n^{-\theta(e^\beta - 1)} \frac{(\theta e^\beta)^{(n)}}{\theta^{(n)}} = n^{-\theta(e^\beta - 1)} \frac{\Gamma(\theta e^\beta + n)\Gamma(\theta)}{\Gamma(\theta e^\beta)\Gamma(\theta + n)} \underset{n\to\infty}{\longrightarrow} \frac{\Gamma(\theta)}{\Gamma(\theta e^\beta)} =: W_\infty(\beta) \end{aligned}$$

locally uniformly in $\beta \in \mathscr{D}$ with a rate of convergence which is polynomial in n^{-1}. Hence Conditions A1–A3 are satisfied. In order to check A4 it is enough to show that for every $a > 0$, $r \in \mathbb{N}$ and every compact subset K_1 of $\mathbb{R}$

$$\sup_{\beta \in K_1} \sup_{a \le u \le \pi} \left(n^{-\theta(e^\beta - 1)} \left| \frac{\Gamma(\theta e^{\beta + iu} + n)\Gamma(\theta)}{\Gamma(\theta + n)\Gamma(\theta e^{\beta + iu})} \right| \right) = o(\log^{-r} n), \quad n \to \infty.$$

But this easily follows from

$$\begin{aligned} &\sup_{\beta \in K_1} \left(n^{-\theta(e^\beta - 1)} \sup_{a \le u \le \pi} \left| \frac{\Gamma(\theta e^{\beta + iu} + n)\Gamma(\theta)}{\Gamma(\theta + n)\Gamma(\theta e^{\beta + iu})} \right| \right) \\ &\le C \sup_{\beta \in K_1} \left(n^{-\theta(e^\beta - 1)} \sup_{a \le u \le \pi} \left| \frac{\Gamma(\theta e^{\beta + iu} + n)}{\Gamma(\theta + n)} \right| \right) \le C_1 \sup_{\beta \in K_1} n^{\theta e^\beta (\cos a - 1)}, \end{aligned}$$

with constants C, C_1 depending on K_1, θ and a. Therefore, Theorem 2.1 of [16] is applicable for the Ewens distribution with arbitrary fixed $\theta > 0$. In particular, for $\theta = 1$, we obtain

$$(\log n)^{\frac{r+1}{2}} \sup_{\beta \in K} \sup_{1 \le k \le n} \left| \frac{\Gamma(e^\beta) e^{\beta k}}{n^{e^\beta - 1} n!} \begin{bmatrix} n \\ k \end{bmatrix} - \frac{e^{-\frac{1}{2} x_n^2(k, e^\beta)}}{\sqrt{2\pi e^\beta \log n}} \sum_{j=0}^{r} \frac{G_j(x_n(k, e^\beta); \beta)}{(\log n)^{j/2}} \right| \underset{n \to \infty}{\longrightarrow} 0, \tag{10}$$

where K is a compact subset of $\mathbb{R}$, and the polynomials $G_0, G_1, \ldots$ are defined as in Theorem 2.1 of [16]: for $j \in \mathbb{N}_0$, we have

$$G_j(x; \beta) = \frac{(-1)^j}{j!} e^{\frac{1}{2}x^2} B_j(D_1, \ldots, D_j) e^{-\frac{1}{2}x^2} \tag{11}$$

with the differential operators

$$D_j := D_j(\beta) = e^{-\frac{1}{2}\beta j} \left(\frac{1}{(j+1)(j+2)} \left(\frac{\mathrm{d}}{\mathrm{d}x} \right)^{j+2} + \chi_j(\beta) \left(\frac{\mathrm{d}}{\mathrm{d}x} \right)^{j} \right), \tag{12}$$

where

$$\chi_j(\beta) = -\left(\frac{\mathrm{d}}{\mathrm{d}\beta} \right)^j \log \Gamma(e^\beta).$$

Now, if $L \subseteq (0, \infty)$ is compact, then $K := \log L$ is compact in $\mathbb{R}$. Applying (10) with $K = \log L$ and $\beta = \log \theta \in K$, we obtain

$$(\log n)^{\frac{r+1}{2}} \sup_{\theta \in L} \sup_{1 \le k \le n} \left| \frac{\Gamma(\theta) \theta^k}{n^{\theta - 1} n!} \begin{bmatrix} n \\ k \end{bmatrix} - \frac{e^{-\frac{1}{2} x_n^2(k, \theta)}}{\sqrt{2\pi \theta \log n}} \sum_{j=0}^{r} \frac{G_j(x_n(k, \theta); \log \theta)}{(\log n)^{j/2}} \right| \underset{n \to \infty}{\longrightarrow} 0.$$

By Stirling's formula, uniformly in $\theta \in L$, $n \in \mathbb{N}$ and $1 \le k \le n$, we have

$$\frac{\Gamma(\theta)\theta^k}{n^{\theta-1} n!} \begin{bmatrix} n \\ k \end{bmatrix} = \frac{\theta^k}{\theta^{(n)}} \begin{bmatrix} n \\ k \end{bmatrix} (1 + O(n^{-1})) = \frac{\theta^k}{\theta^{(n)}} \begin{bmatrix} n \\ k \end{bmatrix} + O(n^{-1}).$$

We conclude the proof by noting that $G_j(x; \log \theta) = \theta^{-j/2} H_j(x)$ which follows directly from $\widetilde{\chi}_j(0) = \chi_j(\log \theta)$. Indeed, by comparing (6) and (12), we obtain

$$D_j(\log \theta) = \theta^{-j/2} \widetilde{D_j}(\theta),$$

which implies that

$$B_j(D_1(\log \theta), \ldots, D_j(\log \theta)) = \theta^{-j/2} B_j(\widetilde{D_1}(\theta), \ldots, \widetilde{D_j}(\theta))$$

since $B_j(z_1, \ldots, z_j)$ is a sum of terms of the form $c \cdot z_1^{i_1} z_2^{i_2} \cdots z_j^{i_j}$ with $1i_1 + 2i_2 + \cdots + ji_j = j$; see (2). Comparing (5) and (11), we obtain the required identity $G_j(x; \log \theta) = \theta^{-j/2} H_j(x)$.

To see that $\widetilde{\chi}_j(0) = \chi_j(\log\theta)$, one can easily show by induction over $j \geq 1$ that, both

$$\chi_j(\beta) = -\sum_{\ell=1}^{j} \left\{ j \atop \ell \right\} \psi^{(\ell-1)}(e^{\beta}) e^{\ell\beta},$$

and

$$\widetilde{\chi}_j(\beta) = -\sum_{\ell=1}^{j} \left\{ j \atop \ell \right\} \psi^{(\ell-1)}(\theta e^{\beta})(\theta e^{\beta})^{\ell}. \tag{13}$$

Here $\psi^{(j)}(x) = (\log\Gamma(x))^{(j+1)}$ denotes the polygamma function and $\left\{ n \atop k \right\}$ is the Stirling number of the second kind satisfying the recurrence

$$\left\{ n+1 \atop k \right\} = \left\{ n \atop k-1 \right\} + k \left\{ n \atop k \right\}, \quad 1 \leq k \leq n, \quad n \in \mathbb{N},$$

with initial conditions $\left\{ 0 \atop 0 \right\} = 1$, $\left\{ n \atop 0 \right\} = \left\{ 0 \atop n \right\} = 0$. □

Proof of Theorem 5. It follows from Theorems 2.10 in [16] that for sufficiently large n, the maximizers of the function $k \mapsto \mathbb{P}(K_n(\theta) = k)$ must be of the form $\lfloor u_n^* \rfloor$ or $\lceil u_n^* \rceil$.

Next we prove that the maximizer is unique (for sufficiently large n) by following a method of Erdős [5] who considered the case $\theta = 1$. Thanks to (8), the uniqueness is evident if θ is irrational. Hence, we assume that $\theta = Q_1/Q_2$ is rational with Q_1, Q_2 being integer. We have, by (1),

$$\left[n \atop k \right] = \sum_{1 \leq a_1 < \ldots < a_{n-k} \leq n-1} a_1 \cdots a_{n-k}.$$

Put $k_n = \lceil u_n^*(\theta) \rceil = \theta \log n + O(1)$ as $n \to \infty$. By (8), it is sufficient to show that

$$\theta^{k_n} \left[n \atop k_n \right] \neq \theta^{k_n - 1} \left[n \atop k_n - 1 \right]. \tag{14}$$

By Erdős' argument relying on the prime number theorem with an appropriate error term [5, p. 233], for all sufficiently large n, there is a prime number p satisfying $(n-1)/k_n < p < (n-1)/(k_n - 1)$. Then,

$$\left[n \atop k_n \right] \not\equiv 0 \pmod p, \qquad \left[n \atop k_n - 1 \right] \equiv 0 \pmod p$$

because in the representation of the former Stirling number all products except one are divisible by p, whereas in the latter all products are divisible by p. If n is large, p is not among the prime factors of Q_1 and Q_2. Hence (14) follows and the mode of $K_n(\theta)$ is unique. Finally, the formula for M_n follows from Theorem 2.13 of [16]. □

Proof of Proposition 6. Recall Hammersley's formula (9):

$$u_n(1) = \left\lfloor \log n + \gamma + \frac{\zeta(2) - \zeta(3)}{\log n + \gamma - \frac{3}{2}} + \frac{h(n)}{(\log n + \gamma - \frac{3}{2})^2} \right\rfloor$$

with some $-1.1 < h(n) < 1.44$. It is easy to check that

$$\frac{\zeta(2) - \zeta(3)}{x} - \frac{1.1}{x^2} > -\frac{1}{2} \text{ and } \frac{\zeta(2) - \zeta(3)}{x} + \frac{1.44}{x^2} < \frac{1}{2}$$

for $x > 2.5$. Hence, the proposition is true for $\log n + \gamma - \frac{3}{2} > 2.5$, that is for $n \geq 31$. For $n = 1, 2, \dots, 30$ the statement is easy to verify using Mathematica 9. □

Proof of Theorem 7 (i) and (ii). Part (i) follows essentially from Theorem 2.10 in [16] and its proof. Namely, by [16, Equation (90)], for $k = k(n) = u_n^*(\theta) + g \in \mathbb{Z}$ with $g = O(1)$, we have

$$\sqrt{2\pi\theta \log n}\,(\mathbb{P}(K_n(\theta) = k + 1) - \mathbb{P}(K_n(\theta) = k)) = -\frac{2g + 1}{2\theta \log n} + o\left(\frac{1}{\log n}\right).$$

The same relation, but with a better remainder term $O(\frac{1}{\log^2 n})$, follows from (16) which we shall prove below. Taking $g = -\{u_n^*(\theta)\}$, so that $k = \lfloor u_n^*(\theta) \rfloor$ and $k + 1 = \lceil u_n^*(\theta) \rceil$, yields

$$\mathbb{P}(K_n(\theta) = \lceil u_n^*(\theta) \rceil) - \mathbb{P}(K_n(\theta) = \lfloor u_n^*(\theta) \rfloor) = \frac{1}{\sqrt{2\pi\theta \log n}} \left(\frac{\{u_n^*(\theta)\} - \frac{1}{2}}{\theta \log n} + O\left(\frac{1}{\log^2 n}\right) \right).$$

It follows that there is a sufficiently large constant $C_0 > 0$ such that, if $\{u_n^*(\theta)\} > \frac{1}{2} + \frac{C_0}{\log n}$, then the right-hand side is positive, and the mode equals $\lceil u_n^*(\theta) \rceil$. Similarly, if $\{u_n^*(\theta)\} < \frac{1}{2} - \frac{C_0}{\log n}$, then the right-hand side is negative, and the mode equals $\lfloor u_n^*(\theta) \rfloor$.

The proof of part (ii) follows immediately from part (i) and the fact that, for every fixed $L > 0$, we have $\log(n + L) - \log n \to 0$ as $n \to \infty$. □

Proof of Theorem 7 (iii). In view of part (i) it suffices to show that

$$\limsup_{\varepsilon \to 0} \limsup_{n \to \infty} \frac{\#\{1 \leq k \leq n : \operatorname{dist}(u_k^*(\theta), \mathbb{Z} + 1/2) < \varepsilon\}}{n} = 0,$$

which, in turn, follows from the fact that

$$\limsup_{\varepsilon \to 0} \limsup_{n \to \infty} \frac{\#\{1 \leq k \leq n : \operatorname{dist}(\log k, \alpha\mathbb{Z} + \beta) < \varepsilon\}}{n} = 0, \tag{15}$$

for all $\alpha > 0$ and $\beta \in \mathbb{R}$. Equation (15) would be true if the sequence of fractional parts of $\alpha^{-1} \log k$, $k \in \mathbb{N}$, were uniformly distributed on $[0, 1]$. However, the latter claim is unfortunately not true [17, Examples 2.4 and 2.5, pp. 8–9]. Let us prove (15). We have, assuming that $\varepsilon < \alpha/2$,

$$\begin{aligned}\#\{1 \le k \le n : \operatorname{dist}(\log k, \alpha\mathbb{Z}+\beta) < \varepsilon\} &= \sum_{k=1}^{n} \#\{j \in \mathbb{Z} : \operatorname{dist}(\log k, \alpha j + \beta) < \varepsilon\} \\ &= \sum_{j\in\mathbb{Z}} \#\{1 \le k \le n : e^{\alpha j+\beta-\varepsilon} < k < e^{\alpha j+\beta+\varepsilon}\} \\ &\le \sum_{j\in\mathbb{Z}} \#\{k \in \mathbb{N} : e^{\alpha j+\beta-\varepsilon} \vee 1 \le k \le e^{\alpha j+\beta+\varepsilon} \wedge n\}.\end{aligned}$$

The summand on the right-hand side is the number of integers in the interval $[e^{\alpha j+\beta-\varepsilon} \vee 1, e^{\alpha j+\beta+\varepsilon} \wedge n]$ (which is empty if either $e^{\alpha j+\beta-\varepsilon} > n$ or $e^{\alpha j+\beta+\varepsilon} < 1$). Hence, it is bounded from above by $\left(e^{\alpha j+\beta+\varepsilon} \wedge n - e^{\alpha j+\beta-\varepsilon} \vee 1 + 1\right)_+$. Therefore,

$$\#\{1 \le k \le n : \operatorname{dist}(\log k, \alpha\mathbb{Z}+\beta) < \varepsilon\} \le \sum_{j\in\mathbb{Z}} \left(e^{\alpha j+\beta+\varepsilon} \wedge n - e^{\alpha j+\beta-\varepsilon} \vee 1 + 1\right)_+ .$$

Further,

$$\begin{aligned}&\sum_{j\in\mathbb{Z}} \left(e^{\alpha j+\beta+\varepsilon} \wedge n - e^{\alpha j+\beta-\varepsilon} \vee 1 + 1\right)_+ \\ &= \sum_{j\in\mathbb{Z}} e^{\alpha j+\beta+\varepsilon} \mathbb{1}_{\{\alpha j+\beta+\varepsilon<0\}} + \sum_{j\in\mathbb{Z}} e^{\alpha j+\beta+\varepsilon} \mathbb{1}_{\{\alpha j+\beta-\varepsilon<0, 0\le\alpha j+\beta+\varepsilon<\log n\}} \\ &+ \sum_{j\in\mathbb{Z}} n \mathbb{1}_{\{\alpha j+\beta-\varepsilon<0, \log n\le\alpha j+\beta+\varepsilon\}} \\ &+ \sum_{j\in\mathbb{Z}} \left(e^{\alpha j+\beta+\varepsilon} - e^{\alpha j+\beta-\varepsilon} + 1\right) \mathbb{1}_{\{\alpha j+\beta-\varepsilon\ge 0, \alpha j+\beta+\varepsilon<\log n\}} \\ &+ \sum_{j\in\mathbb{Z}} \left(n - e^{\alpha j+\beta-\varepsilon} + 1\right)_+ \mathbb{1}_{\{\alpha j+\beta-\varepsilon\ge 0, \log n\le\alpha j+\beta+\varepsilon\}}.\end{aligned}$$

Note that the first series converges, the second contains at most one summand since we assume $\varepsilon < \alpha/2$, and the third vanishes for n large enough. It can be checked that

$$\sum_{j\in\mathbb{Z}} \left(e^{\alpha j+\beta+\varepsilon} - e^{\alpha j+\beta-\varepsilon} + 1\right) \mathbb{1}_{\{\alpha j+\beta-\varepsilon\ge 0, \alpha j+\beta+\varepsilon<\log n\}} \le C(\alpha,\beta)(e^{\beta+\varepsilon} - e^{\beta-\varepsilon})n$$

with an absolute constant $C(\alpha, \beta)$. Further, for n sufficiently large, we have

$$\sum_{j\in\mathbb{Z}} \left(n - e^{\alpha j+\beta-\varepsilon} + 1\right)_+ \mathbb{1}_{\{\alpha j+\beta-\varepsilon\ge 0, \log n\le\alpha j+\beta+\varepsilon\}} \le n(1 - e^{-2\varepsilon}) + 1.$$

Putting pieces together gives (15). □

Proof of Theorem 7 (iv). Recall the notation $w_n = \theta \log n$ and $x_n(k) = x_n(k, \theta) = (k - w_n)/\sqrt{w_n}$. Using Theorem 1 with $r = 4$, we obtain

$$\sqrt{2\pi w_n}\,\mathbb{P}(K_n(\theta) = k) = e^{-\frac{1}{2}x_n^2(k)} \times \left(1 + \frac{H_1(x_n(k))}{w_n^{1/2}} + \frac{H_2(x_n(k))}{w_n} + \frac{H_3(x_n(k))}{w_n^{3/2}} + \frac{H_4(x_n(k))}{w_n^2} + o\left(\frac{1}{\log^2 n}\right)\right),$$

as $n \to \infty$ uniformly in $1 \le k \le n$. Now let $k = \theta \log n + a$, where $a = O(1)$ as $n \to \infty$, so that $x_n(k) = a/w_n^{1/2}$. We have

$$\begin{aligned} H_1(x_n(k)) &= A_{11}(\theta)\frac{a}{w_n^{1/2}} + A_{12}(\theta)\frac{a^3}{w_n^{3/2}}, \\ H_2(x_n(k)) &= A_{21}(\theta) + A_{22}(\theta)\frac{a^2}{w_n} + o\left(\frac{1}{w_n}\right), \\ H_3(x_n(k)) &= A_{31}(\theta)\frac{a}{w_n^{1/2}} + o\left(\frac{1}{w_n^{1/2}}\right), \\ H_4(x_n(k)) &= A_{41}(\theta) + o(1), \end{aligned}$$

where $A_{11}(\theta), \dots, A_{41}(\theta)$ are some polynomials in $\widetilde{\chi_1}(0), \widetilde{\chi_2}(0), \widetilde{\chi_3}(0)$ and $\widetilde{\chi_4}(0)$; see Remark 2. Plugging these expressions into the asymptotic expansion above and using the expansion $e^y = 1 + y + y^2/2 + o(y^2)$, as $y \to 0$, yields

$$\sqrt{2\pi w_n}\,\mathbb{P}(K_n(\theta) = k) = 1 - \left(\frac{a^2}{2} - A_{11}(\theta)a - A_{21}(\theta)\right)\frac{1}{w_n} + \frac{P_\theta(a)}{w_n^2} + o\left(\frac{1}{\log^2 n}\right),$$

where

$$P_\theta(a) := \frac{1}{8}a^4 + \left(A_{12}(\theta) - \frac{1}{2}A_{11}(\theta)\right)a^3 + \left(A_{22}(\theta) - \frac{1}{2}A_{21}(\theta)\right)a^2 + A_{31}(\theta)a + A_{41}(\theta).$$

Now let us write $k = \theta \log n + a^* + g$, where $a^* := A_{11}(\theta) = -\frac{\theta\Gamma'(\theta)}{\Gamma(\theta)} - \frac{1}{2}$, yielding

$$\sqrt{2\pi w_n}\,\mathbb{P}(K_n(\theta) = k) = 1 - \left(\frac{g^2 - (a^*)^2}{2} - A_{21}(\theta)\right)\frac{1}{w_n} + \frac{P_\theta(a^* + g)}{w_n^2} + o\left(\frac{1}{\log^2 n}\right). \quad (16)$$

We are interested in g being either $\lfloor u_n^*(\theta) \rfloor - u_n^*(\theta) =: g_n'$ or $\lceil u_n^*(\theta) \rceil - u_n^*(\theta) =: g_n''$. Let M be the set of natural numbers n with $\{u_n^*(\theta)\} < 1/2 < \{u_{n+1}^*(\theta)\}$. Note that M has infinitely many elements because $\log n \to \infty$ and $\log(n+1) - \log n \to 0$. In the remainder of the proof, we always consider $n \in M$. Since $u_{n+1}^*(\theta) - u_n^*(\theta) = O(n^{-1})$, we have

$$g_n' = -1/2 + O(n^{-1}), \quad g_n'' = 1/2 + O(n^{-1}).$$

Putting $k = \lfloor u_n^*(\theta) \rfloor$ into (16) yields

$$\begin{aligned}
&\sqrt{2\pi w_n}\,\mathbb{P}(K_n(\theta) = \lfloor u_n^*(\theta) \rfloor) \\
&= 1 - \left(\frac{(g_n')^2 - (a^*)^2}{2} - A_{21}(\theta) \right) \frac{1}{w_n} + \frac{P_\theta(a^* + g_n')}{w_n^2} + o\left(\frac{1}{\log^2 n} \right) \\
&= 1 - \left(\frac{1 - 4(a^*)^2}{8} - A_{21}(\theta) \right) \frac{1}{w_n} + \frac{P_\theta(a^* - 1/2)}{w_n^2} + o\left(\frac{1}{\log^2 n} \right).
\end{aligned}$$

Analogously, putting $k = \lceil u_n^*(\theta) \rceil$ gives

$$\sqrt{2\pi w_n}\,\mathbb{P}(K_n(\theta) = \lceil u_n^*(\theta) \rceil) = 1 - \left(\frac{1 - 4(a^*)^2}{8} - A_{21}(\theta) \right) \frac{1}{w_n} + \frac{P_\theta(a^* + 1/2)}{w_n^2} + o\left(\frac{1}{\log^2 n} \right).$$

For sufficiently large n the mode $u_n(\theta)$ equals either $\lfloor u_n^*(\theta) \rfloor$ or $\lceil u_n^*(\theta) \rceil$ depending on the sign of

$$s^*(\theta) := P_\theta(a^* + 1/2) - P_\theta(a^* - 1/2).$$

In the following we shall show that $s^*(\theta) > 0$, hence $u_n(\theta) = \lceil u_n^*(\theta) \rceil$, while $\mathrm{nint}(u_n(\theta)) = \lfloor u_n^*(\theta) \rfloor$, so that $u_n(\theta) \neq \mathrm{nint}(u_n^*(\theta))$. Recalling the polygamma function $\psi^{(m)}(\theta) = (\log \Gamma(\theta))^{(m+1)}$, the authors [15] checked with the help of Mathematica 9 that

$$s^*(\theta) = \frac{\theta^2}{2} \left(2\psi^{(1)}(\theta) + \theta \psi^{(2)}(\theta) \right).$$

Using the well-known formula for the polygamma function [1, 6.4.10]

$$\psi^{(m)}(\theta) = (\log \Gamma(\theta))^{(m+1)} = (-1)^{m+1} m! \sum_{k=0}^{\infty} \frac{1}{(\theta + k)^{m+1}}, \quad -\theta \notin \mathbb{N}_0, \quad m \geq 1,$$

we finally obtain

$$s^*(\theta) = \theta^2 \sum_{k=1}^{\infty} \frac{k}{(\theta + k)^3}, \quad \theta > 0,$$

yielding positivity of $s^*(\theta)$ for all $\theta > 0$. The proof of part (iv), as well as of the whole theorem, is complete. □

Remark 8. For $\theta = 1$ we have $s^*(1) = \zeta(2) - \zeta(3)$, a term appearing in Hammersley's formula (9). In fact, in the special case $\theta = 1$ part (iv) could be deduced directly from (9).

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