NEARLY TIGHT UNIVERSAL BOUNDS FOR THE BINOMIAL TAIL PROBABILITIES

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We derive simple but nearly tight upper and lower bounds for the binomial lower tail probability (with straightforward generalization to the upper tail probability) that apply to the whole parameter regime. These bounds are easy to compute and are tight within a constant factor of $89/44$. Moreover, they are asymptotically tight in the regimes of large deviation and moderate deviation. By virtue of a surprising connection with Ramanujan’s equation, we also provide strong evidences suggesting that the lower bound is tight within a factor of $1.26434$. It may even be regarded as the natural lower bound, given its simplicity and appealing properties. Our bounds significantly outperform the familiar Chernoff bound and reverse Chernoff bounds known in the literature and may find applications in various research areas.

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1. Introduction. The evaluation of tail probabilities is one of central topics in probability theory because it is tied to many important applications, including hypothesis testing, statistical inference, information theory, statistical physics, machine learning, insurance, and risk management. However, it is in general not easy to derive accurate bounds for tail probabilities even for many simple probability distributions. Here we are particularly interested in the binomial distribution, which is one of the oldest probability distributions studied in the literature \([5, 15, 19, 30]\). It characterizes the probability of obtaining \(k\) successes after \(n\) independent Bernoulli trials, assuming that the success probability of each trial is \(p\). To be concrete this probability and the probability of obtaining at most \(k\) successes are give by

\[
b_{n,k}(p) := \binom{n}{k} p^k q^{n-k}, \quad B_{n,k}(p) := \sum_{j=0}^{k} b_{n,j}(p) = \sum_{j=0}^{k} \binom{n}{j} p^j q^{n-j},
\]

where \(q = 1 - p\). To avoid trivial exceptions, we assume that \(0 < p < 1\) (so \(0 < q < 1\)) unless stated otherwise. When \(k \leq np\), the probability \(B_{n,k}(p)\) is referred to as a lower tail probability, which has been studied by numerous researchers in various research areas for a long history \([3, 5, 9, 12, 13, 15, 19, 20, 26, 29, 30, 31, 32, 33, 36]\).

One of the most popular upper bounds for \(B_{n,k}(p)\) is the Chernoff bound \([9, 26]\),

\[
B_{n,k}(p) \leq e^{-nD(\frac{k}{n}||p)} \quad \forall k \leq np,
\]

which correctly characterizes the exponential decay rate of the tail probability. Here

\[
D(f||p) := f \ln \frac{f}{p} + (1 - f) \ln \frac{1 - f}{1 - p}
\]
is the familiar relative entropy (information divergence). Two popular reverse Chernoff bounds are given by

\[
\frac{1}{n+1} e^{-nD(\frac{k}{n}\|p)} \leq b_{n,k}(p) \leq B_{n,k}(p),
\]

\[
\frac{\sqrt{n}}{\sqrt{8k(n-k)}} e^{-nD(\frac{k}{n}\|p)} \leq b_{n,k}(p) \leq B_{n,k}(p).
\]

Here the first bound can be derived with the method of types [12, 13]; the second bound follows from Lemma 4.7.1 in Ref. [3] and from [Chapter 10, Lemma 7] in Ref. [32]. Unfortunately, the Chernoff bound has a major drawback: its ratio over the tail probability is not bounded by any given constant. This is the case even if we only consider the asymptotic regime in which \( k,n \to \infty \). The two reverse Chernoff bounds in Eqs. (4) and (5) have a similar problem. Although many alternative bounds are known in the literature [3, 12, 13, 20, 29, 32], almost all bounds share the same problem unfortunately. Can we construct much better bounds?

The main goal of the current study is to establish good upper bound \( B_{n,k}^\uparrow(p) \) and lower bound \( B_{n,k}^\downarrow(p) \) for the tail probability \( B_{n,k}(p) \) that bear certain desired properties. To be concrete, such bounds should satisfy the following three reasonable criteria, which are related to criteria in Ref. [48]. Our criteria are applicable when both upper and lower bounds are available, but it is straightforward to formulate similar criteria for the upper bound or lower bound alone by replacing \( B_{n,k}^\downarrow(p) \) or \( B_{n,k}^\uparrow(p) \) with \( B_{n,k}(p) \).

(C1) Computability: The bounds have computational complexity \( O(1) \); in other words, they are \( O(1) \)-computable.

(C2) Universal boundedness: the ratio \( B_{n,k}^\uparrow(p)/B_{n,k}^\downarrow(p) \) with \( k \leq pn \) is bounded by a universal constant.

(C3) Asymptotic tightness: The bounds are tight in the limit \( n \to \infty \) when \( 0 < k/n < p \) is fixed, that is,

\[
\lim_{n \to \infty} \frac{B_{n,fn}^\uparrow(p)}{B_{n,fn}^\downarrow(p)} = 1 \quad \forall 0 < f < p.
\]

Here we assume that elementary operations, such as addition and multiplication, are \( O(1) \) when evaluating the computational complexity. Besides computability, we prefer bounds that are simple and explicit functions that do not involve integration because merely numerical bounds for the tail probability are not enough for many applications.

To better understand the criterion of asymptotic tightness, we need to introduce some additional concepts. Let \( \mathbb{N} \) be the set of natural numbers (positive integers) and \( \mathbb{N}_0 \) the set of nonnegative integers. Given a real number \( f \), define

\[
\mathbb{N}_f := \{ n \in \mathbb{N}_0 \mid fn \in \mathbb{N}_0 \}.
\]

When \( f \) is a rational number that satisfies \( 0 < f < p \) and \( n \in \mathbb{N}_f \), as a simple corollary of Theorem 2 in Ref. [2] we can deduce that

\[
\lim_{n \to \infty} \sqrt{n} B_{n,fn}(p) e^{n D(f\|p)} = \frac{1}{(1-r) \sqrt{2\pi f(1-f)}} = \frac{\sqrt{(1-f)} p}{\sqrt{2\pi f (p-f)}},
\]

where

\[
r = r(f,p) := \frac{fq}{(1-f)p}
\]
is the odds ratio. This result can also be derived by virtue of the theory of strong large deviation [4, 7, 16] as shown in Appendix A. Compared with the theory of large deviation [9, 11, 16, 47], which characterizes the exponential decay rate, strong large deviation focuses on more accurate expansion of the tail probability that is beyond conventional large deviation.

In view of Eq. (8), the condition of asymptotic tightness in Eq. (6) can also be formulated as follows,

\[
\lim_{n \to \infty} \sqrt{nB_{n,fn}^\dagger (p)e^{\alpha D(f\|p)}} = \lim_{n \to \infty} \sqrt{nB_{n,fn}^\dagger (p)e^{\alpha D(f\|p)}} = \frac{\sqrt{(1-f)p}}{2\pi f (p-f)}.
\]

Such bounds are of special interest in the study of strong large deviation [4, 7, 16]. Recently such bounds have found numerous applications in classical and quantum information theory, including finite-length analysis for channel coding [17], channel coding with higher orders [21, 35], security analysis with higher orders [21, 22], quantum thermodynamics [27, 45], and local discrimination [23]. Unfortunately, it is in general not easy to derive bounds that satisfy the condition of asymptotic tightness, that is, criterion (C3). Actually, most bounds for this regime [3, 9, 12, 13, 26, 29, 32, 48] known in the literature satisfy criterion (C1), but few bounds satisfy criterion (C2) or (C3). Notably, the Chernoff and reverse Chernoff bounds reproduced in Eqs. (2), (4), and (5) satisfy neither (C2) nor (C3). As exceptions, the bounds derived by McKay [33] satisfy criteria (C2) and (C3), but does not satisfy (C1) because the bounds involve the probability \(b_{n-1,k-1}(p)\); in addition, the bounds involve integrals and are not so explicit compared with the Chernoff and reverse Chernoff bounds mentioned above. The bounds derived recently by Ferrante [17] satisfy criteria (C1) and (C3), but do not satisfy criterion (C2).

In addition to the regime of large deviation, the regime of moderate deviation [14, 16, 48, 50] is of independent interest. Here \(k\) behaves as \(pn - \alpha_n\) with the sequence \(\alpha_n\) satisfying the conditions \(\alpha_n/n \to 0\) and \(\alpha_n/\sqrt{n} \to \infty\). This regime interpolates between the regime of large deviation and the regime of central limit theorem (CLT). The asymptotics of this regime is useful to the analysis of various types of information processing [1, 8, 10, 24, 25, 37, 46]. Although several works have studied the exponential decay rate of the tail probability in this regime [14, 16, 48, 50], few papers have derived its asymptotic behavior up to constant multiplicative factors.

In this paper, to find the desired upper and lower bounds for \(B_{n,k}(p)\), we derive nearly tight upper and lower bounds for the ratio \(B_{n,k}(p)/b_{n,k}(p)\) in the first step. Then, we prepare various nearly tight upper and lower bounds for the probability \(b_{n,k}(p)\). Combining these results, we derive nearly tight upper and lower bounds for the tail probability \(B_{n,k}(p)\) that satisfy criteria (C1-C3). Notably, our bounds are tight within a constant factor of 89/44 and are asymptotically tight in the regime of moderate deviation besides the regime of large deviation. In addition, we conjecture that our lower bound for the ratio \(B_{n,k}(p)/b_{n,k}(p)\) is tight within a factor of 180451625/143327232. If this conjecture holds, then our lower bound \(B_{n,k}^\dagger(p)\) for the tail probability \(B_{n,k}(p)\) is tight within a factor of 1.26434. Furthermore we prove this conjecture in a special case by virtue of a surprising connection with Ramanujan's equation [28, 40]. This connection indicates that our work is of interest beyond probability theory.

The rest of this paper is organized as follows. Section 2 summarizes the main results. Section 3 prepares fundamental knowledges on the binomial distribution. Section 4 proposes nearly tight upper and lower bounds for the ratio \(B_{n,k}(p)/b_{n,k}(p)\). Section 5 proposes nearly tight upper and lower bounds for the tail probability \(B_{n,k}(p)\) by virtue of good bounds for \(b_{n,k}(p)\) and \(B_{n,k}(p)/b_{n,k}(p)\). Section 6 presents a conjecture on the tail probability and provides strong evidences based on a connection with Ramanujan's equation [28, 40]. Section 7 concludes this paper.
2. Summary of results.

2.1. Evaluation of the ratio \( B_{n,k}(p)/b_{n,k}(p) \). In the first step, to evaluate the ratio \( B_{n,k}(p)/b_{n,k}(p) \) we define the following functions, assuming that \( n \geq 0, 0 < p < 1, \) and \( 0 \leq k \leq pn \). It is not necessary to assume that \( k \) and \( n \) are integers in the following definitions.

\[
L(n,k,p) := \frac{k + 1 - pn + \sqrt{(pn-k+1)^2 + 4qk}}{2},
\]

\[
\kappa_1(n,p) := p(n+1) - \sqrt{pq(n+1)},
\]

\[
V(n,k,p,a) := a + \frac{p(n-k+a+1)}{pn+p-k+a},
\]

\[
U(n,k,p) := \min_{a \in \mathbb{N}_0} V(n,k,p,a) = \begin{cases} V(n,k,p,0) & k < \kappa_1(n,p), \\ \min \{V(n,k,p,\lceil\tilde{a}\rceil), V(n,k,p,\lfloor\tilde{a}\rfloor)\} & k \geq \kappa_1(n,p), \end{cases}
\]

where \( q = 1-p, \tilde{a} = k - \kappa_1(n,p) \). The second equality in Eq. (14) follows from the fact that \( V(n,k,p,x) \) is strictly convex in \( x \) for \( x \geq k - pn - p \) and has a unique minimum point at \( x = \tilde{a} \). In addition, it is easy to verify that

\[
V(n,k,p,\lceil\tilde{a}\rceil) \leq 1 + V(n,k,p,\tilde{a}) = 1 + k - pn + 2\sqrt{pq(n+1)}.
\]

If \( 0 \leq f < p \) and \( n \) is sufficiently large; then \( k, fn < \kappa_1(n,p), \) so Eq. (14) yields

\[
U(n,k,p) = V(n,k,p,0), \quad U(n,fn,p) = V(n,fn,p,0).
\]

Then, as shown in Sec. 4, we have the following theorem.

**Theorem 2.1.** Suppose \( k \in \mathbb{N}_0, n \in \mathbb{N}, 0 < p < 1, k \leq pn, \) and \( f = k/n \). Then

\[
1 \leq L(n,k,p) \leq \frac{B_{n,k}(p)}{b_{n,k}(p)} \leq U(n,k,p) < 2L(n,k,p),
\]

where all inequalities are strict when \( k \geq 1 \). If in addition \( 0 < f < p \), then

\[
1 < L(n,k,p) \leq \frac{B_{n,k}(p)}{b_{n,k}(p)} < U(n,k,p) \leq V(n,k,p,0) < \frac{(1-f)p}{p-f} = \frac{1}{1-r}.
\]

Here \( r \) is the odds ratio defined in Eq. (9). The upper bound \( U(n,k,p) \) and lower bound \( L(n,k,p) \) can be computed in \( O(1) \) time by definitions, assuming that elementary operations, such as addition and multiplication, are \( O(1) \). In addition, they are tight within a factor of 2 by Eq. (17). Furthermore, the two bounds \( U(n,k,p) \) and \( L(n,k,p) \) are asymptotically tight according to the following equations,

\[
\lim_{n \to \infty} L(n,k,p) = \lim_{n \to \infty} U(n,k,p) = \lim_{n \to \infty} V(n,k,p,0) = 1,
\]

\[
\lim_{n \to \infty} L(n,fn,p) = \lim_{n \to \infty} U(n,fn,p) = \lim_{n \to \infty} V(n,fn,p,0) = \frac{(1-f)p}{p-f} \quad \forall 0 \leq f < p < 1,
\]

which follow from Eqs. (11)-(14) and (16). Note that Eq. (20) still holds if \( fn \) is replaced by \( \lfloor fn \rfloor \). Numerical calculation illustrated in Fig. 1 further shows that the lower bound \( L(n,k,p) \) is more accurate than what can be proved rigorously (cf. Conjecture 1 in Sec. 6 for potential improvement). The combination of Eqs. (18) and (20) also implies the following result

\[
\lim_{n \to \infty} \frac{B_{n,\lfloor fn \rfloor}(p)}{b_{n,\lfloor fn \rfloor}(p)} = \frac{(1-f)p}{p-f} = \frac{1}{1-r} \quad \forall 0 \leq f < p < 1.
\]
2.2. Evaluation of the tail probability $B_{n,k}(p)$. In the next step, to describe our upper and lower bounds for the binomial tail probability $B_{n,k}(p)$, we introduce two quantities, assuming that $0 < p < 1$ and $1 \leq k \leq n - 1$,

\begin{align}
B_{n,k}^\downarrow(p) &= \frac{\sqrt{n} L(n, k, p)}{\sqrt{2\pi k(n - k)}} e^{-nD(\frac{p}{n} || p)} e^{\frac{1}{12n} - \frac{1}{12k} - \frac{1}{12(n - k)}}, \\
B_{n,k}^\uparrow(p) &= \frac{\sqrt{n} U(n, k, p)}{\sqrt{2\pi k(n - k)}} e^{-nD(\frac{p}{n} || p)} e^{\frac{1}{12n + 1} - \frac{1}{12k + 1} - \frac{1}{12(n - k) + 1}}.
\end{align}

With the above definition, the limit formulas in Eq. (20) guarantee that $B_{n,k}^\downarrow(p)$ and $B_{n,k}^\uparrow(p)$ satisfy the condition of asymptotic tightness in Eqs. (6) and (10). Then, as shown in Sec. 5, we have the following theorem.

**THEOREM 2.2.** Suppose $n, k \in \mathbb{N}$, $0 < p < 1$, $k \leq pn$, and $f = k/n$. Then

\begin{align}
\frac{\sqrt{n} L(n, k, p)}{\sqrt{8k(n - k)}} e^{-nD(\frac{p}{n} || p)} < B_{n,k}(p) < \frac{\sqrt{n} U(n, k, p)}{\sqrt{2\pi k(n - k)}} e^{-nD(\frac{p}{n} || p)}, \\
B_{n,k}^\downarrow(p) < B_{n,k}(p) < B_{n,k}^\uparrow(p) < \frac{89}{44} B_{n,k}^\uparrow(p), \\
B_{n,k}(p) < B_{n,k}^\uparrow(p) < \frac{\sqrt{(1 - f)p}}{\sqrt{2\pi f(p - f)}} e^{-nD(f || p)}, \quad k < pn.
\end{align}

The upper and lower bounds in Eq. (23) are tight within a factor of $4/\sqrt{\pi} \approx 2.25676$ given that $U(n, k, p) \leq 2L(n, k, p)$ by Theorem 2.1; the lower bound improves over the popular reverse Chernoff bound in Eq. (5) given that $L(n, k, p) > 1$ under the assumptions in Theorem 2.2. By definitions the bounds $B_{n,k}^\downarrow(p)$ and $B_{n,k}^\uparrow(p)$ are $O(1)$-computable and thus

**FIG 1.** The ratios $B_{n,k}(p)/[b_{n,k}(p)L(n,k,p)]$ and $B_{n,fn}(p)/[b_{n,fn}(p)L(n,fn,p)]$.
comply with criterion (C1). In addition, they are tight within a factor of 89/44 by Eq. (24) and thus comply with criterion (C2). Furthermore, they are asymptotically tight because they satisfy Eqs. (6) and (10) and thus comply with criterion (C3), which also yields another proof of Eq. (8). In a word, the bounds $B_{n,k}^{\downarrow}(p)$ and $B_{n,k}^{\uparrow}(p)$ satisfy all three criteria of good bounds. The second upper bound in Eq. (25) is equivalent to an upper bound derived in Ref. [17]. Alternatively bounds for $B_{n,k}(p)$ can be constructed from Theorem 5.6 in Sec. 5.

In addition, Theorem 2.2 implies the following result in the regime of moderate deviation.

**Corollary 2.3.** Suppose $n \in \mathbb{N}$ and $\alpha_n$ is a sequence with the properties $\alpha_n/n \to 0$ and $\alpha_n/\sqrt{n} \to \infty$ when $n \to \infty$. Let $k_n = pn - \alpha_n$ and $f_n = k_n/n$; then

$$
\lim_{n \to \infty} B_{n,k_n}(p) \frac{\alpha_n}{\sqrt{n}} e^{nD(f_n || p)} = \lim_{n \to \infty} B_{n,k_n}(p) \frac{\alpha_n}{\sqrt{n}} e^{nD(f_n || p)} = \lim_{n \to \infty} B_{n,k_n}(p) \frac{\alpha_n}{\sqrt{n}} e^{nD(f_n || p)} = \sqrt{\frac{pq}{2\pi}}.
$$

Corollary 2.3 shows that

$$
B_{n,k_n}(p) = \left[ \sqrt{\frac{pq}{2\pi}} + o(1) \right] \frac{\alpha_n}{\sqrt{n}} e^{-nD(k_n || p)}.
$$

This corollary follows from Theorem 2.2 and the following equations [cf. Eq. (20)]:

$$
\lim_{n \to \infty} \left[ nD(k_n/n || p) - nD(f_n || p) \right] = 0,
$$

$$
\lim_{n \to \infty} L(n,k_n,p) \frac{\alpha_n}{n} = \lim_{n \to \infty} L(n,k_n,p) \frac{\alpha_n}{n} = \lim_{n \to \infty} U(n,k_n,p) \frac{\alpha_n}{n} = pq.
$$

### 3. Binomial Probabilities.

**3.1. Preliminary results.** To obtain upper and lower bounds for the tail probability $B_{n,k}(p)$, here we prepare several preliminary results on $b_{n,k}(p)$ and $B_{n,k}(p)$ as well as their relations, assuming that $k,n \in \mathbb{N}_0$, $k \leq n$, and $0 < p < 1$. If there is no danger of confusion, we shall use $b_{n,k}$ and $B_{n,k}$ as shorthands for $b_{n,k}(p)$ and $B_{n,k}(p)$, respectively.

The definitions in Eq. (1) imply that

$$
B_{n,k} = B_{n,k-1} + b_{n,k}, \quad B_{n+1,k} = pB_{n,k-1} + qB_{n,k},
$$

$$
B_{n,k} - B_{n+1,k} = p(B_{n,k} - B_{n,k-1}) = pb_{n,k},
$$

$$
\frac{b_{n,k-1}}{b_{n,k}} = \frac{qk}{p(n-k+1)}, \quad \frac{b_{n,k}}{b_{n,k}} \geq 1 + \frac{b_{n,k-1}}{b_{n,k}} \geq 1 + \frac{qk}{pn},
$$

$$
\frac{b_{n+1,k}}{b_{n,k}} = \frac{(n+1)q}{n+1-k}.
$$

Here it is understood that $B_{n,k-1} = b_{n,k-1} = 0$ whenever $k = 0$. Based on these simple observations we can derive various preliminary results on $b_{n,k}$ and $B_{n,k}$ as follows.

**Lemma 3.1.** Suppose $j,k,n \in \mathbb{N}_0$ satisfy $0 \leq j \leq k \leq n$ and $k \geq 1$, and $0 < p < 1$. Then $B_{n,k-j}(p) / b_{n,k}(p)$ is strictly increasing in $k$, but strictly decreasing in $n$ and $p$. If in addition
\[ j \geq 1, \text{ then } b_{n,k-j}(p)/b_{n,k}(p) \text{ and } B_{n,k-j}(p)/B_{n,k}(p) \text{ are strictly increasing in } k, \text{ but strictly decreasing in } n \text{ and } p. \] Furthermore,

\[
\lim_{n \to \infty} \frac{b_{n,k-j}(p)}{b_{n,k}(p)} = \lim_{n \to \infty} \frac{B_{n,k-j}(p)}{B_{n,k}(p)} = \lim_{n \to \infty} \frac{B_{n,k-j}(p)}{B_{n,k}(p)} = \begin{cases} 1 & j = 0, \\ 0 & j \geq 1. \end{cases}
\]

Here we assume that \( n, k, p \) can vary independently under the constraint specified in the lemma. To be concrete, the monotonicity of \( B_{n,k-j}(p)/b_{n,k}(p) \) with respect to \( k \) means

\[
\frac{B_{n,k-j}}{b_{n,k}} < \frac{B_{n,k'-j}}{b_{n,k'}}, \quad 0 \leq j \leq k < k' \leq n.
\]

Similar remarks apply to other conclusions concerning monotonicity properties.

**PROOF.** From Eq. (32) we can deduce that

\[
\frac{b_{n,k-j}}{b_{n,k}} = \prod_{i=0}^{j-1} \frac{b_{n,k-i-1}}{b_{n,k-i}} = \prod_{i=0}^{j-1} \frac{q(k-i)}{p(n-k+i+1)}, \quad 1 \leq j \leq k,
\]

which implies that \( b_{n,k-j}/b_{n,k} \) is strictly increasing in \( k \), but strictly decreasing in \( n \) and \( p \) when \( 1 \leq j \leq k \). Then, according to the following equation,

\[
\frac{B_{n,k-j}}{b_{n,k}} = \sum_{i=j}^{k} \frac{b_{n,k-i}}{b_{n,k}} = 1 + \sum_{i=0}^{j-1} \frac{b_{n,k-i}}{b_{n,k-j}},
\]

\( B_{n,k-j}/b_{n,k} \) is strictly increasing in \( k \), but strictly decreasing in \( n \) and \( p \) when \( 0 \leq j \leq k \); by contrast, \( B_{n,k-j}/B_{n,k} \) is strictly increasing in \( k \), but strictly decreasing in \( n \) and \( p \) when \( 1 \leq j \leq k \).

Furthermore, Eq. (36) implies that

\[
\lim_{n \to \infty} \frac{b_{n,k-j}}{b_{n,k}} = \begin{cases} 1 & j = 0, \\ 0 & j \geq 1, \end{cases}
\]

which in turn implies Eq. (34).

**LEMMA 3.2.** Suppose \( k, n \in \mathbb{N}_0 \) satisfy \( 0 \leq k \leq n \) and \( 0 < p < 1 \). Then \( B_{n,k}(p) \) is strictly increasing in \( k \), but strictly decreasing in \( n \). In addition, \( B_{n,k}(p) \) is strictly decreasing in \( p \) when \( k < n \).

If \( 0 \leq p \leq 1 \) instead, then \( B_{n,k}(p) \) is nondecreasing in \( k \) and nonincreasing in \( n \) and \( p \) by continuity.

**PROOF.** According to Eqs. (30) and (31), \( B_{n,k}(p) \) is strictly increasing in \( k \), but strictly decreasing in \( n \). When \( k < n \), \( B_{n,k}(p) = B_{n,k}(p)/B_{n,n}(p) \) is strictly decreasing in \( p \) according to Lemma 3.1.

**LEMMA 3.3.** Suppose \( 0 \leq f \leq 1, 0 < p < 1 \), and \( n \in \mathbb{N} \). Then \( B_{n,f_n}(p)/b_{n,f_n}(p) = 1 \) is independent of \( n \) when \( f = 0 \), but is strictly increasing in \( n \in \mathbb{N}_f \) when \( f > 0 \). If in addition \( f < p \), then

\[
\frac{B_{n,f_n}(p)}{b_{n,f_n}(p)} \leq \frac{1}{1-r} = \frac{(1-f)p}{p-f}, \quad \lim_{n \to \infty} \frac{B_{n,f_n}(p)}{b_{n,f_n}(p)} = \frac{1}{1-r} = \frac{(1-f)p}{p-f},
\]

and the inequality is saturated iff \( f = 0 \).
Here \( N_f \) is defined in Eq. (7) and \( r = f q / [(1 − f) p] \) is the odds ratio defined in Eq. (9). The limit in Eq. (39) recovers Eq. (21).

**PROOF.** If \( f = 0 \), then \( r = 0 \) and \( B_{n,fn}/b_{n,fn} = 1 \) is independent of \( n \), so Eq. (39) holds and the inequality is saturated.

Next, we suppose \( f > 0 \) and \( fn < 1 \); then \( \lceil fn \rceil = 0 \) and \( B_{n,[fn]}/b_{n,[fn]} = 1 \). In addition, \( 0 < r < 1 \) when \( 0 < f < p \), so the inequality in Eq. (39) holds and is strict.

Next, suppose \( f > 0 \) and \( fn \geq 1 \); then \( B_{n,[fn]}/b_{n,[fn]} > 1 = B_{n,0}/b_{n,0} \). Let \( j \) be a non-negative integer that satisfies \( j \leq \lceil fn \rceil - 1 \). By virtue of Eq. (32) we can deduce that

\[
\frac{b_{n,[fn]−j−1}}{b_{n,[fn]−j}} = \frac{q(\lceil fn \rceil − j)}{p(n − \lceil fn \rceil + j + 1)} \leq \frac{q(fn − j)}{p(n − fn + j + 1)}.
\]

If in addition \( n \in N_f \), then \( \lceil fn \rceil = fn \) and \( b_{n,fn−j−1}/b_{n,fn−j} \) is strictly increasing in \( n \), so \( B_{n,fn}/b_{n,fn} \) is strictly increasing in \( n \).

If in addition \( 0 < f < 1 \) (it is not necessary to assume that \( n \in N_f \)), then Eq. (40) implies that

\[
\frac{b_{n,[fn]−j−1}}{b_{n,[fn]−j}} < \frac{fq}{(1 − f)p} = r, \quad \lim_{n \to \infty} \frac{b_{n,[fn]−j−1}}{b_{n,[fn]−j}} = \frac{fq}{(1 − f)p} = r.
\]

If in addition \( 0 < f < p \), then \( 0 < r < 1 \) and Eq. (41) implies that

\[
\frac{B_{n,[fn]}}{b_{n,[fn]}} < \sum_{l=0}^{\infty} r^l = \frac{1}{1 − r} = \frac{(1 − f)p}{p − f}, \quad \lim_{n \to \infty} \frac{B_{n,[fn]}}{b_{n,[fn]}} \leq \frac{1}{1 − r} = \frac{(1 − f)p}{p − f},
\]

\[
\lim_{n \to \infty} \frac{B_{n,[fn]}}{b_{n,[fn]}} \geq \lim_{n \to \infty} \frac{B_{n,[fn]−j−1}}{b_{n,[fn]−j}} = \sum_{l=0}^{j−1} r^l = \frac{(1 − f)p}{p − f}(1 − r^j) \quad \forall j \in \mathbb{N}.
\]

The two equations above imply Eq. (39), and the inequality in Eq. (39) is saturated iff \( f = 0 \) given the above discussion.

**LEMMA 3.4.** Suppose \( k, m, n \in \mathbb{N}_0 \) satisfy \( 0 \leq k \leq n \) and \( m \geq 1 \), and \( 0 < p < 1 \). Then \( b_{n+m,k}(p)/b_{n,k}(p) \) and \( B_{n+m,k}(p)/B_{n,k}(p) \) are strictly increasing in \( k \) and strictly decreasing in \( p \). In addition, \( b_{n+m,k}(p)/b_{n,k}(p) = B_{n+m,k}(p)/B_{n,k}(p) = q^m \) is independent of \( n \) when \( k = 0 \), but \( b_{n+m,k}(p)/b_{n,k}(p) \) and \( B_{n+m,k}(p)/B_{n,k}(p) \) are strictly decreasing in \( n \) when \( k \geq 1 \). Furthermore,

\[
q^m = \frac{b_{n+m,0}(p)}{b_{n,0}(p)} \leq \frac{B_{n+m,k}(p)}{B_{n,k}(p)} \leq \frac{b_{n+m,k}(p)}{b_{n,k}(p)} \leq q^m \left( \frac{n + 1}{n + 1 − k} \right)^m.
\]

**PROOF.** From Eq. (33) we can deduce that

\[
\frac{b_{n+m,k}}{b_{n,k}} = \prod_{l=0}^{m−1} \frac{b_{n+l+1,k}}{b_{n+l,k}} = q^m \prod_{l=0}^{m−1} \frac{(n + l + 1)}{n + l + 1 − k} \leq q^m \left( \frac{n + 1}{n + 1 − k} \right)^m,
\]

which implies that \( b_{n+m,k}/b_{n,k} \) is strictly increasing \( k \), but strictly decreasing in \( p \). In addition, \( b_{n+m,k}/b_{n,k} = B_{n+m,k}/B_{n,k} = q^m \) is independent of \( n \) when \( k = 0 \), but \( b_{n+m,k}/b_{n,k} \) is strictly decreasing in \( n \) when \( k \geq 1 \).

From Eq. (30) we can deduce that

\[
\frac{B_{n+1,k}}{B_{n,k}} = \frac{pB_{n,k−1} + qB_{n,k}}{B_{n,k}} = q + p \frac{B_{n,k−1}}{B_{n,k}} = 1 − p \left( 1 − \frac{B_{n,k−1}}{B_{n,k}} \right).
\]
According to Lemma 3.1, \( B_{n+1,k}/B_{n,k} \) is strictly increasing in \( k \), but strictly decreasing in \( p \), and so does \( B_{n+m,k}/B_{n,k} \). If in addition \( k \geq 1 \), then \( B_{n+1,k}/B_{n,k} \) is strictly decreasing in \( n \), and so does \( B_{n+m,k}/B_{n,k} \). In the special case \( k = 0 \), \( B_{n+m,k}/B_{n,k} = b_{n+m,k}/b_{n,k} = q^n \) is independent of \( n \); note that \( B_{n,-1} = 0 \).

Next, we consider Eq. (44). The equality and third inequality in Eq. (44) follow from Eq. (45). The first and second inequalities in Eq. (44) follow from the following equation

\[
B_{n+m,k}/B_{n,k} = \sum_{j=0}^{k} b_{n+m,j} \sum_{j=0}^{k} b_{n,j} = \sum_{j=0}^{k} b_{n+m,j} b_{n,j} / \sum_{j=0}^{k} b_{n,j}
\]

and the fact that \( b_{n+m,j}/b_{n,j} \) is strictly increasing in \( j \) as proved above. In addition, both inequalities are strict when \( k \geq 1 \).

3.2. Connection with the partial mean. The partial mean is defined as

\[
\mu_{n,k}(p) := \sum_{j=0}^{k} j b_{n,j}(p) / B_{n,k}(p),
\]

which is abbreviated as \( \mu_{n,k} \) if there is no danger of confusion. Here we establish a simple but important connection between the ratio \( B_{n,k}/b_{n,k} \) and the partial mean \( \mu_{n,k} \), which will play a crucial role in evaluating the the tail probability \( B_{n,k} \) as we shall see later.

By definition the partial mean \( \mu_{n,k} \) satisfies \( 0 \leq \mu_{n,k} \leq k \), where both inequalities are saturated when \( k = 0 \), but are strict when \( k \geq 1 \). Additional properties of the partial mean is summarized in the following lemma.

**Lemma 3.5.** Suppose \( k, n \in \mathbb{N}_0 \), \( k \leq n \), and \( 0 < p < 1 \). Then \( \mu_{n,k}(p) \) and \( k - \mu_{n,k}(p) \) are strictly increasing in \( k \). In addition, \( \mu_{n,k}(p) = 0 \) for \( k = 0 \), while \( \mu_{n,k}(p) \) is strictly increasing in \( n \) and \( p \) for \( k \geq 1 \). Moreover,

\[
k + 1 - \frac{B_{n,k}(p)}{b_{n,k}(p)} \leq \mu_{n,k}(p) \leq p n,
\]

where the lower bound is saturated iff \( k = 0 \), while the upper bound is saturated iff \( k = n \).

**Proof of Lemma 3.5.** According to the following equation,

\[
\mu_{n,k+1} = \sum_{j=0}^{k+1} j b_{n,j} / B_{n,k+1} = (k+1) b_{n,k+1} + \sum_{j=0}^{k} j b_{n,j} / B_{n,k+1} > \sum_{j=0}^{k} j b_{n,j} / B_{n,k} = \mu_{n,k},
\]

\( \mu_{n,k} \) is strictly increasing in \( k \). When \( k = 0 \), \( \mu_{n,k} = k - \mu_{n,k} = 0 \) are independent of \( n \) and \( p \). When \( k \geq 1 \), we have \( 0 < \mu_{n,k}, k - \mu_{n,k} < k \). In addition, according to Lemma 3.1 and the following equation,

\[
k - \mu_{n,k} = \sum_{j=0}^{k} (k-j) b_{n,j} / B_{n,k} = \sum_{j=0}^{k-1} \sum_{i=0}^{j} b_{n,i} / B_{n,k} = \sum_{j=0}^{k-1} B_{n,j} / B_{n,k} = \sum_{j=1}^{k-1} B_{n,k-j} / B_{n,k},
\]

\( k - \mu_{n,k} \) is strictly increasing in \( k \), but strictly decreasing in \( n \) and \( p \), so \( \mu_{n,k} \) is strictly increasing in \( n \) and \( p \).

The upper bound in Eq. (49) follows from the facts that \( \mu_{n,k} \leq \mu_{n,n} \) and \( \mu_{n,n} = p n \); it is saturated iff \( k = n \) since the inequality \( \mu_{n,k} \leq \mu_{n,n} \) is saturated iff \( k = n \).
Finally, we turn to the lower bound in Eq. (49). If \( k = 0 \), then \( \mu_{n,k} = 0 \), \( B_{n,k} = b_{n,k} \), and \( B_{n,k}/b_{n,k} = 1 \), so the lower bound in Eq. (49) is saturated.

If \( k \geq 1 \), let \( s = b_{n,k}/B_{n,k} \), then \( 0 < s < 1 \). In addition, Lemma 3.1 implies that \( b_{n,i}/B_{n,i} > s \) for \( 0 \leq i < k \), which in turn implies that

\[
(52) \quad \frac{B_{n,i-1}}{B_{n,i}} = 1 - \frac{b_{n,i}}{B_{n,i}} \leq 1 - s, \quad \frac{B_{n,i-1}}{B_{n,k}} \leq (1 - s)^{k-i+1} \quad \forall 1 \leq i \leq k,
\]

where both inequalities are strict when \( i < k \). Therefore,

\[
(53) \quad k - \mu_{n,k} = \sum_{j=0}^{k-1} \frac{B_{n,j}}{B_{n,k}} \leq \sum_{j=0}^{k-1} (1 - s)^{k-j} = \frac{1 - s - (1 - s)^{k+1}}{s} < \frac{1 - s}{s} = \frac{1}{s} - 1,
\]

which implies that

\[
(54) \quad \mu_{n,k} > k + 1 - \frac{1}{s} = k + 1 - \frac{B_{n,k}}{b_{n,k}}
\]

and confirms the lower bound in Eq. (49) with strict inequality. This observation completes the proof of Lemma 3.5.

Next, we clarify the relations between the partial mean and the ratios \( B_{n,k}/B_{n+1,k} \), \( B_{n,k}/b_{n,k} \). By definitions in Eq. (1) we can deduce that

\[
(55) \quad \frac{B_{n,k}}{B_{n+1,k}} = \frac{\sum_{j=0}^{k} b_{n,j}}{\sum_{j=0}^{k} b_{n+1,j}} = \frac{\sum_{j=0}^{k} (n+1-j)q b_{n+1,j}}{\sum_{j=0}^{k} b_{n+1,j}} = \frac{n+1 - \mu_{n+1,k}}{(n+1)q}.
\]

On the other hand, by virtue of Eq. (30) we can deduce that

\[
(56) \quad \frac{B_{n,k}}{B_{n+1,k}} = \frac{B_{n,k}}{pB_{n,k-1} + qB_{n,k}} = \frac{B_{n,k} - pb_{n,k}}{B_{n,k} - pb_{n,k}} = \frac{B_{n,k}}{b_{n,k}} - p.
\]

The two equations above together imply that

\[
(57) \quad \frac{B_{n,k}}{b_{n,k}} = \frac{p(n+1 - \mu_{n+1,k})}{p(n+1) - \mu_{n+1,k}} \iff \mu_{n+1,k} = \frac{p(n+1)\left(\frac{B_{n,k}}{b_{n,k}} - 1\right)}{B_{n,k} - pb_{n,k}}.
\]

4. Nearly tight Bounds for the ratio \( B_{n,k}(p)/b_{n,k}(p) \).

4.1. Upper and lower bounds for \( B_{n,k}(p)/b_{n,k}(p) \). In this section, we evaluate the ratio \( B_{n,k}/b_{n,k} \) in preparation for the study of the tail probability \( B_{n,k}(p) \). The main goal of this section is to prove Theorem 2.1. To this end, we recall the functions \( L(n,k,p) \), \( \kappa_1(n,p) \), \( V(n,k,p,a) \), and \( U(n,k,p) \) defined in Eqs. (11)-(14), and here we may consider wider parameter ranges. In addition, we prepare the following two lemmas, which are proved in Sec. 4.3.

**Lemma 4.1.** Suppose \( k \in \mathbb{N}_0 \), \( n \in \mathbb{N} \), \( k \leq n \), \( f = k/n \), and \( 0 < p < 1 \). Then

\[
(58) \quad \frac{B_{n,k}(p)}{b_{n,k}(p)} \geq L(n,k,p) \geq 1,
\]

where both inequalities are saturated when \( k = 0 \), but are strict when \( k \geq 1 \). In addition, the lower bound \( L(n,k,p) \) satisfies

\[
(59) \quad L(n,k,p) \geq \begin{cases} 
\max \left\{ 1, \frac{(1-f)p}{p-f} - \frac{fpg(1-f)}{(p-f)^2n} \right\} & k < pn, \\
\frac{1}{2}(1 + \sqrt{4qk + 1}) & k \geq pn.
\end{cases}
\]
**Lemma 4.2.** Suppose \( k, n \in \mathbb{N}_0, 0 < p < 1, \) and \( k \leq pn. \) Then

\[
B_{n,k}(p) \quad \frac{b_{n,k}(p)}{b_{n,k}(p)} \leq U(n,k,p) < 2L(n,k,p),
\]

where the first inequality is saturated iff \( k = 0, \) and the upper bound \( U(n,k,p) \) satisfies

\[
U(n,k,p) \leq 1 + 2\sqrt{q(k+p)}.
\]

By virtue of the two lemmas, we can establish Theorem 2.1 as follows.

**Proof of Theorem 2.1.** Equation (17) in Theorem 2.1 follows from Eq. (58) in Lemma 4.1 and Eq. (60) in Lemma 4.2, note that all the inequalities in these equations are strict when \( k \geq 1. \) The first three inequalities in Eq. (18) follow from Eq. (17), the fourth inequality follows from the definition in Eq. (14), and the fifth inequality follows from the limit formulas in Eq. (20) and the fact that \( V(n,fn,p,0) \) is strictly increasing in \( n \) given that \( 0 < f < p. \)

When \( 0 < f < p \) and \( n \) is sufficiently large, the bounds in Theorem 2.1 [cf. Eqs. (11)-(14)] can be approximated as follows,

\[
L(n,k,p) = 1 + \frac{kp}{pn} + \frac{qk(k-1)}{p^2n^2} + O(n^{-3}),
\]

\[
U(n,k,p) = V(n,k,p,0) = 1 + \frac{kp}{pn} + \frac{qk(k-p)}{p^2n^2} + O(n^{-3}),
\]

\[
L(n,fn,0) = \frac{(1-f)p}{p-f} - \frac{fp(1-f)q}{(p-f)^2n} + O(n^{-2}),
\]

\[
U(n,fn,0) = V(n,fn,p,0) = \frac{(1-f)p}{p-f} - \frac{fpq}{(p-f)^2n} + O(n^{-2}).
\]

These results complement the limit formulas in Eqs. (19) and (20). Together with Theorem 2.1 they imply that

\[
B_{n,k}(p) \quad \frac{b_{n,k}(p)}{b_{n,k}(p)} = 1 + \frac{kp}{pn} + O(n^{-2}), \quad B_{n,\lfloor fn \rfloor}(p) \quad \frac{b_{n,\lfloor fn \rfloor}(p)}{b_{n,\lfloor fn \rfloor}(p)} = \frac{(1-f)p}{p-f} + O(n^{-1}).
\]

**4.2. Properties of upper and lower bounds.** In this section we clarify the properties of upper and lower bounds for the ratio \( B_{n,k}/b_{n,k} \) that appear in Theorem 2.1 (and Lemmas 4.1, 4.2). Recall that the bounds \( L(n,k,p), V(n,k,p,a), \) and \( U(n,k,p) \) are defined explicitly in Eqs. (11)-(14). As we shall see shortly, many properties of these bounds match the counterparts of the ratio \( B_{n,k}/b_{n,k}, \) which further corroborates the significance of Theorem 2.1. Here we will focus on these bounds directly and do not consider \( b_{n,k} \) and \( B_{n,k} \) explicitly. Accordingly, we may consider wider parameter ranges and do not assume that \( k \) and \( n \) are integers, unlike Theorem 2.1, because technically it is easier to deal with continuous variables than discrete variables. Notably, taking derivatives is very useful in technical analysis. The proofs of Lemmas 4.3-4.9 below are relegated to Appendix B. Some of the following lemmas will be used in the proofs of Lemmas 4.1 and 4.2. Other lemmas will be useful to deriving auxiliary results later. Nevertheless, only Lemma 4.3 is required to prove our key result Theorem 2.1.

**Lemma 4.3.** Suppose \( n \geq 0, 0 < p < 1 \) and \( 0 \leq k \leq pn; \) then

\[
U(n,k,p) < 2L(n,k,p).
\]
LEMMA 4.4. Suppose \( n \geq -1, k \geq 0, \text{ and } 0 \leq p \leq 1. \) Then \( L(n, k, p) \) is nonincreasing and convex in \( n \) and is nondecreasing and convex in \( k. \) In addition, \( L(n, k, p) \) is nonincreasing and convex in \( p \) when \( n \geq k. \) Furthermore,

\[
1 \leq L(n, k, p) \leq 1 + k,
\]

\[
L(n, k, p) \leq \frac{1}{2} (1 + \sqrt{4kq + 1}) \quad \text{if} \quad pm \geq k,
\]

\[
L(n, k, p) \geq \frac{1}{2} (1 + \sqrt{4kq + 1}) \quad \text{if} \quad pm \leq k.
\]

LEMMA 4.5. Suppose \( n > 0, 0 < p < 1, \) and \( 0 \leq k \leq pn. \) Then

\[
\frac{k(\sqrt{1 + 4k} - 1)}{2pn} + 1 \leq L(n, k, p) \leq \frac{qk}{pn} + 1 \quad \text{if} \quad 0 \leq k \leq 1,
\]

\[
\min \left\{ \frac{qk}{pn}, \frac{k(\sqrt{1 + 4k} - 1)}{2pn} \right\} + 1 \leq L(n, k, p) \leq \frac{k\sqrt{qk}}{pn} + 1 \quad \text{if} \quad 1 \leq k \leq pn,
\]

where

\[
\min \left\{ \frac{qk}{pn}, \frac{k(\sqrt{1 + 4k} - 1)}{2pn} \right\} = \begin{cases} \frac{qk}{pn} & k \geq 1 + q, \\ \frac{k(\sqrt{1 + 4k} - 1)}{2pn} & k \leq 1 + q. \end{cases}
\]

LEMMA 4.6. Suppose \( 0 \leq f, p \leq 1 \) and \( n \geq 0. \) Then \( L(n, f n, p) \) is nondecreasing and concave in \( n, \) nondecreasing and convex in \( f, \) and nonincreasing and convex in \( p. \) If in addition \( 0 < f, p < 1, \) then \( L(n, f n, p) \) is strictly increasing and strictly concave in \( n, \) and both inequalities are strict when \( f > 0. \)

LEMMA 4.7. Suppose \( n \geq 0, 0 < p < 1, \) and \( 0 \leq k \leq pn; \) then

\[
U(n, k, p) = \min_{a \in \mathbb{N}_0, a < k+1} V(n, k, p, a).
\]

If in addition \( p(n + 2) \geq 2, k = 0, \) or \( k \geq 1, \) then

\[
U(n, k, p) = \min_{a \in \mathbb{N}_0, a \leq k} V(n, k, p, a).
\]

LEMMA 4.8. Suppose \( n \geq 0, 0 < p < 1, \) and \( 0 \leq k \leq pn. \) Then \( U(n, k, p) \) is strictly increasing in \( k \) and

\[
U(n, k, p) \leq 1 + 2 \sqrt{pq(n + 1)}.
\]

If in addition \( p(n + 2) \geq 2, k = 0, \) or \( k \geq 1, \) then \( U(n, k, p) \) is nonincreasing in \( n \) and \( p, \) and

\[
U(n, k, p) \leq 1 + 2 \sqrt{q(k + p)}.
\]

LEMMA 4.9. Suppose \( 0 < f \leq p < 1 \) and \( n \geq 0. \) Then \( U(n, f n, p) \) is strictly increasing in \( n \) for \( n \geq 0 \) and is strictly increasing in \( f \) when \( n > 0. \) If in addition \( p(n + 2) \geq 2, f n = 0, \) or \( f n \geq 1, \) then \( U(n, f n, p) \) is nonincreasing in \( p. \) If in addition \( f < p, \) then

\[
U(n, f n, p) \leq V(n, f n, p, 0) < \frac{(1 - f)p}{p - f} = \frac{1}{1 - r}.
\]
4.3. Proofs of Lemmas 4.1 and 4.2.

PROOF OF LEMMA 4.1. Let $\gamma = B_{n,k}/b_{n,k}$. Then Eq. (57) implies that

$$\gamma = \frac{p(n + 1 - \mu_{n+1,k})}{p(n + 1) - \mu_{n+1,k}}, \quad \mu_{n+1,k} = \frac{p(n + 1)(\gamma - 1)}{\gamma - p}. \tag{79}$$

By virtue of Lemma 3.5 we can further deduce that

$$k + 1 \leq \gamma + \mu_{n,k} \leq \gamma + \mu_{n+1,k} = \gamma + \frac{p(n + 1)(\gamma - 1)}{\gamma - p}, \tag{80}$$

which means

$$\gamma^2 + (pn - k - 1)\gamma - (n - k)p \geq 0, \tag{81}$$

given that $\gamma = B_{n,k}/b_{n,k} \geq 1 > p$. Solving this equation yields

$$\gamma \geq \frac{k + 1 - pn + \sqrt{(pn - k - 1)^2 + 4(n - k)p}}{2} = L(n, k, p), \tag{82}$$

which confirms the first inequality in Eq. (58). If $k = 0$, then $B_{n,k}/b_{n,k} = L(n, k, p) = 1$, so this inequality is saturated. If $k \geq 1$, then both inequalities in Eq. (80) are strict, and so are the inequalities in Eqs. (81) and (82), which means the first inequality in Eq. (58) is strict.

The second inequality in Eq. (58) follows from the following equation,

$$L(n, k, p) - 1 = \frac{-\left((pn - k + 1) + \sqrt{(pn - k - 1)^2 + 4qk}\right)}{2} \geq 0, \tag{83}$$

where the inequality is saturated iff $k = 0$.

Equation (59) follows from Lemmas 4.4 and 4.6. \hfill \square

PROOF OF LEMMA 4.2. If $k = 0$, then $B_{n,k}/b_{n,k} = 1$. In addition, $V(n, k, p, 0) = 1$ and $V(n, k, p, a) > 1$ when $a \geq 1$, which means $U(n, k, p) = 1$. So the first inequality in Eq. (60) holds and is saturated.

Next, suppose $k \geq 1$ and let $j, a$ be nonnegative integers. By Eq. (32), $b_{n,j-1}/b_{n,j} < 1$ for $1 \leq j \leq pn$, so $B_{n,k}/b_{n,k} < k + 1$ given the assumption that $k \leq pn$. In addition,

$$V(n, k, p, a) \geq k + 1 > \frac{B_{n,k}}{b_{n,k}} \quad \forall a \geq k, \quad \min_{a \in \mathbb{N}, a \geq k} V(n, k, p, a) \geq k + 1 > \frac{B_{n,k}}{b_{n,k}}. \tag{84}$$

If $0 \leq a \leq k - 1$, then $b_{n,k-a-1}/b_{n,k-a}$ is strictly decreasing in $a$ and satisfies the inequalities $0 < b_{n,k-a-1}/b_{n,k-a} < 1$ by Eq. (32). Therefore,

$$\frac{B_{n,k}}{b_{n,k}} = \sum_{j=0}^{k} \frac{b_{n,j}}{b_{n,k}} \leq a + \sum_{j=0}^{k-a} \frac{b_{n,j}}{b_{n,k}} \leq a + \sum_{j=0}^{k-a} \left( \frac{b_{n,k-a-1}}{b_{n,k-a}} \right) = a + \left( 1 - \frac{b_{n,k-a-1}}{b_{n,k-a}} \right)^{-1} = a + \frac{p(n - k + a + 1)}{pn + p - k + a} = V(n, k, p, a). \tag{85}$$

In conjunction with Eq. (84), this equation shows that the first inequality in Eq. (60) holds and is strict when $k \geq 1$.

The second inequality in Eq. (60) follows from Lemma 4.3. Equation (61) follows from Eq. (77) in Lemma 4.8. \hfill \square
4.4. Bounds for the partial mean \( \mu_{n,k} \) and the ratio \( B_{n,k} / B_{n+1,k} \). The partial mean \( \mu_{n,k} \) defined in Eq. (48) plays a crucial role in the proof of Lemma 4.1 and Theorem 2.1, which reflects the importance of this quantity. On the other hand, by virtue of Lemma 4.1, we can derive pretty good bounds for the partial mean \( \mu_{n,k} \) and the ratio \( B_{n,k} / B_{n+1,k} \) as shown in the following proposition and proved in Appendix C. This result will be useful in studying statistical sampling and quantum verification\(^1\).

**Proposition 4.10.** Suppose \( k \in \mathbb{N}_0, \ n \in \mathbb{N}, \ k \leq n, \) and \( 0 < p < 1 \). Then

\[
\mu_{n,k}(p) \geq k + 1 - L(n-1,k,p) = \frac{pn + k + q - \sqrt{(pn + k + q)^2 + 4qk}}{2},
\]

and

\[
\frac{n - k + 1}{(n + 1)q} \leq \frac{B_{n,k}(p)}{B_{n+1,k}(p)} \leq \frac{n - k + L(n,k,p)}{(n + 1)q} = \frac{(2 - p)n - k + 1 + \sqrt{(pn - k + 1)^2 + 4qk}}{2(n + 1)q}.
\]

If in addition \( k \leq pn \), then

\[
\mu_{n,k}(p) \geq k + 1 - \frac{q}{2} - \frac{1}{2} \sqrt{q(4k + q)} \geq k - \sqrt{qk},
\]

and

\[
\frac{n - k + 1}{(n + 1)q} \leq \frac{B_{n,k}(p)}{B_{n+1,k}(p)} \leq \frac{n - k + 1 + \frac{k\sqrt{qk}}{pn}}{(n + 1)q} \leq \frac{n - k + 1 + \sqrt{qk}}{(n + 1)q}.
\]

If in addition \( f = k/n < p \), then

\[
\frac{n - k + 1}{(n + 1)q} \leq \frac{B_{n,k}(p)}{B_{n+1,k}(p)} \leq \frac{n - k + \frac{(1-f)p}{p-f}}{(n + 1)q}.
\]

5. Nearly tight bounds for the tail probabilities.

5.1. Bounds for the probability \( b_{n,k}(p) \). To evaluate the tail probability \( B_{n,k} \), we need to clarify the properties of the probability \( b_{n,k} \) in this section. Similar to Sec. 4.2, here we do not assume that \( k \) and \( n \) are integers except for Propositions 5.1 and 5.4, because technically it is easier to deal with continuous variables than discrete variables. The proofs of Lemmas 5.2 and 5.3 below are relegated to Sec. 5.5.

To start with we define the following functions for \( n > 0 \) and \( 0 \leq k \leq n \).

\[
\rho(n) := \frac{e^n \Gamma(n + 1)}{n^n}, \quad \varrho(n) := \frac{n^{n+1/2}}{e^n \Gamma(n + 1)},
\]

\[
\phi(n, k) := \frac{\rho(n)}{\rho(k) \varrho(n-k)} = \frac{\Gamma(n+1)}{\Gamma(k+1) \Gamma(n-k+1)} \frac{k^k (n-k)^{n-k}}{n^n},
\]

\[
\varphi(n, k) := \frac{\varrho(k) \varrho(n-k)}{\varrho(n)} = \frac{\Gamma(n+1)}{\Gamma(k+1) \Gamma(n-k+1)} \frac{k^{k+1/2} (n-k)^{n-k+1/2}}{n^{n+1/2}},
\]

where it is understood that \( 0^0 = 1 \). The following proposition clarifies the relation between \( b_{n,k} \) and the functions \( \phi(n, k) \) and \( \varphi(n, k) \), which can be verified by simple calculation.

\(^1\)Quantum verification is actually the original motivation that leads to this work.
Proposition 5.1. Suppose $n, k \in \mathbb{N}$; then

$$\phi(n, k) = \left(\begin{array}{c} n \\ k \end{array}\right) \frac{k^k(n-k)^{n-k}}{n^n}, \quad \varphi(n, k) = \left(\begin{array}{c} n \\ k \end{array}\right) \frac{k^{k+1/2}(n-k)^{n-k+1/2}}{n^{n+1/2}},$$

$$\left(\begin{array}{c} n \\ k \end{array}\right) = \frac{n^n}{k^k(n-k)^n-k} \phi(n, k) = \frac{n^{n+1/2}}{k^{k+1/2}(n-k)^{n-k+1/2}} \varphi(n, k),$$

$$b_{n,k}(p)e^{nD(p||p)} = \phi(n, k) = \frac{\sqrt{n}}{\sqrt{k(n-k)}} \varphi(n, k).$$

Thanks to this proposition, $b_{n,k}$ can be evaluated by using $\phi(n, k)$ and $\varphi(n, k)$. As upper and lower bounds for $\varphi(n, k)$ (cf. Lemma 5.2 below), we define

$$\varphi_+(n, k) := \frac{1}{\sqrt{2\pi}} e^{\frac{1}{12(k+1)} - \frac{1}{12(n-k)+1}}, \quad \varphi_-(n, k) := \frac{1}{\sqrt{2\pi}} e^{\frac{1}{12(k+1)} - \frac{1}{12(n-k)}}.$$

By virtue of the Stirling approximation [34, 41]

$$\sqrt{2\pi} x^{x+1/2} e^{-x} e^{\frac{1}{12x+1}} < \Gamma(x+1) < \sqrt{2\pi} x^{x+1/2} e^{-x} e^{\frac{1}{12x}} \quad \forall x > 0,$$

it is straightforward to prove that

$$\lim_{n \to \infty} n^{-1/2} \rho(n) = \sqrt{2\pi}, \quad \lim_{n \to \infty} g(n) = \frac{1}{\sqrt{2\pi}},$$

$$\lim_{n \to \infty} \phi(n, k) = \frac{1}{\rho(k)} = \frac{k^k}{e^k \Gamma(k+1)}, \quad \lim_{n \to \infty} \varphi(n, k) = \varphi(k) = \frac{k^{k+1/2}}{e^k \Gamma(k+1)},$$

$$\lim_{n \to \infty} \varphi(n, f n) = \lim_{n \to \infty} \varphi_+(n, f n) = \lim_{n \to \infty} \varphi_-(n, f n) = \frac{1}{\sqrt{2\pi}} \quad \forall 0 < f < 1.$$

When $n$ is large, $\varphi(n, f n)$ can be expressed as

$$\varphi(n, f n) = \frac{1}{\sqrt{2\pi}} \left(1 - \frac{1 - f + f^2}{12 f (1 - f)n}\right) + O(n^{-2}).$$

Additional useful properties of $\phi(n, k)$ and $\varphi(n, k)$ are summarized in the following lemma, which is proved in Sec. 5.5.

Lemma 5.2. Suppose $0 < k < n$ and $0 < f < 1$. Then $\phi(n, k)$ is strictly decreasing in $n$ and strictly logarithmically convex in $n$ and $k$, while $\phi(n, n/k)$ is strictly decreasing in $n$. By contrast, $\varphi(n, k)$ is strictly increasing in $n$ and strictly logarithmically concave in $n$ and $k$, while $\varphi(n, f n)$ is strictly increasing in $n$. Furthermore,

$$0 < \frac{k^k e^{-k}}{\Gamma(k+1)} < \phi(n, k) < 1,$$

$$0 < \varphi(n, k) < \frac{k^{k+1/2} e^{-k}}{\Gamma(k+1)} < \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{12x+1}} < \frac{1}{\sqrt{2\pi}}.$$

$$\varphi_-(n, k) < \varphi(n, k) < \varphi_+(n, k) \leq \varphi_+(n, n/2) = \frac{1}{\sqrt{2\pi}} e^{-\frac{18n+1}{6n+1} \frac{1}{(12n+1)}}.$$

If in addition $k \geq 1$, then

$$\phi(n, k) > \frac{k^k e^{-k}}{\Gamma(k+1)} \geq \frac{1}{e \sqrt{k}}.$$
If in addition \( j \leq k \leq n - j \) with \( j \geq 1 \), then

\[
\frac{1}{\sqrt{8}} \leq \varphi(2j, j) \leq \varphi(n, k) < \frac{1}{\sqrt{2\pi}}.
\]

Note that (strict) logarithmic convexity implies (strict) convexity. In addition, \( \phi(n, k) = \phi(n, n-k) \) and \( \varphi(n, k) = \varphi(n, n-k) \) by definition, so Lemma 5.2 implies that \( \phi(n, k) \) is strictly decreasing in \( k \) when \( 0 < k \leq n/2 \) and strictly increasing in \( k \) when \( n/2 \leq k < n \); by contrast, \( \varphi(n, k) \) is strictly increasing in \( k \) when \( 0 < k \leq n/2 \) and strictly decreasing in \( k \) when \( n/2 \leq k < n \). The following lemma formalizes the intuition that the bounds \( \varphi_{\pm}(n, k) \) in Eq. (104) become more and more accurate when \( n \) increases and \( k \) approaches \( n/2 \).

**Lemma 5.3.** Suppose \( 0 < k < n \) and \( 0 < f < 1 \). Then the functions \( \varphi(n, k)/\varphi_-(n, k) \), \( \varphi_+(n, k)/\varphi(n, k) \), and \( \varphi_+(n, k)/\varphi_-(n, k) \) are strictly decreasing in \( n \) and strictly logarithmically convex in \( n \) and \( k \). Meanwhile, \( \varphi(n, fn)/\varphi_-(n, fn) \), \( \varphi_+(n, fn)/\varphi(n, fn) \), and \( \varphi_+(n, fn)/\varphi_-(n, fn) \) are strictly decreasing in \( n \) and strictly logarithmically convex in \( f \). If in addition \( 1 \leq k \leq n - 1 \), then

\[
1 < \frac{\varphi(n, n/2)}{\varphi_-(n, n/2)} \leq \frac{\varphi(n, k)}{\varphi_-(n, k)} \leq \frac{\varphi(2, 1)}{\varphi_-(2, 1)} = \frac{\sqrt{\pi} e^{1/8}}{2},
\]

\[
1 < \frac{\varphi_+(n, n/2)}{\varphi(n, n/2)} \leq \frac{\varphi_+(n, k)}{\varphi(n, k)} \leq \frac{\varphi_+(2, 1)}{\varphi(2, 1)} = \frac{2}{\sqrt{\pi} e^{37/325}},
\]

\[
1 < \frac{\varphi_+(n, n/2)}{\varphi_-(n, n/2)} \leq \frac{\varphi_+(n, k)}{\varphi_-(n, k)} \leq \frac{\varphi_+(2, 1)}{\varphi_-(2, 1)} = e^{29/2600}.
\]

By virtue of Lemma 5.2 we can evaluate the probability \( b_{n,k} \) as follows.

**Proposition 5.4.** Suppose \( k, n \in \mathbb{N}, 1 \leq k \leq n \), and \( 0 < p < 1 \). Then \( b_{n,k}(p)e^{nD(\frac{1}{k}||p)} \) is strictly decreasing in \( n \), but is independent of \( p \). If in addition \( k \leq n - 1 \), then

\[
\frac{1}{\sqrt{k}} e^{-nD(\frac{1}{k}||p)} \leq \frac{k^k}{e^{k!}} e^{-nD(\frac{1}{k}||p)} < b_{n,k}(p) < \frac{n}{n-k} \frac{k^k}{e^{k!}} e^{-nD(\frac{1}{k}||p)},
\]

\[
\frac{1}{\sqrt{2n}} e^{-nD(\frac{1}{k}||p)} \leq \frac{\sqrt{n}}{\sqrt{8k(n-k)}} e^{-nD(\frac{1}{k}||p)} \leq b_{n,k}(p) < \frac{\sqrt{n}}{\sqrt{2\pi k(n-k)}} e^{-nD(\frac{1}{k}||p)},
\]

\[
\frac{\sqrt{n} \varphi_-(n, k)}{\sqrt{k(n-k)}} e^{-nD(\frac{1}{k}||p)} < b_{n,k}(p) < \frac{\sqrt{n} \varphi_+(n, k)}{\sqrt{k(n-k)}} e^{-nD(\frac{1}{k}||p)}.
\]

The constants in the three equations in Proposition 5.4 cannot be improved without further assumptions. Incidentally, \( b_{n,k}e^{nD(\frac{1}{k}||p)} = 1 \) is independent of \( n \) and \( p \) when \( k = 0 \) or \( k = n \). Note that this observation does not contradict the monotonicity property stated in Proposition 5.4 because here \( k \) is proportional to \( n \), but \( k \) is fixed as a constant in Proposition 5.4. The lower bound in Eq. (110) still holds when \( k = n \) given that \( k^k/(e^k!) < 1 \) for \( k > 0 \) according to Theorem 1.1 in Ref. [18]. Here Eq. (111) follows from Lemma 4.7.1 in Ref. [3] and from Chapter 10, Lemma 7 in Ref. [32]; it implies the reverse Chernoff bound in Eq. (5). The lower bound \( e^{-nD(\frac{1}{k}||p)}/\sqrt{2n} \) for \( b_{n,k} \) is applicable whenever \( n \geq 1 \) and implies the reverse Chernoff bound in Eq. (4). In addition, Proposition 5.4 provides several other alternative reverse Chernoff bounds, which improve slightly over reverse Chernoff bounds presented in Refs. [12, 13, 20, 48].
Proof of Proposition 5.4. When \( n > k \geq 1 \), according to Lemma 5.2 and Eq. (96), \( b_{n,k}e^{-\|n\|p} < 1 \) is strictly decreasing in \( n \), but is independent of \( p \). When \( n = k \), we have \( b_{n,k}e^{-\|n\|p} = 1 \). So \( b_{n,k}e^{-\|n\|p} \) is strictly decreasing in \( n \), but is independent of \( p \) when \( n \geq k \geq 1 \).

Equation (110) follows from Eqs. (96), (103), and (105). Equation (111) follows from Eqs. (96) and (106). Equation (112) follows from Eqs. (96) and (104).

5.2. Nearly tight bounds for the lower tail probability \( B_{n,k}(p) \). The main aim of this section is to prove Theorem 2.2, that is, to derive nearly tight bounds for the lower tail probability \( B_{n,k} \). Before presenting our main results, we point out that the discussions in the previous sections can easily reproduce two existing results, the asymptotic limit in Eq. (8) \([2, 4, 7, 16]\) and an upper bound for \( B_{n,k} \) that is asymptotically tight \([17]\), as follows.

Proposition 5.5. Suppose \( 0 < f < 1 \) and \( n \in \mathbb{N} \), then \( \sqrt{n}B_{n,f}(p)e^{-\|n\|p} \) is strictly increasing in \( n \). In addition,

\[
\text{(113)} \quad b_{n,f}(p) \leq B_{n,f}(p) < \frac{e^{-\|n\|p}}{\sqrt{2\pi f(1-f)}} \frac{(1-f)p}{p-f} = \sqrt{\frac{1-f}{2\pi f}} \frac{1}{p-f} e^{-\|n\|p},
\]

\[
\text{(114)} \quad \lim_{n \to \infty} \sqrt{n}B_{n,f}(p)e^{-\|n\|p} = \frac{1}{\sqrt{2\pi f(1-f)}} \frac{(1-f)p}{p-f} = \sqrt{\frac{1-f}{2\pi f}} \frac{1}{p-f}.
\]

Proof of Proposition 5.5. According to Eq. (96) and Lemma 5.2, \( \sqrt{n}b_{n,f}e^{-\|n\|p} \) is strictly increasing in \( n \). Meanwhile, \( B_{n,f}/b_{n,f} \) is strictly increasing in \( n \) according to Lemma 3.3 in Sec. 3, so \( \sqrt{n}B_{n,f}(p)e^{-\|n\|p} \) is strictly increasing in \( n \).

Equation (113) follows from Eqs. (39) and (111). Equation (114) follows from Eqs. (39), (100), and (112).

Equation (113) reproduces Eq. (14) in Ref. [17], which improves the familiar Chernoff bound for \( B_{n,k} \) presented in Eq. (2). Although this bound is asymptotically tight, it is not so accurate when \( n \) is not so large. To construct much better bounds, we need to introduce several additional functions. Define

\[
\text{(115)} \quad \tilde{L}(n,k,p) := \frac{n\varphi(n,k)}{\sqrt{k(n-k)}} \sqrt{n}(n,k)L(n,k,p) = \sqrt{n}\phi(n,k)L(n,k,p),
\]

\[
\text{(116)} \quad \tilde{L}_{-}(n,k,p) := \frac{n\varphi_{-}(n,k)}{\sqrt{k(n-k)}} \sqrt{n}(n,k)L(n,k,p) = \frac{nL(n,k,p)}{\sqrt{2\pi k(n-k)}} e^{\frac{1}{12n+1} - \frac{3}{12k+1} - \frac{1}{12(n-k)+1}},
\]

\[
\text{(117)} \quad \tilde{U}(n,k,p) := \frac{n\varphi(n,k)}{\sqrt{k(n-k)}} U(n,k,p) = \sqrt{n}\phi(n,k)U(n,k,p),
\]

\[
\text{(118)} \quad \tilde{U}_{+}(n,k,p) := \frac{n\varphi_{+}(n,k)}{\sqrt{k(n-k)}} U(n,k,p) = \frac{nU(n,k,p)}{\sqrt{2\pi k(n-k)}} e^{\frac{1}{12n+1} - \frac{3}{12k+1} - \frac{1}{12(n-k)+1}},
\]

where \( L(n,k,p) \) and \( U(n,k,p) \) are defined in Sec. 2. Then, using Theorem 2.1, Lemmas 5.2, 5.3, and Proposition 5.4 we can show the following evaluation of \( B_{n,k} \) as a refinement of Theorem 2.2.
Theorem 5.6. Suppose $k, n \in \mathbb{N}$, $0 < p < 1$, $k \leq pn$, and $f = k/n$. Then

\begin{align}
\frac{1}{e\sqrt{k}} &< \frac{L(n, k, p)}{\sqrt{8}} \leq \frac{k^k L(n, k, p)}{e^k k!} \leq B_n(k)(p)e^{nD(\frac{e}{n})|p|} < \sqrt{\frac{n}{n-k}} \frac{k^k U(n, k, p)}{e^k k!}, \\
\sqrt{\frac{1}{8}} &< \frac{L(n, k, p)}{\sqrt{8}} < \sqrt{\frac{k(n-k)}{n}} B_n(k)(p)e^{nD(\frac{e}{n})|p|} \leq \frac{U(n, k, p)}{\sqrt{2\pi}} < \frac{2L(n, k, p)}{\sqrt{2\pi}}, \\
\tilde{L}_-(n, k, p) &< L(n, k, p) < \sqrt{n} B_n(k)(p)e^{nD(\frac{e}{n})|p|} < \tilde{U}(n, k, p) \\
< \tilde{U}_+(n, k, p) &< \frac{89}{44} \tilde{L}_-(n, k, p).
\end{align}

If in addition $f < p$, then

\begin{align}
\sqrt{n} B_n(k)(p)e^{nD(\frac{e}{n})|p|} < \tilde{U}(n, k, p) < \tilde{U}_+(n, k, p) < \frac{1-f}{2nf} \frac{p}{p-f}.
\end{align}

The bounds $L(n, k, p)/\sqrt{8}$ and $U(n, k, p)/\sqrt{2\pi}$ are tight within a factor of $4/\sqrt{\pi} \approx 2.25676$ by Eq. (120). The bounds $\tilde{L}(n, k, p)$ and $\tilde{U}(n, k, p)$ are tight within a factor of 2 according to their definitions above and the inequality $U(n, k, p) < 2L(n, k, p)$ in Eq. (17) in Theorem 2.1 (cf. Lemma 4.3). The bounds $\tilde{L}_-(n, k, p)$ and $\tilde{U}_+(n, k, p)$ are tight within a factor of $89/44$ by Eq. (121). In conjunction with Eq. (107), we can actually deduce that the bound $\tilde{L}_-(n, k, p)$ is tight within a factor of $\sqrt{\pi} e^{1/8} \approx 2.00845$. In addition, the four bounds $\tilde{L}(n, k, p)$, $\tilde{U}(n, k, p)$, $\tilde{L}_-(n, k, p)$, and $\tilde{U}_+(n, k, p)$ are asymptotically tight.

Note that Eqs. (23)-(25) in Theorem 2.2 are simple corollaries of Eqs. (120)-(122), respectively. In conjunction with Eqs. (19) and (20) in Sec. 2, Theorem 5.6 yields the following corollary.

Corollary 5.7. Suppose $k, n \in \mathbb{N}$ and $0 < f < p < 1$. Then

\begin{align}
\lim_{n \to \infty} \frac{L(n, k, p)}{(e/k)^k k!} = \lim_{n \to \infty} B_n(k)(p)e^{nD(\frac{e}{n})|p|} = \lim_{n \to \infty} \sqrt{n} \frac{U(n, k, p)}{n-k} \frac{e^k}{(e/k)^k k!} = k^k e^k k!, \\
\lim_{n \to \infty} \tilde{L}_-(n, f n, p) = \lim_{n \to \infty} \tilde{U}_+(n, f n, p) = \sqrt{\frac{1-f}{2nf}} \frac{p}{p-f}.
\end{align}

In conjunction with Eq. (121), Eq. (124) yields an alternative proof of Eq. (114). It implies that the bounds $\tilde{B}_n^\pm(k)(p)$ and $\tilde{B}_n^\pm(k)(p)$ defined in Eq. (22) satisfy the condition of asymptotic tightness in Eqs. (6) and (10).

Proof of Corollary 5.7. Equation (123) is a simple corollary of Eqs. (19) and (119). Equation (124) is a simple corollary of Eq. (20) in addition to the definitions in Eqs. (116) and (118).

Proof of Theorem 5.6. Thanks to Eq. (96), $B_n(k) e^{nD(\frac{e}{n})|p|}$ can be expressed as follows,

\begin{align}
B_n(k) e^{nD(\frac{e}{n})|p|} = \frac{B_n(k) b_n(k) e^{nD(\frac{e}{n})|p|}}{B_n(k) b_n(k) e^{nD(\frac{e}{n})|p|}} = \frac{B_n(k)}{b_n(k)} \phi(n, k) = \frac{B_n(k)}{b_n(k)} \sqrt{n} (n-k)^\gamma(n, k),
\end{align}

so Theorem 5.6 follows from Theorem 2.1, Lemmas 5.2, 5.3, and Proposition 5.4. More specifically, Eq. (119) follows from Eqs. (17) and (110), note that all inequalities in Eq. (17) are strict given the assumption $k \geq 1$. Equation (120) follows from Eqs. (17) and (111).
The first and fourth inequalities in Eq. (121) follow from Eq. (104) in addition to the definitions in Eqs. (115)-(118). The second and third inequalities in Eq. (121) follow from Eqs. (18) and (96). The last inequality in Eq. (121) can be proved as follows, 

\[ \tilde{\bar{U}}_+(n, k, p) \leq 2\varphi_+(n, k) \varphi_-(n, k) \tilde{L}_-(n, k, p) \leq 2e^{\frac{29}{44}} \tilde{L}_-(n, k, p) < \frac{89}{44} L_-(n, k, p), \]

where the first inequality follows from the last inequality in Eq. (17) and the definitions in Eqs. (116) and (118), while the second inequality follows from Eq. (109).

The first two inequalities in Eq. (122) follow from Eq. (121), and the last inequality in Eq. (122) follows from Eq. (18) and the fact that \( \varphi_+(n, k) < 1/\sqrt{2\pi}. \)

5.3. Auxiliary results. Equation (121) in Theorem 5.6 offers four bounds for the quantity \( \sqrt{nB_{n,k}D(\frac{k}{n}||p}) \) that are universally bounded and asymptotically tight. Here we discuss the properties of these bounds, which may be useful in certain applications. As in Sec. 4.2, here we do not assume that \( k \) and \( n \) are integers.

**Proposition 5.8.** Suppose \( 0 < f \leq p < 1 \) and \( n \geq 0 \). Then \( \tilde{L}(n, fn, p), \tilde{L}_-(n, fn, p), \tilde{U}(n, fn, p), \) and \( \tilde{U}_+(n, fn, p) \) are strictly increasing in \( n \).

**Proof of Proposition 5.8.** By Lemmas 4.6 and 4.9, \( L(n, fn, p) \) and \( U(n, fn, p) \) are strictly increasing in \( n \). In addition, \( \varphi(n, fn) \) is strictly increasing in \( n \) by Lemma 5.2, while \( \varphi_+(n, fn) \) and \( \varphi_-(n, fn) \) are strictly increasing in \( n \) by straightforward calculation. Therefore, \( \tilde{L}(n, fn, p), \tilde{L}_-(n, fn, p), \tilde{U}(n, fn, p), \) and \( \tilde{U}_+(n, fp, p) \) are strictly increasing in \( n \) given their definitions in Eqs. (115)-(118).

When \( 0 < f < p < 1 \) and \( n \) is sufficiently large, \( \tilde{L}(n, fn, p), \tilde{L}_-(n, fn, p), \tilde{U}(n, fn, p), \) and \( \tilde{U}_+(n, fn, p) \) can be approximated as follows according to their definitions:

\[ \tilde{L}_-(n, fn, p) = \tilde{L}(n, fn, p) + O(n^{-2}) = \sqrt{1 - \frac{f}{p}} \frac{1}{2\pi f} \frac{p}{p - f} - \frac{\beta_1}{n} + O(n^{-2}), \]

\[ \tilde{U}_+(n, fn, p) = \tilde{U}(n, fn, p) + O(n^{-2}) = \sqrt{1 - \frac{f}{p}} \frac{1}{2\pi f} \frac{p}{p - f} - \frac{\beta_2}{n} + O(n^{-2}), \]

where the coefficients \( \beta_1 \) and \( \beta_2 \) are defined as

\[ \beta_1 := \frac{p[13f^2 - 13f^3 + f^4 + (-2f - 10f^2 + 10f^3)p + (1 - f + f^2)p^2]}{12\sqrt{2\pi f(1 - f)} f(p - f)^3}, \]

\[ \beta_2 := \frac{p[-f + 13f^2 - f^3 + (1 - f - 11f^2)p]}{12\sqrt{2\pi f(1 - f)} f(p - f)^2}. \]

For all these bounds, the deviations from the asymptotic limits have order \( O(1/n) \).

5.4. Nearly tight bounds for the upper tail probability \( \tilde{B}_{n,k}(p) \). Here we clarify the properties of the upper tail probability \( \tilde{B}_{n,k}(p) \) defined as follows,

\[ \tilde{B}_{n,k}(p) := \sum_{j=k}^{n} b_{n,j}(p) = \sum_{j=k}^{n} \binom{n}{j} p^j q^{n-j} = B_{n,n-k}(q) = 1 - B_{n,k-1}(p), \]
where \( q = 1 - p \). Thanks to this equation, most results on the lower tail probability \( B_{n,k} \) have analogs for the upper tail probability \( \bar{B}_{n,k} \). For simplicity here we present a few main results. The odds ratio tied to the upper tail probability is defined as

\[
\bar{r} := \frac{(1 - f)p}{fq} = \frac{1}{r},
\]

where \( r \) is the odds ratio tied to the lower tail probability as presented in Eq. (9). By virtue of Eqs. (11)-(14) we can define

\[
\bar{L}(n,k,p) := L(n,n-k,q) = \frac{pm - k + 1 + \sqrt{(pm - k + 1)^2 + 4qk}}{2}
\]

and define \( \bar{V}(n,k,p,a) \) and \( \bar{U}(n,k,p) \) in a similar way. The following theorem is a simple corollary of Eq. (131) and Theorem 2.1.

**Theorem 5.9.** Suppose \( k, n \in \mathbb{N}, 0 < p < 1, pn \leq k \leq n, \) and \( f = k/n \). Then

\[
1 \leq \bar{L}(n,k,p) \leq \frac{\bar{B}_{n,k}(p)}{b_{n,k}(p)} \leq \bar{U}(n,k,p) < 2\bar{L}(n,k,p),
\]

where all inequalities are strict when \( k \leq n - 1 \). If in addition \( p < f < 1 \), then

\[
1 < \bar{L}(n,k,p) < \frac{\bar{B}_{n,k}(p)}{b_{n,k}(p)} < \bar{U}(n,k,p) \leq \bar{V}(n,k,p,0) < \frac{fq}{f - p} = \frac{1}{1 - \bar{r}} = \frac{r}{r - 1}.
\]

In analogy to Theorem 2.1, here the upper bound \( \bar{U}(n,k,p) \) and lower bound \( \bar{L}(n,k,p) \) are tight within a factor of 2 and are asymptotically tight; in addition, they can be computed in \( O(1) \) time. Previously, McKay also derived good upper and lower bounds for the ratio \( \bar{B}_{n,k}(p)/b_{n,k}(p) \) based on a completely different approach [33]. Comparison between our bounds and his bounds is presented in Appendix E.

Next, by virtue of Eqs. (115)-(118) we can define

\[
\hat{L}(n,k,p) := \bar{L}(n,n-k,q)
\]

and define \( \hat{L}_{-}(n,k,p), \hat{U}(n,k,p), \hat{U}_{+}(n,k,p) \) in a similar way. Thanks to Eq. (131) and the equality \( D(f\|p) = D(1 - f\|q) \), Theorem 5.10 and Corollary 5.11 below are simple corollaries of Theorem 5.6 and Corollary 5.7, respectively.

**Theorem 5.10.** Suppose \( k, n \in \mathbb{N}, 0 < p < 1, pn \leq k < n, \) and \( f = k/n \). Then

\[
\frac{1}{e\sqrt{m}} < \frac{\hat{L}(n,k,p)}{e\sqrt{m}} \leq \frac{m^m \hat{L}(n,k,p)}{e^m m!} < \frac{\bar{B}_{n,k}(p)e^{nD(\frac{k}{n}\|p)}}{k} < \frac{m^m \bar{U}(n,k,p)}{e^m m!} < \frac{1}{e\sqrt{m}}
\]

\[
\frac{1}{\sqrt{8}} < \frac{\bar{L}(n,k,p)}{\sqrt{8}} < \frac{\sqrt{kn} \bar{B}_{n,k}(p)e^{nD(\frac{k}{n}\|p)}}{\sqrt{2\pi}} < \frac{\bar{U}(n,k,p)}{\sqrt{2\pi}} < \frac{2\bar{L}(n,k,p)}{\sqrt{2\pi}}.
\]

\[
\hat{L}_{-}(n,k,p) < \hat{L}(n,k,p) < \sqrt{n} \bar{B}_{n,k}(p)e^{nD(\frac{k}{n}\|p)} < \hat{U}(n,k,p) \quad \hat{U}_{+}(n,k,p) < \frac{89}{44} \hat{L}_{-}(n,k,p),
\]

where \( m = n - k \). If in addition \( f > p \), then

\[
\sqrt{n} \bar{B}_{n,k}(p)e^{nD(\frac{k}{n}\|p)} < \bar{U}(n,k,p) < \hat{U}_{+}(n,k,p) < \sqrt{\frac{f}{2\pi(1 - f)}} \frac{q}{f - p}.
\]
In analogy to Theorem 5.6, the bounds \( \bar{L}(n, k, p)/\sqrt{8} \) and \( \bar{U}(n, k, p)/\sqrt{2\pi} \) are tight within a factor of \( 4/\sqrt{\pi} \). The bounds \( \hat{L}(n, k, p) \) and \( \hat{U}(n, k, p) \) are tight within a factor of 2. The bounds \( \hat{L}_-(n, k, p) \) and \( \hat{U}_+(n, k, p) \) are tight within a factor of 89/44. In addition, the four bounds \( \hat{L}(n, k, p), \hat{U}(n, k, p), \hat{L}_-(n, k, p), \) and \( \hat{U}_+(n, k, p) \) are asymptotically tight.

**Corollary 5.11.** Suppose \( k, n \in \mathbb{N} \) and \( 0 < p < f < 1 \); then

\[
\lim_{n \to \infty} \frac{k^L(n, k, p)}{e^{k!}} = \lim_{n \to \infty} \hat{B}_{n, n-k}(q)e^{nD(\hat{\omega}(x))} = \lim_{n \to \infty} \sqrt{n} k^U(n, k, p) = \frac{k^k}{e^{k!}}.
\]

\[
\lim_{n \to \infty} \hat{L}_-(n, f, n, p) = \lim_{n \to \infty} \hat{U}_+(n, f, n, p) = \sqrt{\frac{f}{2\pi(1-f)}} \cdot \frac{q}{f-p}.
\]

If \( f \) is a rational number that satisfies \( p < f < 1 \) and \( n \in \mathbb{N}_f \), then Eqs. (139) and (142) imply the following result [2, 4, 7, 16]:

\[
\lim_{n \to \infty} \sqrt{n} \hat{B}_{n, f, n}(p)e^{nD(f||p)} = \sqrt{\frac{f}{2\pi(1-f)}} \cdot \frac{q}{f-p}.
\]

Thanks to Eq. (131) again, the following two propositions are simple corollaries of Propositions 5.5 and 5.8, respectively.

**Proposition 5.12.** Suppose \( 0 < f < 1 \) and \( n \in \mathbb{N}_f \), then \( \sqrt{n} \hat{B}_{n, f, n}(p)e^{nD(f||p)} \) is strictly increasing in \( n \).

**Proposition 5.13.** Suppose \( 0 < p < f < 1 \) and \( n \geq 0 \). Then \( \hat{L}(n, f, n, p), \hat{L}_-(n, f, n, p), \hat{U}(n, f, n, p), \) and \( \hat{U}_+(n, f, n, p) \) are strictly increasing in \( n \).

### 5.5. Proofs of Lemmas 5.2 and 5.3

Similar to Sec. 5.1, in this section we do not assume that \( k \) and \( n \) are integers.

To prove Lemma 5.2, we need to prepare several auxiliary lemmas. Recall that a function \( \omega(x) \) is completely monotonic [43] over an open interval \( I \) if it has derivatives of all orders and

\[
(-1)^m \omega^{(m)}(x) \geq 0 \quad \forall x \in I, \quad m = 0, 1, 2, \ldots.
\]

The function \( \omega(x) \) is strictly completely monotonic if the inequality in Eq. (144) is always strict. Note that a (strictly) completely monotonic function is in particular (strictly) decreasing and (strictly) convex. A function \( g(x) \) is (strictly) logarithmically completely monotonic if \(-\left[ \ln g(x) \right]' \) is (strictly) completely monotonic [43]. It is known that any function that is (strictly) logarithmically completely monotonic is (strictly) completely monotonic [39]. By definition the sum of two (strictly) completely monotonic functions is (strictly) completely monotonic; the product of two (strictly) logarithmically completely monotonic functions is (strictly) logarithmically completely monotonic. The following lemma is also a simple corollary of the above definitions.

**Lemma 5.14.** Suppose \( \omega(y) \) is (strictly) completely monotonic in \( y \in (0, \infty) \) and \( 0 < f < 1 \); then \( \omega(fy) + \omega((1-f)y) - \omega(y) \) is (strictly) decreasing in \( y \in (0, \infty) \) and (strictly) convex in \( f \). If in addition \( 0 < x < y \), then \( \omega(y-x) - \omega(y) \) and \( \omega(x) + \omega(y-x) - \omega(y) \) are (strictly) completely monotonic in \( y \) and (strictly) convex in \( x \).
Define
\[
\omega_-(x) := \ln \Gamma(x+1) - \ln \sqrt{2\pi} - \left( x + \frac{1}{2} \right) \ln x + x - \frac{1}{12x}, \tag{145}
\]
\[
\omega_+(x) := \ln \Gamma(x+1) - \ln \sqrt{2\pi} - \left( x + \frac{1}{2} \right) \ln x + x - \frac{1}{12x+1}, \tag{146}
\]
\[
\psi_+(x) := \frac{1}{\sqrt{2\pi}} e^{-\omega_-(x)}, \quad \psi_-(x) := \frac{1}{\sqrt{2\pi}} e^{-\omega_+(x)}, \tag{147}
\]
where \(\psi(x)\) is defined in Eq. (99).

**Lemma 5.15.** The functions \(\omega_+(x)\) and \(-\omega_-(x)\) are strictly completely monotonic over \(x \in (0, \infty)\).

This lemma is a combination of Theorems 1 and 2 in Ref. [34], which state that \(-\omega_-(x)\) and \(\omega_+(x)\) are completely monotonic over \(x \in (0, \infty)\). The proof of Theorem 1 in Ref. [34] actually shows that \(-\omega_-(x)\) is strictly completely monotonic. A mistake in the proof of Theorem 2 in Ref. [34] is corrected in Appendix D. Note that the Stirling approximation in Eq. (98) is a simple corollary of Lemma 5.15. The following lemma is also proved in Appendix D.

**Lemma 5.16.** Suppose \(y > 0\), then \(1/\rho(y), 1/\psi(y), 1/\psi_-(y), \) and \(\psi_+(y)\) are strictly logarithmically completely monotonic and strictly completely monotonic in \(y\). If in addition \(0 < x < y\), then
\[
\frac{e^{14y} - e^{12x}}{e^{12x}} < \frac{\psi(x)}{\psi(y)} = \frac{x^{y+1/2} e^{y \Gamma(y+1)}}{y^{y+1/2} e^{x \Gamma(x+1)}} < e^{14y+1} - e^{12x+1}. \tag{148}
\]

This lemma in particular implies that \(\rho(y)\) and \(\psi(y)\) defined in Eq. (91) are strictly increasing and strictly logarithmically concave in \(y\) for \(y > 0\) [18].

**Proof of Lemma 5.2.** To prove Lemma 5.2, we first establish the monotonicity and convexity/concavity properties of \(\phi(n, k), \phi(n, fn), \varphi(n, k), \) and \(\varphi(n, fn)\). The definitions in Eqs. (92) and (93) imply that
\[
\ln \phi(n, k) = \ln \rho(n) - \ln \rho(k) - \ln \rho(n - k), \quad \ln \varphi(n, k) = \ln \varphi(n, k) - \ln \varphi(n - k) - \ln \rho(n). \tag{149}
\]
In addition, \([\ln \rho(n)]'\) and \([\ln \varphi(n)]'\) are strictly completely monotonic by Lemma 5.16, from which it is straightforward to deduce the monotonicity and convexity/concavity properties of \(\phi(n, k), \phi(n, fn), \varphi(n, k), \) and \(\varphi(n, fn)\) stated in Lemma 5.2 (cf. Lemma 5.14).

Equation (102) follows from the limits in Eq. (100) and the fact that \(\lim_{n \to k} \phi(n, k) = 1\), and that \(\varphi(n, k)\) is strictly decreasing in \(n\). The first and fourth inequalities in Eq. (103) are obvious; the second inequality follows from Eq. (100), given that \(\varphi(n, k)\) is strictly increasing in \(n\); the third inequality follows from the Stirling approximation in Eq. (98).

The first and second inequalities in Eq. (104) follow from the Stirling approximation in Eq. (98) and Lemma 5.16; the third inequality in Eq. (104) is straightforward to verify and is saturated when \(k = n/2\).

Finally, we consider Eqs. (105) and (106). The first inequality in Eq. (105) follows from Eq. (102); the second inequality follows from the fact that \(\varphi(k)\) is strictly increasing in \(k\).
by Lemma 5.16 and the fact that \( g(1) = 1/e \). The third inequality in Eq. \((106)\) follows from Eq. \((103)\); the second and first inequalities in Eq. \((106)\) can be proved as follows,

\[
\varphi(n, k) \geq \varphi(j + k, k) = \varphi(j + k, j) \geq \varphi(2j, j) \geq \varphi(j + 1, j)
\]

(150)

Here all the inequalities follow from the assumption \( 1 \leq j \leq k \leq n - j \) and the fact that \( \varphi(n, k) \) is strictly increasing in \( n \); the first two equalities follow from the fact that \( \varphi(n, k) = \varphi(n, n - k) \). Incidentally, the first inequality in Eq. \((106)\) can also be regarded as a special case of the second inequality.

To prove Lemma 5.3, we need to introduce one more auxiliary lemma. Define

\[
\tau(n) := \frac{1}{12n} - \frac{1}{12n + 1} = \frac{1}{12n(12n + 1)}, \quad \xi(n, k) := \tau(k) + \tau(n - k) - \tau(n).
\]

Lemma 5.17. Suppose \( 0 < k < n \) and \( 0 < f < 1 \); then \( \tau(n) \) is strictly completely monotonic. Meanwhile, \( \xi(n, k) \) is strictly completely monotonic in \( n \) and strictly convex in \( k \), while \( \xi(n, fn) \) is strictly decreasing in \( n \) and strictly convex in \( f \). If in addition \( 1 \leq k \leq n - 1 \), then

\[
0 < \xi(n, k) \leq \frac{29}{2600}
\]

Proof of Lemma 5.17. By definition it is easy to verify that the function \( 1/(12n) \) is strictly completely monotonic, so \( \tau(n) \) is strictly completely monotonic according to Lemma 5.14. Thanks to Lemma 5.14 again, \( \xi(n, k) \) is strictly completely monotonic in \( n \) and strictly convex in \( k \), while \( \xi(n, fn) \) is strictly decreasing in \( n \) and strictly convex in \( f \).

If in addition \( 1 \leq k \leq n - 1 \), then

\[
\xi(n, k) \leq \xi(k + 1, k) = \xi(k + 1, 1) \leq \xi(2, 1) = \frac{29}{2600},
\]

given that \( \xi(n, k) \) is strictly decreasing in \( n \) and that \( \xi(n, k) = \xi(n, n - k) \).

Proof of Lemma 5.3. Straightforward calculation shows that

\[
\frac{\varphi(n, k)}{\varphi_-(n, k)} = \frac{\sqrt{2\pi} \varphi_+(k) \varphi_+(n - k)}{\varphi_+(n)} = e^{\omega_-(n) - \omega_-(k) - \omega_-(n - k)},
\]

(154)

\[
\frac{\varphi_+(n, k)}{\varphi(n, k)} = \frac{\varphi_-(n)}{\sqrt{2\pi} \varphi_-(k) \varphi_-(n - k)} = e^{-\omega_+(n) + \omega_+(k) + \omega_+(n - k)}.
\]

(155)

In addition, \( \omega_+(x) \) and \(-\omega_-(x)\) are strictly completely monotonic over \( x \in (0, \infty) \) according to Lemma 5.15, so \( \omega_-(n) - \omega_-(k) - \omega_-(n - k) \) and \( -\omega_+(n) + \omega_+(k) + \omega_+(n - k) \) are strictly completely monotonic in \( n \) and strictly convex in \( k \) by Lemma 5.14. It follows that \( \varphi(n, k)/\varphi_-(n, k) \) and \( \varphi_+(n, k)/\varphi(n, k) \) are strictly logarithmically completely monotonic in \( n \) and strictly logarithmically convex in \( k \); in particular, they are strictly decreasing in \( n \) and strictly logarithmically convex in \( n \) and \( k \). Meanwhile, \( \varphi(n, fn)/\varphi_-(n, fn) \) and \( \varphi_+(n, fn)/\varphi(n, fn) \) are strictly decreasing in \( n \) and strictly logarithmically convex in \( f \).

According to Lemma 5.17 and the following equation

\[
\frac{\varphi_+(n, k)}{\varphi_-(n, k)} = e^{\xi(n, k)},
\]

(156)
the function $\varphi_+ (n, k)/\varphi_- (n, k)$ is strictly logarithmically completely monotonic in $n$ and strictly logarithmically convex in $k$; in particular, it is strictly decreasing in $n$ and strictly logarithmically convex in $n$ and $k$. Meanwhile, $\varphi_+ (n, fn)/\varphi_- (n, fn)$ is strictly decreasing in $n$ and strictly logarithmically convex in $f$.

As a corollary of the above discussions, the functions $\varphi(n, k)/\varphi_-(n, k)$, $\varphi_+(n, k)/\varphi(n, k)$, and $\varphi_+(n, k)/\varphi_-(n, k)$ are strictly decreasing in $k$ when $0 < k \leq n/2$ and strictly increasing in $k$ when $n/2 < k < n$, given that these functions are invariant when $k$ is replaced by $n - k$.

The first inequality in Eq. (107) follows from Eq. (104), and the second inequality follows from the monotonicity property of $\varphi(n, k)/\varphi_-(n, k)$ with respect to $k$ as established above. The third inequality in Eq. (107) can be proved as follows,

$$
\frac{\varphi(n, k)}{\varphi_-(n, k)} \leq \frac{\varphi(k + 1, k)}{\varphi_-(k + 1, k)} \leq \frac{\varphi(k + 1, 1)}{\varphi_-(k + 1, 1)} \leq \frac{\varphi(2, 1)}{\varphi_-(2, 1)},
$$

and the equality in Eq. (107) can be verified by straightforward calculation. Equations (108) and (109) follow from a similar reasoning.

6. A conjecture on the tail probability.

6.1. The conjecture. Theorem 2.1 establishes upper and lower bounds for the ratio $B_{n,k}(p)/b_{n,k}(p)$ that are tight within a factor of 2, which lead to nearly tight upper and lower bounds for the tail probability $B_{n,k}(p)$ itself. Numerical calculation illustrated in Fig. 1 shows that the lower bound $\bar{L}(n, k, p)$ in Theorem 2.1 is tight within a factor of $180451625/143327232 \approx 1.25902$. To stimulate further progresses, here we formulate the conjecture and prove this conjecture in a special case by virtue of a surprising connection with Ramanujan’s equation [28, 40].

CONJECTURE 1. Suppose $k, n \in \mathbb{N}_0$, $k \leq n$, $0 < p < 1$. Then $B_{n,k}(p)/[b_{n,k}(p)L(n, k, p)]$ is nondecreasing in $k$ and nonincreasing in $n$ and $p$. In addition,

$$
\frac{B_{n,k}(p)}{b_{n,k}(p)} < \frac{180451625}{143327232} L(n, k, p) \quad \forall k \leq pn,
$$

$$
\frac{B_{n,k}(p)}{b_{n,k}(p)} < \sqrt{\frac{\pi}{2}} L(n, k, p) \quad \forall k \leq pn - 1.
$$

Incidentally,

$$
1.25901 < \frac{180451625}{143327232} = \frac{5^3 \times 1443613}{2^{16} \times 3^7} < 1.25902, \quad 1.25331 < \sqrt{\frac{\pi}{2}} < 1.25332.
$$

If Conjecture 1 holds, then by virtue of Eq. (131) we can deduce that

$$
\frac{\bar{B}_{n,k}(p)}{b_{n,k}(p)} < \frac{180451625}{143327232} \bar{L}(n, k, p) \quad \forall k \geq pn,
$$

$$
\frac{\bar{B}_{n,k}(p)}{b_{n,k}(p)} < \sqrt{\frac{\pi}{2}} \bar{L}(n, k, p) \quad \forall k \geq pn + 1.
$$

In addition, many results in Theorems 2.1, 2.2, 5.6, and 5.10 can be improved. Notably, the lower bound $\bar{L}(n, k, p)$ in Theorem 5.6 will be tight within a factor of $180451625/143327232$, and the lower bound $\bar{L}_-(n, k, p)$ will be tight within a factor of

$$
\frac{180451625 \sqrt{\pi^{1/8}}}{143327232} < 1.26434.
$$
thanks to Eq. (107). Accordingly, the lower bound $B_{n,k}^+(p)$ in Theorem 2.2 will be tight within this factor, that is,

$$B_{n,k}^+(p) < B_{n,k}(p) < \frac{180451625 \sqrt{\pi} e^{1/8}}{2} B_{n,k}^+(p) < 1.26434 B_{n,k}^+(p).$$

Equations (158) and (159) will hold if $B_{n,k}(p)/[b_{n,k}(p)L(n,k,p)]$ is indeed nonincreasing in $p$. In that case we have

$$\frac{B_{n,k}(p)}{b_{n,k}(p)L(n,k,p)} \leq \frac{B_{n,k}(k/n)}{b_{n,k}(k/n)L(n,k,k/n)} < \frac{180451625}{143327232} \forall k \leq pn,$$

$$\frac{B_{n,k-1}(p)}{b_{n,k-1}(p)L(n,k-1,p)} \leq \frac{B_{n,k-1}(k/n)}{b_{n,k-1}(k/n)L(n,k-1,k/n)} < \sqrt{\frac{\pi}{2}} \forall 1 \leq k \leq pn,$$

which imply Eqs. (158) and (159). Here the second inequality in Eq. (165) follows from Lemma 6.3 below, and the second inequality in Eq. (166) follows from Lemma 6.2 below.

6.2. Evidences for Conjecture 1. Next, provide three lemmas that resolve Conjecture 1 in certain special case. The proofs of Lemmas 6.1-6.3 below are relegated to Appendices F and G. Our analysis also shows that the constants in the two equations in Conjecture 1 are best possible.

**Lemma 6.1.** Suppose $j \in \mathbb{N}_0$ and $k, n \in \mathbb{N}$ satisfy $j \leq k \leq n - 1$, and $0 < f < 1$; then $B_{n,j}(k/n)/b_{n,j}(k/n)$ is equal to 1 when $j = 0$ and is strictly increasing in $n$ when $j \geq 1$. In addition,

$$\lim_{n \to \infty} \frac{B_{n,j}(k/n)}{b_{n,j}(k/n)} = \sum_{l=0}^{j} \frac{\Gamma(j+1)}{k! \Gamma(j-l+1)},$$

$$\lim_{n \to \infty} \frac{B_{n,k-1}(k/n)}{b_{n,k-1}(k/n)} = \sum_{l=0}^{k-1} \frac{\Gamma(k)}{k! \Gamma(k-l)} = \frac{e^{k} k!}{2k^{k}} - \theta_{k} \leq \sqrt{\frac{\pi k}{2}} - \sqrt{\frac{\pi}{2}} + 1,$$

$$\lim_{n \to \infty} \frac{B_{n,k}(k/n)}{b_{n,k}(k/n)} = 1 + \sum_{l=0}^{k-1} \frac{\Gamma(k)}{k! \Gamma(k-l)} = \frac{e^{k} k!}{2k^{k}} + 1 - \theta_{k} \leq \sqrt{\frac{\pi k}{2}} - \sqrt{\frac{\pi}{2}} + 2,$$

$$\lim_{n \to \infty} \frac{B_{n,[jn-f]}(f)}{b_{n,[jn-f]}(f)L(n,fn-j,f)} = \sqrt{\frac{\pi}{2}}.$$ 

where $\theta_{k}$ is defined by Ramanujan’s equation [28, 40]:

$$\frac{e^{k}}{k!} = \theta_{k} k^{k} + \sum_{i=0}^{k-1} \frac{k^{i}}{i!}.$$ 

According to Ref. [44, 49], $\theta_{k}$ is strictly decreasing in $k$ and satisfies

$$\frac{1}{3} < \theta_{k} \leq \theta_{1} = \frac{e - 2}{2}.$$ 

Lemma 6.1 implies that (given the assumptions in the lemma)

$$\frac{B_{n,j}(k/n)}{b_{n,j}(k/n)} \leq \sum_{l=0}^{j} \frac{\Gamma(j+1)}{k! \Gamma(j-l+1)}.$$
implies that by considering the regime of small deviation in connection with the CLT we can deduce that

\[ \frac{B_{n,k-1}(k/n)}{b_{n,k-1}(k/n)} \leq \sum_{l=0}^{k-1} \frac{\Gamma(k)}{k!\Gamma(k-l)} \cdot \frac{e^{k!k!}}{2k^{k}} - \theta_{k} \leq \sqrt{\frac{\pi k}{2}} - \sqrt{\frac{\pi}{2}} + 1, \]

and the inequality in Eq. (173) is strict when \( j \geq 1. \)

**Lemma 6.2.** Suppose \( k, n \in \mathbb{N} \) satisfy \( 1 \leq k \leq n - 1; \) then

\[ \frac{B_{n,k-1}(k/n)}{b_{n,k-1}(k/n)} < \sqrt{\frac{\pi}{2}}L(n, k-1, k/n). \]

**Lemma 6.3.** Suppose \( k, n \in \mathbb{N} \) satisfy \( 1 \leq k \leq n - 1; \) then

\[ \frac{B_{n,k}(k/n)}{b_{n,k}(k/n)} < \frac{180451625}{14332732}L(n, k, k/n). \]

If in addition \( n \leq 2k, \) then

\[ \frac{B_{n,k}(k/n)}{b_{n,k}(k/n)} < \sqrt{\frac{\pi}{2}}L(n, k, k/n). \]

Equation (170) shows that the constants in Eqs. (176) and (178) cannot be improved. It turns out the constant in Eq. (177) cannot be improved either. To see this, note that

\[ \lim_{n \to \infty} L(n, k, k/n) = \lim_{n \to \infty} \frac{1}{2} \left( 1 + \sqrt{1 + \frac{4k(n-k)}{n}} \right) = \frac{1}{2} \left( 1 + \sqrt{1 + 4k} \right). \]

In conjunction with Lemma 6.1 we can deduce that

\[ \lim_{n \to \infty} \frac{B_{n,k}}{b_{n,k}L(n, k, k/n)} = \frac{e^{k!k!}}{k^{k}(1 + \sqrt{1 + 4k})} + \frac{2(1 - \theta_{k})}{1 + \sqrt{1 + 4k}}. \]

Now, direct calculation shows that this limit is equal to the constant in Eq. (177), that is, \( \frac{180451625}{14332732}, \) when \( k = 12. \) However, this value cannot be approached when \( k \) deviates from 12, in sharp contrast with Eqs. (176) and (178).

### 6.3. Additional evidence for Conjecture 1

Here we provide an additional evidence for Conjecture 1 by considering the regime of small deviation in connection with the CLT theorem. Let \( k_{n} = pn - x\sqrt{pqn} \) with \( x \geq 0, \) then by definitions in Eqs. (11)-(14) and (22) we can deduce that

\[ \lim_{n \to \infty} B_{n,k,n,k_{n}}(p) = \lim_{n \to \infty} B_{n,k,n,k_{n}}^{+}(p) = \lim_{n \to \infty} \frac{L(n,k_{n},p)}{\sqrt{2\pi pqn}}e^{-x^{2}/2} = \ell(x)e^{-x^{2}/2}, \]

\[ \lim_{n \to \infty} B_{n,k,n,k_{n}}^{+}(p) = \lim_{n \to \infty} B_{n,k,n,k_{n}}^{+}(p) = \lim_{n \to \infty} \frac{U(n,k_{n},p)}{\sqrt{2\pi pqn}}e^{-x^{2}/2} = \nu(x)e^{-x^{2}/2}, \]

where

\[ \ell(x) := \frac{1}{2\sqrt{2\pi}} \left( \sqrt{4 + x^{2} - x} \right), \quad \nu(x) := \frac{1}{\sqrt{2\pi}} \left\{ \begin{array}{ll} 2 - x & x \leq 1, \\
\frac{1}{x} & x \geq 1. \end{array} \right. \]

So Theorem 2.2 implies that

\[ \ell(x)e^{-x^{2}/2} \leq \lim_{n \to \infty} B_{n,k,n,k_{n}}(p) \leq \nu(x)e^{-x^{2}/2}. \]
On the other hand, the CLT implies that
\begin{equation}
\lim_{n \to \infty} B_{n,\lfloor k_n \rfloor}(p) = \Phi(-x) := \int_{-\infty}^{-x} \frac{1}{\sqrt{2\pi}} e^{-t^2/2} dt = \int_x^{\infty} \frac{1}{\sqrt{2\pi}} e^{-t^2/2} dt,
\end{equation}
where \( \Phi(x) \) is the cumulative distribution function of the standard Gaussian distribution. The two equations above together imply that
\begin{equation}
\ell(x) e^{-x^2/2} \leq \Phi(-x) \leq v(x) e^{-x^2/2}.
\end{equation}
Here the lower bound was originally derived by Birnbaum [6], but we are not aware of any previous derivation that is based on lower bounds for the binomial distribution, note that it is much more common to derive bounds for the binomial distribution based on the counterparts for the Gaussian distribution, but not in the other way.

To see the connection between the above discussion and Conjecture 1, note that
\begin{equation}
\lim_{n \to \infty} \sqrt{n} b_{n,\lfloor k_n \rfloor}(p) = \frac{1}{\sqrt{2\pi pq}} e^{-x^2/2}
\end{equation}
according to Eqs. (100) and (112). In conjunction with Eqs. (181) and (185) we can deduce that
\begin{equation}
\lim_{n \to \infty} \frac{B_{n,\lfloor k_n \rfloor}(p)}{b_{n,\lfloor k_n \rfloor}(p) L(n, k_n, p)} = \frac{\Phi(-x)}{\ell(x) e^{-x^2/2}},
\end{equation}
so the properties of the ratio \( \Phi(-x) e^{x^2/2}/\ell(x) \) are suggestive of the properties of the ratio \( B_{n,\lfloor k_n \rfloor}(p)/[b_{n,\lfloor k_n \rfloor}(p) L(n, k_n, p)] \).

According to Eqs. (181) and (182) and the inequality \( U(n, k, p) < 2L(n, k, p) \) in Theorem 2.1, the upper and lower bounds in Eqs. (184) and (186) are tight within a factor of 2. The following proposition proved in Appendix H further shows that these bounds are asymptotically tight and that the lower bound in each equation is actually tight within a factor of \( \sqrt{\pi}/2 \), which together with Eq. (188) offers an additional evidence for Eq. (159) in Conjecture 1. In addition, \( \Phi(-x) e^{x^2/2}/\ell(x) \) is strictly decreasing in \( x \), so the lower bound \( \ell(x) e^{-x^2/2} \) becomes more and more accurate as \( x \) increases, which is also reminiscent of the monotonicity properties stated in Conjecture 1.

**PROPOSITION 6.4.** Suppose \( x \geq 0 \); then \( v(x)/\ell(x) \) and \( \Phi(-x) e^{x^2/2}/\ell(x) \) are strictly decreasing in \( x \). In addition,
\begin{align}
\lim_{x \to \infty} \frac{\Phi(-x) e^{x^2/2}}{\ell(x)} &= \lim_{x \to \infty} \frac{v(x)}{\ell(x)} = \lim_{x \to \infty} \sqrt{2\pi x} \ell(x) = 1, \\
\ell(x) < v(x) \leq 2\ell(x), \\
\ell(x) e^{-x^2/2} < \Phi(-x) \leq \sqrt{\frac{\pi}{2}} \ell(x) e^{-x^2/2},
\end{align}
where the second inequality in Eq. (190) and that in Eq. (191) are saturated iff \( x = 0 \).

**7. Conclusion.** We derived simple but nearly tight upper bound \( B_{n,k}^{\uparrow}(p) \) and lower bound \( B_{n,k}^{\downarrow}(p) \) for the binomial tail probability \( B_{n,k}(p) \). These bounds have a number of appealing properties, including (C1) \( O(1) \)-computability, (C2) Universal boundedness of the ratio \( B_{n,k}^{\uparrow}(p)/B_{n,k}^{\downarrow}(p) \), (C3) Asymptotic tightness in the regime of large deviation, and (C3') Asymptotic tightness in the regime of moderate deviation. To the best of our knowledge, no
bounds for the tail probability $B_{n,k}(p)$ known in the literature satisfy these criteria simultaneously. By virtue of these universal bounds, we derived the asymptotic expansion of the tail probability $B_{n,k}(p)$ up to a constant multiplicative factor. In the course of study, we derived nearly tight upper and lower bounds for the ratio $B_{n,k}(p)/b_{n,k}(p)$, which are of independent interest. Furthermore, we believe that our lower bound for the ratio $B_{n,k}(p)/b_{n,k}(p)$ is more accurate than what can be proved rigorously, as stated in Conjecture 1 and supported by strong evidences. If this conjecture holds, then the lower bound $B_{n,k}(p)$ will be tight within a factor of $1.26434$. We hope that our work can stimulate further progresses in this direction.

In the future, it would be desirable to generalize our results to other probability distributions, such as multinomial distributions. Such extension, if available, may find diverse applications in various research areas, including statistical sampling, quantum verification, channel coding with higher order [17, 21, 35], security analysis with higher order [21, 22], quantum thermodynamics [27, 45], and local discrimination [23].

APPENDIX A: DERIVATION OF EQ. (8)

The references [7, Theorem 4], [4, Case 2], [16, Theorem 3.7.4] derived general formulas for strong large deviation, but did not give the explicit formula for the binomial distribution. The aim of this appendix is to derive the explicit formula of strong large deviation for the binomial distribution as presented in Eq. (8) from general results mentioned above. Here our derivation is mainly based on [16, Theorem 3.7.4], which yields the following proposition in the lattice case with lattice span $d$. Note that the lattice span is 1 in the case of the binomial distribution. Incidentally, a simple alternative derivation of Eq. (8) is presented in the proof of Proposition 5.5.

We define the cumulant generating function $\Lambda(s) := \ln E[e^{sX}]$, where $E[X]$ expresses the expectation of the random variable $X$. The inverse function of the derivative $\Lambda'(s)$ is denoted by $\eta$.

**Proposition A.1.** Suppose $X$ is a lattice variable with lattice span $d$ and its cumulant generating function $\Lambda(s)$ is finite in some neighborhood of 0. If $R < E[X]$, then the $n$-iid sum $X_n$ of the random variable $X$ satisfies

\[
\Pr\{X_n \geq nR\} = e^{-n\chi_0(R)} \frac{d}{\sqrt{2\pi n \Lambda''(\eta(R))}} \left(1 - e^{-d\eta(R)}\right) \left[1 + O(n^{-1})\right],
\]

where

\[
\chi_0(R) := R\eta(R) - \Lambda(\eta(R)).
\]

Now, we apply the above proposition to the binomial upper tail probability $\bar{B}_{n,f_n}(p)$ defined in Eq. (131), assuming that $f$ is a rational number and $n \in \mathbb{N}_f$. In this case, we have

\[
\Lambda(s) = \ln(1 - p + pe^s), \quad \Lambda'(s) = \frac{pe^s}{1 - p + pe^s}.
\]

The inverse function of $\Lambda'$ reads

\[
\eta(f) = \ln \frac{f(1 - p)}{(1 - f)p},
\]

from which we can deduce that

\[
\Lambda''(\eta(f)) = \eta'(f)^{-1} = f(1 - f).
\]
In addition, the definition (A.2) implies that

\[(A.6) \quad \chi_0(f) = f \eta(f) - \Lambda(\eta(f)) = f \ln \frac{f(1 - p)}{(1 - f)p} - \ln \left(1 - p + \frac{f(1 - p)}{(1 - f)p}\right) = D(f||p).\]

Substituting Eqs. (A.4)-(A.6) into (A.1), we can deduce that

\[(A.7) \quad \lim_{n \to \infty} \sqrt{n} B_{n,(1-f)n}(q) e^{nD(q||f)} = \frac{1}{\sqrt{2\pi f(1 - f) f - p}} \frac{f(1 - p)}{f - p},\]

where \(q = 1 - p\). As a simple corollary this equation yields

\[(A.8) \quad \lim_{n \to \infty} \sqrt{n} B_{n,f_n(p)} e^{nD(f||p)} \sqrt{n} = \lim_{n \to \infty} \sqrt{n} B_{n,(1-f)n}(q) e^{nD(1-f||q)} = \sqrt{\frac{1 - f}{2\pi f}} \frac{p}{p - f},\]

which confirms Eq. (8).

Incidentally, reference [35, (5.41)] derived a limit for \(\sqrt{n} B_{n,f_n} e^{nD(f||p)}\) that is different from Eq. (A.7) because its derivation is problematic.

**APPENDIX B: PROOFS OF LEMMAS 4.3-4.9**

**B.1. Proof of Lemma 4.3.** To prove Lemma 4.3, we need to consider two different parameter ranges depending on the value of \(k\) in comparison with \(\kappa_1(n,p)\) defined in Eq. (12) and the following function

\[(B.1) \quad \kappa_2(n,p) := p(n + 1) - \frac{q}{4} - \frac{1}{4} \sqrt{q(8pn + 7p + 1)},\]

where \(q = 1 - p\). Here we first prepare an auxiliary lemma to clarify the properties of \(\kappa_1(n,p)\) and \(\kappa_2(n,p)\) as well as their relations.

**Lemma B.1.** Suppose \(n \geq -1\) and \(0 < p < 1\). Then \(\kappa_1(n,p)\) is strictly convex in \(n\); it is strictly decreasing in \(n\) for \(-1 \leq n \leq [q/(4p)] - 1\), but strictly increasing for \(n \geq [q/(4p)] - 1\). Meanwhile, \(\kappa_2(n,p)\) and \(\kappa_2(n,p) - \kappa_1(n,p)\) are strictly increasing in \(n\). In addition,

\[(B.2) \quad \kappa_1(n,p) \geq -\frac{q}{4}, \quad \kappa_2(n,p) - \kappa_1(n,p) \geq -\frac{q}{2}, \quad \kappa_2(n,p) - \kappa_1(n,p) \geq -\frac{q}{2}\]

Furthermore, the following four conditions are equivalent:

1. \(n > (1/p) - 2\);
2. \(\kappa_1(n,p) > 0\);
3. \(\kappa_2(n,p) > 0\);
4. \(\kappa_2(n,p) - \kappa_1(n,p) > 0\).

**Proof of Lemma B.1.** According to the following equation,

\[(B.3) \quad \frac{\partial \kappa_1(n,p)}{\partial n} = p \left(1 - \frac{q}{2\sqrt{pq(n+1)}}\right), \quad \frac{\partial^2 \kappa_1(n,p)}{\partial n^2} = \frac{\sqrt{pq(n+1)}}{4(n+1)^2} \quad \forall n > -1,\]

\(\kappa_1(n,p)\) is strictly decreasing in \(n\) for \(-1 \leq n \leq [q/(4p)] - 1\), but is strictly increasing in \(n\) for \(n \geq [q/(4p)] - 1\), given that \(\kappa_1(n,p)\) is continuous in \(n\) when \(n \geq -1\). At \(n = [q/(4p)] - 1\), \(\kappa_1(n,p)\) attains its minimum value \(-q/4\), which implies the first inequality in Eq. (B.2). In
addition, $\kappa_1(n,p)$ is strictly convex in $n$, which is also clear from its definition in Eq. (12). Furthermore, $\kappa_1(n,p) = 0$ when $n = -1$ or $n = (1/p) - 2$. So $\kappa_1(n,p) > 0$ iff $n > (1/p) - 2$ given that $\kappa_1(n,p)$ is strictly convex.

According to the following equations,

\begin{equation}
\frac{\partial \kappa_2(n,p)}{\partial n} = p \left( 1 - \frac{q}{\sqrt{q(8pn + 7p + 1)}} \right) > 0 \quad \forall n \geq -1, \tag{B.4}
\end{equation}

\begin{equation}
\frac{\partial [\kappa_2(n,p) - \kappa_1(n,p)]}{\partial n} = pq \left[ \sqrt{q(8pn + 7p + 1)} - 2\sqrt{pq(n + 1)} \right] > 0 \quad \forall n > -1, \tag{B.5}
\end{equation}

$\kappa_2(n,p)$ and $\kappa_2(n,p) - \kappa_1(n,p)$ are strictly increasing in $n$ for $n \geq -1$, given that they are continuous in $n$ for $n \geq -1$. Now the second and third inequalities in Eq. (B.2) follow from this fact and the following equation

\begin{equation}
\kappa_1(-1,p) = 0, \quad \kappa_2(-1,p) - \kappa_1(-1,p) = \kappa_2(-1,p) = -\frac{q}{2}. \tag{B.6}
\end{equation}

When $n = (1/p) - 2$, calculation shows that

\begin{equation}
\kappa_2(n,p) - \kappa_1(n,p) = \kappa_2(n,p) = \kappa_1(n,p) = 0. \tag{B.7}
\end{equation}

Therefore, $\kappa_2(n,p) > 0$ iff $n > (1/p) - 2$; similarly, $\kappa_2(n,p) - \kappa_1(n,p) > 0$ iff $n > (1/p) - 2$. This observation completes the proof of Lemma B.1.

**Proof of Lemma 4.3.** If $\kappa_1(n,p) \leq k \leq pm$, then the definition in Eq. (14) implies that

\begin{equation}
U(n,k,p) = V(n,k,p, [\tilde{a}]) < W(n,k,p), \tag{B.8}
\end{equation}

where $\tilde{a} = k - \kappa_1(n,p)$ and

\begin{equation}
W(n,k,p) := 1 + V(n,k,p, \tilde{a}) = 1 + k - pn + 2\sqrt{pq(n + 1)}. \tag{B.9}
\end{equation}

In conjunction with Eq. (11) we can deduce that

\begin{equation}
2L(n,k,p) - W(n,k,p) = \sqrt{(pn - k + 1)^2 + 4qk} - 2\sqrt{pq(n + 1)} \geq 0, \tag{B.10}
\end{equation}

which implies Eq. (67). Here the inequality follows from the following equation

\begin{equation}
(pm - k + 1)^2 + 4qk - 4pq(n + 1) = [p(n + 2) - k - 1]^2 \geq 0. \tag{B.11}
\end{equation}

If $0 \leq k < \kappa_1(n,p)$ and $k \leq pm$, then $\kappa_2(n,p) > \kappa_1(n,p) > k \geq 0$ and $n > (1/p) - 2$ by Lemma B.1. In addition, the definition in Eq. (14) implies that $U(n,k,p) = V(n,k,p,0)$. Let

\begin{equation}
\Delta = 2L(n,k,p) - 1 - V(n,k,p,0) = k - pn + \sqrt{(pn - k + 1)^2 + 4qk} - \frac{p(n + 1 - k)}{p(n + 1) - k}; \tag{B.12}
\end{equation}

then to prove Eq. (67) it suffices to prove the inequality $\Delta \geq 0$. Solving the equation $\Delta = 0$ yields two solutions for $k$ that are not larger than $pn + p$, that is, $k = 0$ or $k = \kappa_2(n,p)$. In addition, the inequality $n > (1/p) - 2$ means

\begin{equation}
\frac{\partial \Delta}{\partial k} |_{k=0} = \frac{qp(n + 2p - 1)}{p(n + 1)(1 + pn)} > 0. \tag{B.13}
\end{equation}

Note that $\Delta$ is continuous in $k$ for $0 \leq k \leq \kappa_2(n,p)$ and has no zero in this interval except for the end points. So $\Delta \geq 0$ for $0 \leq k \leq \kappa_2(n,p)$, which implies Eq. (67) and completes the proof of Lemma 4.3.
B.2. Proof of Lemma 4.4. Equation (11) implies that

\[ L(n, k, p) - 1 = \frac{-(pn - k + 1) + \sqrt{(pn - k + 1)^2 + 4qk}}{2} \geq 0, \]

so \( L(n, k, p) \geq 1 \), and this inequality is strict when \( 0 < p < 1 \) and \( k > 0 \). Meanwhile, \( L(n, k, p) \) is continuous in \( n, k, p \) in the parameter range specified in Lemma 4.4, so in the following discussion we can focus on the interior of this parameter range, that is, \( n > -1 \), \( k > 0 \), and \( 0 < p < 1 \). Then \( L(n, k, p) \) is the solution to the following equation that is larger than 1 [cf. Eq. (80)],

\[ L + \frac{p(n + 1)(L - 1)}{L - p} = k + 1. \]  

(B.15)

This equation shows that \( k \) is strictly increasing and concave in \( L \), so \( L \) is strictly increasing and convex in \( k \).

From Eq. (B.15) we can deduce that

\[ n = \frac{kL + L - L^2 - pk}{p(L - 1)} = \frac{k - L}{p} + \frac{kq}{p(L - 1)}, \]

which implies that \( n \) is strictly decreasing and convex in \( L \), so \( L \) is strictly decreasing and convex in \( n \). Now Eqs. (68) and (69) follow from Eq. (B.14) and the following equation,

\[ L(-1, k, p) = 1 + k, \quad L(k/p, k, p) = \frac{1}{2} \left(1 + \sqrt{4qk + 1}\right). \]  

(B.17)

If in addition \( n = k > 0 \), then \( L(n, k, p) = 1 + k - pk \), which is strictly decreasing and linear in \( p \). If \( n > k > 0 \), then from Eq. (B.15) we can deduce that

\[ p = \frac{L(k + 1 - L)}{n(L - 1) + k} = \frac{kn + k - nL}{n^2} + \frac{k(n - k)(n + 1)}{n^2[n(L - 1) + k]}, \]

which implies that \( p \) is strictly decreasing and convex in \( L \), so \( L \) is strictly decreasing and convex in \( p \).

B.3. Proof of Lemma 4.5. The proof is divided into three steps: In the first step we prove Eq. (70), in the second step we prove the lower bound in Eq. (71), and in the third step we prove the upper bound in Eq. (71).

Step 1: Proof of Eq. (70). Modifying the function \( L(n, k, p) \), we define

\[ g(n, k, p) := n[L(n, k, p) - 1], \quad g(\infty, k, p) := \lim_{n \to \infty} g(n, k, p) = \frac{qk}{p}. \]

Then

\[ \frac{\partial g(n, k, p)}{\partial n} = \frac{s_2 + (k - 1 - 2pn)\sqrt{s_1}}{2\sqrt{s_1}}, \]

(B.20)

where \( s_1 \) and \( s_2 \) are defined as follows,

\[ s_1 := (pn - k + 1)^2 + 4qk > 0, \]

(B.21)

\[ s_2 := s_1 + pn(1 - k + pn) = 2p^2n^2 + 3p(1 - k)n + (k + 1)^2 - 4pk, \]

(B.22)

which satisfy

\[ s_2^2 - (k - 1 - 2pn)^2s_1 = 4qk[(k - 1)^2 + 4qk - 2p(k - 1)n]. \]  

(B.23)
When $0 \leq k \leq 1$, we have $s_2 \geq 0$ and $s_2^2 - (k - 1 - 2pn)^2s_1 \geq 0$, which implies that $\partial g(n,k,p)/\partial n \geq 0$, so $g(n,k,p)$ is nondecreasing in $n$. In conjunction with Eq. (B.19) we conclude that $g(n,k,p) \leq qk/p$, which implies the upper bound in Eq. (70). Note that this upper bound holds even if $pn < k$. If $pn \geq k$ as stated in the assumption, then

$$g(n,k,p) \geq g(k/p,k,p) = \frac{k(\sqrt{1 + 4qk} - 1)}{2p},$$

which implies the lower bound in Eq. (70).

**Step 2:** Proof of the lower bound in Eq. (71). We first assume that $1 < k \leq pn$ to start with. Then $\partial g(n,k,p)/\partial n$ has a unique zero at

$$n = n_0 := \frac{(k - 1)^2 + 4qk}{2p(k - 1)}.$$

Note that

$$k - 1 - 2pn_0 = \frac{4qk}{k - 1} \leq 0, \quad s_2|_{n = n_0} = \frac{2qk[(k - 1)^2 + 4qk]}{(k - 1)^2} \geq 0.$$

Meanwhile,

$$\left. \frac{\partial g(n,k,p)}{\partial n} \right|_{n = 0} = \frac{1}{2} \sqrt{(k - 1)^2 + 4qk + k - 1} > 0,$$

while $\partial g(n,k,p)/\partial n < 0$ when $n$ is sufficiently large, given that

$$k - 1 - 2pn < 0, \quad s_2^2 - (k - 1 - 2pn)^2s_1 < 0$$

in that case. Therefore, $\partial g(n,k,p)/\partial n \geq 0$ when $0 \leq n \leq n_0$ and $\partial g(n,k,p)/\partial n \leq 0$ when $n \geq n_0$, which means

$$g(n,k,p) \geq \min\{g(\infty,k,p),g(k/p,k,p)\} = \min\left\{ \frac{qk}{p}, \frac{k(\sqrt{1 + 4qk} - 1)}{2p} \right\}$$

and confirms the lower bound in Eq. (71) given the assumption $1 < k \leq pn$. By continuity the lower bound holds when $1 \leq k \leq pn$.

**Step 3:** Proof of the upper bound in Eq. (71). We also assume that $1 < k \leq pn$ to start with. Then the above analysis implies that

$$g(n,k,p) \leq g(n_0,k) = \frac{(k - 1)^2 + 4qk}{4p}, \quad n_0 - k = \frac{4qk - (k^2 - 1)}{2(k - 1)p}.$$

If $k \geq 2 + \sqrt{3}$, then $(k^2 - 1)/(4k) \geq 1 \geq q$. Therefore, $n_0 \leq k/p$, and $g(n,k,p)$ is nonincreasing in $n$ for $n \geq k/p$, which means

$$g(n,k,p) \leq g(k/p,k,p) = \frac{k(\sqrt{1 + 4qk} - 1)}{2p} \leq \frac{k\sqrt{qk}}{p} \quad \text{if} \quad pn \geq k.$$

If $1 < k < 2 + \sqrt{3}$ and $0 < q \leq (k^2 - 1)/(4k)$, then Eq. (B.31) holds due to a similar reason.

It remains to consider the case with $1 < k < 2 + \sqrt{3}$ and $(k^2 - 1)/(4k) < q < 1$. Let

$$s_3 := 4k\sqrt{qk} - 4pg(n_0,k,p) = 4k\sqrt{qk} - (k - 1)^2 - 4qk;$$
then $s_3$ is concave in $q$ for $0 < q < 1$. In addition,

\[(B.33) \quad s_3 = 2k\left[\sqrt{k^2 - 1} - (k - 1)\right] \geq 0 \quad \text{if} \quad q = \frac{k^2 - 1}{4k},\]

\[(B.34) \quad \lim_{q \to 1} s_3 = 4k^{3/2} - (k + 1)^2 \geq 0,\]

given that $1 < k < 2 + \sqrt{5}$. Therefore,

\[(B.35) \quad s_3 \geq 0, \quad g(n, k, p) \leq g(n_0, k, p) \leq k\sqrt{qk}p \quad \text{if} \quad 1 < k < 2 + \sqrt{5}, \quad k^2 - 1 < q < 1.\]

In summary, we have

\[(B.36) \quad g(n, k, p) \leq k\sqrt{qk}p \quad \text{if} \quad 1 < k \leq pn.\]

By continuity this upper bound holds when $1 \leq k \leq pn$, which implies the upper bound in Eq. (71) and completes the proof of Lemma 4.5.

**B.4. Proof of Lemma 4.6.** The proof is divided into two steps: In the first step we prove the monotonicity and convexity/concavity properties of $L(n, fn, p)$ and in the second step we prove Eq. (73).

**Step 1:** Proofs of the monotonicity and convexity/concavity properties of $L(n, fn, p)$. Note that $L(n, fn, p)$ is continuous in $n, f, p$ in the parameter range specified in Lemma 4.6, so we can focus on the interior of this parameter range, that is, $n > 0$ and $0 < f, p < 1$. Then $L(n, fn, p) > 1$ [cf. Eq. (B.14)] and $L(n, fn, p)$ is the solution to the following equation that is larger than 1 [cf. Eqs. (80) and (B.15)],

\[(B.37) \quad L + \frac{p(n+1)(L-1)}{L-p} = fn + 1.\]

This equation shows that $f$ is strictly increasing and concave in $L$, so $L$ is strictly increasing and convex in $f$. Alternatively, this conclusion follows from Lemma 4.4 and its proof. Meanwhile, Lemma 4.4 implies that $L$ is nonincreasing and convex in $p$.

According to the following equation,

\[(B.38) \quad \frac{2\partial L(n, fn, p)}{\partial n} = f - p + \frac{(p-f)^2n + f + p - 2fp}{\sqrt{(pn - fn + 1)^2 + 4qfn}} > 0,\]

$L(n, fn, p)$ is strictly increasing in $n$. Here the inequality holds because

\[(B.39) \quad (p-f)^2n + f + p - 2fp > 0,\]

\[(B.40) \quad [(p-f)^2n + f + p - 2fp]^2 - (f-p)^2[(pn - fn + 1)^2 + 4qfn] = 4f(1-f)pq > 0.\]

In addition, by virtue of Eq. (B.37) we can deduce that

\[(B.41) \quad n = \frac{L(L-1)}{p(1-f) - (p-f)L}, \quad \frac{\partial^2 n}{\partial L^2} = \frac{2f(1-f)pq}{[p(1-f) - (p-f)L]^3} > 0,\]

which implies that $p(1-f) > (p-f)L$ and $n$ is strictly convex in $L$, so $L$ is strictly concave in $n$ given that it is strictly increasing in $n$.\]
Step 2: Proof of Eq. (73), assuming that \( n > 0 \) and \( 0 < f < p < 1 \). If \( f = 0 \), then both bounds in Eq. (73) are equal to 1 and \( L(n, f, p) = 1 \), so Eq. (73) holds and both inequalities are saturated.

If \( n > 0 \) and \( 0 < f < p < 1 \), then \( L(n, f, p) \) is strictly increasing in \( n \) as proved above. In conjunction with Eq. (20) and the equality \( L(0, 0, p) = 1 \) we can deduce that

\[
(B.42) \quad 1 < L(n, f, p) < \frac{(1 - f)p}{p - f} = \frac{1}{1 - r}.
\]

Alternatively, the upper bound follows from Eq. (B.41).

Next, we turn to the lower bound in Eq. (73), assuming that \( n > 0 \) and \( 0 < f < p < 1 \). Let

\[
(B.43) \quad h(n, f, p) := n \left[ \frac{(1 - f)p}{p - f} - L(n, f, p) \right], \quad h(\infty, f, p) := \lim_{n \to \infty} h(n, f, p) = \frac{fpq(1 - f)}{(p - f)^3}.
\]

Calculation shows that

\[
(B.44) \quad \frac{\partial h(n, f, p)}{\partial n} = \frac{t_2\sqrt{1 - t_3}}{2\sqrt{t_1}},
\]

where \( t_1, t_2, \) and \( t_3 \) are defined as follows:

\[
(B.45) \quad t_1 := (pn - fn + 1)^2 + 4qfn, \quad t_2 := \frac{f + p - 2fp + 2(p - f)^2n}{p - f},
\]

\[
(B.46) \quad t_3 := n[f + p - 2fp + (p - f)^2n] + t_1 = 2(p - f)^2n^2 + 3(f + p - 2fp)n + 1.
\]

which satisfy \( t_1, t_2, t_3 > 0 \). In addition,

\[
(B.47) \quad t_2^2t_1 - t_3^2 = \frac{4fpq(1 - f)[1 + 2(f + p - 2fp)n]}{(p - f)^2} > 0,
\]

which implies that \( \partial h(n, f, p)/\partial n > 0 \) and that \( h(n, f, p) \) is strictly increasing in \( n \). So

\[
(B.48) \quad h(n, f, p) < h(\infty, f, p) = \frac{fpq(1 - f)}{(p - f)^3},
\]

\[
(B.49) \quad L(n, f, p) > \frac{(1 - f)p}{p - f} - \frac{fpq(1 - f)}{(p - f)^3n},
\]

which implies Eq. (73) given Eq. (B.42). Moreover, both inequalities in Eq. (73) are strict when \( n, f > 0 \).

B.5. Proof of Lemma 4.7. The proof is divided into two steps, in the first step we prove Eq. (74) and in the second step we prove Eq. (75).

Step 1: Proof of Eq. (74). From Eq. (13) we can deduce that

\[
(B.50) \quad \frac{\partial V(n, k, p, x)}{\partial x} = 1 - \frac{pq(n + 1)}{(pn + p - k + x)^2}, \quad \frac{\partial^2 V(n, k, p, x)}{\partial x^2} = \frac{2qp(n + 1)}{(pn + p - k + x)^3},
\]

which means \( V(n, k, p, x) \) is strictly convex in \( x \) for \( x \geq k - pn - p \) and has a unique minimum point at \( x = \tilde{a} = k - \kappa_1(n, p) \), where \( \kappa_1(n, p) \) is defined in Eq. (12). In addition, \( V(n, k, p, x) \) is strictly decreasing in \( x \) when \( k - pn - p < x \leq \tilde{a} \) and strictly increasing in \( x \) when \( x \geq \tilde{a} \). In conjunction with the following equation

\[
(B.51) \quad V(n, k, p, k + 1) - V(n, k, p, k) = \frac{p(n + 2)}{pn + p + 1} > 0,
\]
we can deduce that the minimum of $V(n,k,p,a)$ over $a \in \mathbb{N}_0$ is attained when $a < k + 1$, which implies Eq. (74).

**Step 2:** Proof of Eq. (75). If in addition $k$ is a nonnegative integer, say $k = 0$, then Eq. (B.51) implies that the minimum of $V(n,k,p,a)$ over $a \in \mathbb{N}_0$ is attained when $a \leq k$, which implies Eq. (75).

If $p(n + 2) \geq 2$, then

$$V(n,k,p) - V(n,k,p,k - 1) = \frac{p(n + 2) - 2}{pn + p - 1} \geq 0,$$

so the minimum of $V(n,k,p,a)$ over $a \in \mathbb{N}_0$ is attained when $a \leq k$, which implies Eq. (75). If $k \geq 2$, then $p(n + 2) > pn \geq k \geq 2$, so Eq. (75) holds.

Finally, we consider the case $1 \leq k < 2$. If $pn \geq 2$, then Eq. (75) holds according to the above discussion, so we can assume that $1 \leq k \leq pn < 2$ in the following discussion. Calculation shows that

$$V(n,k,p,2) - V(n,k,p,1) = \frac{k^2 - k[3 + 2p(n + 1)] + p^2(n^2 + 3n + 2) + 2p(n + 1) + 2}{(pn + p - k + 1)(pn + p - k + 2)}.$$

Here the denominator is positive; the numerator is strictly decreasing in $k$ for $0 \leq k < 2$ and is equal to

$$2 + 2p - pn + p^2(n + 2) > 0 \quad \text{if} \quad k = pn.$$

Therefore, $V(n,k,p,2) - V(n,k,p,1) \geq 0$ when $1 \leq k \leq pn \leq 2$, which implies Eq. (75) and completes the proof of Lemma 4.7.

**B.6. Proof of Lemma 4.8.** From Eq. (13) we can deduce that

$$\frac{\partial V(n,k,p,a)}{\partial k} = \frac{pq(n + 1)}{(pn + p - k + a)^2},$$

which implies that $V(n,k,p,a)$ is strictly increasing in $k$ when $a \geq 0$ given that $k \leq pn$ by assumption. So $U(n,k,p)$ is strictly increasing in $k$ according to the definition in Eq. (14) and Lemma 4.7. Consequently,

$$U(n,k,p) \leq U(n,pn,p) \leq V(n,pn,p,[\tilde{a}]) \leq 1 + U(n,pn,p,\tilde{a}) = 1 + 2\sqrt{pq(n + 1)},$$

where $\tilde{a} = pn - \kappa_1(n,p) = \sqrt{pq(n + 1)} - p > -1$.

According to the following equation,

$$\frac{\partial V(n,k,p,a)}{\partial n} = \frac{pq(a - k)}{(pn + p - k + a)^2}, \quad \frac{\partial V(n,k,p,a)}{\partial p} = \frac{(a - k)(n - k + a + 1)}{(pn + p - k + a)^2},$$

$V(n,k,p,a)$ is nonincreasing in $n$ and $p$ when $0 \leq a \leq k$. If in addition $p(n + 2) \geq 2$, $k = 0$, or $k \geq 1$, then $U(n,k,p) = \min_{\tilde{a} \in \mathbb{N}_0, a \leq k} V(n,k,p,a)$ according to Eq. (75) in Lemma 4.7, so $U(n,k,p)$ is nonincreasing in $n$ and $p$. Consequently,

$$U(n,k,p) \leq U(k/p,k,p) \leq V(k/p,k,p,[\tilde{a}]) \leq 1 + V(k/p,k,p,\tilde{a}) = 1 + 2\sqrt{q(k + p)},$$

where $\tilde{a} = k - \kappa_1(k/p,p) = \sqrt{q(k + p)} - p > -1$. 
\textbf{B.7. Proof of Lemma 4.9.} From Eq. (13) we can deduce that

\begin{equation}
\frac{\partial V(n, fn, p, a)}{\partial n} = \frac{pq(f + a)}{(pn - fn + p + a)^2}, \quad \frac{\partial V(n, fn, p, a)}{\partial f} = \frac{pqn(n + 1)}{(pn - fn + p + a)^2},
\end{equation}

which implies that $V(n, fn, p, a)$ is strictly increasing in $n$ when $a \geq 0$. So $U(n, fn, p)$ is strictly increasing in $n$ according to the definition in Eq. (14) and Eq. (74) in Lemma 4.7. If in addition $n > 0$, then $V(n, fn, p, a)$ is strictly increasing in $f$ when $a \geq 0$, so $U(n, fn, p)$ is strictly increasing in $f$. Alternatively, this conclusion follows from Lemma 4.8.

From Eq. (13) we can deduce that

\begin{equation}
\frac{\partial V(n, fn, p, a)}{\partial p} = -\frac{(f - a)(fn + a + 1)}{(pn - fn + p + a)^2},
\end{equation}

so $V(n, fn, p, a)$ is nonincreasing in $p$ when $fn \geq a$. If in addition $p(n + 2) \geq 2$, $fn = 0$, or $fn \geq 1$, then $U(n, fn, p) = \min_{a \in [0, a \leq fn]} V(n, fn, p, a)$ by Eq. (75) in Lemma 4.7, so $U(n, fn, p)$ is nonincreasing in $p$. Alternatively, this conclusion follows from Lemma 4.8.

Next, suppose $0 < f < p < 1$. The first inequality in Eq. (78) follows from the definition in Eq. (14); the second inequality in Eq. (78) follows from Eq. (20) and the fact that $V(n, fn, p, 0)$ is strictly increasing in $n$.

\textbf{APPENDIX C: PROOF OF PROPOSITION 4.10}

By virtue of Eqs. (57) and (58) we can deduce that

\begin{equation}
\mu_{n+1, k} \geq \frac{p(n + 1)[L(n, k, p) - 1]}{L(n, k, p) - p} = \frac{pn + k + 1 - \sqrt{(pn - k + 1)^2 + 4qk}}{2},
\end{equation}

This equation also holds when $k = n + 1$ given that $\mu_{n+1, n+1} = p(n + 1)$ and

\begin{equation}
k + 1 - L(n, n + 1, p) = \frac{1}{2}[2 + n + pn - \sqrt{q\left(qn^2 + 4n + 4\right)}] \\
\leq \frac{1}{2}[2 + n + pn - (qn + 2q)] = p(n + 1).
\end{equation}

Therefore,

\begin{equation}
\mu_{n, k} \geq k + 1 - L(n - 1, k, p) \quad \forall k = 0, 1, \ldots, n,
\end{equation}

which confirms Eq. (86).

The lower bound in Eq. (87) follows from Lemma 3.4, and the upper bound follows from Eqs. (55) and (C.1).

Next, we assume that $k \leq pn$. Then

\begin{equation}
\mu_{n, k} \geq k + 1 - L(n - 1, k, p) \geq k + 1 - L((k/p) - 1, k, p) \\
= k + \frac{q}{2} - \frac{1}{2}\sqrt{q(4k + q)} \geq k - \sqrt{qk},
\end{equation}

which confirms Eq. (88). Here the first inequality follows from Eq. (C.3), and the second inequality follows from the assumption that $k \leq pn$ and the fact that $L(n - 1, k, p)$ is nonincreasing in $n$ for $n \geq 0$ by Lemma 4.4 presented in Sec. 4.2.

Equation (89) follows from Eq. (71) in Lemma 4.5 and Eq. (87). Equation (90) follows from Eq. (73) in Lemma 4.6 and Eq. (87).
APPENDIX D: PROOFS OF LEMMAS 5.15 AND 5.16

D.1. Proof of Lemma 5.15. Before proving Lemma 5.15, we need to prepare an auxiliary result. Define

\[
\nu(t) := t - \left( 1 + \frac{t}{2} + \frac{t^2}{12} e^{-t/12} \right) (1 - e^{-t}).
\]

**Lemma D.1.** Suppose \( t > 0 \), then \( \nu(t) > 0 \).

**Proof.** Straightforward calculation shows that

\[
\nu(t)e^t = te^t - \left( 1 + \frac{t}{2} + \frac{t^2}{12} e^{-t/12} \right) (e^t - 1) = \sum_{j=0}^{\infty} \frac{a_j t^j}{j!},
\]

where the second equality is derived by considering the tailor expansion of the exponential function and \( a_j \) reads

\[
a_j = \frac{j}{2} - 1 - \frac{j(j - 1)}{12} \left( \frac{11}{12} \right)^{j-2} + \frac{j(j - 1)}{12} \left( -\frac{1}{12} \right)^{j-2}.
\]

When \( 4 \leq j \leq 12 \), it is straightforward to verify that \( a_j > 0 \). When \( j \geq 13 \), the function \( j(1/12)^{j-2} + j(1/12)^{j-2} \) decreases monotonically with \( j \) and is bounded from above by 5, which implies that

\[
a_j \geq \frac{j}{2} - 1 - \frac{j(j - 1)}{12} \left( \frac{11}{12} \right)^{j-2} \geq \frac{j}{2} - 1 - \frac{5(j - 1)}{12} = \frac{j - 7}{12} > 0.
\]

In a word, \( a_j > 0 \) for \( j \geq 4 \), which means \( \nu(t)e^t > 0 \) and \( \nu(t) > 0 \) for \( t > 0 \).

**Proof of Lemma 5.15.** According to Theorem 1 in Ref. [34] and its proof, \(-\omega_- (x)\) is strictly completely monotonic. So it remains to prove that \( \omega_+ (x) \) is strictly completely monotonic. Here our proof follows the proof of Theorem 2 in Ref. [34] with a mistake corrected. Calculation shows that

\[
\omega'_+(x) = \psi(x) + \frac{1}{2x} - \ln x + \frac{1}{12} \left( \frac{1}{x + \frac{1}{12}} \right)^2;
\]

\[
\omega''_+(x) = \psi'(x) - \frac{1}{2x^2} - \frac{1}{x} \ln x + \frac{1}{6} \left( \frac{1}{x + \frac{1}{12}} \right)^2 \int_0^\infty \frac{e^{-xt}}{1 - e^{-t}} \nu(t) dt;
\]

\[
\omega_+^{(m)}(x) = (-1)^m \int_0^\infty \frac{e^{-xt}}{1 - e^{-t}} t^{m-2} \nu(t) dt \quad \forall m = 2, 3, 4, \ldots,
\]

where \( \psi(x) \) is the digamma function, that is, the logarithmic derivative of the gamma function, and \( \nu(t) \) is defined in Eq. (D.1). According to Lemma D.1, we have \( \nu(t) > 0 \) for \( t > 0 \) (the proof of this fact in Ref. [34] is problematic), which implies that \( \omega''_+(x) \) is strictly completely monotonic. In particular, we have \( \omega''_+(x) > 0 \) for \( x > 0 \).

In addition,

\[
\lim_{x \to \infty} \omega'_+(x) = \lim_{x \to \infty} \omega_+(x) = 0.
\]

Therefore, \( \omega'_+(x) < 0 \) for \( x > 0 \) given that \( \omega''_+(x) > 0 \) for \( x > 0 \). This result in turn implies that \( \omega_+(x) > 0 \) for \( x > 0 \), so \( \omega_+(x) \) is strictly completely monotonic.
D.2. Proof of Lemma 5.16. Direct calculation shows that
\begin{align}
\ln \rho(y) & = \psi(y) + \frac{1}{y} - \ln y, \\
\ln \varrho(y) & = \ln y - \psi(y) - \frac{1}{2y},
\end{align}
where \( \psi(y) \) is the digamma function. Both \( \psi(y) + (1/y) - \ln y \) and \( \ln y - \psi(y) - [1/(2y)] \) are strictly completely monotonic according to Theorem 1.3 in Ref. [38] (in the theorem the word "strictly" is not mentioned explicitly, but its proof actually shows this stronger result), so \( \ln \rho(y) \)' and \( \ln \varrho(y) \)' are strictly completely monotonic, which imply that \( 1/\rho(y) \) and \( 1/\varrho(y) \) are strictly logarithmically completely monotonic.

Next, according to Lemma 5.15 and the definitions in Eq. (147), \( 1/\varrho(y) \), and \( \varrho_+(y) \) are strictly logarithmically completely monotonic.

Recall that any function that is strictly logarithmically completely monotonic is strictly completely monotonic. So \( 1/\rho(y) \), \( 1/\varrho(y) \), and \( \varrho_+(y) \) are strictly completely monotonic given that they are strictly logarithmically completely monotonic as shown above.

Finally, Eq. (148) follows from the following equation
\begin{align}
\varrho_+(y) < \varrho_+(x), \quad \varrho_-(y) > \varrho_-(x),
\end{align}
given that \( \varrho_+(y) \) is strictly decreasing, while \( \varrho_-(y) \) is strictly increasing.

APPENDIX E: COMPARISON WITH BOUNDS OF MCKAY [33]

E.1. Comparison of asymptotic bounds for the ratio \( \bar{B}_{n,k}(p)/b_{n,k}(p) \). Here we compare bounds for the ratio \( \bar{B}_{n,k}(p)/b_{n,k}(p) \) presented in Theorem 5.9 with the counterparts derived by McKay [33], assuming that \( n, k \in \mathbb{N} \), \( 0 < p < 1 \), and \( pm < k \leq n \). To simplify the discussion we will focus on the ratio of the upper bound over the lower bound in the large-\( n \) limit.

Theorem 2 in Ref. [33] states that
\begin{align}
\sigma Y(x) \leq \bar{B}_{n,k}(p)/b_{n-1,k-1}(p) \leq \sigma Y(x)e^{E_{n,k}(p)},
\end{align}
where
\begin{align}
\sigma = \sqrt{npq}, \quad q = 1-p, \quad x = \frac{|k - pn|}{\sigma},
\end{align}
and
\begin{align}
Y(x) = e^{x^2/2} \int_{x}^{\infty} e^{-t^2/2} dt, \quad E_{n,k}(p) = \min \left\{ \frac{\pi}{8npq}, \frac{1}{|k - pn|} \right\}.
\end{align}
Thanks to the equality \( b_{n-1,k-1}(p) = (k/pn)b_{n,k}(p) \), which follows from the definition in Eq. (1), Eq. (E.1) implies that
\begin{align}
k\sqrt{\frac{q}{pm}} Y(x) \leq \bar{B}_{n,k}(p)/b_{n,k}(p) \leq k\sqrt{\frac{q}{pm}} Y(x)e^{E_{n,k}(p)}.
\end{align}
Suppose \( k = fn \) with \( p < f \leq 1 \) and \( n \) is sufficiently large; then the ratio of the upper bound over the lower bound in Eq. (E.4) reads
\begin{align}
\exp \left( \frac{1}{(f-p) n} \right) = 1 + \frac{\gamma_1}{n} + O(n^{-2}), \quad \gamma_1 = \frac{1}{f-p}.
\end{align}
By contrast, our Theorem 5.9 yields the following bounds,
\begin{align}
\bar{L}(n, fn, p) \leq \frac{\bar{B}_{n,fn}(p)}{b_{n,fn}(p)} \leq \bar{U}(n, fn, p).
\end{align}
Comparison between our bounds for the ratio $\bar{B}_{n,fn}(p)/b_{n,fn}(p)$ presented in Theorem 5.9 and the counterparts derived by McKay [33] in the large-$n$ limit, where $\bar{B}_{n,fn}(p)$ is the upper tail probability. In the green region (with $\gamma_2 > \gamma_1$) the bounds in Ref. [33] are more accurate; in the red region (with $\gamma_2 < \gamma_1$), our bounds are more accurate. The boundary is determined by Eq. (E.8).

The ratio of the upper bound over the lower bound reads

\[
\frac{U(n,fn,p)}{L(n,fn,p)} = \frac{U(n,(1-f)n,q)}{L(n,(1-f)n,q)} = 1 + \frac{\gamma_2}{n} + O(n^{-2}), \quad \gamma_2 = \frac{(1-f)p^2}{f(f-p)^2}.
\]

Note that $\gamma_2/\gamma_1 = (1-f)p^2/[f(f-p)]$ decreases monotonically with $f$ for $p < f \leq 1$. In addition, $\gamma_2 = \gamma_1$ iff $f = f^*$ with

\[
f^* = \frac{p}{2}(q + \sqrt{4 + q^2}).
\]

If $p < f < f^*$ ($f$ is close to $p$), then $\gamma_2 > \gamma_1$, so the bounds in Ref. [33] are more accurate. If instead $f^* < f \leq 1$ ($f$ is not so close to $p$), then $\gamma_2 < \gamma_1$, so our bounds are more accurate. The two parameter ranges are illustrated in Fig. 2. In addition, our bounds do not involve integrals and are more explicit than the bounds in Ref. [33].

**E.2. Derived bounds based on Ref. [33].** Here we derive a number of related bounds for the ratio $B_{n,k}(p)/b_{n,k}(p)$ and the upper tail probability $\bar{B}_{n,k}(p)$ that are of independent interest.

First, we present a simple upper bound for the function $E_{n,k}(p)$, assuming that $n, k \in \mathbb{N}$, $0 < p < 1$, and $pn < k \leq n - 1$ (the special case with $k = n$ is not essential).

**PROPOSITION E.1.** If $n, k \in \mathbb{N}$, $0 < p < 1$, and $pn < k \leq n - 1$, then $E_{n,k}(p) \leq 3/2$.

**PROOF.** By assumption we have $p \leq 1 - (1/n)$. If in addition $p \geq 1/(3n)$, then

\[
E_{n,k}(p) \leq \sqrt{\frac{\pi}{8npq}} \leq \sqrt{\frac{\pi}{3(1-1/3n)}} \leq \frac{3}{4}\sqrt{\pi} < \frac{3}{2}.
\]

If $p < 1/(3n)$ instead, then

\[
E_{n,k}(p) \leq \frac{1}{k-pn} < \frac{1}{1-\frac{1}{3}} = \frac{3}{2}.
\]

\[\square\]
Next, we provide upper and lower bounds for the function $Y(x)$ by virtue of Eqs. (183), (185), and (186) in Sec. 6,

\[(E.11) \quad \tilde{\ell}(x) \leq Y(x) \leq \tilde{\nu}(x) \quad \forall x \geq 0,\]

where

\[(E.12) \quad \tilde{\ell}(x) := \sqrt{2\pi} \ell(x) = \frac{1}{2} \left( \sqrt{4 + x^2} - x \right), \quad \tilde{\nu}(x) := \sqrt{2\pi} \nu(x) = \begin{cases} 2 - x & x \leq 1, \\ \frac{1}{2} & x \geq 1. \end{cases}\]

Combining Eqs. (E.4) and (E.11) we can obtain bounds for $\bar{B}_{n,k}(p)/b_{n,k}(p)$ that do not involve integrals and are easy to compute,

\[(E.13) \quad k \sqrt{\frac{q}{pn}} \tilde{\ell}(x) \leq \frac{\bar{B}_{n,k}(p)}{b_{n,k}(p)} \leq k \sqrt{\frac{q}{pn}} \tilde{\nu}(x)e^{E_{n,k}(p)} \leq 2e^{3/2}k \sqrt{\frac{q}{pn}} \tilde{\ell}(x),\]

where the last inequality follows from Proposition E.1 above and Eq. (190) in Proposition 6.4. The two propositions also show that the lower bound and the first upper bound for $\bar{B}_{n,k}(p)/b_{n,k}(p)$ in this equation are asymptotically tight and universally bounded.

Combining Eqs. (E.4) and (E.11) with Eq. (112) in Proposition 5.4, we can further deduce upper and lower bounds for the upper tail probability $\bar{B}_{n,k}(p)$ as follows,

\[(E.14) \quad \sqrt{\frac{qk}{pm}} \varphi_-(n,k)\tilde{\ell}(x)e^{-nD(\frac{x}{n})||p||} \leq \sqrt{\frac{qk}{pm}} \varphi_-(n,k)Y(x)e^{-nD(\frac{x}{n})||p||} < \bar{B}_{n,k}(p)\]

\[< \sqrt{\frac{qk}{pm}} \varphi_+(n,k)Y(x)e^{E_{n,k}(p)}e^{-nD(\frac{x}{n})||p||} \leq \sqrt{\frac{qk}{pm}} \varphi_+(n,k)\tilde{\nu}(x)e^{E_{n,k}(p)}e^{-nD(\frac{x}{n})||p||},\]

where $m = n - k$ and $\varphi_\pm(n,k)$ are defined in Eq. (97). It is not difficult to verify that the final upper bound and the final lower bound in Eq. (E.14) satisfy criteria (C1-C3) presented in the introduction. To be specific, the ratio of the upper bound over the lower bound reads

\[(E.15) \quad \frac{\varphi_+(n,k)\tilde{\nu}(x)e^{E_{n,k}(p)}}{\varphi_-(n,k)\tilde{\ell}(x)} \leq 2e^{\frac{3}{2} + \frac{2n}{2600}} = 2e^{\frac{3929}{2600}} \approx 9.06391,\]

where the inequality follows from Eq. (109) in Lemma 5.3, Eq. (190) in Proposition 6.4, and Proposition E.1. This bound is much larger than the upper bound 89/44 that appears in Theorem 5.10 (cf. Theorem 5.6).

Thanks to the relation between the upper and lower tail probabilities presented in Eq. (131), all the above results have analogs for the lower tail probability $\bar{B}_{n,k}(p)$. Notably, Eq. (E.14) has the following analog, assuming that $n, k \in \mathbb{N}$, $0 < p < 1$, and $1 \leq k < pn$,

\[(E.16) \quad \sqrt{\frac{pm}{qk}} \varphi_-(n,k)\tilde{\ell}(x)e^{-nD(\frac{x}{n})||p||} \leq \sqrt{\frac{pm}{qk}} \varphi_-(n,k)Y(x)e^{-nD(\frac{x}{n})||p||} < \bar{B}_{n,k}(p)\]

\[< \sqrt{\frac{pm}{qk}} \varphi_+(n,k)Y(x)e^{E_{n,k}(p)}e^{-nD(\frac{x}{n})||p||} \leq \sqrt{\frac{pm}{qk}} \varphi_+(n,k)\tilde{\nu}(x)e^{E_{n,k}(p)}e^{-nD(\frac{x}{n})||p||},\]

where all the functions involved are defined as before.

**APPENDIX F: PROOFS OF LEMMAS 6.1 AND 6.2**

**F.1. Proof of Lemma 6.1.** When $j = 0$, we have $B_{n,j}(k/n)/b_{n,j}(k/n) = 1$ by definition and Eq. (167) holds.
When \( j \geq 1 \), from Eq. (32) we can deduce that
\[
\frac{b_{n,j-1}(k/n)}{b_{n,j}(k/n)} = \frac{j(n-k)}{k(n-j+1)},
\]
which implies that \( b_{n,j-1}(k/n)/b_{n,j}(k/n) \) and \( B_{n,j}(k/n)/b_{n,j}(k/n) \) for \( j = 1, 2, \ldots, k \) are strictly increasing in \( n \). In addition, the above equation implies that
\[
\lim_{n \to \infty} \frac{b_{n,j-1}(k/n)}{b_{n,j}(k/n)} = \frac{j}{k}, \quad \lim_{n \to \infty} \frac{B_{n,j}(k/n)}{b_{n,j}(k/n)} = \sum_{l=0}^{j} \frac{\Gamma(j+1)}{\Gamma(j-l+1)},
\]
which confirms Eq. (167).

The equalities in Eqs. (168) and (169) follow from Eq. (167) and the definition of \( \theta_k \) in Eq. (171). When \( k = 1 \), the inequality in Eq. (168) can be verified directly. When \( k \geq 2 \), the inequality can be proved by virtue of the Stirling approximation in Eq. (98) and the lower bound for \( \theta_k \) in Eq. (172) as follows,
\[
\frac{e^k}{2k} - \theta_k - \sqrt{\frac{\pi k}{2}} < \sqrt{\frac{\pi k}{2}} \left[ \exp \left( \frac{1}{12k} \right) - 1 \right] - \theta_k < \frac{\pi 2\sqrt{k}}{2} - \frac{1}{3} < 1 - \sqrt{\frac{\pi}{2}}.
\]
The inequality in Eq. (169) follows from the counterpart in Eq. (168).

Next, by virtue of Eqs. (11), (100), and (112) we can deduce that
\[
\lim_{n \to \infty} \frac{L(n, \lfloor fn - j \rfloor, f)}{\sqrt{n}} = \lim_{n \to \infty} \frac{L(n, fn - j, f)}{\sqrt{n}} = \sqrt{f(1-f)},
\]
which imply Eq. (170), given that \( \lim_{n \to \infty} B_{n, \lfloor fn - j \rfloor}(f) = 1/2. \)

**F.2. Proof of Lemma 6.2.** The proof is divided into two steps: In the first step we prove Eq. (176) in the four special cases \( k = 1, 2, n - 1, n - 2 \) and in the second step we prove Eq. (176) in the case \( 3 \leq k \leq n - 3 \).

**Step 1:** Proof of Eq. (176) in the four special cases \( k = 1, 2, n - 1, n - 2 \). If \( k = 1 \), then \( n \geq 2 \) and
\[
B_{n,1-1}(k/n) = b_{n,1-1}(k/n) = \left( \frac{n-1}{n} \right)^n, \quad L(n, k-1, k/n) = 1,
\]
so Eq. (176) holds in the case \( k = 1 \).

If \( k = 2 \), then \( n \geq 3 \) and
\[
B_{n,2-1}(k/n) = \frac{3n-2}{n-2} \left( \frac{n-2}{n} \right)^n, \quad b_{n,2-1}(k/n) = 2 \left( \frac{n-2}{n} \right)^{n-1},
\]
\[
L(n, k-1, k/n) = \sqrt{\frac{2n-2}{n}}.
\]
Therefore,
\[
\frac{B_{n,2-1}(k/n)}{b_{n,2-1}(k/n)L(n, k-1, k/n)} = \frac{3n-2}{\sqrt{8n(n-1)}} \leq \sqrt{\frac{9}{8}} < \sqrt{\frac{\pi}{2}},
\]
which confirms Eq. (176) in the case \( k = 2 \).
If \( k = n - 1 \), then

\[
B_{n,k-1}(k/n) = 1 - \left( \frac{k}{k+1} \right)^{k+1} - \left( \frac{k}{k+1} \right)^k,
\]

(F.10)

\[
b_{n,k-1}(k/n) = \frac{1}{2} \left( \frac{k}{k+1} \right)^k,
\]

(F.11)

\[
L(n, k-1, k/n) = \sqrt{\frac{2k}{k+1}}.
\]

Therefore,

\[
\frac{B_{n,k-1}(k/n)}{b_{n,k-1}(k/n)L(n, k-1, k/n)} = \sqrt{2} \left[ \left( \frac{k}{k+1} \right)^{k+\frac{1}{2}} - \sqrt{\frac{k}{k+1}} - \sqrt{\frac{k+1}{k}} \right]
\]

\[
\leq 4 - 2\sqrt{2} < \frac{\pi}{2},
\]

which confirms Eq. (176) in the case \( k = n - 1 \).

If \( k = n - 2 \), then

\[
B_{n,k-1}(k/n) = 1 - \left( \frac{k}{k+2} \right)^{k+2} - 2 \left( \frac{k}{k+2} \right)^{k+1} - 2 \frac{k+1}{k+2} \left( \frac{k}{k+2} \right)^k,
\]

(F.13)

\[
b_{n,k-1}(k/n) = \frac{4k+1}{3k+2} \left( \frac{k}{k+2} \right)^k,
\]

(F.14)

\[
L(n, k-1, k/n) = \sqrt{\frac{3k}{k+2}}.
\]

Therefore,

\[
\frac{B_{n,k-1}(k/n)}{b_{n,k-1}(k/n)L(n, k-1, k/n)} = \frac{\sqrt{3}}{4} \left[ \frac{k+2}{k+1} \left( \frac{k+2}{k} \right)^{k+\frac{1}{2}} - \frac{3k+4}{k+1} \sqrt{\frac{k}{k+2}} - 2 \frac{k+2}{k} \right]
\]

\[
\leq \frac{\sqrt{3}}{4} (\frac{9\sqrt{3}}{2} - 5) = \frac{27}{8} - \frac{5\sqrt{3}}{4} < \frac{\pi}{2},
\]

which confirms Eq. (176) in the case \( k = n - 2 \). Here the first inequality follows from the following inequalities:

\[
\frac{k+2}{k+1} \left( \frac{k+2}{k} \right)^{k+\frac{1}{2}} \leq \frac{9\sqrt{3}}{2}, \quad \frac{3k+4}{k+1} \sqrt{\frac{k}{k+2}} + 2 \frac{k+2}{k} \geq 5.
\]

(F.16)

Above analysis shows that Eq. (176) holds when \( k = 1, 2, n - 1, \) or \( n - 2 \), so we can exclude these cases in the following discussion.

**Step 2:** Proof of Eq. (176) in the case \( 3 \leq k \leq n - 3 \). Define \( \zeta_{n,k} \) by the following equation

\[
\frac{1}{2} = B_{n,k-1}(k/n) + \zeta_{n,k} b_{n,k}(k/n);
\]

(F.17)

then

\[
B_{n,k-1}(k/n) = \frac{1}{2} - \zeta_{n,k} b_{n,k}(k/n).
\]

(F.18)

It is known that [28]

\[
\frac{1}{3} < \zeta_{n,k} \leq \frac{1}{2} \quad \text{if} \quad n \geq 2k,
\]

(F.19)

\[
\frac{1}{2} \leq \zeta_{n,k} < \frac{2}{3} \quad \text{if} \quad n \leq 2k.
\]
By definition in Eq. (1) and the Stirling approximation in Eq. (98) (cf. Proposition 5.4) we can deduce that

\[
(F.20) \quad b_{n,k}(k/n) \geq \frac{n}{2\pi k(n-k)} \exp \left[ -\frac{1}{12n+1} - \frac{1}{12k} - \frac{1}{12(n-k)} \right].
\]

In addition, Eqs. (11) and (32) yield

\[
(F.21) \quad L(n,k-1,k/n) = \frac{\sqrt{k(n-k+1)}}{n}, \quad b_{n,k-1}(k/n) = \frac{n-k}{n-k+1} b_{n,k}(k/n).
\]

The above two equations together imply that

\[
(F.22) \quad \frac{B_{n,k-1}(k/n)}{\sqrt{\pi} b_{n,k-1}(k/n)L(n,k-1,k/n)} = \sqrt{\frac{2}{\pi}} \sqrt{\frac{n(n-k+1)}{k(n-k)^2}} \left( \frac{1}{2b_{n,k}(k/n)} - \zeta_{n,k} \right)
\]

\[
\leq \sqrt{\frac{n-k+1}{n-k}} \left\{ \exp \left[ \frac{1}{12k} + \frac{1}{12(n-k)} - \frac{1}{12n+1} \right] - \sqrt{\frac{2}{\pi}} \sqrt{\frac{n}{k(n-k)}} \zeta_{n,k} \right\}
\]

\[
\leq \left( 1 + \frac{1}{2(n-k)} \right) \left( 1 + \frac{n}{11k(n-k)} \right) - \sqrt{\frac{2}{\pi}} \sqrt{\frac{n}{k(n-k)}} \zeta_{n,k}
\]

\[
\leq 1 + \frac{n}{k(n-k)} \left( \frac{1}{2\sqrt{n-k}} + \frac{7\sqrt{6}}{198} \right) - \sqrt{\frac{2}{\pi}} \zeta_{n,k}.
\]

Here the first equality follows from Eqs. (F.18) and (F.21). The first inequality follows from Eq. (F.20). The second inequality follows from the following equation

\[
(F.23) \quad 1 < \sqrt{\frac{n-k+1}{n-k}} < 1 + \frac{1}{2(n-k)}, \quad \exp \left[ \frac{1}{12k} + \frac{1}{12(n-k)} - \frac{1}{12n+1} \right] < 1 + \frac{n}{11k(n-k)}.
\]

The third inequality in Eq. (F.22) follows from the following equation

\[
(F.24) \quad \left( 1 + \frac{1}{2(n-k)} \right) \frac{n}{11k(n-k)} \leq \frac{7\sqrt{6}}{66} \sqrt{\frac{n}{k(n-k)}} \sqrt{\frac{n}{k(n-k)}} \leq \frac{7\sqrt{6}}{198} \sqrt{\frac{n}{k(n-k)}},
\]

\[
\frac{1}{n-k} \leq \sqrt{\frac{n}{k(n-k)}} \frac{1}{\sqrt{n-k}},
\]

given that 3 \(\leq k \leq n-3\), so that \(n/[k(n-k)] \leq 2/3\).

If \(n/2 \leq k \leq n-3\), that is, \(3 \leq n-k \leq k\), then \(\zeta_{n,k} \geq 1/2\) by Eq. (F.19), which implies that

\[
(F.25) \quad \frac{1}{2\sqrt{n-k}} + \frac{7\sqrt{6}}{198} - \sqrt{\frac{2}{\pi}} \zeta_{n,k} \leq \frac{1}{2\sqrt{3}} + \frac{7\sqrt{6}}{198} - \frac{1}{2} \sqrt{\frac{2}{\pi}} < 0.
\]

If \(k \leq n-8\), that is, \(n-k \geq 8\), then \(\zeta_{n,k} > 1/3\) by Eq. (F.19), which implies that

\[
(F.26) \quad \frac{1}{2\sqrt{n-k}} + \frac{7\sqrt{6}}{198} - \sqrt{\frac{2}{\pi}} \zeta_{n,k} < \frac{1}{2\sqrt{8}} + \frac{7\sqrt{6}}{198} - \frac{1}{3} \sqrt{\frac{2}{\pi}} < 0.
\]

In both cases Eq. (176) holds. In the remaining case with \(n-7 \leq k < n/2\), Eq. (176) can be verified by direct calculation because such a case can happen only when \(n \leq 13\). This observation completes the proof of Lemma 6.2.
APPENDIX G: PROOF OF LEMMA 6.3

G.1. Auxiliary lemmas. Here we prove two auxiliary lemmas that are required to prove Lemma 6.3, without assuming that \( k \) and \( n \) are integers.

**Lemma G.1.** Suppose \( k \geq 2/7 \) and \( n \geq 5k/3 \). Then

\[
\exp \left[ \frac{1}{12k} + \frac{1}{12(n-k)} - \frac{1}{12n+1} \right] \leq 1 + \frac{n}{n-k} \exp \left( \frac{1}{12k} \right) - 1.
\]

**Proof of Lemma G.1.** The inequality in Eq. (G.1) is equivalent to the following inequality,

\[
k \exp \left( -\frac{1}{12k} \right) + (n-k) \exp \left[ \frac{1}{12(n-k)} - \frac{1}{12n+1} \right] \leq n.
\]

By assumption we can deduce that

\[
\frac{1}{12(n-k)} - \frac{1}{12n+1} \leq \frac{1}{12k},
\]

\[
\exp \left[ \frac{1}{12(n-k)} - \frac{1}{12n+1} \right] \leq 1 + 12k \left[ \exp \left( \frac{1}{12k} \right) - 1 \right] \left[ \frac{1}{12(n-k)} - \frac{1}{12n+1} \right].
\]

Therefore,

\[
k \exp \left( -\frac{1}{12k} \right) + (n-k) \exp \left[ \frac{1}{12(n-k)} - \frac{1}{12n+1} \right] \\
\leq k \exp \left( -\frac{1}{12k} \right) + n-k + 12k(n-k) \left[ \exp \left( \frac{1}{12k} \right) - 1 \right] \left[ \frac{1}{12(n-k)} - \frac{1}{12n+1} \right] \\
= n + k \left[ \exp \left( \frac{1}{12k} \right) + \exp \left( -\frac{1}{12k} \right) - 2 \right] - \frac{12k(n-k)}{12n+1} \left[ \exp \left( \frac{1}{12k} \right) - 1 \right] \\
\leq n + \frac{1}{40} - \frac{n-k}{12n+1} \leq n + \frac{1}{40} - \frac{2k}{3(20k+1)} \leq n + \frac{1}{40} - \frac{4}{141} < n,
\]

which confirms Eq. (G.2) and implies Eq. (G.1). Here the first inequality follows from Eq. (G.4); the second inequality follows from the following two inequalities

\[
\exp \left( \frac{1}{12k} \right) + \exp \left( -\frac{1}{12k} \right) - 2 \leq \frac{1}{40k}, \quad \exp \left( \frac{1}{12k} \right) - 1 \geq \frac{1}{12k},
\]

given that \( k \geq 2/7 \) and \( 1/(12k) \leq 7/24 \); the third and fourth inequalities in Eq. (G.5) follow from the assumption that \( k \geq 2/7 \) and \( n \geq 5k/3 \). \( \square \)

**Lemma G.2.** Suppose \( k \geq 1 \) and \( n \geq k \). Then

\[
\frac{1 + \sqrt{1+4k}}{2L(n,k,k/n)} \sqrt{\frac{n-k}{n}} \leq 1 - \frac{k}{2n\sqrt{1+4k}}.
\]

Meanwhile, the function

\[
n \left[ \frac{1 + \sqrt{1+4k}}{2L(n,k,k/n)} - 1 \right]
\]

is strictly decreasing in \( n \). If in addition \( n \geq jk \) with \( j \geq 1 \), then

\[
\frac{1 + \sqrt{1+4k}}{2L(n,k,k/n)} \leq 1 + \frac{jk}{n} \left[ \sqrt{\frac{1 + \sqrt{1+4k}}{j + \sqrt{j + 4(j-1)k} - 1}} \right].
\]
**Proof of Lemma G.2.** Let

\[ s(k, x) := \frac{1 + \sqrt{1 + 4k}}{1 + \sqrt{1 + 4k - 4kx}} \sqrt{1 - x}, \quad 0 \leq x \leq 1; \]

then \( s(k, x) \) is continuous in \( x \) for \( 0 \leq x \leq 1 \). In addition, \( s(k, 0) = 1 \) and

\[ \frac{\partial s}{\partial x} = \frac{1 + \sqrt{1 + 4k}}{2\sqrt{1 - x}(1 + 4y + \sqrt{1 + 4y})} < 0 \quad \forall 0 \leq x < 1, \quad \left. \frac{\partial s}{\partial x} \right|_{x=0} = -\frac{1}{2\sqrt{1 + 4k}}, \]

where \( y = k(1 - x) \). Therefore, \( s(k, x) \) is strictly decreasing and concave in \( x \) for \( 0 \leq x \leq 1 \), which means

\[ s(k, x) \leq 1 - \frac{x}{2\sqrt{1 + 4k}} \quad \forall 0 \leq x \leq 1. \]

This equation in turn implies Eq. (G.7), given that the left hand side in Eq. (G.7) is equal to \( s(k, k/n) \).

To prove the monotonicity of the function defined in Eq. (G.8), it suffices to prove that

\[ n_1 \left[ \frac{1 + \sqrt{1 + 4k}}{2L(n, k, k/n_1)} - 1 \right] > n_2 \left[ \frac{1 + \sqrt{1 + 4k}}{2L(n, k, k/n_2)} - 1 \right] \quad \forall n_2 > n_1 \geq k. \]

Let \( x_1 := k/n_1 \) and \( x_2 := k/n_2 \); then the above equation is equivalent to

\[ \frac{1}{x_1} \left[ \frac{1 + \sqrt{1 + 4k}}{1 + \sqrt{1 + 4k - 4kx_1}} - 1 \right] > \frac{1}{x_2} \left[ \frac{1 + \sqrt{1 + 4k}}{1 + \sqrt{1 + 4k - 4kx_2}} - 1 \right] \]

for \( 0 < x_2 < x_1 \leq 1 \). Now this conclusion follows from the fact that the function

\[ \frac{1 + \sqrt{1 + 4k}}{1 + \sqrt{1 + 4k - 4kx}} - 1 \]

is strictly increasing and strictly convex in \( x \) for \( 0 \leq x \leq 1 \) and is equal to 0 when \( x = 0 \). Therefore, the function defined in Eq. (G.8) is strictly decreasing in \( n \).

If in addition \( n \geq jk \) with \( j \geq 1 \), then

\[ n \left[ \frac{1 + \sqrt{1 + 4k}}{2L(n, k, k/n)} - 1 \right] \leq jk \left[ \frac{1 + \sqrt{1 + 4k}}{2L(jk, k, 1/j)} - 1 \right] = jk \left[ \frac{\sqrt{j} (1 + \sqrt{1 + 4k})}{\sqrt{j} + \sqrt{j + 4(j-1)k} - 1} \right], \]

which implies Eq. (G.9).

**G.2. Proof of Lemma 6.3.** The proof is divided into three steps: In the first step we prove Eq. (178), in the second step we prove Eq. (177) for the case \( k \geq 16 \), and in the third step we prove Eq. (177) for the case \( k \leq 15 \). To simplify the notation, \( B_{n,k}(k/n) \) and \( b_{n,k}(k/n) \) are abbreviated as \( B_{n,k} \) and \( b_{n,k} \), respectively, in the following proof. Several auxiliary functions defined in the proof are independent of those functions defined in the proofs of previous results.
Step 1: Proof of Eq. (178), assuming that $n \leq 2k$. By definitions in Eqs. (1) and (11) and the Stirling approximation in Eq. (98) we can deduce that

\begin{equation}
B_{n,k} = B_{n,k-1}(k/n) + b_{n,k} = \frac{1}{2} + (1 - \zeta_{n,k})b_{n,k},
\end{equation}

\begin{equation}
L(n, k, k/n) = \frac{1}{2} \left(1 + \sqrt{1 + \frac{4k(n-k)}{n}}\right),
\end{equation}

where the two inequalities in Eq. (G.18) follow from the Stirling approximation in Eq. (98), and $\zeta_{n,k}$ is defined in Eq. (F.17). Therefore,

\begin{equation}
\frac{B_{n,k}}{b_{n,k}} = \frac{1}{2b_{n,k}} + 1 - \zeta_{n,k}
\end{equation}

\begin{equation}
\leq \frac{e^{k} \Gamma(k+1)}{2k^{k}} \sqrt{\frac{n-k}{n}} \exp \left[\frac{1}{12n+1} - \frac{1}{12(n-k)}\right] + 1 - \zeta_{n,k}
\end{equation}

\begin{equation}
\leq \sqrt{\frac{\pi k(n-k)}{2n}} \exp \left[\frac{1}{12k} + \frac{1}{12(n-k)} - \frac{1}{12n+1}\right] + 1 - \zeta_{n,k}
\end{equation}

\begin{equation}
\leq \sqrt{\frac{\pi k(n-k)}{2n}} \left[1 + \frac{n}{11k(n-k)}\right] + 1 - \zeta_{n,k}.
\end{equation}

If $\zeta_{n,k} \geq 1 - \sqrt{\pi/8}$, which holds when $n \leq 2k$ by Eq. (F.19), then Eq. (G.20) and the third inequality in Eq. (G.21) yield

\begin{equation}
\frac{B_{n,k}}{b_{n,k}} \leq \left(1 + \frac{1}{11z}\right) \sqrt{\frac{\pi z}{2}} + 1 - \zeta_{n,k} \leq \left(1 + \frac{1}{11z}\right) \sqrt{\frac{\pi z}{2}} + \sqrt{\frac{\pi}{8}},
\end{equation}

\begin{equation}
\frac{B_{n,k}}{b_{n,k}L(n, k, k/n)} = \frac{2B_{n,k}}{(1 + \sqrt{1 + 4z})b_{n,k}} \leq \frac{\pi}{2} g(z),
\end{equation}

where

\begin{equation}
z := \frac{k(n-k)}{n}, \quad g(z) := \frac{2(1 + \frac{1}{11z})\sqrt{z} + 1}{1 + \sqrt{1 + 4z}}.
\end{equation}

The derivative of $g(z)$ over $z$ reads

\begin{equation}
g'(z) = \frac{(11z - 1)\sqrt{1+4z} + 3z - 22z^{3/2} - 1}{11z^{3/2}\sqrt{1+4z}(1 + \sqrt{1+4z})^{2}}.
\end{equation}

By assumption we have $z \geq 1/2$ and

\begin{equation}
(11z - 1)\sqrt{1+4z} + 3z - 22z^{3/2} - 1
\end{equation}

\begin{equation}
\geq (11z - 1)2\sqrt{z}\left(1 + \frac{\sqrt{6} - 2}{4z}\right) + 3z - 22z^{3/2} - 1
\end{equation}
\[
\frac{B_{n,k}}{b_{n,k} L(n, k, k/n)} \leq \sqrt{\frac{\pi z}{2}} \left( 1 + \frac{c_k}{z} \right) + 1 - \zeta_{n,k} \leq \sqrt{\frac{\pi}{2}} \left( 1 + \frac{c_k}{z} \right) \sqrt{z} + 1 - \theta_k,
\]
which confirms Eq. (178).

**Step 2:** Proof of Eq. (177) in the case \( k \geq 16 \). Thanks to Eq. (178) proved above, we can assume that \( n > 2k \), which means \( n - k > k \) and \( 1/2 < k/2 < z < k \) given the assumption \( 1 \leq k \leq n - 1 \). Then Lemma G.1 implies that

\[
\exp \left[ \frac{1}{12k} + \frac{1}{12(n-k)} - \frac{1}{12n+1} \right] \leq 1 + c_k \frac{n}{k(n-k)} = 1 + \frac{c_k}{z},
\]
where the coefficient \( c_k \) is defined as

\[
c_k := k \exp \left( \frac{1}{12k} \right) - k,
\]
which is strictly decreasing in \( k \) and satisfies

\[
\frac{1}{12} < c_k \leq \exp \left( \frac{1}{12} \right) - 1 < \frac{1}{11}.
\]
In addition, it is known that \( \zeta_{n,k} \geq \theta_k \), where \( \theta_k \) is defined by Ramanujan’s equation in Eq. (171) [28]. Therefore, the second inequality of Eq. (G.21) and Eq. (G.28) imply that

\[
\frac{B_{n,k}}{b_{n,k} L(n, k, k/n)} = \frac{2B_{n,k}}{(1 + \sqrt{1+4z})b_{n,k}} \leq \sqrt{\frac{\pi}{2}} h_k(z),
\]
where the function \( h_k(z) \) is defined as

\[
h_k(z) := \frac{2(1 + \frac{a_k}{z}) \sqrt{z} + a_k}{1 + \sqrt{1+4z}}, \quad a_k := 2 \sqrt{\frac{2}{\pi}} (1 - \theta_k).
\]
Here \( \theta_k \) is strictly decreasing in \( k \) and satisfies Eq. (172) [44, 49], so \( a_k \) is strictly increasing in \( k \) and satisfies

\[
1.02266 \approx \sqrt{\frac{2}{\pi}(4 - e)} = a_1 < a_k < \frac{4}{3} \sqrt{\frac{2}{\pi}} \approx 1.06385.
\]
Calculation shows that

\[
h'_k(z) = \frac{u_k(z)}{z^{3/2} \sqrt{1+4z} (1 + \sqrt{1+4z})^2},
\]
where the function \( u_k(z) \) is defined as

\[
u_k(z) := (z - c_k) \sqrt{1+4z} - 2a_k z^{3/2} + (1 - 8c_k) z - c_k
\]
\[
\leq (z - c_k) 2\sqrt{z} \left( 1 + \frac{1}{8z} \right) - 2a_k z^{3/2} + (1 - 8c_k) z - c_k
\]
\[
= -2(a_k - 1) z^{3/2} + (1 - 8c_k) z + \frac{1 - 8c_k}{4} \sqrt{z} - c_k - \frac{c_k}{4 \sqrt{z}} \leq v_k(z).
\]
Here the function \( v_k(z) \) is defined as
\[
(G.37) \quad v_k(z) := -2(a_k - 1)z^{3/2} + \frac{1}{3}z + \frac{1}{12}\sqrt{z} - \frac{1}{12} - \frac{1}{48\sqrt{z}},
\]
and its derivative over \( z \) reads
\[
(G.38) \quad v'_k(z) = -3(a_k - 1)\sqrt{z} + \frac{1}{3} + \frac{1}{24\sqrt{z}} + \frac{1}{96z^{3/2}}.
\]
If \( z \geq 9 \) and \( k \geq 9 \), then
\[
(G.39) \quad v'_k(z) \leq -9(a_k - 1) + \frac{1}{3} + \frac{1}{72} + \frac{1}{2592} < 0, \quad u_k(z) \leq v_k(z) \leq v_k(9) \leq v_9(9) < 0,
\]
which means \( h_k(z) \) is strictly decreasing in \( z \).

If in addition \( z, k \geq 20 \), then
\[
(G.40) \quad \frac{B_{n,k}}{b_{n,k}L(n,k,k/n)} \leq \sqrt{\frac{\pi}{2}} h_k(z) \leq \sqrt{\frac{\pi}{2}} h_k(20) \leq \sqrt{\frac{\pi}{2}}2(1 + \frac{z}{20})\sqrt{20 + a_\infty} < \frac{180451625}{143327232},
\]
where \( a_\infty = \lim_{k \to \infty} a_k = 4\sqrt{2/\pi}/3 \), given that \( a_k \) is strictly decreasing in \( k \), while \( a_k \) is strictly increasing in \( k \). Therefore, Eq. (177) holds when \( k \geq 40 \) and \( n \geq 2k \), in which case \( z \geq k/2 = 20 \) given the definition of \( z \) in Eq. (G.24).

When \( 25 \leq k \leq 39 \) and \( z \geq 2k/3 \), direct calculation shows that
\[
(G.41) \quad \sqrt{\frac{\pi}{2}} h_k(z) \leq \sqrt{\frac{\pi}{2}} h_k(2k/3) < \frac{180451625}{143327232},
\]
so Eq. (177) also holds when \( 25 \leq k \leq 39 \) and \( n \geq 3k \). When \( 25 \leq k \leq 39 \) and \( n < 3k \), Eq. (177) can be verified by direct calculation.

When \( 16 \leq k \leq 24 \) and \( z \geq 9k/10 \), direct calculation shows that
\[
(G.42) \quad \sqrt{\frac{\pi}{2}} h_k(z) \leq \sqrt{\frac{\pi}{2}} h_k(9k/10) < \frac{180451625}{143327232},
\]
so Eq. (177) also holds when \( 16 \leq k \leq 24 \) and \( n \geq 10k \). When \( 16 \leq k \leq 24 \) and \( n < 10k \), Eq. (177) can be verified by direct calculation.

The above analysis shows that Eq. (177) holds when \( k \geq 16 \).

**Step 3:** Proof of Eq. (177) in the case \( k \leq 15 \). First, suppose \( n \geq jk \) with \( j \geq 2 \). By virtue of Eq. (G.21), Lemma G.2, and the following equation
\[
(G.43) \quad \exp \left[ \frac{1}{12(n - k)} - \frac{1}{12n + 1} \right] \leq \exp \left[ \frac{1}{11(n - k)} - \frac{1}{11n} \right] \leq 1 + \frac{1}{10(j - 1)n},
\]
we can deduce that
\[
(G.44) \quad \frac{B_{n,k}}{b_{n,k}L(n,k,k/n)} \leq \frac{e^{\kappa}(k + 1)}{2k^{\kappa}L(n,k,k/n)} \sqrt{\frac{n - k}{n}} \exp \left[ \frac{1}{12(n - k)} - \frac{1}{12n + 1} \right] + \frac{1 - \theta_k}{L(n,k,k/n)}
\]
\[
\leq \frac{e^{\kappa}(k + 1)}{k^{\kappa}(1 + \sqrt{1 + 4k})} \left( 1 - \frac{k}{2n\sqrt{1 + 4k}} \right) \left[ 1 + \frac{1}{10(j - 1)n} \right]
\]
\[
+ \frac{2(1 - \theta_k)}{1 + \sqrt{1 + 4k}} \left\{ 1 + \frac{jk}{n} \left[ \sqrt{\frac{1}{j + \sqrt{j + 4(j - 1)k}} - 1} \right] \right\}
\]
\[ \leq \frac{e^k \Gamma(k + 1)}{k^k(1 + \sqrt{1+4k})} + \frac{2(1 - \theta_k)}{1 + \sqrt{1+4k}} + \frac{w_k}{n}, \]

where \( \theta_k \) is defined by Ramanujan’s equation in Eq. (171) and \( w_k \) is defined as

\[(G.45) \quad w_k := \frac{e^k \Gamma(k + 1)}{k^k(1 + \sqrt{1+4k}) \left[ \frac{1}{10(j-1)} - \frac{k}{2\sqrt{1+4k}} \right] + 2jk(1-\theta_k)}{1 + \sqrt{1+4k} \left[ \sqrt{j}(1+\sqrt{1+4k}) \sqrt{\frac{j}{j+4(j-1)k}} - 1 \right]}.\]

Here the first inequality in Eq. (G.44) follows from the first inequality in Eq. (G.21) and the inequality \( \varsigma_{n,k} \geq \theta_k \) \cite{28}; the second inequality in Eq. (G.44) follows from Eqs. (G.7) and (G.9) in Lemma G.2 and Eq. (G.43), given that \( 1 - \theta_k \) by Eq. (172); the third inequality in Eq. (G.44) follows from straightforward calculation.

Now we choose \( j = 11 \), then direct calculation shows that \( w_k < 0 \) for \( k = 1, 2, \ldots, 15 \), so

\[(G.46) \quad \frac{B_{n,k}}{b_{n,k}L(n,k,k/n)} \leq \frac{e^k \Gamma(k + 1)}{k^k(1 + \sqrt{1+4k})} + \frac{2(1 - \theta_k)}{1 + \sqrt{1+4k}} \leq \frac{180451625}{143327232} \]

for \( k = 1, 2, \ldots, 15 \) and \( n \geq 11k \), which confirms Eq. (177). When \( 1 \leq k \leq 15 \) and \( n < 11k \), Eq. (177) can be verified directly. This observation completes the proof of Lemma 6.3.

APPENDIX H: PROOF OF PROPOSITION 6.4

By the definitions of \( \ell(x) \) and \( v(x) \) in Eq. (183) we can deduce that

\[(H.1) \quad \frac{d}{dx} \left[ \frac{\ell(x)}{v(x)} \right] = \begin{cases} \frac{2 + x - \sqrt{4 + x^2}}{(2-x)\sqrt{4 + x^2}} & 0 \leq x \leq 1, \\ \frac{2}{\sqrt{4 + x^2}} & x \geq 1, \end{cases} \]

which shows that the derivative is positive when \( x > 0 \). Since \( \ell(x), v(x) > 0 \) are continuous in \( x \) for \( x \geq 0 \). It follows that \( \ell(x)/v(x) \) is strictly increasing in \( x \), and \( v(x)/\ell(x) \) is strictly decreasing in \( x \). By definition it is also straightforward to verify that

\[(H.2) \quad \frac{v(0)}{\ell(0)} = 2, \quad \lim_{x \to \infty} \frac{v(x)}{\ell(x)} = \lim_{x \to \infty} \sqrt{2\pi} x \ell(x) = 1, \]

which implies Eq. (190) given that \( v(x)/\ell(x) \) is strictly decreasing in \( x \); in addition, the second inequality in Eq. (190) is saturated iff \( x = 0 \). In conjunction with Eq. (186) we can then deduce that

\[(H.3) \quad \lim_{x \to \infty} \frac{\Phi(-x)e^{x^2/2}}{\ell(x)} = 1. \]

The two equations above together confirm Eq. (189).

Finally, we are ready to prove Eq. (191). Direct calculation yields

\[(H.4) \quad \frac{d}{dx} \left[ \frac{\Phi(-x)e^{x^2/2}}{\ell(x)} \right] = \frac{1}{\ell(x)} \left[ \left( x + \frac{1}{\sqrt{x^2+4}} \right) e^{x^2/2} \Phi(-x) - \frac{1}{\sqrt{2\pi}} \right] \leq \frac{1}{\sqrt{2\pi} \ell(x)} \left[ \left( x + \frac{1}{\sqrt{x^2+4}} \right) \frac{4}{3x + \sqrt{8 + x^2}} - 1 \right] < 0 \quad \forall x \geq 0, \]

so \( \Phi(-x)e^{x^2/2}/\ell(x) \) is strictly decreasing in \( x \) for \( x \geq 0 \). Here the first inequality follows from the following inequality proved by Sampford \cite{42},

\[(H.5) \quad \Phi(-x) < \frac{4}{3x + \sqrt{8 + x^2}} e^{-x^2/2} \quad \forall x \geq 0, \]
and the second inequality can be proved as follows, assuming that \( x \geq 0 \),
\[
\left( \frac{1}{\sqrt{x^2 + 4}} \right) - 1 < 0 \quad \Leftrightarrow \quad x < \frac{4}{3x + \sqrt{8 + x^2}} - \frac{4}{\sqrt{x^2 + 4}}
\]
\( (H.6) \)
\[
\Leftrightarrow \quad x^2 < 8 + x^2 + \frac{16}{x^2 + 4} - 8 \sqrt{\frac{x^2 + 8}{x^2 + 4}} \quad \Leftrightarrow \quad 1 + \frac{2}{x^2 + 4} > \sqrt{\frac{x^2 + 8}{x^2 + 4}}
\]
\[
\Leftrightarrow \quad 1 + \frac{4}{x^2 + 4} + \left( \frac{2}{x^2 + 4} \right)^2 > \frac{x^2 + 8}{x^2 + 4} \quad \Leftrightarrow \quad \left( \frac{2}{x^2 + 4} \right)^2 > 0.
\]

Now Eq. (191) follows from Eq. (189) and the equality \( \Phi(0) = \sqrt{\pi/2} \ell(0) \), given that the function \( \Phi(-x)e^{x^2/2}/\ell(x) \) is strictly decreasing in \( x \) for \( x \geq 0 \). In addition, the second inequality in Eq. (191) is saturated iff \( x = 0 \).

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