A continuation of counting: The Lambert W function and asymptotics

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Introduction

These notes extend the previous notes on counting. In particular, we introduce the Lagrange inversion theorem and, for the asymptotic analysis of integrals, the Laplace method. Our starting point is the Lambert W function, defined as the multivalued inverse of the function

$$z \mapsto ze^z$$

for $z \in \mathbb{C}$ (see Figure 1 for the real branches). In other words, it holds that $z = W(z)e^{W(z)}$. Notice that while also using complex methods, we mostly restrict our considerations to the real-valued branches of W throughout these notes; see Corless et al. [3] for the complex case.

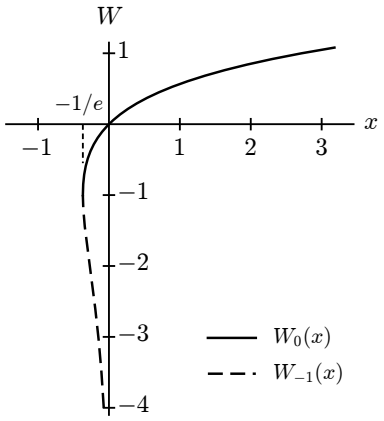


Figure 1: The two real branches of $W(x)$.

The W function tends to show up in unexpected circumstances. Let us tackle the problem [8, 3] of solving $x^y = y^x$ for positive and unequal $x, y \in \mathbb{R}$. Indeed, taking roots leads to $x^{1/x} = y^{1/y}$, which means that one wants to find two distinct points with the same value for $g(x) = x^{1/x}$; the function g is displayed in Figure 2. Writing $z = g(x)$ and exponentiating led Euler [5] to consider the *power tower*

$$h(z) = z^{z^{z^{\cdot^{\cdot^{\cdot}}}}} = z^{h(z)}, \tag{1}$$

where he found that the iterated exponential converges for $e^{-e} \leq z \leq e^{1/e}$. Given that the function converges, it is known that (1) admits a solution in terms of W [4]. Indeed, taking logarithms, one gets that

$$h(z) = \frac{W(-\ln z)}{-\ln z}.$$

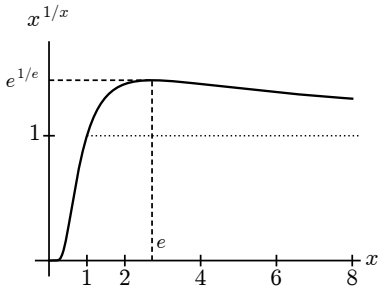


Figure 2: The function $g(x) = x^{1/x}$.

Before we continue with our investigations of further occurrences of W, let us fix some notation. Indeed, formal power series

$$A(z) = a_0 + a_1 z + a_2 z^2 + \cdots = \sum_{k \geq 0} a_k z^k,$$

$$B(z) = a_0 + a_1 \frac{z}{1!} + a_2 \frac{z^2}{2!} + \cdots = \sum_{k \geq 0} a_k \frac{z^k}{k!}$$

in the indeterminate z (with real or complex coefficients) are called ordinary generating function (OGF) and exponential generating function (EGF), respectively. We write $[z^n]A(z) = a_n$. As is customary, i denotes the imaginary unit.

We start by counting trees.

Rooted trees with labelled nodes

Recall that a rooted tree is a tree with one node designated as *root*. A tree is labelled if to every of the n nodes there is an associated label uniquely identifying the node. With these conventions, let t_n be the number of rooted trees on n labelled nodes. Then, the exponential generating function corresponding to t_n is known [10] to satisfy the functional equation[1]

$$T(z) = \sum_{k\geq 1} t_k \frac{z^k}{k!} = z e^{T(z)},$$

which in terms of W is expressed as $T(z) = -W(-z)$.

[1] See Sedgewick and Flajolet [11] and Flajolet and Sedgewick [6] for an 'automatic' method to derive results of this and similar problems.

Our first goal is to find a closed form for the t_n-s, for which we use the following fundamental result.

Theorem 1 (Lagrange inversion formula; LIF)**.** *Let ϕ be holomorphic in a neighborhood of the origin with $\phi(0) \neq 0$. Then there exist $a, b > 0$ such that for $|w| < a$, the equation*

$$w = z/\phi(z) \tag{2}$$

has exactly one solution $z = z(w)$ with $|z| < b$. The function $z(w)$ is holomorphic in $|w| < a$ and is given by

$$z(w) = \sum_{k\geq 1} c_k w^k, \qquad c_k = \frac{1}{k!} \frac{\mathrm{d}^{k-1}}{\mathrm{d}z^{k-1}} \big(\phi(z)^k\big)\Big|_{z=0}.$$

Moreover, if f is holomorphic in a neighborhood of the origin, then for $|w|$ sufficiently small,

$$f\big(z(w)\big) = f(0) + \sum_{k\geq 1} d_k w^k, \qquad d_k = \frac{1}{k!} \frac{\mathrm{d}^{k-1}}{\mathrm{d}z^{k-1}} \big(f'(z)\phi(z)^k\big)\Big|_{z=0}.$$

Our proof follows Wilf [13, Theorem 5.1.1], considering holomorphic functions instead of formal power series.

Proof (of Theorem 1). We prove the second part of the statement. The first part then follows by considering $f(z) = z$. To start, notice that by the inverse function theorem, $z = z(w)$ exists and is holomorphic in a sufficiently small neighborhood of the origin, as $w'(0) = 1/\phi(0) \neq 0$.

Using these observations, we have the chain of equalities

$$\begin{aligned}
k\,d_k &= \big[z^{k-1}\big]\big\{f'(z)\phi(z)^k\big\} && \text{(extracting coefficients)}\\
&= \big[z^{k-1}\big]\big\{f'(z)(z/w)^k\big\} && \text{(by (2))}\\
&= \big[z^{-1}\big]\big\{f'(z)/w^k\big\}\\
&= \frac{1}{2\pi i}\int \frac{f'(z)}{w(z)^k}\,\mathrm{d}z && \text{(residue formula)}\\
&= \frac{1}{2\pi i}\int w^{-k} f'(z(w))\,z'(w)\,\mathrm{d}w && \text{(set } z = z(w)\text{)}\\
&= \big[w^k\big]\big\{w(\mathrm{d}/\,\mathrm{d}w)f(z(w))\big\} && \text{(Cauchy integral formula)}\\
&= k\big[w^k\big]f(z(w)),
\end{aligned}$$

which gives the statement upon dividing by k. □

With the above result in place, we notice that if ϕ and f are formal power series and $\phi(0) \neq 0$, there exists a unique formal solution to (2) in terms of a power series. The coefficient identity follows by applying Theorem 1 to the formal series of ϕ and f, truncated at a fixed $k > 0$, which is possible as the resulting polynomials are entire, and by noticing that terms of degree exceeding k do not influence the result.

The application of the LIF to the functional equation for enumerating rooted labelled trees $T(z) = ze^{T(z)}$ (by setting $\phi(u) = e^u$) yields that

$$\begin{aligned}
\big[z^n\big]T(z) &= (1/n)\big[u^{n-1}\big]\big\{\phi(u)^n\big\}\\
&= (1/n)\big[u^{n-1}\big]\big\{e^{nu}\big\}\\
&= (1/n)\frac{n^{n-1}}{(n-1)!}\\
&= \frac{n^{n-1}}{n!}.
\end{aligned}$$

Hence,

$$\frac{t_n}{n!} = \frac{n^{n-1}}{n!},$$

and $t_n = n^{n-1}$, a result already known to Cayley [2] in 1889.

Together with the facts that $W_0(z)$ is analytic[2] at $z = 0$ and that $W(z) = -T(-z)$, the above derivation implies the series expansions

$$\begin{aligned}
T(z) &= \sum_{k\geq 1} k^{k-1}\frac{z^k}{k!} = z + z^2 + \frac{3}{2}z^3 + \frac{8}{3}z^4 + \frac{125}{24}z^5 + \cdots,\\
W_0(z) &= \sum_{k\geq 1} (-k)^{k-1}\frac{z^k}{k!} = z - z^2 + \frac{3}{2}z^3 - \frac{8}{3}z^4 + \frac{125}{24}z^5 - \cdots
\end{aligned}$$

around $z = 0$.

[2] As $F(z) = ze^z$ satisfies $F(0) = 0$ and $F'(0) = 1 \neq 0$, the existence of a holomorphic local inverse around 0 is guaranteed by the inverse function theorem.

Birthday problem 1

Our next step is tackling two famous flavours of the birthday problem, which allows us to recall and introduce some asymptotics. The first one is as follows.

> What is the least number of persons required if the probability exceeds $\frac{1}{2}$ that two or more of them have the same birthday? (Year of birth need not match.)
>
> —Mosteller [9, Problem 31]

The solution to this puzzle is well known. For some generality, let us assume that a year has n days and let us compute the probability of having a repetition in d uniform draws from $\{1, \dots, n\}$ with replacement. We then find d such that the probability exceeds $\frac{1}{2}$. Thinking in terms of complements, we get

$$\begin{aligned}\Pr(\text{no repeats after } d \text{ draws}) &= \frac{n}{n}\,\frac{n-1}{n} \cdots \frac{n-d+1}{n} \\ &= \frac{n(n-1)\cdots(n-d+1)}{n^d};\end{aligned}$$

notice that for $d > n$ the product is zero.[3] Hence,

[3] A fact also implied by the pigeonhole principle.

$$\begin{aligned}\Pr(\text{at least one repeat in } d \text{ draws}) &= 1 - \Pr(\text{no repeats after } d \text{ draws}) \\ &= 1 - \frac{n(n-1)\cdots(n-d+1)}{n^d},\end{aligned}$$

and, after some experimentation, one finds that for $n = 365$, taking at least $d = 23$ suffices for the probability to exceed $\frac{1}{2}$.

To approximate the solution, we use that the series expansion of the exponential function

$$e^{-x} = 1 - x + O\big(x^2\big) \quad (0 \le x \le 1)$$

implies that $1 - x = e^{-x} + O\big(x^2\big)$. Using this fact[4] and rewriting the complement yields

[4] More specifically, we are using that every $x_k = k/n$ satisfies $0 \le x_k \le 1$ and that there exists an absolute $M > 0$ such that $0 \le e^{-x_k} - (1 - x_k) \le M x_k^2$.

$$\begin{aligned}\Pr(\text{no repeats after } d \text{ draws}) &= \left(1 - \frac{1}{n}\right) \cdots \left(1 - \frac{d-1}{n}\right) \\ &= e^{-\left(\frac{1}{n} + \cdots + \frac{d-1}{n}\right)} + O\big(d^3/n^2\big) \\ &= e^{-d(d-1)/(2n)} + O\big(d^3/n^2\big).\end{aligned}$$

Now setting $e^{-d(d-1)/(2n)} = \frac{1}{2}$ and $n = 365$ gives $d \approx 22.9999$, which reproduces that at least $d = 23$ persons are needed.

Birthday problem 2

After this warm-up, we are ready to tackle a second flavour of the birthday problem.

> What is the expected number of persons it takes in order to find two having the same birth date (when the year has n days!)?
>
> —Flajolet et al. [7, p. 105]

Again, we model this problem as drawing uniformly with replacement from a set $\{1,\dots,n\}$, but now ask what the expected number of draws until a repetition is. We have

$$\text{expected number of draws} = \sum_{k\geq 1} k \Pr(\text{first repetition in } k\text{-th draw}),$$

and the only challenge is computing the probabilities in the sum. We illustrate the situation in Figure 3 for $n = 3$. In this case, denoting by A_k the event "first repetition in k-th draw", we compute

$$\Pr(A_1) = 0, \qquad \Pr(A_2) = \frac{3}{3^2},$$
$$\Pr(A_3) = \frac{12}{3^3}, \qquad \Pr(A_4) = \frac{18}{3^4},$$

and notice that all other $\Pr(A_k)$-s are zero. Now multiplying each $\Pr(A_k)$ by k and summing yields an expected number of draws of $\frac{26}{9} \approx 2.89$.

We next address the general case. Indeed, let t_k and t'_k be the number of repeated and non-repeated nodes at depth k, that is, after k draws from $\{1,\dots,n\}$, respectively. Every non-repeated node at depth k corresponds to a unique sequence of k distinct elements and has n children, of which k are repeats and $n-k$ are non-repeats. Hence,

$$t'_0 = 1, \qquad t'_{k+1} = (n-k)\, t'_k, \qquad \text{and} \qquad t_{k+1} = k\, t'_k.$$

In particular, $t'_k = n(n-1)\cdots(n-k+1)$. Combining the above, we find that

$$\text{expected number of draws} = \sum_{2\leq k\leq n+1} k\,\frac{t_k}{n^k} = \sum_{1\leq k\leq n} (k+1)\,\frac{t_{k+1}}{n^{k+1}},$$

which we simplify next. Indeed, recall that for any sequences $(a_k)_k$ and $(b_k)_k$ summation by parts gives

$$\sum_{k=m}^{N} a_k\,(b_k - b_{k+1}) = \big(a_m b_m - a_{N+1} b_{N+1}\big) + \sum_{k=m}^{N} b_{k+1}\,(a_{k+1} - a_k).$$

Setting $a_k = k+1$, $b_k = \frac{t'_k}{n^k}$, $m = 1$, and $N = n$ in this expression, noting that $b_1 = 1$ and $b_{n+1} = 0$, and using $\frac{t_{k+1}}{n^{k+1}} = \frac{k}{n}\,\frac{t'_k}{n^k} = b_k - b_{k+1}$ shows

$$\sum_{1\leq k\leq n} (k+1)\,\frac{t_{k+1}}{n^{k+1}} = 2 + \frac{n-1}{n} + \frac{n-1}{n}\,\frac{n-2}{n} + \cdots$$
$$= 1 + \sum_{1\leq k\leq n} \frac{n!}{(n-k)!\,n^k} = 1 + Q(n),$$

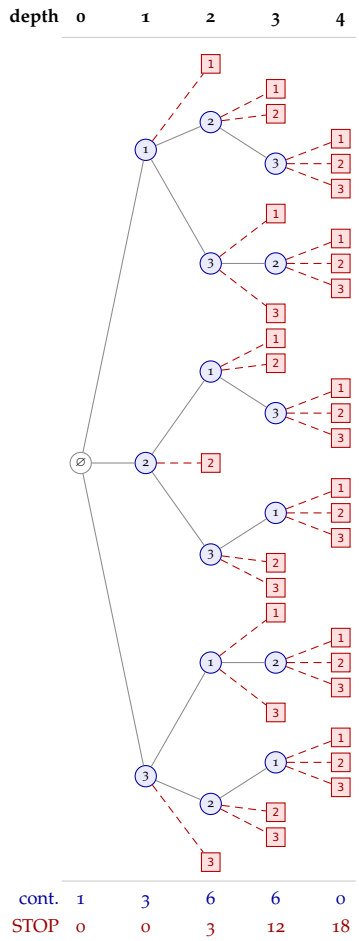


Figure 3: Drawing with replacement from $n = 3$ items until an item repeats. Blue: new item, red: repeated item.

where

$$Q(n) = \sum_{1 \le k \le n} \frac{n!}{(n-k)!\, n^k}$$

denotes the Ramanujan–Knuth Q-function.

We next introduce the Laplace method, which we afterwards apply to analyse the asymptotic behaviour of $Q(n)$ as $n \to \infty$.

Laplace method

The Laplace method for the asymptotic analysis of integrals deals with the behaviour as $t \to \infty$ of integrals of the form

$$I(t) = \int_{-\infty}^{\infty} \varphi(x,t)\, \mathrm{d}x$$

where $x \mapsto \varphi(x,t)$ has a peak whose neighborhood is the main contributor to the integral.[5] The idea is then to approximate φ by simpler functions in this neighborhood, which allow the evaluation of the integral [1].

To illustrate the idea, following essentially Stein and Shakarchi [12, Appendix A], we consider

$$I(t) = \int_0^{\infty} e^{-t\Phi(x)} \psi(x)\, \mathrm{d}x,$$

and assume that Φ and ψ are real-analytic on $[0,\infty)$, $\Phi(0) = \Phi'(0) = 0$, $\Phi''(0) > 0$, $\psi \ge 0$ on $[0,\infty)$, $\inf_{x \ge \epsilon} \Phi(x) > 0$ for every $\epsilon > 0$, and

$$\int_0^{\infty} e^{-t_0\Phi(x)} \psi(x)\, \mathrm{d}x < \infty \tag{3}$$

for some $t_0 \ge 0$. Figure 4 illustrates the situation.

As Φ is real-analytic with $\Phi(0) = \Phi'(0) = 0$ and $\Phi''(0) > 0$, we get

$$\Phi(x) = \frac{\Phi''(0)}{2}\, x^2 g(x),$$

where g is real-analytic on $[0,\infty)$ with $g(0) = 1$, in particular, $g(x) = 1 + O(x)$ as $x \to 0^+$. By continuity of g and Φ'', there exists $\epsilon > 0$ such that $g > 0$ and $\Phi'' > 0$ on $[0,\epsilon]$; in particular, $\Phi' > 0$ on $(0,\epsilon]$, since $\Phi'(0) = 0$. We split the integral

$$I(t) = \int_0^{\epsilon} e^{-t\Phi(x)} \psi(x)\, \mathrm{d}x + \int_{\epsilon}^{\infty} e^{-t\Phi(x)} \psi(x)\, \mathrm{d}x = I_1(t) + I_2(t),$$

and treat both terms separately.

For the second term, let $c := \inf_{x \ge \epsilon} \Phi(x) > 0$. For $t \ge t_0$ and $x \ge \epsilon$ we have

$$e^{-t\Phi(x)} = e^{-(t-t_0)\Phi(x)}\, e^{-t_0\Phi(x)} \le e^{-(t-t_0)c}\, e^{-t_0\Phi(x)},$$

[5] Integrals over intervals fit into this setting by setting φ to zero outside of the interval, so that the perspective is sufficiently general.

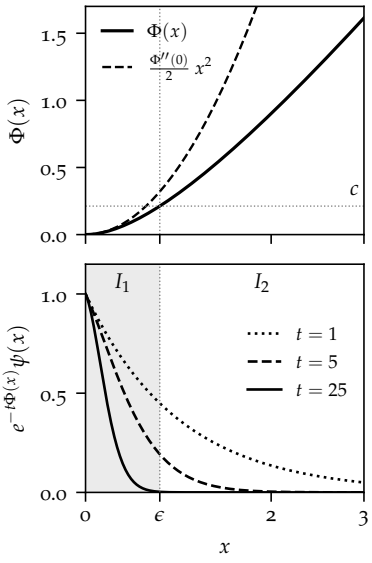


Figure 4: Top: $\Phi(x) = x - \ln(1+x)$ (solid) and $\frac{\Phi''(0)}{2} x^2$ (dashed). Bottom: $e^{-t\Phi(x)}\psi(x)$ for $\psi(x) = 1/(1+x)$.

since $t - t_0 \geq 0$ and $\Phi(x) \geq c$. As $\psi \geq 0$, it follows with (3) that

$$I_2(t) = O\big(e^{-ct}\big) \qquad (t \to \infty).$$

To obtain a known integral, we substitute

$$u(x) := x\sqrt{g(x)} = \sqrt{\frac{2\Phi(x)}{\Phi''(0)}}, \qquad 0 \leq x \leq \epsilon,$$

so that

$$\Phi(x) = \frac{\Phi''(0)}{2}\, u(x)^2.$$

Since g is real-analytic and positive on $[0,\epsilon]$, u is real-analytic there, with $u(0) = 0$ and $u'(0) = \sqrt{g(0)} = 1$. For $0 < x \leq \epsilon$, differentiating $\frac{\Phi''(0)}{2}u^2 = \Phi$ gives

$$u'(x) = \frac{\Phi'(x)}{\Phi''(0)\, u(x)} > 0.$$

Hence u is a strictly increasing bijection from $[0,\epsilon]$ onto $[0,\delta]$, where $\delta := u(\epsilon) > 0$, and $u' > 0$ on $[0,\epsilon]$. By the inverse function theorem, its inverse $x = x(u)$ is real-analytic on $[0,\delta]$ with $x(0) = 0$ and $x'(0) = 1$. Substituting $x = x(u)$ in I_1 yields

$$I_1(t) = \int_0^\delta e^{-t\frac{\Phi''(0)}{2}u^2}\, G(u)\,\mathrm{d}u, \qquad G(u) := \psi\big(x(u)\big)\, x'(u).$$

The function G is real-analytic on $[0,\delta]$ and by Taylor's theorem on the compact interval $[0,\delta]$,

$$G(u) = \sum_{k=0}^{N-1} a_k u^k + O(u^N) \qquad \text{uniformly for } 0 \leq u \leq \delta,$$

with $a_0 = \psi(0)$. Write $\lambda := \Phi''(0)/2$. Inserting this into I_1 and exchanging the finite sum with the integral gives

$$I_1(t) = \sum_{k=0}^{N-1} a_k\, M_k(t) + O\big(M_N(t)\big), \qquad M_k(t) := \int_0^\delta e^{-\lambda t u^2} u^k\,\mathrm{d}u.$$

The M_k are truncated moments of a half-Gaussian. For the full moments, with the substitution $v = \lambda t u^2$, we get

$$\int_0^\infty e^{-\lambda t u^2} u^k\,\mathrm{d}u = \frac{1}{2\,(\lambda t)^{\frac{k+1}{2}}} \int_0^\infty e^{-v}\, v^{\frac{k+1}{2}-1}\,\mathrm{d}v = \frac{\Gamma\left(\frac{k+1}{2}\right)}{2\,(\lambda t)^{\frac{k+1}{2}}}.$$

Extending the integration interval from $[0,\delta]$ to $[0,\infty)$ incurs only a negligible error. Indeed, for $t \geq 1$,

$$\int_\delta^\infty e^{-\lambda t u^2} u^k\,\mathrm{d}u \leq e^{-\lambda(t-1)\delta^2} \int_0^\infty e^{-\lambda u^2} u^k\,\mathrm{d}u = O\Big(e^{-\lambda\delta^2 t}\Big),$$

so that

$$M_k(t) = \frac{\Gamma\left(\frac{k+1}{2}\right)}{2\,(\lambda t)^{\frac{k+1}{2}}} + O\left(e^{-\lambda\delta^2 t}\right).$$

In particular, $M_N(t) = O\left(t^{-\frac{N+1}{2}}\right)$. Combining this with $I_2(t) = O(e^{-ct})$, we obtain for every $N \geq 1$

$$I(t) = \sum_{k=0}^{N-1} a_k \frac{\Gamma\left(\frac{k+1}{2}\right)}{2\,(\lambda t)^{\frac{k+1}{2}}} + O\left(t^{-\frac{N+1}{2}}\right) \qquad (t \to \infty),$$

which has the first term $\psi(0)\sqrt{\pi/(2\Phi''(0)\,t)}$. Note that the asymptotic expansion holds for each fixed N; the full series is in general divergent.

Asymptotic analysis

We now use the result of the previous section to analyse the Q-function showing up in the second birthday problem. As already observed by Ramanujan, it holds that

$$Q(n) = \int_0^\infty e^{-y}\left(1 + \frac{y}{n}\right)^{n-1} \mathrm{d}y. \tag{4}$$

Indeed, expanding by the binomial theorem and using

$$\Gamma(z+1) = \int_0^\infty s^z e^{-s}\,\mathrm{d}s, \qquad \mathrm{Re}(z) > -1,$$

together with $\Gamma(j+1) = j!$ for every nonnegative integer j,[6] the right-hand side of (4) equals

$$\sum_{j=0}^{n-1} \binom{n-1}{j} \frac{j!}{n^j} = \sum_{j=0}^{n-1} \frac{(n-1)!}{(n-1-j)!\,n^j} = Q(n).$$

[6] A result easily obtained through integration by parts and induction.

Substituting $y = nx$ in (4) yields

$$\begin{aligned} Q(n) &= n\int_0^\infty e^{-nx}(1+x)^{n-1}\,\mathrm{d}x = n\int_0^\infty e^{-nx+n\ln(1+x)}\,\frac{\mathrm{d}x}{1+x} \\ &= n\int_0^\infty e^{-n\Phi(x)}\psi(x)\,\mathrm{d}x = n\,I(n), \end{aligned}$$

where

$$\Phi(x) = x - \ln(1+x), \qquad \psi(x) = \frac{1}{1+x},$$

and I is as in the previous section.[7]

[7] Curiously, the Lambert W function shows up again: substituting $v = \Phi(x)$, i.e. $x = -1 - W_{-1}\left(-e^{-1-v}\right)$, one gets

$$Q(n) = -n\int_0^\infty \frac{e^{-nv}}{1 + W_{-1}\left(-e^{-1-v}\right)}\,\mathrm{d}v.$$

Notice that Φ and ψ satisfy the assumptions of the previous section: both are real-analytic on $(-1,\infty)$, $\Phi(0) = \Phi'(0) = 0$, $\Phi''(0) = 1$, $\psi > 0$, $\Phi'(x) = \frac{x}{1+x} > 0$ for $x > 0$, so that $\inf_{x\geq\epsilon}\Phi(x) = \epsilon - \ln(1+\epsilon) > 0$, and (3) holds with $t_0 = 1$, since $e^{-\Phi(x)}\psi(x) = e^{-x}$. Hence, by the Laplace method,

$$Q(n) \sim n\sqrt{\frac{\pi}{2\Phi''(0)\,n}}\,\psi(0) = \sqrt{\frac{\pi n}{2}} \qquad (n \to \infty).$$

To obtain further terms, we need the coefficients a_k of G. As $u(x) = x\sqrt{g(x)}$, by LIF

$$a_k = [x^k]\ \psi(x)\left(\frac{x}{u(x)}\right)^{k+1} = [x^k]\ \psi(x)\, g(x)^{-\frac{k+1}{2}}.$$

In our case,

$$g(x) = \frac{2\Phi(x)}{x^2} = 1 - \frac{2x}{3} + \frac{x^2}{2} + O(x^3), \qquad \psi(x) = 1 - x + x^2 + O(x^3),$$

and thus, by the binomial series,

$$g(x)^{-1} = 1 + \frac{2x}{3} + O(x^2), \qquad g(x)^{-3/2} = 1 + x + \frac{x^2}{12} + O(x^3).$$

This yields

$$a_0 = 1, \qquad a_1 = -\frac{1}{3}, \qquad a_2 = \frac{1}{12}.$$

With $\lambda = \frac{1}{2}$, the k-th term of the expansion of $I(n)$ is seen to be $a_k\, 2^{\frac{k-1}{2}}\, \Gamma\left(\frac{k+1}{2}\right) n^{-\frac{k+1}{2}}$. Taking $N = 3$ and multiplying by n, we obtain

$$Q(n) = \sqrt{\frac{\pi n}{2}} - \frac{1}{3} + \frac{1}{12}\sqrt{\frac{\pi}{2n}} + O\left(\frac{1}{n}\right) \qquad (n \to \infty),$$

so that the expected number of draws until the first repetition is

$$1 + Q(n) = \sqrt{\frac{\pi n}{2}} + \frac{2}{3} + O\left(\frac{1}{\sqrt{n}}\right) \qquad (n \to \infty).$$

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