ON THE ASYMPTOTICS OF TAKEUCHI NUMBERS

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Abstract

I present a conjectured asymptotic formula for the Takeuchi numbers T_n . In particular, I give compelling numerical evidence and present a heuristic argument showing that

$$T_n \sim C_T B_n \exp \frac{1}{2} W(n)^2$$

as n tends to infinity, where B_n are the Bell numbers, W(n) is Lambert's W function, and $C_T = 2.239...$ is a constant. Moreover, I show that the method presented here can be generalized to derive conjectures for related problems.

Keywords: Takeuchi numbers, enumerative combinatorics, asymptotic enumeration, asymptotic combinatorics, recursion, iterative functional equations, indifferent fixed point, generating functions

1. INTRODUCTION

In a paper entitled "Textbook Examples of Recursion," Donald E. Knuth discusses recurrence equations related to the properties of recursive programs [4], among them Takeuchi's function [7, 8]

$$t(x, y, z) =$$
if $x \le y$ then y else $t(t(x - 1, y, z), t(y - 1, z, x), t(z - 1, x, y))$. (1)

Let T(x, y, z) denote the number of times the **else** clause is invoked when t(x, y, z) is evaluated recursively.¹ For non-negative integers n, the Takeuchi

¹Note that it is the recursive evaluation of t(x, y, z) rather than the actual value of t(x, y, z) that is of interest. See Knuth's paper for an explicit expression of t(x, y, z).

numbers T_n are defined as $T_n = T(n, 0, n+1)$. The first few values of T_n for $n = 0, 1, 2, \ldots$ are

$$0, 1, 4, 14, 53, 223, 1034, 5221, 28437, 165859, \dots$$
 (2)

Knuth gives the recurrence

$$T_{n+1} = \sum_{k=0}^{n} \left\{ \binom{n+k}{n} - \binom{n+k}{n+1} \right\} T_{n-k} + \sum_{k=1}^{n+1} \binom{2k}{k} \frac{1}{k+1} , n \ge 0, \quad (3)$$

and deduces a functional equation for the generating function $T(z) = \sum_{n=0}^{\infty} T_n z^n$:

$$T(z) = \frac{C(z) - 1}{1 - z} + \frac{z(2 - C(z))}{\sqrt{1 - 4z}} T(zC(z)), \qquad (4)$$

where

$$C(z) = \frac{1}{2z}(1 - \sqrt{1 - 4z}) = \sum_{n=0}^{\infty} {2n \choose n} \frac{z^n}{n+1}$$
 (5)

is the generating function for the Catalan numbers $C_n = \binom{2n}{n} \frac{1}{n+1}$. Lastly, he gives asymptotically valid bounds for T_n ,

$$e^{n\log n - n\log\log n - n} < T_n < e^{n\log n - n + \log n} \tag{6}$$

for all sufficiently large n, and poses obtaining further information about the asymptotic properties of T_n as an open problem.

In this paper I give arguments leading to two conjectures about the asymptotic behaviour of the Takeuchi numbers T_n . In Section 2, I present an explicit asymptotic formula for T_n which improves upon the bounds (6) based on numerical evidence and a heuristic argument. For this, I briefly discuss the related asymptotic behavior of the Bell numbers and give an argument based on a numerical observation which leads directly to an explicit asymptotic formula for T_n as n tends to infinity. The formula, as described in Conjecture 1, is exact up to $O((\log n/n)^2)$ and contains a constant C_T which is numerically determined to 25 significant digits. Section 3 presents a heuristic analytic argument which gives the asymptotic behavior up to o(1) and enables one to identify the constant C_T in terms of an explicit expression, as stated in Conjecture 2. In the final section I show that the method developed in Section 3 can give insight into the asymptotic behavior of a larger class of problems.

I conclude this introduction by briefly discussing the structure of the recurrence (3) and the related functional equation (4). It is clear from the asymptotic bounds (6) for T_n , that the generating function T(z), defined as a formal power series, does not converge, and is therefore at best only an asymptotic expansion to an actual solution of the functional equation. This is also evident from the structure of the functional equation. This structure becomes clearer upon a change of variables, which gives

$$T(z) = \frac{1}{z}T(z-z^2) - \frac{1}{(1-z)(1-z+z^2)},$$
 (7)

where one sees directly that the transformation involved is $g(z) = z - z^2$, which is only marginally contracting at its fixed point z = 0. While functional equations with a transformation g(z) that has an expanding or contracting fixed point $(|g'(0)| \neq 1)$ are very well understood [5], it is precisely the fact that |g'(0)| = 1 which is at the root of the underlying difficulty of the problem discussed in this paper.

Finally, I mention that trying to find an exponential generating function for T_n leads to

$$\frac{d}{dz} \sum_{n=0}^{\infty} \frac{z^n}{n!} (T_n - V_n) = \sum_{n=0}^{\infty} \frac{z^n}{n!} T_n \sum_{k=0}^{\infty} \frac{z^k}{k!} \frac{\binom{n+2k}{k}}{\binom{n+k+1}{k}} , \qquad (8)$$

where $V_n = \sum_{k=1}^n C_n$, and the sum over the index k can be identified with the hypergeometric function ${}_2F_2(\frac{n+2}{2},\frac{n+1}{2};n+2,n+1;4z)$.

2. NUMERICAL OBSERVATIONS

My starting point is Knuth's observation [4] that for n > 0 the Bell numbers B_n are a lower bound to T_n . Here, B_n is defined as

$$B_{n+1} = \sum_{k=0}^{n} \binom{n}{k} B_{n-k} , \qquad B_0 = 1 .$$
 (9)

The asymptotics of B_n is discussed in great detail by de Bruijn [1]. In [6] one finds a systematic way of generating higher order terms in the asymptotic expansion by means of a contour integral representation using the well-known fact that

$$\sum_{n=0}^{\infty} B_n \frac{z^n}{n!} = \exp(e^z - 1) \ . \tag{10}$$

Alternatively, one can also expand the right-hand side of (10) in z to get

$$B_n = \frac{1}{e} \sum_{m=0}^{\infty} \frac{m^n}{m!} \,, \tag{11}$$

which can then be evaluated asymptotically by use of the Euler-MacLaurin formula. Either way, in the course of the computation of the asymptotics of B_n it turns out that a convenient asymptotic scale is given in terms of W(n) rather than in terms of n, where W(x) is Lambert's W function, which is defined as the real solution of

$$W(x) \exp W(x) = x . (12)$$

The sum (11) is dominated by terms around $m = e^{W(n)}$, and one can easily calculate that, written in terms of w = W(n), the Bell numbers B_n behave asymptotically as

$$\log B_n = e^w (w^2 - w + 1) - \frac{1}{2} \log(1 + w) - 1$$

$$- \frac{w(2w^2 + 7w + 10)}{24(1 + w)^3} e^{-w}$$

$$- \frac{w(2w^4 + 12w^3 + 29w^2 + 40w + 36)}{48(1 + w)^6} e^{-2w} + O(e^{-3w}) ,$$
(13)

and it is straightforward to calculate additional terms. It is more conventional to state this formula with the exponentials e^{kw} replaced by $(n/w)^k$, but this obscures the fact that the asymptotic expansion is obtained in terms of w rather than n.

Having rather explicit control over this lower bound, it is natural to now try to compare B_n and T_n more closely. There is a principal difficulty coming from the fact that the asymptotic scale presumably also involves w = W(n), which grows more slowly than $\log n$. (As an example, $W(1000) \approx 5.2496$ and $W(10000) \approx 7.2318$.) Thus, one would expect that a direct numerical investigation of T_n/B_n is not very insightful, due to the presence of slowly varying correction terms of unknown form.

However, as Figure 1 shows, if one compares the growth rates T_n/T_{n-1} and B_n/B_{n-1} instead, one is led to observe the surprisingly simple relationship

$$\lim_{n \to \infty} \left(\frac{T_{n+1}}{T_n} - \frac{B_n}{B_{n-1}} \right) = 1 . \tag{14}$$

In fact, the left hand side approaches 1 rather quickly,

$$\frac{B_n}{B_{n-1}} + 1 \le \frac{T_{n+1}}{T_n} \le \frac{B_n}{B_{n-1}} + 1 + O(e^{-w}) . \tag{15}$$

This (unproven) numerical observation leads to a straightforward derivation of an asymptotic formula. From (13) it follows easily that $B_{n-1}/B_n =$

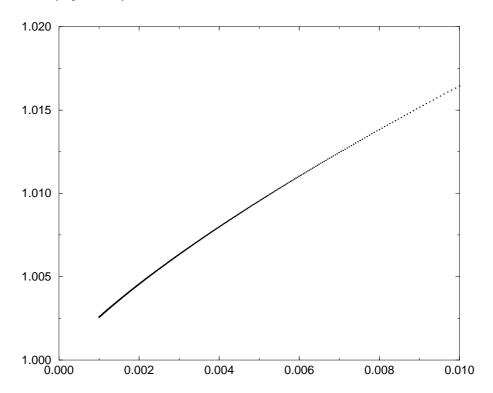


Figure 1. $T_{n+1}/T_n - B_n/B_{n-1}$ plotted versus 1/n for $n \le 1000$

 $e^{-w}+O(e^{-2w}).$ Now one takes logarithms and sums up successively, from whence it follows that

$$\log T_{n+1} = \log B_n + \frac{1}{2}w^2 + w + O(1) . \tag{16}$$

Now that I have guessed the leading asymptotic form, I can again resort to numerical work to try to improve upon it. In fact, numerically it appears that the convergence is even better than expected due to a chance cancellation of higher order correction terms. Figure 2 seems to indicate that the quotient $T_{n+1}/[B_n \exp(\frac{1}{2}w^2 + w)]$ approaches a limiting value C_T as $n \to \infty$. A closer numerical analysis reveals that

$$T_{n+1} = C_T B_n \exp(\frac{1}{2}w^2 + w + O(e^{-2w})),$$
 (17)

and from the first 1000 terms of the sequence I am able to deduce by iterative application of standard series extrapolation methods that

$$C_T = 2.23943\ 31040\ 05260\ 73175\ 4785\ (1)\ .$$
 (18)

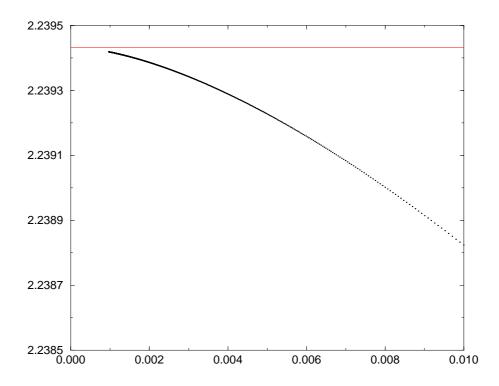


Figure 2. $T_{n+1}/[B_n \exp(\frac{1}{2}w^2 + w)]$ plotted versus 1/n for $n \le 1000$. The horizontal line is at $C_T = 2.2394331040...$

Using the known asymptotic form of the Bell numbers, I can now give an explicit asymptotic expression for T_n in terms of w = W(n) alone, as stated in the following conjecture.

Conjecture 1. As n tends to infinity, one has

$$\log T_n = e^w (w^2 - w + 1) + \frac{1}{2} w^2 - \frac{1}{2} \log(1 + w) + + \log C_T - 1 - \frac{w(26w^2 + 67w + 46)}{24(1 + w)^3} e^{-w} + O(e^{-2w}).$$
(19)

Here w = W(n) and the constant C_T is some positive real number.

Numerically, $\log C_T - 1 = -0.19377~72447~31916~75890~1157~(1)$. Of course it would be desirable to find an analytic expression for this number. In the next section I shall present a heuristic argument giving such an expression.

Dropping one correction term and comparing with the asymptotic expression (13) for the Bell numbers, Conjecture 1 implies the nice formula given

in the abstract,

$$T_n \sim C_T B_n \exp \frac{1}{2} W(n)^2 . \tag{20}$$

Asymptotic expansions of W(n) in terms of more elementary functions are given in [2].

3. ANALYTIC RESULTS

In view of the previous section it seems promising to exploit the apparent affinity between Takeuchi numbers T_n and Bell numbers B_n . Given a recurrence of the general form

$$a_n = \sum_{k=1}^n c_{n,k} a_{n-k} + b_n , \qquad (21)$$

I choose to write

$$a_n = \frac{1}{e} \sum_{m=0}^{\infty} \frac{1}{m!} f_{m,n}$$
 and $b_n = \frac{1}{e} \sum_{m=0}^{\infty} \frac{1}{m!} b_n$. (22)

Inserting (22) into the recurrence (21) and shifting the summation index by one, I next equate terms to get

$$f_{m,n} = m \sum_{k=1}^{n} c_{n,k} f_{m-1,n-k} + b_n , \qquad (23)$$

This Ansatz might seem less arbitrary when considering that in the case of Bell numbers it reduces to $f_{m,n} = m^n$. In general, one observes that $f_{m,n}$ must be a polynomial in m of at most degree n, which I write as

$$f_{m,n} = m^n \sum_{k=0}^n d_{n,k} m^{-k} . (24)$$

If one further requires the coefficients $c_{n,k}$ in the recurrence to be polynomials of degree k in n, it follows that $d_{n,k}$ are polynomials of degree k in n, which I write as

$$d_{n,k} = n^k \sum_{l=0}^k r_{k,l} n^{-l} . (25)$$

Combining equations (24) and (25) gives

$$m^{-n} f_{m,n} = \sum_{k=0}^{n} \sum_{l=0}^{k} r_{k,l} n^{k-l} m^{-k} = \sum_{l=0}^{n} m^{-l} \sum_{k=0}^{n-l} r_{l+k,l} (n/m)^{k} .$$
 (26)

In order to get an idea about the asymptotic behavior of this double sum, I now replace the quotient n/m by a new variable v and consider the formal limit of taking the summation bounds to infinity, leading to

$$s_m(v) = \sum_{l=0}^{\infty} m^{-l} r_l(v)$$
 with $r_l(v) = \sum_{k=0}^{\infty} r_{l+k,l} v^k$. (27)

Applying this method to Takeuchi numbers, one now inserts $c_{n,k} = \left\{\binom{n+k-2}{n-1} - \binom{n+k-2}{n}\right\}$ and $b_n = \sum_{k=1}^n \binom{2k}{k} \frac{1}{k+1}$. With this choice, $r_0(v)$ is trivially zero as $c_{n,k}$ are polynomials in n of degree k-1, and one gets a rather interesting result for $l \geq 1$. In fact,

$$r_1(v) = e^{\frac{1}{2}v^2 + v} \tag{28}$$

$$r_2(v) = e^{\frac{1}{2}v^2} \left(2e^{2v} - \frac{1}{2}(v^3 + v^2 + 4v + 2)e^v \right)$$
 (29)

$$r_3(v) = e^{\frac{1}{2}v^2} \left(-\frac{1}{8}e^{3v} - (v^3 + 3v^2 + 7v + 6)e^{2v} + \right)$$
(30)

$$+\frac{1}{24}(3v^6+6v^5+47v^4+52v^3+144v^2+74v+51)e^v$$

$$r_4(v) = e^{\frac{1}{2}v^2} \left(-\frac{347}{108}e^{4v} + \frac{1}{16}(v^3 + 5v^2 + 12v + 12)e^{3v} + \frac{1}{12}(3v^6 + 18v^5 + 89v^4 + 226v^3 + 411v^2 + 406v + 195)e^{2v} - \frac{1}{432}(9v^9 + 27v^8 + 315v^7 + 603v^6 + 3024v^5 + 3384v^4 + 8757v^3 + 4707v^2 + 5484v + 772)e^{v} \right).$$

$$(31)$$

From this, I conjecture

$$r_l(v) = e^{\frac{1}{2}v^2} \left(p_{l,0}(v)e^{lv} + p_{l,1}(v)e^{(l-1)v} + \dots + p_{l,l-1}(v)e^v \right) , \qquad (32)$$

where $p_{l,k}(v)$ are polynomials in v of degree 3k. (This pattern has been verified for $l \leq 8$.) For v large, this conjecture implies

$$r_l(v) \sim \lambda_l e^{\frac{1}{2}v^2 + lv} , \qquad (33)$$

and with a little effort one can compute the next values of $\lambda_l = p_{l,0}$. One gets

$$\lambda_0 = 0$$
, $\lambda_1 = 1$, $\lambda_2 = 2$, $\lambda_3 = -\frac{1}{8}$, $\lambda_4 = -\frac{347}{108}$, $\lambda_5 = \frac{28201}{3456}$,

$$\lambda_6 = -\frac{3172987}{216000}, \quad \lambda_7 = \frac{822813607}{93312000}, \quad \lambda_8 = \frac{2183235065857}{16003008000}, \quad \dots,$$

from whence I am led to conjecture that one can write $\lambda_n = \mu_n/[(n-1)!]^3$ where μ_n is integer. (Unfortunately, I did not find a way to compute the coefficients λ_l in a closed form!) One would expect from this behavior that

$$s_m(v) \sim e^{\frac{1}{2}v^2} h(e^v/m) ,$$
 (34)

where h(x) is given in some sense by

$$h(x) = \sum_{l=0}^{\infty} \lambda_l x^l \ . \tag{35}$$

I caution here that the series may be divergent and just valid as an asymptotic expansion.

Keeping in mind that the evidence for the existence of h(x) is rather sketchy, I nevertheless proceed under the assumption that for n >> m >> 1 one can write

$$f_{m,n} \sim m^n e^{\frac{1}{2}(n/m)^2} h(e^{n/m}/m)$$
 (36)

This now enables a heuristic computation of the Takeuchi numbers T_n . I approximate

$$T_n = \frac{1}{e} \sum_{m=0}^{\infty} \frac{1}{m!} f_{m,n} \sim \frac{1}{e} \sum_{m \approx m_{max}(n)} \frac{1}{m!} f_{m,n}$$
 (37)

$$\sim \frac{1}{e} \sum_{m \approx m_{max}(n)} \frac{m^n}{m!} e^{\frac{1}{2}(n/m)^2} h(e^{n/m}/m) ,$$
 (38)

where in the last step it is assumed that $n >> m_{max}(n) >> 1$. This sum is indeed dominated around $m_{max}(n) \sim e^w$, where the argument of h simplifies to 1. A careful asymptotic analysis of

$$\hat{T}_n = \frac{1}{e} \sum_{m \approx m_{max}(n)} \frac{m^n}{m!} e^{\frac{1}{2}(n/m)^2} h(e^{n/m}/m)$$
(39)

gives

$$\log \hat{T}_{n} = e^{w}(w^{2} - w + 1) + \frac{1}{2}w^{2} - \frac{1}{2}\log(1+w) + h_{0} - 1$$

$$+ \frac{w(12w^{5} + 24w^{4} + 36w^{3} + 58w^{2} + 29w - 10)}{24(w+1)^{3}}e^{-w}$$

$$+ \frac{(w+1)(h_{1}^{2} + h_{2}) + (2w^{2} + w + 2)h_{1}}{2}e^{-w} + O(e^{-2w}),$$
(40)

where one has expanded h(x) around x = 1 as $\log h(x) = h_0 + h_1(x-1) + h_2(x-1)^2/2 + O((x-1)^3)$.

As long as the corrections made on passing from T_n to \hat{T}_n are small enough, it follows easily from this that asymptotically

$$T_n \sim B_n e^{\frac{1}{2}w^2} h(1) ,$$
 (41)

and one can identify the constant C_T from equation (20) with h(1). Provided the series expansion of $h(x) = \sum_{k=0}^{\infty} \lambda_k x^k$ converges at x = 1, I can thus conjecture an explicit expression for the constant C_T , which in principle is computable.

Conjecture 2. The constant C_T in Conjecture 1 is given by

$$C_T = h(1) = \sum_{k=0}^{\infty} \lambda_k . (42)$$

While the approximation of T_n by \hat{T}_n may be correct up to $O(e^{-w})$, no choice of h(x) can match the next term in (40) with the expansion of T_n . Thus, one also gets an indication of the size of the error made.

It seems that a careful asymptotic evaluation of the $f_{m,n}$ promises to be a suitable way of providing rigorous proof for the asymptotics of the Takeuchi numbers. Of course one could also try to find a direct proof of our numerically observed equation (14).

4. A GENERALIZATION

In the derivation of the functional equation (4) for the Takeuchi numbers T_n , it is crucial that

$$\sum_{k=0}^{\infty} \binom{n+2k}{k} z^k = C(z)^n / \sqrt{1-4z} , \qquad (43)$$

as this identity allows the explicit summation of the terms in the recurrence (3). The identity used is a special case of the following nice identity

$$\sum_{k=0}^{\infty} \binom{n+(\lambda+1)k}{k} z^k = \left\{ \sum_{k=0}^{\infty} \binom{(\lambda+1)k}{k} z^k \right\} \left\{ \sum_{k=0}^{\infty} \binom{(\lambda+1)k}{k} \frac{z^k}{1+\lambda k} \right\}^n. \tag{44}$$

This identity can be proved by inserting $z = y/(1+y)^{\lambda+1}$, which after expanding leads to

$$\sum_{k=0}^{\infty} {\binom{(\lambda+1)k}{k}} \frac{z^k}{1+\lambda k} = 1+y \tag{45}$$

and

$$\sum_{k=0}^{\infty} \binom{n + (\lambda + 1)k}{k} z^k = \frac{(1+y)^{n+1}}{1 - \lambda y} . \tag{46}$$

This identity can be found in [3]. I use this now as a motivation for the study of the family of recursions (with parameter λ)

$$A_{n+1} = \sum_{k=0}^{n} \binom{n+\lambda k}{k} A_{n-k} , \qquad A_0 = 1 .$$
 (47)

Due to equation (44) one is able to derive a functional equation for the corresponding generating function $A(z) = \sum_{n=0}^{\infty} A_n z^n$:

$$A(z) = 1 + z \frac{1+y}{1-\lambda y} A(z(1+y)) , \quad z = y/(1+y)^{\lambda+1} . \tag{48}$$

For $\lambda = 0$ one recovers the recursion for the Bell numbers, and for $\lambda = 1$ one has something which is at least "morally" related to the Takeuchi numbers.

Inserting the Ansatz (22) into (47), one can easily repeat the analysis of the previous section. The result is now

$$A_n \sim B_n \exp \lambda \left\{ \frac{1}{2} W(n)^2 + W(n) + d(\lambda) \right\}$$
 (49)

for any fixed value of λ . Again, one has an identification of the kind $d(\lambda) = h_{\lambda}(1)$, where the first terms in the series expansion of $h_{\lambda}(x)$ are

$$h_{\lambda}(x) = \frac{1}{2}(\lambda - 1)x - \frac{1}{24}(2\lambda^{2} + 18\lambda - 5)x^{2}$$
$$-\frac{1}{216}(33\lambda^{3} + 90\lambda^{2} - 329\lambda + 54)x^{3}$$
$$-\frac{1}{960}(52\lambda^{4} - 520\lambda^{3} + 4240\lambda - 502)x^{4} + O(x^{5}), \quad (50)$$

and one sees that the kth coefficient is a polynomial in λ of degree k (this has been verified up to k=7). I caution again that convergence of this series expansion is an open question.

Finally, one can establish numerically the next term in the asymptotic expansion of A_n . For any fixed value of λ , one finds

$$\log A_n = \log B_n + \lambda \left(\frac{w^2}{2} + w + d(\lambda) - \frac{\lambda + 1}{2} e^{-w} \right) + O(e^{-2w}) . \tag{51}$$

Indeed, this result even seems to hold for *complex* values of λ .

I conclude with remarking that even though Takeuchi's function has been labelled a "Textbook Example," it provides an exciting open question for asympotic analysis.

Acknowledgements

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