Asymptotic expansions and conjectures related to the exponential integral

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26 Sept 2018

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D-finite series and sequences

A formal power series $f(z) := \sum f_n z^n$ is *D-finite* (or *differentially finite*) if it satisfies a linear differential equation with polynomial coefficients (not all zero), e.g.

$$(1-z)^2 f'' + (4z-5)f' + 2f = 0.$$

Another name is *holonomic*.

If the series $\sum f_n z^n$ converges for sufficiently small $|z|$, then it represents an analytic function $f : \mathbb{C} \to \mathbb{C}$, but we allow the case where the radius of convergence is zero, e.g. $f_n = n!$.

A sequence $(a_n)_{n\geqslant 0}$ is *D-finite* (or *P-recursive*) if, for some N, $(a_n)_{n\geqslant N}$ satisfies a linear recurrence with a fixed number of polynomial coefficients (not all zero), e.g.

$$na_n - (2n-1)a_{n-1} + (n-2)a_{n-2} = 0, \;\; n \geqslant 2.$$

The two concepts are equivalent: the formal power series $\sum f_n z^n$ is D-finite iff the sequence (f_n) is D-finite.

Closure properties of D-finiteness

The set of D-finite power series is closed under addition and (ordinary) multiplication. (Recall that multiplication of power series corresponds to convolution of the corresponding sequences.)

It is also closed under the *Hadamard product* $(f \circ g)_n = f_n \cdot g_n$, which corresponds to pointwise multiplication of sequences.

However, it is not closed under division, e.g. the Maclaurin series for $\tan z = \sin z / \cos z$ and $\sec z = 1/\cos z$ are not D-finite.

Asymptotics of D-finite sequences

We are interested in the asymptotic behaviour of D-finite sequences (a_n) as $n \to \infty$.

For example, it is clear from the polynomial recurrence satisfied by a D-finite sequence (a_n) that, for some constant c, $a_n \ll \exp(cn \log n)$.

Thus, it is not possible for a_n to grow as fast as $\exp(n^2)$.

On the other hand, polynomial growth and exponential growth are certainly possible.

An example of “stretched exponential” growth

There are D-finite sequences (a_n) such that

$$a_n \sim An^g \exp(Bn^\alpha) \;\text{ as }\; n \to \infty,$$

for certain constants $A \neq 0$, $B > 0$, g, and $\alpha \in (0, 1)$.

For example: from a result of Wright (1949), the coefficients in the Maclaurin series for

$$\exp(1/\sqrt{1-z})$$

have this form of asymptotic behaviour, with

$$A = \frac{1}{2^{1/3}\sqrt{3\pi}},\; B = \frac{3}{2^{2/3}},\; g = -\frac{5}{6},\; \alpha = \frac{1}{3}.$$

Another example (our starting point)

From a result of Perron (1914), the coefficients a_n in the Maclaurin series for

$$f_0(z) := \exp(z/(1-z))$$

have the same "stretched exponential" form of asymptotic behaviour, with

$$A = 1/\sqrt{4\pi e},\ B = 2,\ g = -3/4,\ \text{ and }\ \alpha = 1/2,$$

so

$$a_n \sim \frac{e^{2\sqrt{n}}}{2n^{3/4}\sqrt{\pi e}}\,.$$

Salvy's conjecture

Bruno Salvy recently conjectured that similar behaviour was possible with $B < 0$. In particular, he conjectured that the function

$$f_1(z) := e^x E_1(x) = e^x \int_x^\infty \frac{e^{-t}}{t}\, dt, \quad \text{where} \quad x = \frac{1}{1-z}\,,$$

has Maclaurin series coefficients b_n such that

$$b_n \sim A n^{-3/4} \exp(-2n^{1/2}).$$

In the notation on the previous slides,

$$B = -2,\; g = -3/4, \quad \text{and} \quad \alpha = 1/2.$$

We have proved Salvy's conjecture. In fact, we have found a full asymptotic expansion for b_n.

Differential equations for f_0 and f_1

Recall that $f_0(z) = \exp(z/(1-z))$. Differentiating, we see that f_0 satisfies the differential equation

$$(1-z)^2 f_0'(z) - f_0(z) = 0.$$

Similarly, with

$$f_1(z) = e^x E_1(x) = e^x \int_x^\infty \frac{e^{-t}}{t}\, dt, \quad \text{where} \quad x = 1/(1-z),$$

we find that

$$(1-z)^2 f_1'(z) - f_1(z) = z - 1.$$

Only the right-hand sides (and initial conditions) differ. Differentiating twice more, we get a third-order differential equation

$$(1-z)^2 f''' + (4z-5) f'' + 2f' = 0$$

satisfied by both f_0 and f_1.

Recurrence relation for a_n

Putting $f_0(z) = \sum a_n z^n$ in the differential equation satisfied by f_0 and equating coefficients, we get the 3-term recurrence relation

$$na_n - (2n-1)a_{n-1} + (n-2)a_{n-2} = 0 \;\text{ for }\; n \geqslant 2.$$

Initial conditions are $a_0 = a_1 = 1$. Using the recurrence, we can compute $(a_n)_{n\geqslant 0} = (1, 1, 3/2, 13/6, 73/24, 167/40, \ldots)$.

A closed form is

$$a_n = \sum_{k=1}^{n} \frac{1}{k!}\binom{n-1}{k-1} \;(n \geqslant 1).$$

We can also write $a_n = L_n^{(-1)}(-1)$, where the generalised Laguerre polynomials $L_n^{(\alpha)}(x)$ are orthogonal over $[0, \infty)$ with respect to the weight function $x^\alpha e^{-x}$.

Recurrence relation for b_n

The differential equation satisfied by $f_1(z) = \sum b_n z^n$ implies a 3-term recurrence

$$nb_n - (2n-1)b_{n-1} + (n-2)b_{n-2} = 0 \text{ for } n \geqslant 3.$$

This is the same recurrence that is satisfied by (a_n), but the initial conditions are different.

For (b_n), the initial conditions are $b_0 = G$, $b_1 = G - 1$, $b_2 = (3G-2)/2$, where $G := eE_1(1) \approx 0.596$ is the Euler-Gompertz constant.

The recurrence can be used to compute more terms, but it is numerically unstable if used in the forward direction.

Asymptotic expansions of a_n and b_n

Recall that $a_n = [z^n]f_0(z)$ and $b_n = [z^n]f_1(z)$.

Using the recurrence relation satisfied by (a_n) and (b_n), we can prove that a_n and b_n have closely related asymptotic expansions:

$$a_n \sim \frac{e^{2\sqrt{n}}}{2n^{3/4}\sqrt{\pi e}} \sum_{k\geqslant 0} c_k n^{-k/2},$$

$$b_n \sim -\frac{\sqrt{\pi e}}{n^{3/4}e^{2\sqrt{n}}} \sum_{k\geqslant 0} (-1)^k c_k n^{-k/2},$$

for certain constants $c_k \in \mathbb{Q}$, $c_0 = 1$.

The expansion for a_n is known [Perron (1914), Wright (1932)], but the expansion for b_n appears to be new.

The Hadamard product

In the Hadamard product $\rho_n := a_n b_n$, the exponentials and constant $\sqrt{\pi e}$ cancel, giving

$$\rho_n \sim -\frac{1}{2n^{3/2}} \left(c_0 + c_1 h + c_2 h^2 + \cdots\right) \left(c_0 - c_1 h + c_2 h^2 - \cdots\right),$$

where $h = n^{-1/2}$. Observe that

$$\begin{aligned}\left(F(h^2) + hG(h^2)\right)\left(F(h^2) - hG(h^2)\right) \\ &= F(h^2)^2 - h^2 G(h^2)^2 \\ &= F(n^{-1})^2 - n^{-1} G(n^{-1})^2,\end{aligned}$$

so

$$\rho_n \sim -\frac{1}{2n^{3/2}} \left(d_0 + \frac{d_1}{n} + \frac{d_2}{n^2} + \cdots\right)$$

for certain constants $d_k \in \mathbb{Q}$, $d_0 = 1$.

The constants c_k

Let $(\tau)_m$ denote the ascending factorial $\tau(\tau+1)\cdots(\tau+m-1)$.

The constants c_k appearing in the asymptotic expansions of a_n and b_n can be computed from

$$c_k = (-1)^k \sum_{j=0}^{k} [h^{k-j}] \exp(\mu(h)) \, \frac{(k-2j+3/2)_{2j}}{4^j j!} \, ,$$

where

$$\mu(h) = \frac{1}{h} - \frac{1}{e^h - 1} - \frac{1}{2} = -\sum_{m=1}^{\infty} \frac{B_{2m}}{(2m)!} \, h^{2m-1},$$

and the B_{2m} are Bernoulli numbers. This follows from results of Temme (2013).

Numerically,

$$(c_k)_{k\geqslant 0} = \left(1, -\frac{5}{48}, -\frac{479}{4608}, -\frac{15313}{3317760}, \frac{710401}{127401984}, \ldots\right).$$

The constants d_k

The constants d_k appearing in the asymptotic expansion of $\rho_n = a_n b_n$ can be computed from the c_k using

$$d_k = \sum_{j=0}^{2k} (-1)^j c_j c_{2k-j}.$$

This gives the following numerical values:

$$(d_k)_{k \geqslant 0} = \left(1, -\frac{7}{32}, \frac{43}{2048}, -\frac{915}{65536}, -\frac{521101}{8388608}, \ldots\right).$$

We observe that the denominators appear to be powers of two!

In other words, the (d_k) appear to be dyadic rationals.

A conjecture

Let $r_k := 2^{6k} d_k$, so

$$(r_k)_{k \geqslant 0} = (1, -14, 86, -3660, -1042202, -247948260, \ldots).$$

Conjecture: for all $k \geqslant 0$, $r_k \in \mathbb{Z}$.

We have verified the conjecture numerically for all $k \leqslant 1000$.

We also showed that $r_k < 0$ for $k \geqslant 3$, r_k is even for $k > 0$, and $4 | r_k$ unless k is zero or a power of two (all for $k \leqslant 1000$).

Towards the conjecture: we can prove that $k! r_k \in \mathbb{Z}$ (even this weak result is not obvious).

An analogy

The modified Bessel functions $I_0(z)$ and $K_0(z)$ are solutions of the same ordinary differential equation $zy'' + y' - zy = 0$, but $I_0(z)$ increases with z while $K_0(z)$ decreases. $K_0(z)$ is a *minimal solution* of the ODE.

The product $I_0(Z)K_0(z)$ has an asymptotic expansion

$$I_0(z)K_0(z) \sim \frac{1}{2z} \sum_{k \geqslant 0} e_k \, z^{-2k}.$$

Here

$$e_k = \frac{(2k)!^3}{2^{6k} k!^4} = \frac{(2k)!}{2^{6k}} \binom{2k}{k}^2,$$

so clearly $2^{6k} e_k \in \mathbb{Z}$ (in fact $2^{4k} e_k \in \mathbb{Z}$).

Similarly if $(I_0, K_0) \mapsto (I_\nu, K_\nu)$. Here $I_\nu(z)$, $K_\nu(z)$ are independent solutions of the differential equation $z^2y'' + zy' - (z^2 + \nu^2)y = 0$, and we assume that $\nu \in \mathbb{Z}$.

A recurrence for d_k

The rational numbers d_k, and hence the [conjectured] integers $r_k = 2^{6k} d_k$, may be computed as follows, avoiding any mention of the sequence (c_k).

$$d_0 = 1 \text{ and, for all } k \geqslant 1, \; d_k = \frac{1}{8k} \sum_{j=0}^{k-1} \alpha_{j,k} \, d_j .$$

Here the coefficients $\alpha_{j,k}$ are defined by

$$\begin{aligned} \alpha_{j,k} = \; & (-1 + 3 \cdot 2^{m-1} - 2 \cdot 3^m)(\tau)_{m-1}/(m-1)! \\ & + (7 - 17 \cdot 2^m + 17 \cdot 3^m)(\tau)_m/m! \\ & + (-13 + 38 \cdot 2^m - 33 \cdot 3^m)(\tau)_{m+1}/(m+1)! \\ & + 6(1 - 4 \cdot 2^m + 3 \cdot 3^m)(\tau)_{m+2}/(m+2)!, \end{aligned}$$

where $m := k - j$ and $\tau := j + 1/2$.

A recurrence for ρ_n

To prove the result on the previous slide, we use a recurrence satisfied by $\rho_n = a_n b_n$. Since (a_n) and (b_n) are D-finite, so also is (ρ_n), so such a recurrence must exist.

Using $\sigma_n := n\rho_n$, the recurrence may be written as

$$n(n-1)(2n-3)\sigma_n = (2n-1)(3n^2-5n+1)\sigma_{n-1} \\ -(2n-3)(3n^2-5n+1)\sigma_{n-2} + (n-2)(n-3)(2n-1)\sigma_{n-3}$$

(for $n \geqslant 3$), with $\sigma_0 = 0$, $\sigma_1 = G - 1$, $\sigma_2 = 9G/2 - 3$.

The mysterious constants in the definition of $\alpha_{j,k}$ on the previous slide arise in a natural way from the polynomials in the recurrence for σ_n.

Confluent hypergeometric functions

Kummer's differential equation may be written as

$$zw'' + (b - z)w' - aw = 0,$$

with a regular singular point at $z = 0$ and an irregular singular point at $z = \infty$. It has two (usually) linearly independent solutions $M(a, b, z)$ and $U(a, b, z)$. Kummer (1837) considered

$$M(a, b, z) := {}_1F_1(a; b; z) = \sum_{k \geqslant 0} \frac{(a)_k \, z^k}{(b)_k \, k!}, \qquad (1)$$

which is undefined if b is zero or a negative integer. In the case $a \neq b = 0$, we can use the solution

$$zM(a + 1, 2, z) = \lim_{b \to 0} \frac{b}{a} M(a, b, z).$$

A second solution

For a second solution to Kummer's differential equation, Tricomi (1954) introduced

$$U(a,b,z) := \frac{\Gamma(1-b)}{\Gamma(a+1-b)} M(a,b,z) + \frac{\Gamma(b-1)}{\Gamma(a)} z^{1-b} M(a+1-b, 2-b, z),$$

where the right side is undefined if $b \in \mathbb{Z}$, but the definition may be extended by continuity. To avoid this problem, we can use the integral representation (for $\Re(a) > 0, \Re(z) > 0$)

$$U(a,b,z) = \frac{1}{\Gamma(a)} \int_0^\infty e^{-zt}\, t^{a-1}\, (1+t)^{b-a-1}\, dt.$$

We are interested in the case $(a,b,z) = (n,0,1)$.

The connection between a_n, b_n and Kummer functions

Recall that $a_n = [z^n]f_0(z)$ and $b_n = [z^n]f_1(z)$.
We can prove

Theorem

For $n \geqslant 1$,

$$a_n = e^{-1}M(n+1,2,1) \ \ \textit{and} \ \ b_n = -\Gamma(n)U(n,0,1).$$

Sketch of proof. For a_n, we show that a_n and $e^{-1}M(n+1,2,1)$ satisfy the same recurrence (a so-called "connection formula", due to Gauss) and the same initial conditions, so must be equal.

For b_n, we use an integral representation of U to obtain a generating function.

Application to computing the c_k

Slater (1960) and Temme (2013) give asymptotic expansions of the Kummer functions $M(n, b, z)$ and $U(n, b, z)$ for large n. We can use their results to obtain asymptotic expansions of a_n and b_n. However, it is possible to derive the asymptotic expansions of a_n and b_n independently, using the recurrence that both sequences satisfy.

The latter approach has the advantage of showing that the same constants c_k occur in both asymptotic expansions (apart from a change of sign).

Using these two different methods, we obtain two different formulas for the c_k.

Two formulas for the c_k

The direct method gives a recursive formula: $c_0 = 1$ and, for all $k \geqslant 1$,

$$kc_k = [h^{k+3}] \sum_{j=0}^{k-1} c_j h^j \sum_{s \in \{\pm 1\}} (1+sh^2)^{\frac{1-2j}{4}} \exp\left(\frac{2}{h}\left((1+sh^2)^{\frac{1}{2}} - 1\right)\right).$$

The results of Slater and Temme lead to the formula that we mentioned earlier. It does not involve recursion, but does involve Bernoulli numbers:

$$c_m = (-1)^m \sum_{j=0}^{m} [h^{m-j}] \exp(\mu(h)) \, \frac{(m-2j+3/2)_{2j}}{4^j j!} \, ,$$

where $\mu(h) = h^{-1} - (e^h - 1)^{-1} - \frac{1}{2} = -\sum_{k=1}^{\infty} \frac{B_{2k}}{(2k)!} h^{2k-1}$.

Conclusion

I hope that I have given you an interesting conjecture to occupy idle hours – but not, of course, during subsequent talks!

References

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