

# Rounding Error Analysis of Linear Recurrences Using Generating Series

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## A Toy Example

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[Boldo 2009]

$$c_{n+1} = 2c_n - c_{n-1} \quad (c_0 = \diamond(1/3), c_{-1} = 0)$$

	Floating-point arithmetic	Interval arithmetic
n = 0	0.333333333333333	$[0.333333333333333 \pm 1.49e-17]$
5	2.000000000000000	$[2.000000000000000 \pm 3.78e-15]$
10	3.66666666666667	$[3.6666666666667 \pm 5.74e-13]$
15	5.3333333333334	$[5.3333333333 \pm 5.29e-11]$
20	7.00000000000001	$[7.00000000 \pm 1.60e-9]$
25	8.66666666666668	$[8.666667 \pm 4.65e-7]$
30	10.3333333333333	$[10.3333 \pm 4.41e-5]$
35	12.0000000000000	$[12.000 \pm 8.82e-4]$
40	13.6666666666667	$[1.4e+1 \pm 0.406]$
45	15.3333333333334	$[\pm 21.3]$
50	17.0000000000000	$[\pm 5.04e+2]$

## Naïve error analysis

Model:  $\diamond(x \text{ op } y) = x \text{ op } y + \varepsilon_{\text{op}}$  with  $\varepsilon_{\text{op}} \in [-\mathbf{u}, \mathbf{u}]$  ( $\sim$  fixed-point arithmetic)  
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Slightly better: 
$$\begin{aligned}|\tilde{c}_n - c_n| &\leq (\lambda_+ \alpha_+^n + \lambda_- \alpha_-^n - 4) \mathbf{u} \approx 2.4^n \mathbf{u} \\ &\approx 2.4^n \mathbf{u}\end{aligned}$$

$$\alpha_{\pm} = 1 \pm \sqrt{2}$$

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This is what interval evaluation amounts to!

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The error satisfies “the same” recurrence as the computed sequence

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Calculations can become unwieldy (nested sums, determinants...)

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Encode sequences by generating functions



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- + Analytic methods (Cauchy integrals)
- + Fast algorithms
- + Method of majorants
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  $\sum_n \square z^n$

$$z \sum a_n z^n = \sum a_{n-1} z^n$$

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$$|\delta_n| \leq \frac{n(n-1)}{2} \mathbf{u} \quad \text{😊}$$



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## Related work

in the backward direction. There has been less attention devoted to computation which utilizes the difference equation in the forward direction, not because a forward algorithm is more difficult to analyze, but rather for the opposite reason—that its analysis was considered straightforward. Of the above

[Wimp 1972]

### 'Linear' error propagation

- Henrici 1962 finite difference schemes for ODE
- Oliver 1967 linear recurrences

### Explicit bounds (not necessarily easy to compute)

- von Neumann & Goldstine 1947, Turing 1948 triangular system solving
- Elliott 1968 sums of generalized Fourier series
- Wimp 1972 order 2
- Barrio & Melendo & Serrano 2003 order  $n$ ,  $O(u^2)$

### Transfer functions of digital filters

- Liu & Kaneko 1969 random errors
- Hilaire & Lopez 2013 error bounds

# Relative error propagation

Model:  $\diamond(x \text{ op } y) = (x \text{ op } y)(1 + \varepsilon_{\text{op}})$  with  $\varepsilon_{\text{op}} \in [-\mathbf{u}, \mathbf{u}]$  ( $\sim$  floating-point arithmetic)  
 (multiplication by 2 is exact)

Exact rec.:

$$c_{n+1} = 2c_n - c_{n-1} \quad \times(1 + \varepsilon_n)$$

Approx. rec.:

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$$\delta_{n+1} - c_{n+1}\varepsilon_n = (2\delta_n - \delta_{n-1})(1 + \varepsilon_n)$$

$$\delta_{n+1} - 2\delta_n + \delta_{n-1} = \varepsilon_n(c_{n+1} + 2\delta_n - \delta_{n-1})$$

# Relative error propagation

Model:  $\diamond(x \text{ op } y) = (x \text{ op } y)(1 + \varepsilon_{\text{op}})$  with  $\varepsilon_{\text{op}} \in [-\mathbf{u}, \mathbf{u}]$  ( $\sim$  floating-point arithmetic)  
 (multiplication by 2 is exact)

Exact rec.:

$$c_{n+1} = 2c_n - c_{n-1} \quad \times(1 + \varepsilon_n)$$

Approx. rec.:

$$\begin{aligned} \tilde{c}_{n+1} &= \diamond(2\tilde{c}_n - \tilde{c}_{n-1}) \\ &= (2\tilde{c}_n - \tilde{c}_{n-1})(1 + \varepsilon_n) \quad \text{with } |\varepsilon_n| \leq \mathbf{u} \quad \times(-1) \end{aligned}$$

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Translate:

$$\downarrow \sum_n \square z^n$$

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$$\#f(z) = \sum_n |f_n| z^n$$

$$\delta(z) \ll \frac{z(2+z)\mathbf{u}}{(1-z)^2} \# \delta(z) + \frac{\# c(z) \mathbf{u}}{(1-z)^2}$$



# Majorizing equations

 Obtain the bound as a solution of a “similar” equation

$$\delta(z) \ll \frac{z}{(1-z)^2} \# \delta(z) + \frac{\# c(z) u}{(1-z)^2}$$

**Lemma.** [~ Cauchy]

Let  $\hat{a}(z), \hat{b}(z) \in \mathbb{R}_+[[z]]$  with  $\hat{a}(0) = 0$ . Suppose  $y \in \mathbb{R}_+[[z]]$  satisfies

$$y(z) \ll \hat{a}(z) y(z) + \hat{b}(z).$$

Then  $y(z)$  is majorized by the solution of  $\hat{y}(z) = \hat{a}(z) \hat{y}(z) + \hat{b}(z)$ , i.e.,

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**Proof.**

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## Bound on the floating-point error

$$\#\delta(z) \ll \underbrace{\frac{z(2+z)\mathbf{u}}{(1-z)^2} \#\delta(z)}_{\hat{a}(z)} + \underbrace{\frac{\#c(z)\mathbf{u}}{(1-z)^2}}_{\hat{b}(z)}$$

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$$\ll \frac{|c_0|}{(1-z)^2} =: \hat{c}(z)$$

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$$|\delta_n| \leq \frac{|c_0|}{6} (n+3)^3 \alpha^n \mathbf{u}$$

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Exponential for fixed  $\mathbf{u}$ ,  
but  $O(n^3 \mathbf{u})$  if  $n = O(\mathbf{u}^{-1/2})$

# Differential equations

# Evaluation of Legendre polynomials

[Johansson & M. 2018]

**Algorithm 1.** Evaluation of Legendre polynomials in GMP fixed-point arithmetic.

**Input:** An integer  $x$  and  $t \geq 0$  such that  $|2^{-t}x| \leq 1$ , and  $n \geq 1$

**Output:**  $p, q$  such that  $|2^{-t}p - P_{n-1}(2^{-t}x)|, |2^{-t}q - P_n(2^{-t}x)| \leq (0.75(n+1)(n+2)+1)2^{-t}$

```

1: void legendre(mpz_t p, mpz_t q, int n, const mpz_t x, int t) {
2:     mpz_t tmp; int k; mpz_init(tmp);                                ▷ Comments use the notation of
3:     mp_limb_t denlo, den = 1;                                       ▷ the proof of Corollary 6
4:     mpz_set_ui(p, 1); mpz_mul_2exp(p, p, t);                         ▷  $p_0 = 2^t$ 
5:     mpz_set(q, x);                                                 ▷  $q_0 = x$ 
6:     for (k = 1; k < n; k++) {
7:         mpz_mul(tmp, q, x); mpz_tdiv_q_2exp(tmp, tmp, t);           ▷  $\lceil \hat{x} q_{k-1} 2^{-t} \rceil$ 
8:         mpz_mul_si(p, p, -k*k);
9:         mpz_addmul_ui(p, tmp, 2*k+1);                                ▷  $-k^2 p_{k-1} + (2k+1) \text{tmp}$ 
10:        mpz_swap(p, q);
11:        if (mpn_mul_i(&denlo, &den, 1, k+1)) {                      ▷ If multiplication overflows
12:            mpz_tdiv_q_ui(p, p, den);                                 ▷  $\lceil p/d_{k-1} \rceil$ 
13:            mpz_tdiv_q_ui(q, q, den);
14:            den = k+1;                                              ▷  $d_k = k+1$ 
15:        } else den = denlo;                                         ▷  $d_k = (k+1)d_{k-1}$ 
16:    }
17:    mpz_tdiv_q_ui(p, p, den/n); mpz_tdiv_q_ui(q, q, den);
18:    mpz_clear(tmp);
19: }
```

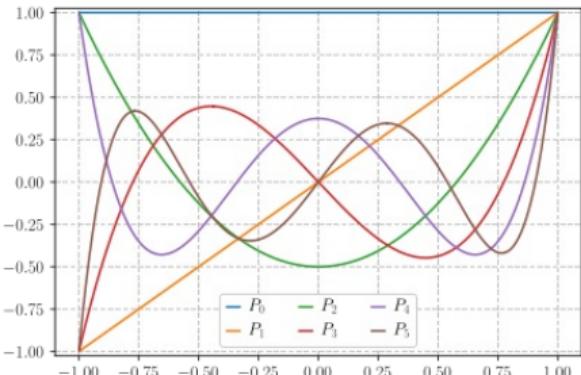
Context: rigorous arbitrary-precision  
 Gauss-Legendre quadrature  
 [Johansson 2018]

$$P_{n+1}(x) = \frac{1}{n+1} [(2n+1)x P_n(x) - n P_{n-1}(x)]$$

$\tilde{p}_n = P_n(x)$  evaluated using this recurrence  
 in  $t$ -bit fixed-point arithmetic



Bound  $|\tilde{p}_n - P_n(x)|$ .



## Legendre polynomials: error analysis

Exact rec.:

$$p_{n+1} = \frac{1}{n+1} [(2n+1)x p_n - n p_{n-1}] \quad p_n := P_n(x)$$

Approx. rec.:

$$\tilde{p}_{n+1} = \frac{1}{n+1} [(2n+1)x \tilde{p}_n - n \tilde{p}_{n-1}] + \varepsilon_{n+1} \quad \text{with } \varepsilon_n \leq 3u$$

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Global error:

$$\delta_n = \tilde{p}_n - p_n \quad (n+1) \delta_{n+1} = (2n+1)x \delta_n - n \delta_{n-1} + (n+1) \varepsilon_{n+1}$$

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Translate:

$$\downarrow \sum_n \square z^n$$

$$(1 - 2x z + z^2) \delta'(z) = z(x - z) \delta(z) + \varepsilon'(z)$$

Solve:

$$\delta(z) = \frac{1}{\sqrt{1 - 2x z + z^2}} \int_0^z \frac{\varepsilon'(w)}{\sqrt{1 - 2x w + w^2}} dw$$

## Legendre polynomials: bound

$$\delta(z) = \frac{1}{\sqrt{1 - 2x z + z^2}} \int_0^z \frac{\varepsilon'(w)}{\sqrt{1 - 2x w + w^2}} dw$$

$$\varepsilon(z) \ll \frac{3u}{1-z}$$

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 \end{aligned}$$

**Proposition.** [Johansson & M.]

For all  $x \in [-1, 1]$  and  $n \in \mathbb{N}$ , the error in the recursive fixed-point computation of Legendre polynomials satisfies

$$|\tilde{p}_n - P_n(x)| \leq \frac{3}{4} (n+1)(n+2) u.$$

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We were lucky that the equation could be solved explicitly

# Partial sums of differentially finite series

$$L(u) = a_r u^{(r)} + \cdots + a_1 u' + a_0 u = 0, \quad a_i \in \mathbb{C}[z]$$



Given the operator  $L$ , initial values  $u_0, \dots, u_{r-1}$ , an evaluation point  $\zeta$ , a truncation order  $N$  compute an **enclosure** of  $\sum_{n=0}^{N-1} u_n \zeta^n$ .

## Assumptions

ordinary point  $a_r(0) \neq 0$

“obvious” geometric convergence  $|\zeta| < \min \{ |\xi| : a_r(\xi) = 0 \}$

## Strategy

- Compute a recurrence on the  $u_n$
- Compute and sum the  $u_n \zeta^n$  iteratively  $\Rightarrow$  need to avoid interval blow-up

## D-finite series: error propagation

Exact rec.:  $u_n = \frac{-1}{b_s(n)} [b_{s-1}(n) u_{n-1} + \dots + b_1(n) u_{n-s+1} + b_0(n) u_{n-s}]$

Approx. rec.:  $\tilde{u}_n = \frac{-1}{b_s(n)} [b_{s-1}(n) \tilde{u}_{n-1} + \dots + b_1(n) \tilde{u}_{n-s+1} + b_0(n) \tilde{u}_{n-s}] + \varepsilon_n$

local error bound  $|\varepsilon_n| \leq \hat{\varepsilon}_n$  computed on the fly

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('running' error analysis)

The global error  $\delta_n = \tilde{u}_n - u_n$  satisfies

$$b_s(n) \delta_n + b_{s-1}(n) \delta_{n-1} + \dots + b_0(n) \delta_{n-s} = b_s(n) \varepsilon_n$$

$$\downarrow \sum_n \square z^n$$

$$a_r(z) \delta^{(r)}(z) + \dots + a_1(z) \delta'(z) + a_0(z) \delta(z) = Q(\theta) \cdot \varepsilon(z) \quad \theta = z \frac{d}{dz}$$

$$Q(\theta) = b_s(0) \theta (\theta - 1) \dots (\theta - s + 1) \text{ (ordinary point)}$$

Compute a bound on  $\delta_n$  given one on  $\varepsilon_n$ ?

## D-finite series: error bound

$$a_r(z) \delta^{(r)}(z) + \cdots + a_1(z) \delta'(z) + a_0(z) \delta(z) = Q(\theta) \cdot \varepsilon(z)$$

**Lemma.** [~ Cauchy]

Let  $a_0, \dots, a_r \in \mathbb{C}[z]$ . Suppose  $y \in \mathbb{C}[[z]]$  satisfies

$$a_r(z) y^{(r)}(z) + \cdots + a_0(z) y(z) = Q(\theta) \cdot \varepsilon(z).$$

Suppose  $\varepsilon(z) \ll \hat{\varepsilon}(z)$ .

One can compute a rational series  $\hat{a}(z) \in \mathbb{R}_+[[z]]$  such that  $y(z)$  is majorized by any solution of

$$\hat{y}'(z) = \hat{a}(z) \hat{y}(z) + \hat{\varepsilon}(z)$$

such that  $|y_0|, \dots, |y_{r-1}| \leq \hat{y}_0$ .

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Solve:

$$\hat{\delta}(z) = \hat{h}(z) \left( \text{cst} + \int_0^z \frac{\hat{\varepsilon}(w)}{\hat{h}(w)} dw \right), \quad \hat{h}(z) = \exp \int_0^z \hat{a}(w) dw$$

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Choose  $\hat{\varepsilon}_n = \bar{\varepsilon} \hat{h}_n$ :

$$= \bar{\varepsilon} z \hat{h}(z)$$

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$$\hat{\delta}(z) = \hat{h}(z) \left( c \text{st} + \int_0^z \frac{\hat{\varepsilon}(w)}{\hat{h}(w)} dw \right), \quad \hat{h}(z) = \exp \int_0^z \hat{a}(w) dw$$

Choose  $\hat{\varepsilon}_n = \bar{\varepsilon} \hat{h}_n$ :

$$= \bar{\varepsilon} z \hat{h}(z)$$



Compute a bound on the truncation error at the same time

# Bernoulli Numbers

## Scaled Bernoulli numbers

$$B_n = 1, \frac{-1}{2}, \frac{1}{6}, 0, \frac{-1}{30}, 0, \frac{1}{42}, 0, \frac{-1}{30}, 0, \frac{5}{66}, 0, \frac{-691}{2730}, 0, \frac{7}{6}, 0, \frac{-3617}{510}, \dots$$

$$|B_{2k}| \sim \frac{2(2k)!}{(2\pi)^{2k}}$$

$$\mathbf{b}_k = \frac{B_{2k}}{(2k)!}$$

$$b(z) = \sum_{k=0}^{\infty} \mathbf{b}_k z^k = \frac{\sqrt{z}/2}{\tanh(\sqrt{z}/2)}$$

**Algorithm.** [Brent 1980, based on a suggestion of Reinsch]

$$\mathbf{b}_k = \frac{1}{(2k)! 4^k} - \sum_{j=0}^{k-1} \frac{\mathbf{b}_j}{(2k+1-2j)! 4^{k-j}}$$

be used with sufficient guard digits, or **a more stable recurrence** must be used. If we multiply both sides of (30) by  $\sinh(x/2)/x$  and equate coefficients, we get the recurrence

$$C_k + \frac{C_{k-1}}{3! 4} + \cdots + \frac{C_1}{(2k-1)! 4^{k-1}} = \frac{2k}{(2k+1)! 4^k} \quad (36)$$

If (36) is used to evaluate  $C_k$ , using precision  $n$  arithmetic, the error is only  $O(k^2 2^{-n})$ . Thus,

[Brent 1980]

## Error in the floating-point computation of $b_k$

$$b_k = \frac{1}{(2k)! 4^k} - \sum_{j=0}^{k-1} \frac{b_j}{(2k+1-2j)! 4^{k-j}}, \quad \tilde{b}_k = \text{computed values}$$

**Exercise 4.35** Prove (or give a plausibility argument for) the statements made in §4.7 that: (a) if a recurrence based on (4.59) is used to evaluate the scaled Bernoulli number  $C_k$ , using precision  $n$  arithmetic, then the relative error is of order  $4^k 2^{-n}$ ; and (b) if a recurrence based on (4.60) is used, then the relative error is  $O(k^2 2^{-n})$ .

[Brent & Zimmermann 2010]

**Conjecture.** [Brent, Zimmermann]

The computed values  $\tilde{b}_k$  satisfy  $\tilde{b}_k = b_k (1 + \eta_k)$  where  $\eta_k = O(k \cdot u)$ .

$u$  = unit roundoff

**Remark.** To be understood as  $\eta_k = O(k \cdot u)$  when  $k = O(u^{-1})$   
 or  $|\eta_k| \leq C_k u$  as  $u \rightarrow 0$  with  $C_k = O(k)$  (resp.  $O(k^2)$ )

## Error analysis

$$b_k = \frac{1}{(2k)! 4^k} - \sum_{j=0}^{k-1} \frac{b_j}{(2k+1-2j)! 4^{k-j}}, \quad \tilde{b}_k = \text{computed values}$$

### Local error analysis.

$$\tilde{b}_k = \frac{1 + s_k}{(2k)! 4^k} - \sum_{j=0}^{k-1} \frac{\tilde{b}_j (1 + t_{k,j})}{(2k+1-2j)! 4^{k-j}}$$

$|s_k| \leq \hat{\theta}_{2k}$   
 $|t_{k,j}| \leq \hat{\theta}_{3(k-j)+2}$   
 where  $\hat{\theta}_n = (1 + u)^n - 1$

# Error analysis

$$b_k = \frac{1}{(2k)! 4^k} - \sum_{j=0}^{k-1} \frac{b_j}{(2k+1-2j)! 4^{k-j}}, \quad \tilde{b}_k = \text{computed values}$$

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**Linearity.**  $\delta_k := \tilde{b}_k - b_k = \text{global error}$

$$\delta_k = \frac{s_k}{(2k)! 4^k} - \sum_{j=0}^{k-1} \frac{\delta_j + (b_j + \delta_j) t_{k,j}}{(2k+1-2j)! 4^{k-j}}$$

# Error analysis

$$b_k = \frac{1}{(2k)! 4^k} - \sum_{j=0}^{k-1} \frac{b_j (1 + t_{k,j})}{(2k+1-2j)! 4^{k-j}}, \quad \tilde{b}_k = \text{computed values}$$

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## Inequation on the global error.

$$\delta(z) \ll \check{S}(z) \tilde{C}(z) + \check{S}(z) \tilde{S}(z) \# \delta(z) + \check{S}(z) \tilde{S}(z) \# b(z)$$

$$\# f(z) = \sum_k |f_k| z^k$$

where

$$C(z) = \cosh(\sqrt{z}/2),$$

$$S(z) = (\sqrt{z}/2)^{-1} \sinh(\sqrt{z}/2),$$

$$\check{S}(z) = \frac{(\sqrt{z}/2)}{\sin(\sqrt{z}/2)},$$

$$\tilde{C}(z) = C(a^2 z) - C(z),$$

$$\tilde{S}(z) = S(a^4 z) - S(z) - (a^2 - 1)$$

$$\text{with } a = 1 + u$$

# Error analysis

$$b_k = \frac{1}{(2k)! 4^k} - \sum_{j=0}^{k-1} \frac{b_j (1 + t_{k,j})}{(2k+1-2j)! 4^{k-j}}, \quad \tilde{b}_k = \text{computed values}$$

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with  $a = 1 + u$

## First-order bound

$$\delta(z) \ll \check{S}(z) \tilde{C}(z) + \check{S}(z) \tilde{S}(z) \# b(z) + \check{S}(z) \tilde{S}(z) \# \delta(z)$$

**'Explicit' majorant.** By the first lemma on majorizing equations

$$\delta(z) \ll \frac{\check{S}(z) \tilde{C}(z) + \check{S}(z) \tilde{S}(z) \# b(z)}{1 - \check{S}(z) \tilde{S}(z)} =: \hat{\delta}(z)$$

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**Asymptotic behavior.**



Series notation → computer algebra

$$\hat{\delta}(z) = \left( \frac{2(1 - \cosh w) \cos(w)}{w^{-2} \sin(w)^2} + \frac{4(\cosh w - 1) + w \sinh w}{w^{-1} \sin w} \right) \mathbf{u} + O(\mathbf{u}^2)$$

$$w = \sqrt{z}/2$$

Unique dominant pole at  $z = 4\pi^2$ ,  
multiplicity (w.r.t.  $z$ ) = 2

$$\Rightarrow \hat{\delta}_k = O(k(2\pi)^{-2k}) \cdot \mathbf{u} + O(\mathbf{u}^2)$$

$$\Rightarrow \eta_k = "O(k \cdot \mathbf{u})"$$

## A 'hard' bound

$$\delta(z) = \hat{\delta}(z) \ll \frac{\check{S}(z) \tilde{C}(z) + \check{S}(z) \tilde{S}(z) \# b(z)}{1 - \check{S}(z) \tilde{S}(z)}$$

### Controlling the dominant pole.

Suppose  $u \leq 2^{-16}$ .

Then  $\hat{\delta}(z)$  has a pole at  $\gamma = \left( \frac{2\pi}{1 + \varphi(u)} \right)^2$  where  $0 \leq \varphi(u) \leq 2(\cosh \pi - 1)u$ .

This is the only pole with  $|z| < 153.7 \approx (3.9\pi)^2$ .

(A little analysis + comparison with the limiting case using Rouché's theorem.)

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### Symbolic-numeric estimate.

$$\hat{\delta}(z) = \frac{2 \text{ explicit } R(u)}{1 - z/\gamma} - \frac{2}{1 - z/(2\pi)^2} + \text{ analytic for } |z| < 153.7$$

$$\hat{\delta}(z) \ll \frac{2 |\text{R}(u) - 1|}{1 - z/\gamma} + \frac{\text{explicit and O}(u)}{(1 - z/\gamma)^2} + \frac{\sup_{|z=\lambda\gamma|} \text{analytic}}{1 - z/(\lambda\gamma)}$$

Cauchy's formula + interval arithmetic.

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Cauchy's formula + interval arithmetic.

## Scaled Bernoulli numbers: conclusion

$$b(z) = \frac{\sqrt{z}/2}{\tanh(\sqrt{z}/2)}$$

$$b_k = \frac{1}{(2k)! 4^k} - \sum_{j=0}^{k-1} \frac{b_j}{(2k+1-2j)! 4^{k-j}}$$

$$\tilde{b}_k = b_k (1 + \eta_k)$$

**Theorem.** The total relative error satisfies

$$|\eta_k| \leq (1 + 21.2 u)^k (1.1 k + 446) u$$

**Corollary.** Assuming  $u < 2^{-16}$  and  $43 k u \leq 1$ , one has  $|\eta_k| \leq (3 k + 1213) u$ .

# Conclusion



Error analyses of linear recurrences can (should!) use generating series



- Local errors → global errors via exact expressions or equations
- Cauchy majorants
- Analytic methods



- Legendre polynomials
- General D-finite functions
- Bernoulli numbers



- Other algorithms for D-finite functions, e.g.,  $O(n M(d)/d)$
- Tighter bounds in practice
- Backward recurrence schemes
- Orthogonal polynomials, numerical integration schemes, ...

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Thank you!

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