High-precision methods for zeta functions
Part 2: derivatives

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Computing derivatives

$$f(a+x) = \sum_{n=0}^{\infty} \frac{f^{(n)}(a)}{n!} x^n$$

Reasons we might want to compute derivatives

- We are interested in the derivatives / Taylor coefficients themselves
- Removing singularities (computing limits)
- Analytic operations (integrals, finding roots or extreme points). Newton's method:

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$$

Numerical differentiation

Finite difference:

$$f^{(n)}(a) \approx \frac{1}{h^n} \sum_{k=0}^{n} (-1)^{k+n} \binom{n}{k} f(a+kh), \quad h \sim 2^{-p}$$

Cauchy integral formula:

$$f^{(n)}(a) = \frac{n!}{2\pi i} \oint_{\gamma} \frac{f(z)}{(z-a)^{n+1}} \, dz$$

Symbolic differentiation

```
sage: diff(1/cos(x), x, 10)

50521/cos(x) + 1326122*sin(x)^2/cos(x)^3 +
6749040*sin(x)^4/cos(x)^5 + 13335840*sin(x)^6/cos(x)^7 +
11491200*sin(x)^8/cos(x)^9 + 3628800*sin(x)^10/cos(x)^11
```

$$\zeta^{(n)}(s) = ???$$

Power series arithmetic (automatic differentiation)

We work with objects

$$f = f_0 + f_1 x + \ldots + f_{n-1} x^{n-1} \quad \in \quad \mathbb{C}[[x]]/\langle x^n \rangle$$

With $n = 2$ (first derivatives):

$$(f_0 + f_1 x) \times (g_0 + g_1 x) = f_0 g_0 + (f_0 g_1 + f_1 g_0) x$$

$$\frac{1}{f_0 + f_1 x} = \frac{1}{f_0} - \frac{f_1}{f_0^2} x$$

$$\sin(f_0 + f_1 x) = \sin(f_0) + \cos(f_1) x$$

Formal and non-formal operations

$$\frac{1}{1-f} = 1 + f + f^2 + f^3 + \dots$$

With $f = x + x^2$:

$$1 + (x + x^2) + (x^2 + 2x^3 + x^4) + (x^3 + 3x^4 + 3x^5 + x^6) + \dots$$

With $f = 0.5 + x$:

$$1 + (0.5 + x) + (0.25 + x + x^2) + (0.125 + 0.75x + 1.5x^2 + x^3) + \dots$$

With $f = 2 + x^2$?

Functions of formal power series

In general, if F is a function and f is a power series, we define

$$F(f) = F(f_0 + x) \circ (f_1 x + f_2 x^2 + \ldots)$$

where

$$F(c + x) = F(c) + F'(c)x + \frac{1}{2}F''(c)x^2 + \ldots$$

and $\circ$ denotes **formal** composition of two power series.

Example:

$$\frac{1}{1-f} = \left(\frac{1}{1-f_0} + \frac{x}{(1-f_0)^2} + \frac{x^2}{(1-f_0)^3} \ldots\right) \circ (f_1 x + f_2 x^3 + \ldots)$$

Fast power series arithmetic

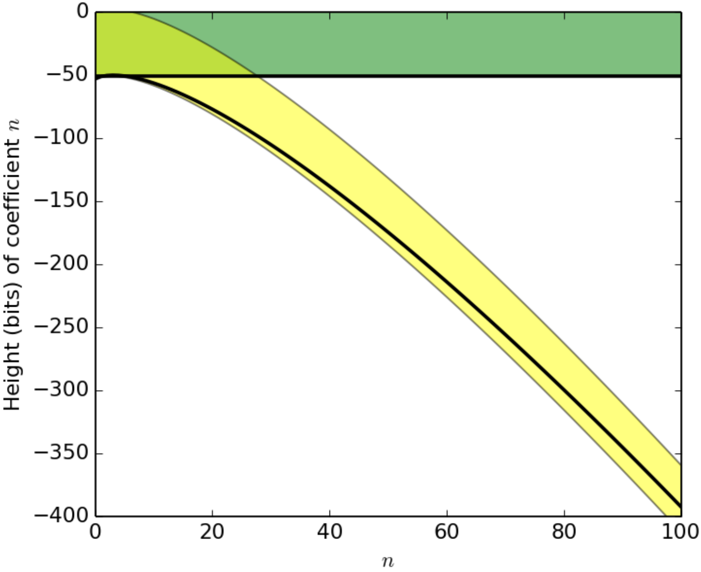
For large n, **reduce everything to multiplication**

- Classical polynomial multiplication: $M(n) = O(n^2)$ arithmetic operations, $\tilde{O}(n^2 p)$ bit operations
- FFT-based polynomial multiplication: $M(n) = \tilde{O}(n)$ arithmetic operations, $\tilde{O}(np)$ bit operations

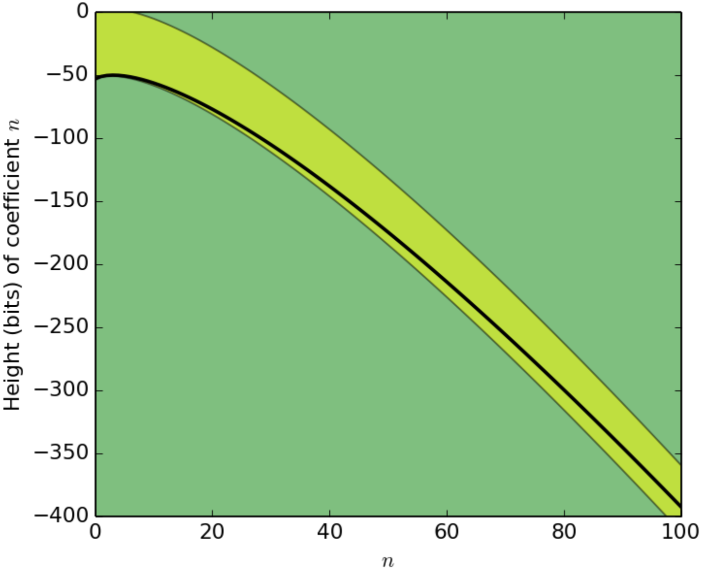
Caveat: When working with numerical data, we often need precision $p \sim n$, so effective bit complexity with FFT is often $\tilde{O}(n^2)$.

Feasible to work with $n \approx 10^5$ ($\approx 10^{10}$ bits of data).

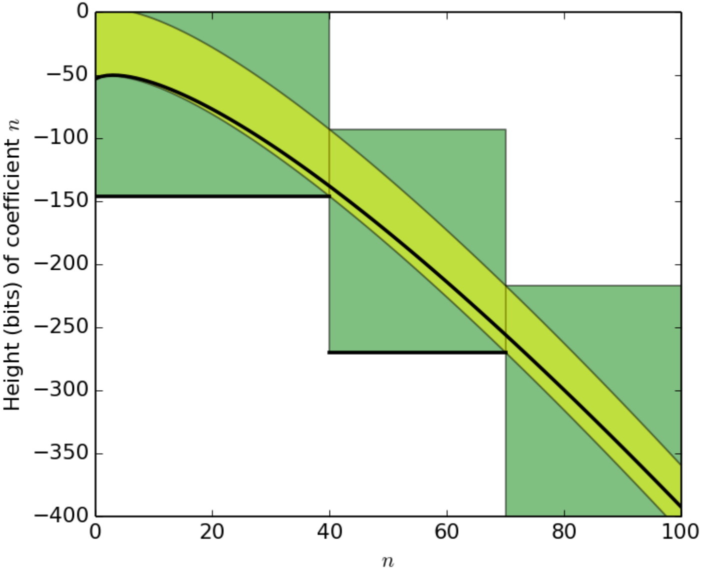
Bad: truncate



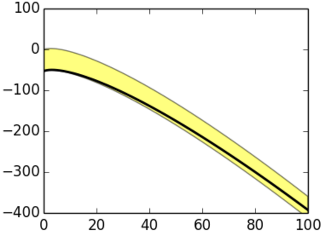
Bad: cover everything



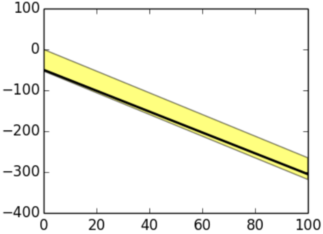
Better: split into blocks



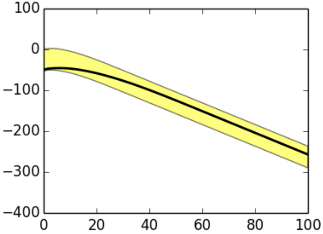
Improving efficiency: scaling



$F(x)$ $\times$

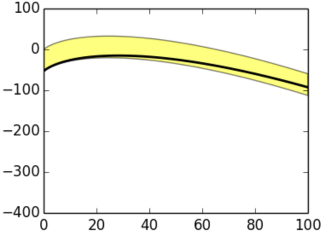


$G(x)$



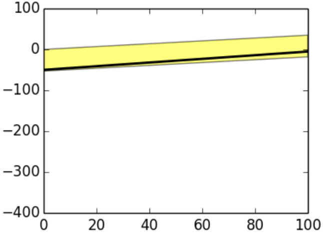
$= H(x)$

Improving efficiency: scaling

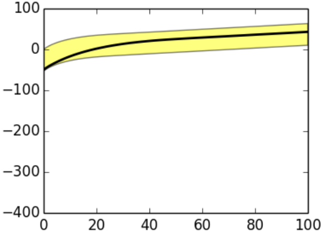


$F(2^c x)$

$\times$



$G(2^c x)$



$= H(2^c x)$

Fast operations on power series

Many operations on power series of length n can all be done in $O(M(n))$ arithmetic operations:

- Multiplication
- Division
- Square root
- Elementary functions (exp, log, sin, ...)
- Solution of some differential equations

Formal Newton iteration

To solve $F(g) = 0$, apply the Newton step

$$g_{new} = g_{old} - \frac{F(g_{old})}{F'(g_{old})}$$

If $F(g_{old}) = O(x^n)$, then $F(g_{new}) = O(x^{2n})$

Example: to compute the reciprocal $1/f$ of a power series, solve

$$F(g) = \frac{1}{g} - f$$

which corresponds to the Newton update

$$g_{new} = 2g_{old} - fg_{old}^2.$$

Fast mass computation of Bernoulli numbers

Using the generating function:

$$\frac{x}{e^x - 1} = \frac{1}{1 + \frac{1}{2}x + \frac{1}{6}x^2 + \ldots} = \sum_{k=0}^{\infty} \frac{B_k}{k!} x^k$$

Cost to compute n Bernoulli numbers exactly (using $\mathbb{Q}[[x]]$ arithmetic):

- $O(M(n)) = \tilde{O}(n)$ arithmetic operations
- $\tilde{O}(n^2)$ bit operations

A slower (but faster) algorithm for Bernoulli numbers

How to generate $B_0, B_1, \ldots, B_{10\,000}$ in two seconds!

$$B_{2n} = (-1)^{n+1} \frac{2(2n)!}{(2\pi)^{2n}} \zeta(2n)$$

$$\zeta(2) = 1 + \frac{1}{2^2} + \frac{1}{3^2} + \frac{1}{4^2} + \ldots$$

$$\zeta(4) = 1 + \frac{1}{2^4} + \frac{1}{3^4} + \frac{1}{4^4} + \ldots$$

$$\zeta(6) = 1 + \frac{1}{2^6} + \frac{1}{3^6} + \frac{1}{4^6} + \ldots$$

Recycle the powers in each column (multiplication by $2^2, 3^2, 4^2, \ldots$)

Complexity is $\tilde{O}(n^3)$, but in practice an order of magnitude faster than the $\tilde{O}(n^2)$ power series algorithm. I first saw this algorithm in a blog by Remco Bloemen `http://2π.com/09/11/even-faster-zeta-calculation`

Elementary functions of power series

Functional equation + formal composition

$$\exp(f) = \exp(f_0)\left(\exp(x) \circ (f_1 x + f_2 x^2 + \ldots)\right)$$

$$\log(f) = \log(f_0) + \log(1+x) \circ \left(\frac{x f_1 + x^2 f_2 + \ldots}{f_0}\right)$$

Fast formal composition ($O(M(n))$ arithmetic operations):

$$\log(1+f) = \int \frac{f'}{1+f}$$

$$\operatorname{atan}(f) = \int \frac{f'}{1+f^2}$$

Newton iteration gives log $\to$ exp, atan $\to$ tan, etc.

Fast composition of arbitrary formal power series

Horner's rule

$$f(g(x)) = f_0 + g(f_1 + g(f_2 + \cdots + g(f_{n-2} + f_{n-1}x)\cdots))$$

Arithmetic complexity: $O(nM(n))$

Brent-Kung 2.1: baby-step, giant-step version of Horner's rule
Arithmetic complexity: $O(n^{1/2}M(n) + n^{1/2}MM(n^{1/2}))$

Brent-Kung 2.2: divide-and-conquer Taylor expansion
Arithmetic complexity: $O((n \log n)^{1/2}M(n))$

Brent-Kung algorithm 2.1

Example with $n = 9$, $m = \lceil \sqrt{n} \rceil = 3$

Computing $f(g)$ where $f = f_0 + f_1 x + \ldots + f_8 x^8$

$$(f_0 + f_1 g + f_2 g^2) + (f_3 + f_4 g + f_5 g^2) g^3 + (f_6 + f_7 g + f_8 g^2) g^6$$

$(m \times m) \times (m \times m^2)$ matrix multiplication:

$$\begin{pmatrix} f_0 & f_1 & f_2 \\ f_3 & f_4 & f_5 \\ f_6 & f_7 & f_8 \end{pmatrix} \times \begin{pmatrix} & 1 & \\ & g & \\ & g^2 & \end{pmatrix}$$

Finally apply Horner's rule to block polynomials.

General functions of power series

If f, g are holomorphic with

$$f(z) \approx g(z)$$

for all z inside some disk, then also

$$f^{(n)}(z) \approx g^{(n)}(z)$$

$$\zeta(s) \approx \sum_{k=1}^{N} \frac{1}{k^s} \quad \Rightarrow \quad \zeta(s+x) \approx \sum_{k=1}^{N} \frac{1}{k^{s+x}}$$

where $\zeta(s+x) = \zeta(s) + \zeta'(s)x + \frac{1}{2}\zeta''(s)x \ldots$

To compute derivatives of $\zeta(s)$, take your favorite approximate formula and evaluate it at $s + x \in \mathbb{C}[[x]]$ instead of s.

Recall: the Euler-Maclaurin formula

$$\sum_{k=N}^{U} f(k) = I + T + R$$

$$I = \int_N^U f(t)\, dt$$

$$T = \frac{1}{2}\left(f(N) + f(U)\right) + \sum_{k=1}^{M} \frac{B_{2k}}{(2k)!}\left(f^{(2k-1)}(U) - f^{(2k-1)}(N)\right)$$

$$R = -\int_N^U \frac{\tilde{B}_{2M}(t)}{(2M)!} f^{(2M)}(t)\, dt$$

Computing $\zeta(s, a)$ using Euler-Maclaurin

$$\zeta(s,a) = \underbrace{\sum_{k=0}^{N-1} f(k)}_{S} + \underbrace{\sum_{k=N}^{\infty} f(k)}_{I+T+R}, \quad f(k) = \frac{1}{(a+k)^s}$$

For derivatives, substitute $s \to s + x \in \mathbb{C}[[x]]$:

$$f(k) = \frac{1}{(a+k)^{s+x}} = \sum_{i=0}^{\infty} \frac{(-1)^i \log^i(a+k)}{i!(a+k)^s} x^i \in \mathbb{C}[[x]]$$

The terms

$$f(1) = \left[\frac{1}{(a+1)^s}\right] + \left[-\frac{\log(a+1)}{(a+1)^s}\right] x + \left[\frac{\log^2(a+1)}{2(a+1)^s}\right] x^2 + \dots$$

$$f(2) = \left[\frac{1}{(a+2)^s}\right] + \left[-\frac{\log(a+2)}{(a+2)^s}\right] x + \left[\frac{\log^2(a+2)}{2(a+2)^s}\right] x^2 + \dots$$

$$f(3) = \left[\frac{1}{(a+3)^s}\right] + \left[-\frac{\log(a+3)}{(a+3)^s}\right] x + \left[\frac{\log^2(a+3)}{2(a+3)^s}\right] x^2 + \dots$$

Parts to evaluate

$$S = \sum_{k=0}^{N-1} \frac{1}{(a+k)^{s+x}}$$

$$I = \int_N^\infty \frac{1}{(a+t)^{s+x}} dt = \frac{(a+N)^{1-(s+x)}}{(s+x)-1}$$

$$T = \frac{1}{(a+N)^{s+x}} \left(\frac{1}{2} + \sum_{k=1}^{M} \frac{B_{2k}}{(2k)!} \frac{(s+x)_{2k-1}}{(a+N)^{2k-1}} \right)$$

$$R = -\int_N^\infty \frac{\tilde{B}_{2M}(t)}{(2M)!} \frac{(s+x)_{2M}}{(a+t)^{(s+x)+2M}} dt \quad \text{(bound)}$$

Bounding the remainder

Define $|f| = |f_0| + |f_1|x + |f_2|x^2 + \ldots$
Then $|f+g| \le |f| + |g|$ and $|fg| \le |f||g|$ (coefficient-wise)

$$|R| = \left| \int_N^\infty \frac{\tilde{B}_{2M}(t)}{(2M)!} \frac{(s+x)_{2M}}{(a+t)^{s+x+2M}} dt \right|$$
$$\le \int_N^\infty \left| \frac{\tilde{B}_{2M}(t)}{(2M)!} \frac{(s+x)_{2M}}{(a+t)^{s+x+2M}} \right| dt$$
$$\le \frac{4\,|(s+x)_{2M}|}{(2\pi)^{2M}} \int_N^\infty \left| \frac{dt}{(a+t)^{s+x+2M}} \right| \in \mathbb{R}[[x]]$$

$$\int_N^\infty \left| \frac{dt}{(a+t)^{s+x+2M}} \right| = \sum_{k=0}^{\infty} \left(\int_N^\infty \frac{dt}{k!} \left| \frac{\log(a+t)^k}{(a+t)^{s+2M}} \right| \right) x^k$$

A sequence of integrals

For $k \in \mathbb{N}$, $A > 0, B > 1, C \geq 0$,

$$J_k(A, B, C) \equiv \int_A^\infty t^{-B}(C + \log t)^k dt = \frac{L_k}{(B-1)^{k+1} A^{B-1}}$$

where

$$L_0 = 1, \; L_k = kL_{k-1} + D^k$$

$$D = (B-1)(C + \log A)$$

Error bound

Given complex numbers $s = \sigma + \tau i$, $a = \alpha + \beta i$ and positive integers N, M such that $\alpha + N > 1$ and $\sigma + 2M > 1$, the error term in the Euler-Maclaurin summation formula applied to $\zeta(s + x, a) \in \mathbb{C}[[x]]$ satisfies

$$|R(s+x)| \le \frac{4\,|(s+x)_{2M}|}{(2\pi)^{2M}} \left| \sum_{k=0}^{\infty} R_k x^k \right| \in \mathbb{R}[[x]]$$

where $R_k \le (K/k!)\, J_k(N + \alpha, \sigma + 2M, C)$, with

$$C = \frac{1}{2} \log\left(1 + \frac{\beta^2}{(\alpha+N)^2}\right) + \operatorname{atan}\left(\frac{|\beta|}{\alpha+N}\right)$$

and

$$K = \exp\left(\max\left(0, \tau \operatorname{atan}\left(\frac{\beta}{\alpha+N}\right)\right)\right).$$

Evaluation steps

To evaluate $\zeta(s+x, a)$ with an error of 2^{-p}:

1. Choose $N, M = O(p)$, bound the error term R
2. Compute the power sum S
3. Compute the integral I
4. Compute the Bernoulli numbers
5. Compute the tail T

Some computational results

Stieltjes constants

The **(generalized) Stieltjes constants** are the coefficients $\gamma_n(a)$ in the Laurent series

$$\zeta(s, a) = \frac{1}{s-1} + \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \gamma_n(a) \, (s-1)^n.$$

The **(classical) Stieltjes constants** $\gamma_n = \gamma_n(1)$ have numerical values

$\gamma_0 \approx +0.577216$	$\gamma_{10} \approx +0.000205$
$\gamma_1 \approx -0.072816$	$\gamma_{100} \approx -4.25340 \times 10^{17}$
$\gamma_2 \approx -0.009690$	$\gamma_{1000} \approx -1.57095 \times 10^{486}$

Asymptotics of Stieltjes constants

One of the best available bounds for γ_n is [Matsuoka, 1985]:

$$|\gamma_n| < 0.0001 e^{n \log \log n}, \; n \geq 10$$

But this is not very accurate.

Actual value: $\gamma_{1000} \approx -1.57095 \times 10^{486}$

Matsuoka: $|\gamma_{1000}| < 2.17242 \times 10^{835}$

Knessl-Coffey approximation

[Knessl and Coffey, *An effective asymptotic formula for the Stieltjes constants*, 2011]

$$\gamma_n \sim \frac{B}{\sqrt{n}} e^{nA} \cos(an + b)$$

$$A = \frac{1}{2}\log(u^2 + v^2) - \frac{u}{u^2 + v^2}, \; B = \frac{2\sqrt{2\pi}\sqrt{u^2 + v^2}}{[(u+1)^2 + v^2]^{1/4}}$$

$$a = \tan^{-1}\left(\frac{v}{u}\right) + \frac{v}{u^2 + v^2}, \; b = \tan^{-1}\left(\frac{v}{u}\right) - \frac{1}{2}\left(\frac{v}{u+1}\right)$$

where $u = v \tan v$, and v is the unique solution of $2\pi \exp(v \tan v) = (n/v)\cos(v)$, $0 < v < \pi/2$. Similar formula for $\gamma_n(a)$, $a \neq 1$.

- Predicts sign oscillations (correct except for $n = 137$?)
- Accurate even for small n
- No explicit error bound

Computations of Stieltjes constants

[Kreminski, *Newton-Cotes integration for approximating Stieltjes (generalized Euler) constants*, 2003]:

- Values up to $n = 8300$ with 200 significant digits
- Heuristic error estimates

Later heuristic computations up to about $n = 35\,000$

[FJ, 2014]:

- All γ_n up to $n = 100\,000$ with more than $10\,000$ digits each
- Rigorous error bounds
- To replicate, simply call the Hurwitz zeta function of a power series in Arb (also for $\gamma_n(a)$)

Data available from:
`http://fredrikj.net/math/hurwitz_zeta.html`

Numerical values

Computed value of γ_{100000}:

$$1.99192730631254109565\ldots \times 10^{83432}$$

Knessl-Coffey approximation:

$$1.9919333 \times 10^{83432}$$

Matsuoka bound: 3.71×10^{106114}

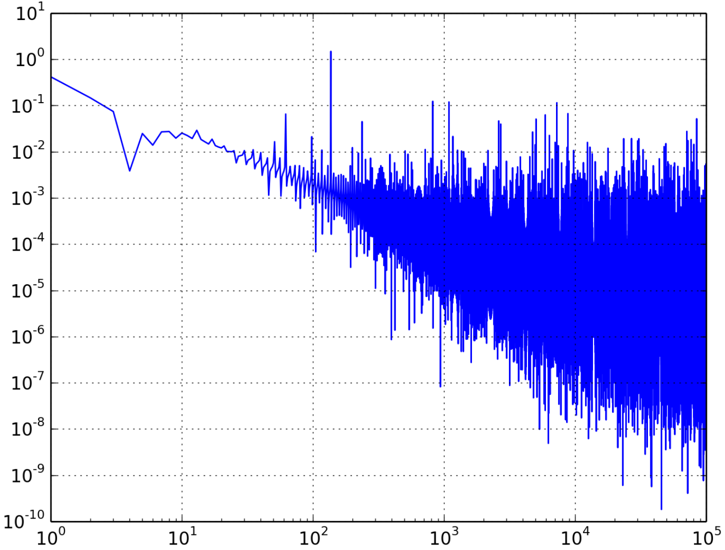
Computed value of $\lambda_{50000}(1+i)$:

$$(1.032502087431\ldots - 1.441962552840\ldots i) \times 10^{39732}$$

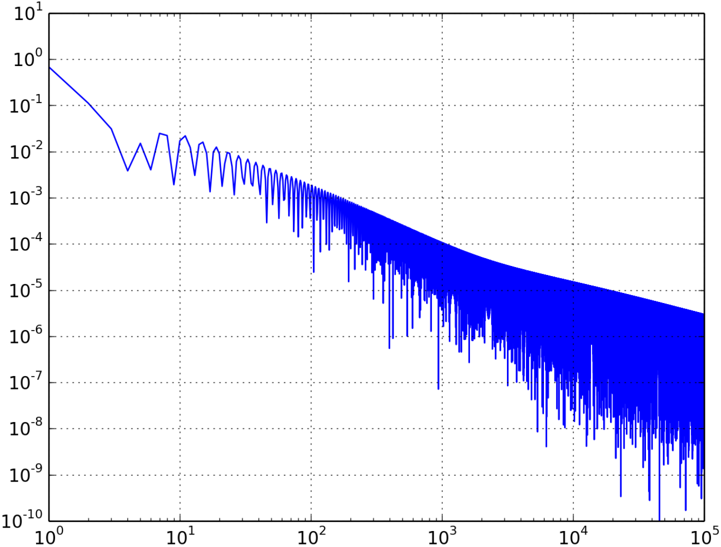
Knessl-Coffey approximation:

$$(1.0324943 - 1.4419586i) \times 10^{39732}$$

Relative error of Knessl-Coffey formula



Relative error of Knessl-Coffey formula



The Keiper-Li coefficients

Define $\{\lambda_n\}_{n=1}^{\infty}$ by

$$\log \xi\left(\frac{1}{1-x}\right) = \log \xi\left(\frac{x}{x-1}\right) = -\log 2 + \sum_{n=1}^{\infty} \lambda_n x^n$$

where $\xi(s) = \frac{1}{2}s(s-1)\pi^{-s/2}\Gamma(s/2)\zeta(s)$.

Keiper (1992): Riemann hypothesis $\Rightarrow \forall n : \lambda_n > 0$
Li (1997): Riemann hypothesis $\Leftarrow \forall n : \lambda_n > 0$

Keiper conjectured $2\lambda_n \approx (\log n - \log(2\pi) + \gamma - 1)$

Evaluating the Keiper-Li coefficients

Evaluate

$$\log \xi(s) = \log(-\zeta(s)) + \log \Gamma(1 + s/2) + \log(1 - s) - s \log(\pi)/2$$

at $s = x \in \mathbb{R}[[x]]$

Ingredients:

1. The series expansion $\zeta(s + x)$ at $s = 0$
2. The logarithm of a power series: $\log f(x) = \int f'(x)/f(x) dx$
3. The series $\log \Gamma(1 + x)$, essentially $\gamma, \zeta(2), \zeta(3), \zeta(4), \ldots$
4. Right-composing by $x/(x - 1)$

A working precision of $\approx n$ bits is needed to get an accurate value for λ_n.

Fast composition

The *binomial transform* of $f = \sum_{k=0}^{\infty} a_k x^k$ is

$$T[f] = \frac{1}{1-x} f\left(\frac{x}{x-1}\right) = \sum_{n=0}^{\infty} \left(\sum_{k=0}^{n} (-1)^k \binom{n}{k} a_k \right) x^n$$

and the *Borel transform* is

$$B[f] = \sum_{k=0}^{\infty} \frac{a_k}{k!} x^k.$$

$T[f(x)] = B^{-1}[e^x B[f(-x)]]$, so we get $f\left(\frac{x}{x-1}\right)$ by a single power series multiplication!

Values of Keiper-Li coefficients

I have computed rigorous values of all λ_n up to $n = 100\,000$ (using Arb, and 110 000 bits of working precision). In particular,

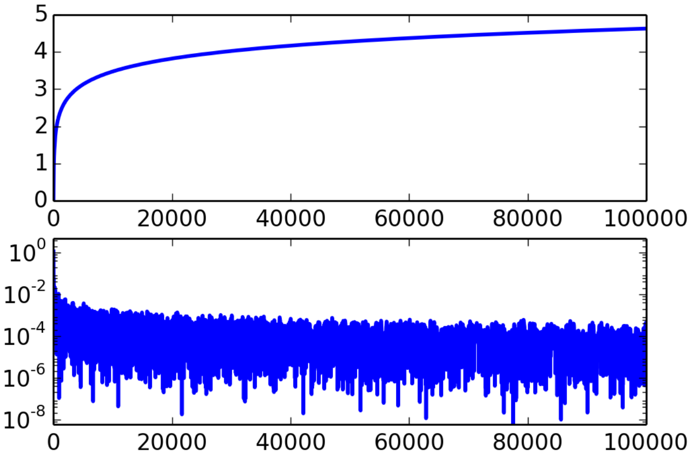
$$\lambda_{100000} = 4.62580782406902231409416038\ldots$$

plus about 2900 more accurate digits.

Keiper's approximation suggests $\lambda_{100000} \approx 4.626132$.

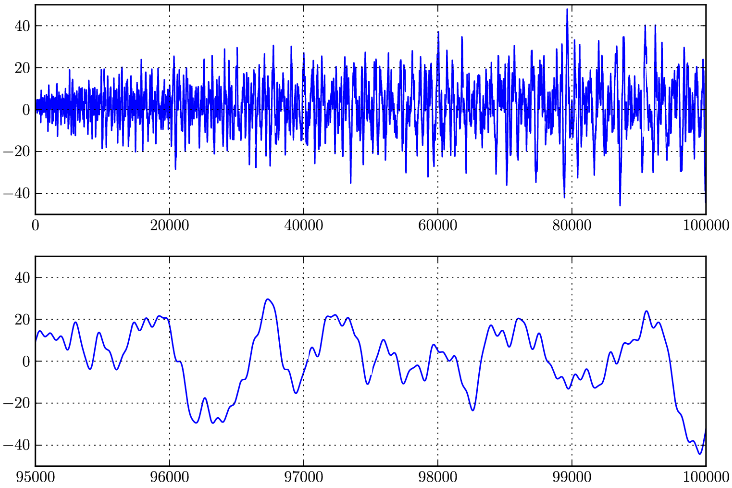
See `examples/keiper_li.c` in Arb and
`http://fredrikj.net/math/hurwitz_zeta.html` for data

Comparison with approximation formula



Plot of λ_n and $\lambda_n - (\log n - \log(2\pi) + \gamma - 1)/2$

Comparison with approximation formula



Plot of $n\,(\lambda_n - (\log n - \log(2\pi) + \gamma - 1)/2)$.

Time to compute Keiper-Li coefficients

(In seconds)

	$n = 1000$	$n = 10000$	$n = 100000$
Error bound R	0.017	1.0	97
Power sum S	0.048	47	65402
(CPU time)	(0.65)	(693)	(1042210)
Bernoulli numbers	0.0020	0.19	59
Tail T	0.058	11	1972
Logarithm of power series	0.047	8.5	1126
$\log \Gamma(1+x)$	0.019	3.0	1610
Composition by $x/(x-1)$	0.022	4.1	593
Total wall time	0.23	84	71051
RAM (MiB)	8	730	48700

Bit complexity is $\tilde{O}(n^2)$ except for the power sum which is $\tilde{O}(n^3)$ ($\tilde{O}(n^2)$ is possible in theory, but not implemented)