

Numerical integration in arbitrary-precision ball arithmetic

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Introduction

Arb (<http://arblib.org>) – C library for arbitrary-precision ball arithmetic (+polynomials, matrices, special functions...)

[3.141592653589793238462643 +/- 4.03e-25]

[-0.200293 +/- 8.48e-7] + [0.979736 +/- 3.44e-7]*I

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New feature (2018): fast rigorous numerical integration

- ▶ Documentation: http://arblib.org/acb_calc.html
- ▶ Demo: `examples/integrals.c`

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- ▶ Demo: `examples/integrals.c`

High-level interfaces in SageMath* and Nemo.jl.

Example: $\int_0^1 \cos(x) \sin(x) dx$

```
sage: C = ComplexBallField(100)
```

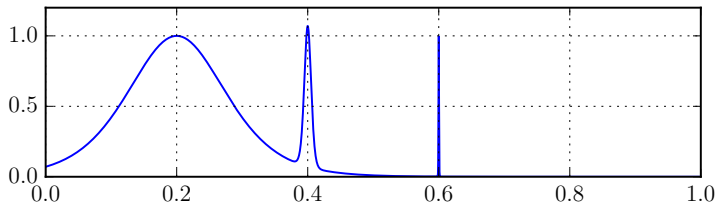
```
sage: C.integral(lambda x, _: cos(x) * sin(x), 0, 1)
```

```
[0.35403670913678559674939205737 +/- 8.89e-30]
```

*Thanks to Marc Mezzarobba and Vincent Delecroix

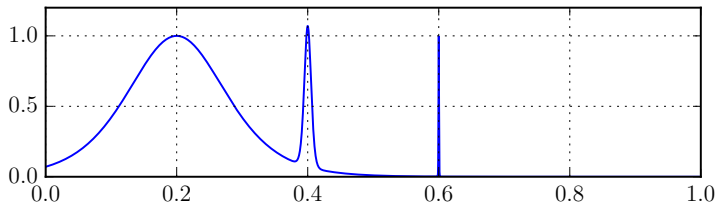
A nice and smooth function (Cranley and Patterson, 1971)

$$\int_0^1 \operatorname{sech}^2(10(x-0.2)) + \operatorname{sech}^4(100(x-0.4)) + \operatorname{sech}^6(1000(x-0.6)) \, dx$$



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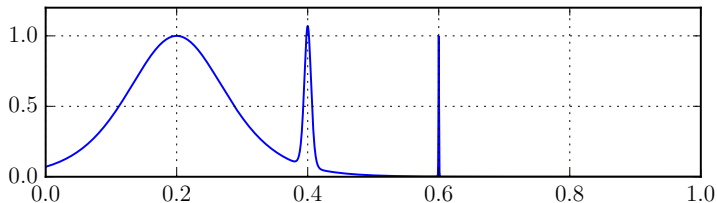
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Mathematica NIntegrate: 0.209736

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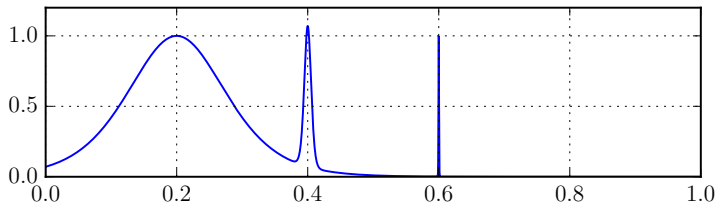


Mathematica NIntegrate: 0.209736

Octave quad: 0.209736, error estimate 10^{-9}

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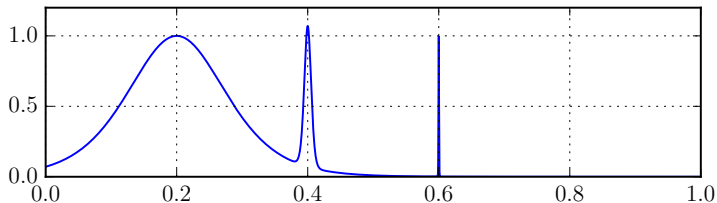
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Sage numerical_integral: 0.209736, error estimate 10^{-14}

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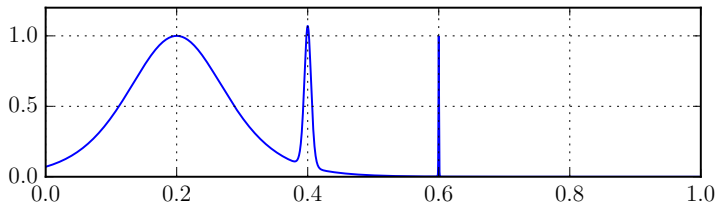
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| | |
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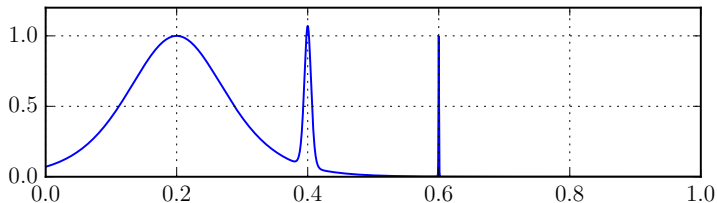
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| mpmath quad: | 0.209819 |

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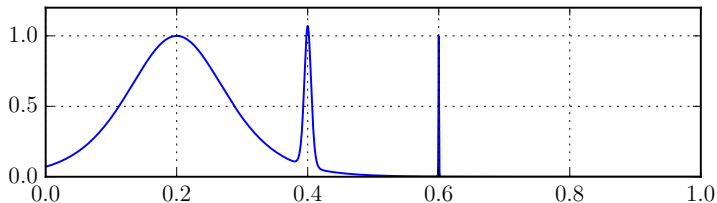
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| Pari/GP intnum: | 0.211316 |

A nice and smooth function (Cranley and Patterson, 1971)

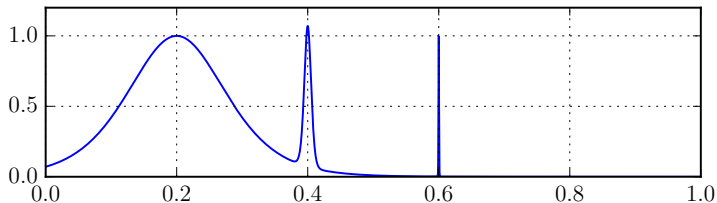
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| mpmath quad: | 0.209819 |
| Pari/GP intnum: | 0.211316 |
| Actual value: | 0.210803 |

A nice and smooth function (Cranley and Patterson, 1971)

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Arb, 64-bit precision:

[0.21080273550054928 +/- 4.55e-18] # time 0.003 s

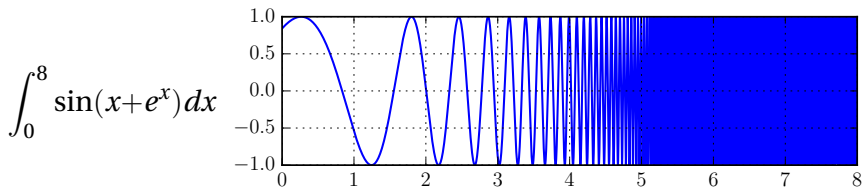
333-bit precision:

[0.2108027355005492773756... +/- 3.67e-99] # 0.02 s

3333-bit precision:

[0.2108027355005492773756... +/- 1.39e-1001] # 5.3 s

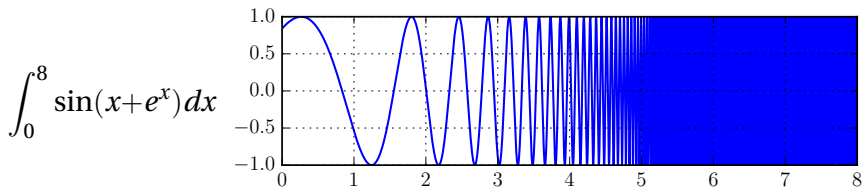
Another example: violent oscillation



S. Rump (2010) noticed that MATLAB's quad returned the incorrect 0.2511 after 1 second of computation.

Rump's INTLAB gives [0.34740016, 0.34740018] in about 1 s

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Arb at 64, 333, and 3333 bits:

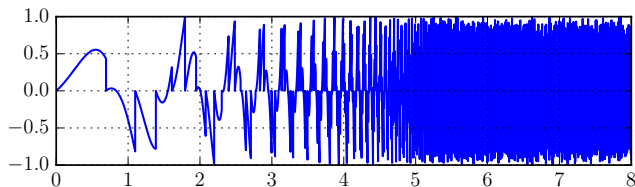
[0.34740017265725 +/- 3.34e-15] # 0.004 s

[0.34740017265... +/- 5.31e-96] # 0.01 s

[0.34740017265... +/- 2.41e-999] # 1 s

Yet another example: a monster

$$\int_0^8 (e^x - \lfloor e^x \rfloor) \sin(x+e^x) dx \quad - \text{ now with 2980 discontinuities!}$$



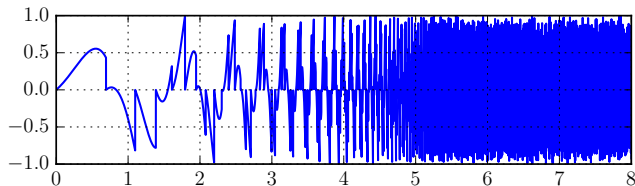
64-bit precision:

[+/- 5.45e+3]

time 0.14 s

Yet another example: a monster

$$\int_0^8 (e^x - \lfloor e^x \rfloor) \sin(x+e^x) dx \quad - \text{now with 2980 discontinuities!}$$



64-bit precision:

[+/- 5.45e+3] # time 0.14 s

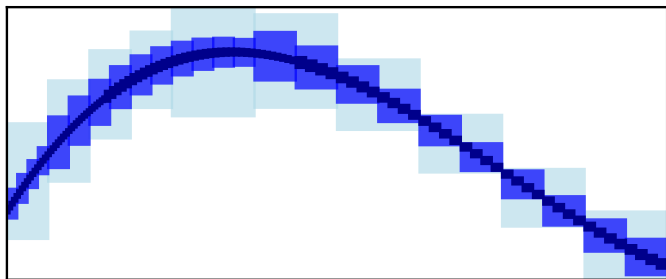
[0.0986517044784 +/- 4.46e-14] # time 5 s

333-bit precision:

[0.09865170447836520611965824976485985650416962079238449145
10919068308266804822906098396240645824 +/- 6.28e-95] # 268 s

Brute force interval integration

$$\int_a^b f(x) dx \in (b-a)f([a, b]) + \text{adaptive subdivision of } [a, b]$$



This is simple and general, but we need $2^{O(p)}$ evaluations to achieve p -bit accuracy!

Efficient integration of analytic functions

We can achieve p -bit accuracy with $n = O(p)$ work.

$2 \times 2 = 4$ potential algorithms:

Approximation:

$O(x^n)$ Taylor series

$$\int \sum_{k=0}^{n-1} a_k x^k = \sum_{k=0}^{n-1} a_k \frac{x^{k+1}}{k+1}$$

n -point quadrature

$$\int f(x) dx \approx \sum_{k=1}^n w_k f(x_k)$$

Error bounds:

Using derivatives $f^{(n)}$ on
 $[a, b]$

Using $|f|$ on a complex
domain around $[a, b]$

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Fast generation of Gauss-Legendre quadrature nodes (x_k, w_k)
due to F.J. and M. Mezzarobba (arxiv.org/abs/1802.03948).

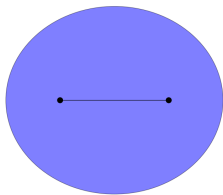
Error bounds for Gauss-Legendre quadrature

If f is analytic with $|f(z)| \leq M$ on an ellipse E with foci $-1, 1$ and semi-axes X, Y with $\rho = X + Y > 1$, then

$$\left| \int_{-1}^1 f(x) dx - \sum_{k=1}^n w_k f(x_k) \right| \leq \frac{M}{\rho^{2n}} \cdot C_\rho$$



$$X = 1.25, Y = 0.75, \rho = 2.00$$



$$X = 2.00, Y = 1.73, \rho = 3.73$$

Fast convergence when no singularities are close to $[a, b]$, but should be combined with subdivision otherwise!

Adaptive integration algorithm

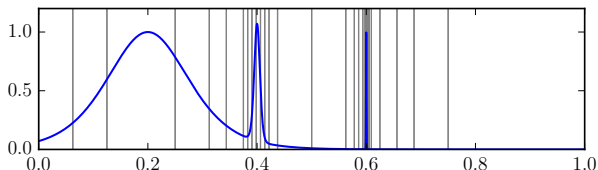
1. Compute $(b - a)f([a, b])$. If the error is $\leq \varepsilon$, done!
2. On an ellipse E around $[a, b]$, bound $|f|$ and check that f is analytic. If the error of Gauss-Legendre quadrature is $\leq \varepsilon$, compute it – done!
3. Split at $m = (a + b)/2$ and integrate on $[a, m]$, $[m, b]$ recursively.

Knut Petras (2002) pointed out that this guarantees rapid convergence for a large class of piecewise analytic functions.

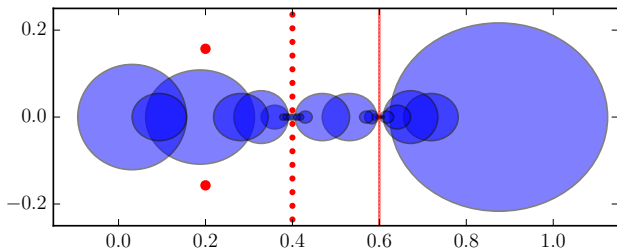
Adaptive subdivision

$$\int_0^1 \operatorname{sech}^2(10(x-0.2)) + \operatorname{sech}^4(100(x-0.4)) + \operatorname{sech}^6(1000(x-0.6)) \, dx$$

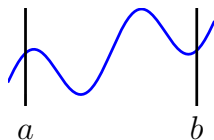
Arb chooses
31 subintervals,
narrowest is 2^{-11}



Complex ellipses
used for bounds
Red dots = poles

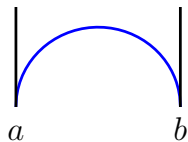


Typical proper integrals



Analytic around $[a, b]$

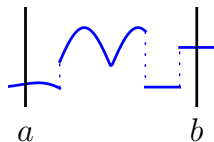
Complexity: $O(p)$



Bounded algebraic-type singularities

Example: $\sqrt{1-x^2}$

Complexity: $O(p^2)$



Piecewise analytic functions*

Examples: $\lfloor x \rfloor$, $\text{sgn}(x)$, $|x|$, $\max(f(x), g(x))$

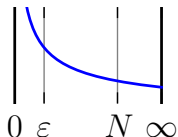
Complexity: $O(p^2)$

* Trick: extend piecewise real functions to the complex plane.

Discontinuities \rightarrow branch cuts.

Typical improper integrals

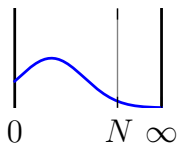
Manual truncation required, e.g. $\int_0^\infty f(x) dx \approx \int_\epsilon^N f(x) dx$
if $|a|$, $|b|$ or $|f| \rightarrow \infty$



Algebraic blow-up or decay

Examples: $\int_0^1 \frac{dx}{\sqrt{x}}$, $\int_0^1 \log(x) dx$, $\int_0^\infty \frac{dx}{1+x^2}$

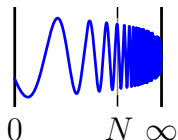
Complexity: $O(p^2)$



Exponential decay

Example: $e^{-x} \sin(x)$

Complexity: $O(p \log p)$



Essential singularity with slow decay

Example: $\int_1^\infty \frac{\sin(x)}{x} dx$

Complexity: $2^{O(p)}$

Timings: f analytic around $[a, b]$

| p | Pari/GP | mpmath | Arb | Sub | Eval | Pari/GP | mpmath | Arb | Sub | Eval |
|------|-----------------------------------------------------------------------------------------|--------------|----------|-----|------|-------------------------------------------------------------------------|-------------|---------|-----|-------|
| | $I_0 = \int_0^1 1/(1+x^2) dx$ | | | | | $I_1 = \int_0^1 \sum_{k=1}^3 \operatorname{sech}^{2k}(10^k(x-0.2k)) dx$ | | | | |
| 64 | 0.00039 | 0.0011 | 0.000036 | 2 | 52 | 0.54 | 5.0 | 0.0031 | 31 | 768 |
| 333 | 0.0043 | 0.0058 | 0.00017 | 2 | 188 | 12 | 38 | 0.023 | 31 | 3086 |
| 3333 | 1.0 | 0.13 | 0.012 | 2 | 2056 | 3385 | - | 5.3 | 31 | 30092 |
| | $I_2 = \int_0^\pi x \sin(x)/(1+\cos^2(x)) dx$ | | | | | $I_3 = \int_0^{1000} W_0(x) dx$ | | | | |
| 64 | 0.00077 | 0.0046 | 0.00022 | 6 | 159 | 0.0037 | 0.032 | 0.00093 | 12 | 273 |
| 333 | 0.0088 | 0.037 | 0.0018 | 6 | 643 | 0.052 | 0.25 | 0.0095 | 12 | 1109 |
| 3333 | 2.2 | 4.4 | 0.43 | 6 | 6171 | 11 | 25 | 1.3 | 12 | 12043 |
| | $I_4 = \int_0^{100} \sin(x) dx$ | | | | | $I_5 = \int_0^8 \sin(x + e^x) dx$ | | | | |
| 64 | 0.0012 | 0.0014 | 0.000070 | 1 | 72 | 0.063 | 0.25 | 0.0035 | 25 | 2239 |
| 333 | 0.015 | 0.018 | 0.00029 | 1 | 139 | 0.22 | 0.58 | 0.013 | 21 | 3940 |
| 3333 | 2.0 | 0.71 | 0.031 | 1 | 526 | 14 | 12 | 0.9 | 6 | 8341 |
| | $I_6 = \int_{-1}^1 e^{-x} \operatorname{erf}\left(\sqrt{1250}x + \frac{3}{2}\right) dx$ | | | | | $I_7 = \int_1^{1+1000i} \Gamma(x) dx$ | | | | |
| 64 | 0.024 | 0.057 | 0.0054 | 6 | 438 | 0.054 | 0.093 | 0.0046 | 12 | 324 |
| 333 | 0.50 | 0.22 | 0.047 | 4 | 791 | 0.65 | 1.1 | 0.091 | 14 | 1456 |
| 3333 | 173 | 466 | 5.7 | 2 | 2923 | 561 | 847 | 48 | 14 | 16535 |

Timings: endpoint singularities and infinite intervals

| p | Pari/GP | mpmath | Arb | Sub | Eval | Pari/GP | mpmath | Arb | Sub | Eval |
|------|---------|----------------------------------------|---------|------|-------|---------|---------------------------------------------------------|---------|------|-------|
| | | $E_0 = \int_0^1 \sqrt{1-x^2} dx$ | | | | | $E_1 = \int_0^\infty 1/(1+x^2) dx$ * | | | |
| 64 | 0.00041 | 0.00067 | 0.00057 | 44 | 674 | 0.00060 | 0.0012 | 0.0022 | 190 | 2887 |
| 333 | 0.0044 | 0.0060 | 0.015 | 223 | 12687 | 0.0068 | 0.011 | 0.048 | 997 | 51900 |
| 3333 | 0.94 | 0.18 | 6.6 | 2223 | 1.2 M | 1.7 | 0.24 | 27 | 9997 | 4.7 M |
| | | $E_2 = \int_0^1 \log(x)/(1+x) dx$ * | | | | | $E_3 = \int_0^\infty \operatorname{sech}(x) dx$ * | | | |
| 64 | 0.00081 | 0.00094 | 0.0012 | 67 | 1026 | 0.0011 | 0.0043 | 0.00022 | 7 | 181 |
| 333 | 0.011 | 0.011 | 0.038 | 336 | 19254 | 0.013 | 0.098 | 0.0019 | 9 | 853 |
| 3333 | 1.7 | 1.08 | 106 | 3336 | 1.8 M | 3.5 | 3.3 | 0.68 | 12 | 12046 |
| | | $E_4 = \int_0^\infty e^{-x^2+ix} dx$ * | | | | | $E_5 = \int_0^\infty e^{-x} \operatorname{Ai}(-x) dx$ * | | | |
| 64 | 0.0014 | 0.016 | 0.00017 | 1 | 98 | - | 0.91 | 0.012 | 9 | 842 |
| 333 | 0.017 | 0.13 | 0.0016 | 2 | 397 | - | 26 | 0.94 | 124 | 24548 |
| 3333 | 4.7 | 7.1 | 0.47 | 4 | 3894 | - | 10167 | 502 | 1205 | 0.7 M |

* For Arb, the path was truncated manually (with error $\leq 2^{-p}$)

Timings: mid-interval jumps/kinks

| p | Arb | Sub | Eval | Arb | Sub | Eval |
|------|-------------------------------------------------------------------------------|-------|----------|-----------------------------------|--------|---------|
| | $\int_0^1 x^4 + 10x^3 + 19x^2 - 6x - 6 e^x dx$ | | | $\int_0^{100} \lceil x \rceil dx$ | | |
| 64 | 0.0016 | 70 | 1093 | 0.014 | 5536 | 16606 |
| 333 | 0.049 | 339 | 18137 | 0.12 | 33512 | 100534 |
| 3333 | 101 | 3339 | 1624951 | 1.6 | 345512 | 1036534 |
| | $\int_0^{10} (x - \lfloor x \rfloor - \frac{1}{2}) \max(\sin(x), \cos(x)) dx$ | | | $\int_{-1-i}^{-1+i} \sqrt{x} dx$ | | |
| 64 | 0.026 | 1257 | 16168 | 0.0021 | 132 | 1462 |
| 333 | 1.2 | 7076 | 394881 | 0.067 | 670 | 28304 |
| 3333 | 2588 | 71984 | 39128525 | 35 | 6670 | 2669940 |

High accuracy with mpmath or Pari/GP is not possible without manually splitting at all the singular points.

Defining functions

The user provides the integrand $f(z)$ as a black-box function that takes two parameters:

- ▶ A complex ball (rectangle) representing z
- ▶ A boolean flag *analytic*
 - ▶ *False* - the function returns an enclosure of $f(z)$. There are no assumptions about analyticity.
 - ▶ *True* - the function returns an enclosure of $f(z)$. It must return non-finite (NaN, $[\pm\infty]$) if the ball z contains any non-analytic point of f .

The user can always ignore the *analytic* flag when f is a composition of meromorphic functions.

Defining functions



The *analytic* flag **must** be handled
when the integrand has branch cuts.



$$\int_1^4 \sqrt{x} dx = \frac{14}{3}$$

```
sage: F1 = lambda x, _: x.sqrt() # WRONG!  
sage: CBF.integral(F1, 1, 4)  
[4.66941489478101 +/- 7.48e-15]
```

```
sage: F2 = lambda x, a: x.sqrt(analytic=a) # correct  
sage: CBF.integral(F2, 1, 4)  
[4.66666666666667 +/- 4.62e-14]
```

Versions of common functions (\sqrt{x} , $\log(x)$, x^y , $|x|$, $\lfloor x \rfloor$, $\max(x,y)$, ...) with builtin branch cut detection are provided in Arb.

Optional settings for the integration algorithm

The user specifies:

- ▶ Working precision p
- ▶ Absolute and relative tolerances ε_{abs} and ε_{rel}

Configurable work limits:

- ▶ Maximum quadrature degree (default: $O(p)$)
- ▶ Number of calls to the integrand (default: $O(p^2)$)
- ▶ Number of queued subintervals (default: $O(p)$)
- ▶ Use stack (default) or global priority queue for the list of subintervals generated by bisection

Applications

- ▶ Special functions:

$$\Gamma(s, z) = \int_z^\infty t^{s-1} e^{-t} dt$$

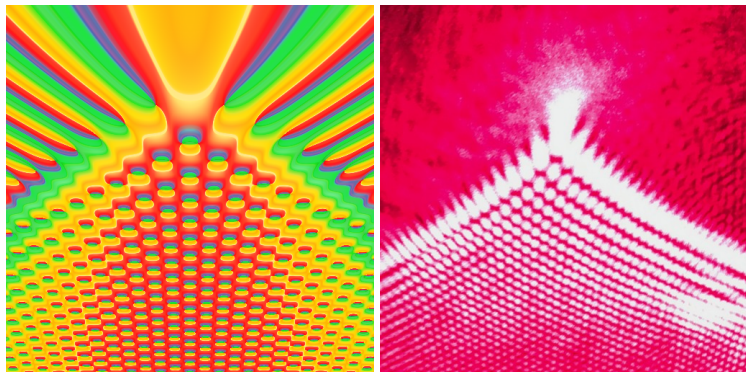
- ▶ (Inverse) Laplace/Fourier/Mellin transforms
- ▶ Taylor/Laurent/Fourier coefficients
- ▶ Counting zeros and poles:

$$N - P = \frac{1}{2\pi i} \oint_C \frac{f'(z)}{f(z)} dz$$

- ▶ Acceleration of series (Euler-Maclaurin summation. . .)

Example: diffraction catastrophe integrals

$$P(x, y) = \int_{-\infty}^{\infty} e^{i(t^4 + yt^2 + xt)} dt = 2 \int_0^{\infty} e^{-t^4 + at^2 + b} \cosh(ct) dt$$



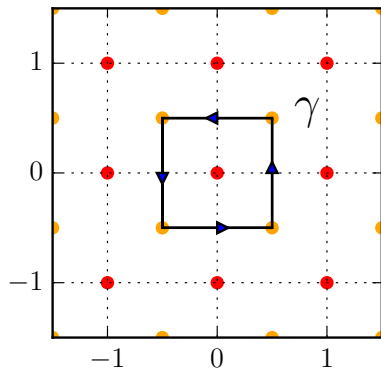
Left: 512×512 image rendered in 15 minutes with Arb ($|x| \leq 12.5$, $-20 \leq y \leq 5$). Using doubling precision (30, 60, ... bits). Near the bottom, $p = 120$ is required.

Right: photo of a cusp caustic produced by illuminating a flat surface with a laser beam through a droplet of water (image credit: Dan Piponi, CC-BY-SA)

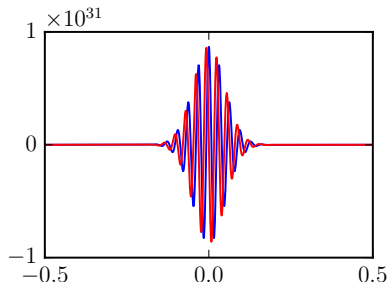
Example: Laurent series of elliptic functions

$$\wp(z; \tau) = \sum_{n=-2}^{\infty} a_n(\tau) z^n, \quad a_n = \frac{1}{2\pi i} \int_{\gamma} \frac{\wp(z)}{z^{n+1}} dz$$

$\wp(z)$ with $\tau = i$ has poles at $z = M + Ni$ ($M, N \in \mathbb{Z}$).



One segment ($n = 100$):



Example: Laurent series of elliptic functions

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a_{-2}, \dots, a_{100} with 333-bit precision (0.8 seconds for each a_n):

```
a[-2] = [1.0000000000000000000 ... 00000 +/- 3.57e-98] + [+/- 1.89e-98]*I
a[-1] =                                     [+/- 4.11e-98] + [+/- 2.57e-98]*I
a[0]  =                                     [+/- 1.02e-97] + [+/- 5.39e-98]*I
a[1]  =                                     [+/- 1.41e-97] + [+/- 1.35e-97]*I
a[2]  = [9.453636006461692 ... 52235 +/- 4.44e-97] + [+/- 2.48e-97]*I
a[3]  =                                     [+/- 4.47e-97] + [+/- 4.60e-97]*I
...
a[94] = [380.000000000000135 ... 63746 +/- 9.24e-70] + [+/- 8.27e-70]*I
a[95] =                                     [+/- 1.37e-69] + [+/- 1.37e-69]*I
a[96] =                                     [+/- 2.93e-69] + [+/- 2.91e-69]*I
a[97] =                                     [+/- 5.81e-69] + [+/- 5.82e-69]*I
a[98] = [395.9999999999996482...46383 +/- 2.90e-68] + [+/- 1.17e-68]*I
a[99] =                                     [+/- 2.32e-68] + [+/- 2.32e-68]*I
a[100] =                                    [+/- 4.95e-68] + [+/- 4.95e-68]*I
```

Example: Laurent series of the Hurwitz zeta function

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

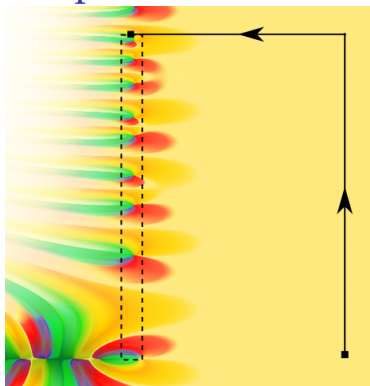
Joint work with I. Blagouchine (arxiv.org/abs/1804.01679)

$$\gamma_n(\nu) = -\frac{\pi}{2(n+1)} \int_{-\infty}^{\infty} \frac{(\log(\nu - \frac{1}{2} + ix))^{n+1}}{\cosh^2(\pi x)} dx$$

$\gamma_{10^{100}}(1) \in [3.18743141870239927999741646993 \pm 2.89 \cdot 10^{-30}] \cdot 10^e$
 $e = 2346394292277254080949367838399091160903447689869$
 $8373852057791115792156640521582344171254175433483694$

Some pen-and-paper analysis (steepest descent contour, tight enclosures near saddle point) needed for large n .

Example: zeros of the Riemann zeta function



Number of zeros of $\zeta(s)$ on
 $R = [0, 1] + [0, T]i$:

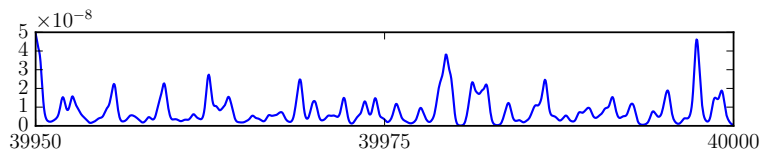
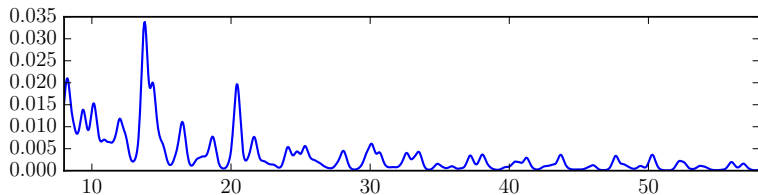
$$N(T) - 1 = \frac{1}{2\pi i} \int_{\gamma} \frac{\zeta'(s)}{\zeta(s)} ds = \frac{\theta(T)}{\pi} +$$

$$\frac{1}{\pi} \operatorname{Im} \left[\int_{1+\varepsilon}^{1+\varepsilon+Ti} \frac{\zeta'(s)}{\zeta(s)} ds + \int_{1+\varepsilon+Ti}^{\frac{1}{2}+Ti} \frac{\zeta'(s)}{\zeta(s)} ds \right]$$

| T | p | Time (s) | Eval | Sub | $N(T)$ |
|--------|-----|----------|------|-----|------------------------------|
| 10^3 | 32 | 0.51 | 1219 | 109 | [649.00000 +/- 7.78e-6] |
| 10^6 | 32 | 16 | 5326 | 440 | [1747146.00 +/- 4.06e-3] |
| 10^9 | 48 | 1590 | 8070 | 677 | [2846548032.000 +/- 1.95e-4] |

Example: $|\zeta(s)|$ -integrals (from Harald Helfgott)

$$\int_{-\frac{1}{4}+8i}^{-\frac{1}{4}+40000i} \left| \frac{F_{19}(s + \frac{1}{2})F_{19}(s + 1)}{s^2} \right| |ds|, \quad F_N(s) = \zeta(s) \prod_{p \leq N} (1 - p^{-s})$$



We compute Taylor models $f(s) = g(s) + h(s)i + \varepsilon$ on subintervals $[a, a + 0.5]$, and integrate $\sqrt{g^2(s) + h^2(s)}$. Total time: a few hours.

Todo

- ▶ Efficient and semi-automatic support for singularities, infinite intervals
 - ▶ User may specify scale, e.g. $|f(x)| \leq x^\alpha e^{\beta x^\gamma}$
 - ▶ Dedicated algorithms: Gauss-Jacobi, double exponential...
 - ▶ Algorithms for oscillatory integrals
- ▶ Symbolic interface
- ▶ Let user choose Taylor/Gauss-Legendre quadrature and bounds based on derivatives / complex magnitudes
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Thank you!