Computing with real numbers
-
Calculer avec les nombres réels

Fredrik Johansson
Inria Bordeaux

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Book chapter

- French version (thanks to Xavier Caruso):
  http://fredrikj.net/math/ejcim2020_joh_fr.pdf

- English version:
  http://fredrikj.net/math/ejcim2020_joh_en.pdf

Recommended: *Calcul mathématique avec Sage / Computational Mathematics with SageMath*

- http://sagebook.gforge.inria.fr/
- http://sagebook.gforge.inria.fr/english.html

The problem

$$\frac{\sqrt{2}}{2} = \frac{1}{\sqrt{2}} \qquad ?$$

```
sage: sqrt(2.0)/2.0 == 1.0/sqrt(2.0)
False
```

```
sage: sqrt(2.0)/2.0; 1.0/sqrt(2.0)
0.707106781186548
0.707106781186547
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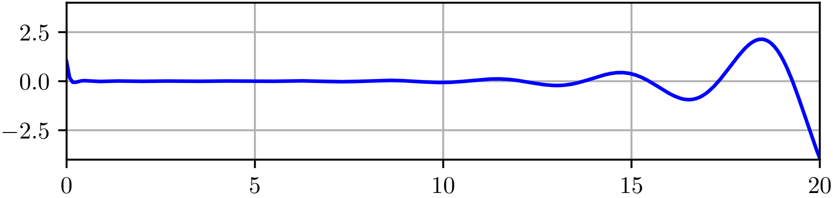
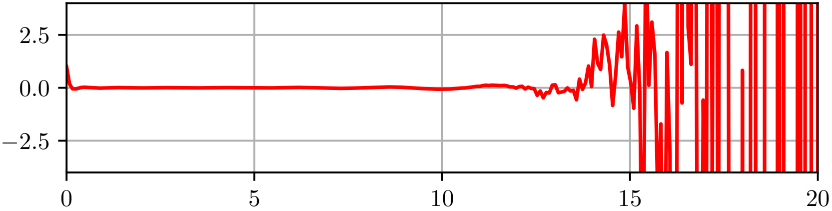
Why?

- Cannot store infinitely many digits on a computer
- Exact results may be impossible
- Exact results may be expensive

Errors can add up...



The hypergeometric function ${}_1F_1(-50, 3, x)$ on $0 \leq x \leq 20$



The function as computed by `scipy.special.hyp1f1`

...or worse

http://www-users.math.umn.edu/~arnold/disasters/disasters.html

Lecture plan

- **Part 1: computability, exact arithmetic**
- Part 2: approximate arithmetic, interval arithmetic

Approaches to computing with real numbers

1. Work with some *effective subset* $S \subset \mathbb{R}$ (or $S \subset \mathbb{C}$)
   - Algebraic structures
     - Rational numbers $\mathbb{Q}$
     - Algebraic numbers $\overline{\mathbb{Q}}$
     - …
   - Computable numbers
   - Symbolic expressions, e.g. $x = e^{\pi} + 2\zeta(3)$

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2. Work with some *approximate model* of $\mathbb{R}$ (or $\mathbb{C}$)
   - Floating-point arithmetic
   - Interval arithmetic

What do we mean by an "effective" set S?

- Represent any element of S by a finite description, and
- Represent any relevant operation on S by a (terminating) algorithm[1]

[1] For example, on a Turing machine, or in C/C++/Python/Julia...

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Warning: it all depends on the needed operations. Even for $\mathbb{Q}$, other operations may not be effective/computable/decidable.

[1] For example, on a Turing machine, or in C/C++/Python/Julia...

“Computable numbers”

Definition

Computable number x: there is an algorithm which, given n, outputs a rational $\tilde{x}$ with $|x - \tilde{x}| < 2^{-n}$
Computable function f: there is an algorithm which, given n and a computable number x, outputs $\tilde{y}$ with $|f(x) - \tilde{y}| < 2^{-n}$

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Example: $\pi = \sum_{k=0}^{\infty} \frac{8}{(4k+1)(4k+3)}$
Example: $f(x, y) = x + y, \quad f(x) = e^x = \sum_{k=0}^{\infty} \frac{x^k}{k!}$

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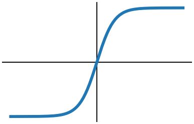
Effective?

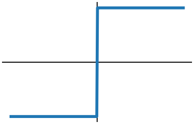
- ✓ Finite representation
- ✓ $\{+, -, \times, /\}$ (except for division by zero)
- × $\{=, <\}$ only semi-decidable (halting problem)

Computability – continuity – well-posedness



Computable

- $f(x,y) = x + y$
- $\sin(x)$
- $|x|$
- $1/x$ (on $\mathbb{R} \setminus \{0\}$)



Not computable

- $\text{sign}(x)$
- $x = y$
- $x < y$
- $\lfloor x \rfloor, \lceil x \rceil$

Example: matrices

Assume A is a computable complex n by n matrix (each entry in A is a computable complex number).

- $\det(A)$ is computable

[2] At least, up to issues with ordering

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- The eigenvalues $\lambda_i(A)$ are computable[2]
- The multiplicity of an eigenvalue is not computable (unless the multiplicity is 1)

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Symbolic expressions

Real numbers encoded as trees or strings (in some fixed language):

$$\sqrt{2} + \tfrac{5}{3}\pi \quad \equiv \quad (+, (\sqrt{\cdot}, 2), (\times, (/, 5, 3), \pi))$$

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  - **Easy**: $\frac{1}{2}\sqrt{2} = \frac{1}{\sqrt{2}}, \ \sin(\pi) = 0$
  - **Harder**: $\pi = \sum_{n=0}^{\infty} \frac{1}{16^n} \left(\frac{4}{8n+1} - \frac{2}{8n+4} - \frac{1}{8n+5} - \frac{1}{8n+6} \right)$

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- Problem: expression may not define a real number $(1/\sin(\pi))$

Cautionary example 1

$$8 \int_0^\infty \cos(2x) \prod_{n=1}^{\infty} \cos(x/n) dx \stackrel{?}{=} \pi$$

```
sage: from mpmath import mp
sage: print(8 * mp.quadosc(lambda x: mp.cos(2*x) *
...       mp.nprod(lambda n: mp.cos(x/n), [1,mp.inf]),
...              [0,mp.inf], omega=1))
3.14159265358979

sage: print(mp.pi)
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sage: print(mp.pi)
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```

In fact, there is a difference of $\approx 10^{-41}$

Cautionary example 2

$$\sum_{n=1}^{\infty} \frac{\lfloor n e^{\pi\sqrt{163/9}} \rfloor}{2^n} \stackrel{?}{=} 1280640$$

```
sage: from mpmath import mp
sage: mp.dps = 10000
sage: print(mp.nsum(lambda n: mp.floor(n*mp.exp(mp.pi*
...     mp.sqrt(163)/mp.sqrt(9)))/2**n, [1,mp.inf]) - 1280640)
0.0
```

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0.0
```

In fact, there is a difference of $< 10^{-500{,}000{,}000}$

More examples:
https://mathworld.wolfram.com/AlmostInteger.html

Cautionary example 3

$$\frac{1}{\pi}\int_0^\infty \log\left(\left|\frac{\zeta\left(\frac{1}{2}+it\right)}{\zeta\left(\frac{1}{2}\right)}\right|\right)\frac{1}{t^2}\,dt \;\stackrel{?}{=}\; \frac{\pi}{8}+\frac{\gamma}{4}+\frac{\log(8\pi)}{4}-2$$

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This is equivalent to the Riemann hypothesis!

Algebraic structures

Special sets of numbers:

- Rational numbers $\mathbb{Q}$
- Algebraic numbers $\overline{\mathbb{Q}}$
- Transcendental number fields, e.g. $\mathbb{Q}(\pi)$
- Elementary numbers
- Periods
- Holonomic constants

Known properties of all numbers in such a ring $\implies$ Effective equality test (at least conjecturally)

Practical problem: coefficient explosion

$$1 + \frac{1}{2} + \frac{1}{3} + \ldots + \frac{1}{50} = \frac{13943237577224054960759}{3099044504245996706400}$$

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Workarounds: fast algorithms, modular arithmetic (+ Chinese remainder theorem, rational reconstruction)

$$\mathbb{Q} \;\to\; \mathbb{Z}/n\mathbb{Z} \text{ or } \mathbb{Z}_p \;\to\; \mathbb{Q}$$

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```
sage: %time random_matrix(QQ, 1000, 1000).det(algorithm=
                                                  "generic")
Wall time: 10min 46s
(...2000 digit answer...)

sage: %time random_matrix(QQ, 1000, 1000).det()
Wall time: 7.77 s
(...2000 digit answer...)
```

Algebraic numbers

$$\overline{\mathbb{Q}} = \{x : x \in \mathbb{C},\ f(x) = 0 \text{ for some } f \in \mathbb{Z}[x] \setminus \{0\}\}$$

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Representation: minimal polynomial + isolating interval

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Arithmetic operations: resultants + polynomial factorisation, operations in a fixed number field $\mathbb{Q}(\alpha)$ where possible

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`QQbar` in Sage:

```
sage: x = QQbar(2)
sage: sqrt(x)/2 == 1/sqrt(x)
True
```

Equality test for algebraic numbers

- Factorisation in $\mathbb{Z}[x] \implies$ unique minimal polynomials, no repeated roots

- Root separation bounds

$$\mathrm{sep}(f) > \frac{\sqrt{3}\Delta(f)}{n^{n/2+1}(\|f\|_2)^{n-1}}$$

- Analytic theorems (numerical analysis)

Practical problem: degree explosion

Minimal polynomial of $x = \sqrt{2} + \sqrt{3}$:

$$x^4 - 10x^2 + 1$$

Minimal polynomial of $x = \sqrt{2} + \sqrt{3} + \sqrt{5}$:

$$x^8 - 40x^6 + 352x^4 - 960x^2 + 576$$

Minimal polynomial of $x = \sqrt{2} + \sqrt{3} + \sqrt{5} + \sqrt{7}$:

$$x^{16} - 136x^{14} + \ldots - 5596840x^2 + 46225$$

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```
sage: x = QQbar(sum(sqrt(nth_prime(n+1)) for n in range(6)))
sage: %time x - (x - 1) - 1 == 0
CPU times: user 8.98 s, sys: 14.4 ms, total: 9 s
Wall time: 9.17 s
True
```

Beyond arithmetic: quantifier elimination

Theorem (M-D-R-P, 1970)

There is no algorithm that can decide for any given $f \in \mathbb{Z}[x_1, \ldots, x_n]$ *whether* $\exists x_1, \ldots, x_n \in \mathbb{Z} : f(x_1, \ldots, x_n) = 0$.

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Theorem (Tarski, 1951)

Any formula in first-order logic (using boolean operations and quantifiers $\forall, \exists$ *) involving n variables* $x_1, \ldots, x_n$ *and polynomial equalities and inequalities over* $R = \overline{\mathbb{Q}} \cap \mathbb{R}$ *is decidable.*

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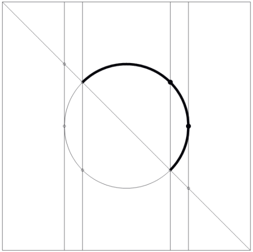
Practical ($2^{2^{O(n)}}$) algorithm: cylindrical algebraic decomposition (CAD) by Collins, 1975.

$x_1^2 + x_2^2 - 1 = 0 \wedge x_1 + x_2 > 0$



Elementary numbers

Definition

The field of (closed-form)[3] *elementary numbers* is the smallest field $E \subset \mathbb{C}$ that is closed with respect to e^x and $\log x$ ($x \neq 0$).

- $\sqrt{2} = e^{\log(2)/2} \in E$
- $\pi = \log(-1)/e^{\log(-1)/2} \in E$
- $\sin(\sin(1)) \in E$

[3] Competing definitions exist; for example, ensuring $\overline{\mathbb{Q}} \subset E$. See "What is a closed-form number?" by T. Chow, https://arxiv.org/abs/math/9805045

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Theorem (Richardson and Fitch, 1994)

Equality of elementary numbers is decidable if Schanuel's conjecture is true.

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Equality test (conjectural)

$x \neq y \implies$ can find difference by numerical computation

$x = y \implies$ can find relation of known type using algebraic computations and integer relation algorithms

Alternatively:
$x = y \implies$ can prove $|x - y| < \varepsilon$ using numerical computation, where ε is a separation bound

Transcendence results

Theorem (Baker, 1966)

If $\{2\pi i, \log(a_1), \ldots, \log(a_n)\}$ *are linearly independent over* $\mathbb{Q}$, $a_i \in \overline{\mathbb{Q}} \setminus \{0\}$, *then they are linearly independent over* $\overline{\mathbb{Q}}$.

In fact, there is an effective separation bound:
$|b_1 \log(a_1) + \ldots + b_n \log(a_n)| > 2^{-C(b_1,\ldots,b_n,a_1,\ldots,a_n)}$

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Example: $\frac{\pi}{4} = \arctan\frac{1}{2} + \arctan\frac{1}{3}$

Conjecture (Schanuel, 1960s)

If the complex numbers $z_1, \ldots, z_n$ *are linearly independent over* $\mathbb{Q}$*, then* $\mathbb{Q}(z_1, \ldots, z_n, e^{z_1}, \ldots, e^{z_n})$ *has transcendence degree at least n over* $\mathbb{Q}$*.*

Undecidability for elementary functions

Theorem (Richardson, 1968)

Given $f : \mathbb{R} \to \mathbb{R}$ *defined using:*

- *rational numbers,* π, $\log(2)$
- *arithmetic operations*
- e^x, $\sin(x)$, *and* $|x|$,

it is undecidable (in general) whether $f(x) = 0$ *holds everywhere.*

Periods

$$C = \int_A F(\mathbf{x})\, d\mathbf{x}$$

$A =$ algebraic set, $F =$ algebraic function

Example: $\pi = \int_0^1 \frac{4}{x^2+1} dx = \int_0^1 4\sqrt{1-x^2} dx = \int_{x^2+y^2\leq 1} 1 dxdy$

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Theorem

Periods are computable.[4]

[4] In fact, very efficiently. See: Lairez, Mezzarobba & Safey El Din, *Computing the volume of compact semi-algebraic sets,* https://arxiv.org/abs/1904.11705

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Theorem

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Conjecture (Kontsevich-Zagier, 2001)

Equality of periods can be decided using repeated use of additivity, change of variables, and the Stokes theorem.

---

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Holonomic constants

Values $f(\alpha)$, $\alpha \in \overline{\mathbb{Q}}$, where f is a D-finite function

$$a_r(z)f^{(r)}(z) + \ldots + a_1(z)f'(z) + a_0(z)f(z) = 0$$

with $a_i \in \overline{\mathbb{Q}}(x)$.

Examples: $\exp(\sqrt{2})$, $J_0(1)$, ${}_2F_1(\frac{1}{3}, \frac{1}{4}, \frac{1}{5}, -1 + 2i)$

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Efficient computation: algorithms by Chudnovsky^2, van der Hoeven, Mezzarobba

- Implementation: https://github.com/mkauers/ore_algebra/

Equality test: ???

Summary

- Computable real numbers
- Barrier to exact computation over $\mathbb{R}$: testing $x = y$
- Effective subsets of $\mathbb{R}$ such as $\overline{\mathbb{Q}}$
- Practical problem: coefficient/expression growth

Summary

- Computable real numbers
- Barrier to exact computation over $\mathbb{R}$: testing $x = y$
- Effective subsets of $\mathbb{R}$ such as $\overline{\mathbb{Q}}$
- Practical problem: coefficient/expression growth

Advertisement: Calcium - `http://fredrikj.net/calcium/`

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Other software:

- `http://irram.uni-trier.de/`
- `https://cs.nyu.edu/exact/core_pages/intro.html`
- `https://github.com/flatsurf/exact-real`
- …

Lecture plan

- Part 1: computability, exact arithmetic
- **Part 2: approximate arithmetic, interval arithmetic**

Approximate arithmetic

$$\underbrace{x}_{\text{True value}} = \underbrace{\hat{x}}_{\text{Approximation}} + \underbrace{\varepsilon}_{\text{Error}}$$

$\hat{x}$ - easy to represent

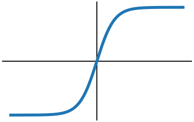
ε - unknown in general, but can often be bounded/estimated

Sources of numerical error

- Rounding error in single arithmetic operation
  - Typically:
    $$\frac{|x - \hat{x}|}{|x|} \approx 2^{-p}$$
- Truncation / discretization error
  - Example: $\sum_{n=0}^{\infty} a_n = \sum_{n=0}^{N} a_n + \varepsilon_N$
  - Example: differential equation approximated by finite difference with step size $h > 0$
- Uncertainty in input data (e.g. measurement error)

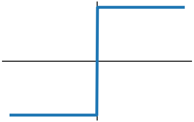
Multiple operations: need to study error propagation

Recall: computability – continuity – well-posedness



Computable

- $f(x, y) = x + y$
- $\sin(x)$
- $|x|$
- $1/x$ (on $\mathbb{R} \setminus \{0\}$)



Not computable

- $\operatorname{sign}(x)$
- $x = y$
- $x < y$
- $\lfloor x \rfloor$, $\lceil x \rceil$

Floating-point numbers

(Binary) floating-point numbers:

$$\hat{x} = a \cdot 2^b, \qquad a, b \in \mathbb{Z}$$

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Precision: p such that $|a| < 2^p$

- IEEE 754 `binary32` (`float`): $p = 24$ (= 7 decimals)
- IEEE 754 `binary64` (`double`): $p = 53$ (= 16 decimals)
- Arbitrary-precision arithmetic (e.g. `MPFR`): any p

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Note: a floating-point system typically also defines an exponent range $E_{\min} \le b \le E_{\max}$ and special values $-0, -\infty, +\infty, \mathrm{NaN}$.

Precision in practice

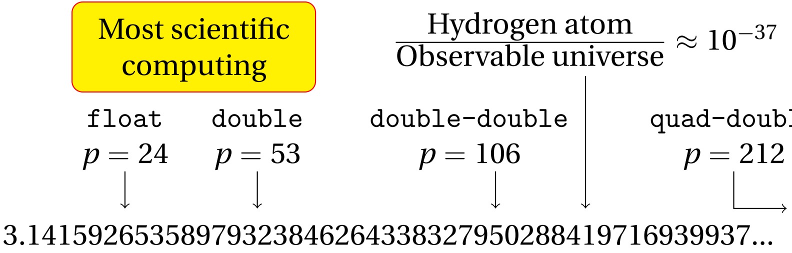
Most scientific computing

`float` $p = 24$

`double` $p = 53$

3.14159265358979323846264338327950288419716939937...

Precision in practice



Precision in practice

Most scientific computing

$$\frac{\text{Hydrogen atom}}{\text{Observable universe}} \approx 10^{-37}$$

`float` $p = 24$ ↓

`double` $p = 53$ ↓

`double-double` $p = 106$ ↓

`quad-double` $p = 212$ →

3.14159265358979323846264338327950288419716939937...

↑ $p = 8$ `bfloat16`

Computer graphics
Machine learning

Precision in practice

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Arbitrary-precision arithmetic

Computer graphics
Machine learning

Unstable algorithms
Ill-conditioned problems
Mathematical problems

Example: inequalities

$$e^{\pi\sqrt{163}} = 640320^3 + 744?$$

```
sage: R = RealField(53)
sage: (R(163).sqrt() * R.pi()).exp(); R(640320**3 + 744)
2.62537412640768e17
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Example: computing discrete objects

$$p(4) = 5 \qquad (4) = (3+1) = (2+2) = (2+1+1) = (1+1+1+1)$$

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Exact formula (Hardy-Ramanujan-Rademacher) for the partition function $p(n)$:

$$p(n) = \sum_{k=1}^{\infty} A_k(n) \frac{\sqrt{k}}{\pi\sqrt{2}} \cdot \frac{d}{dn} \left[\frac{\sinh\left(\frac{\pi}{k}\sqrt{\frac{2}{3}\left(n-\frac{1}{24}\right)}\right)}{\sqrt{n-\frac{1}{24}}} \right]$$

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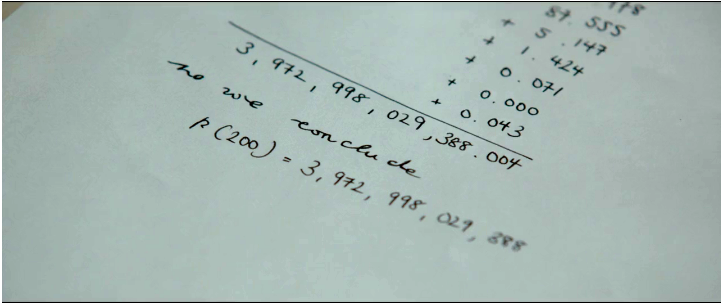

Scene from *The Man Who Knew Infinity*, 2015

Example: guessing

Find the minimal polynomial of $\sqrt{2} + \sqrt{3} + \sqrt{5}$ from a numerical approximation:

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Find the minimal polynomial of $\sqrt{2} + \sqrt{3} + \sqrt{5}$ from a numerical approximation:

```
sage: R = RealField(100)
sage: x = R(2).sqrt() + R(3).sqrt() + R(5).sqrt()
sage: x
5.3823323474417620387383087344
sage: algdep(x, 8)
85*x^8 - 937*x^7 + 2332*x^6 + 1474*x^5 - 359*x^4 - 1935*x^3
    - 268*x^2 + 318*x + 730
```

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Find the minimal polynomial of $\sqrt{2}+\sqrt{3}+\sqrt{5}$ from a numerical approximation:

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sage: R = RealField(200)
sage: x = R(2).sqrt() + R(3).sqrt() + R(5).sqrt()
sage: x
5.3823323474417620387383087344468466809530954887988544255034
sage: algdep(x, 8)
x^8 - 40*x^6 + 352*x^4 - 960*x^2 + 576
```

Complexity of high-precision arithmetic

FFT: $O(n \log n)$ arithmetic operations

$$X_k = \sum_{j=0}^{n-1} x_j e^{-2\pi i k j / n}, \quad k = 0, 1, \ldots, n-1$$

Bit complexity: (number of operations) $\times$ (cost per operation)

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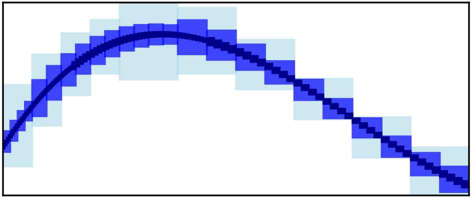
Cost for p-bit operations:

- Multiplication: $M(p) = O(p \log p)$ [Harvey and van der Hoeven, 2019]
- Divison, square root: $O(M(p))$
- Exp, log, π: $O(M(p) \log p)$
- Holonomic constants: $O(M(p) \log^c p)$

Interval arithmetic and ball arithmetic

Definition

Interval extension of $f : A \to B$: given $X \subseteq A$, return some superset (enclosure) of $\{f(x) : x \in X\}$.



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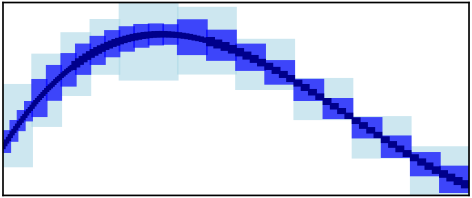

Real intervals: $[3.14, 3.15]$ – `RealIntervalField` (MPFI)

- Better for subdivision of space

Real balls: $[3.14 \pm 0.01]$ – `RealBallField` (Arb)

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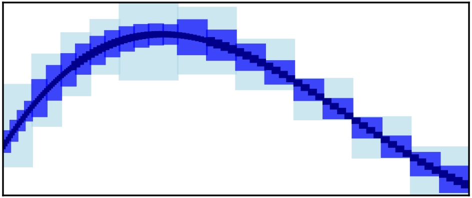

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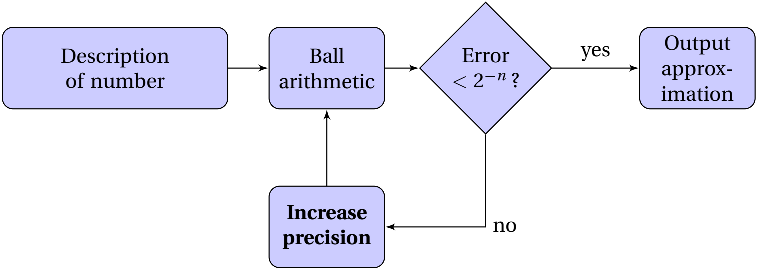
Note: $\sin([0,\pi]) \to [-2, 2]$ just as correct as $\sin([0,\pi]) \to [0, 1]$

Computable numbers using ball arithmetic



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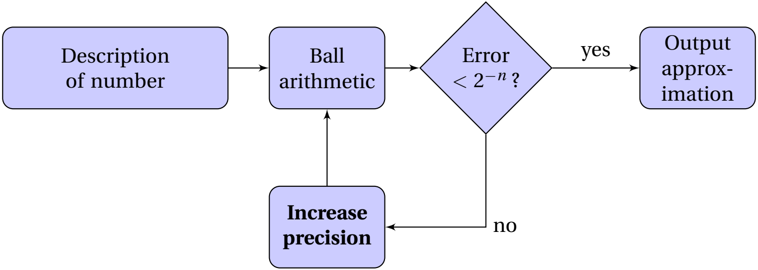

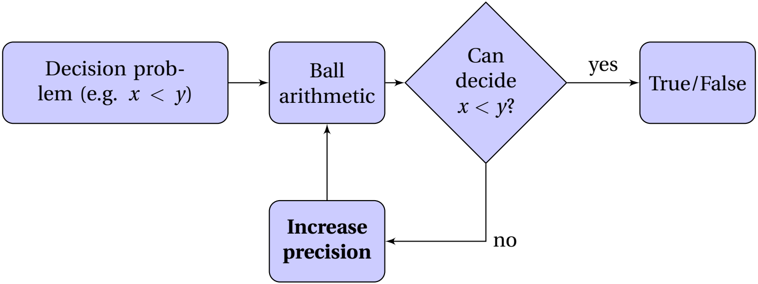

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$$e^{\pi\sqrt{163}} = 640320^3 + 744?$$

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[+/- 7.23e+3]
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[+/- 5.02e-11]

sage: R = RealBallField(128)
sage: (R(163).sqrt() * R.pi()).exp() - R(640320**3 + 744)
[-7.49927e-13 +/- 5.89e-19]
```

Pessimistic error bounds: the dependency problem

Error of sum of N terms?

$$\sum_{n=1}^{N} x_n = \sum_{n=1}^{N} \tilde{x}_n + \varepsilon_n$$

(Let's say $\varepsilon_n = O(2^{-p})$)

- Worst-case bound: $\sum |\varepsilon_n| = O(N \cdot 2^{-p})$
- Expected error: $O(N^{1/2} \cdot 2^{-p})$ (assuming ε_n behave like independent random variables)
- Best case: 0 (errors might cancel out completely!)

Example: linear solving

Solve $Ax = b$

- Well-conditioned A
- Ill-conditioned A

- Floating-point arithmetic
- Ball arithmetic

Well-conditioned matrix, floating-point arithmetic

Solve $Ax = b$, $A =$ size-n DCT matrix, $b = [1, \ldots, 1]^T$

```
n       x_1
----------------------------------------------
1       1.00000000000000
2       1.41421356237310
3       1.69270534084004
4       1.92387953251129
5       2.12756936615424
10      2.93381472087850
20      4.08975996439745
30      4.98358363678481
40      5.73967906112813
50      6.40709547252447
100     9.03226736256870
1000    28.4797579795013
```

Gaussian elimination in floating-point arithmetic ($p = 53$)

Well-conditioned matrix, ball arithmetic

Solve $Ax = b$, $A =$ size-n DCT matrix, $b = [1, \ldots, 1]^T$

```
n       x_1
---------------------------------------------
1       1.00000000000000
2       [1.41421356237310 +/- 5.53e-15]
3       [1.69270534084004 +/- 6.07e-15]
4       [1.9238795325113 +/- 2.18e-14]
5       [2.1275693661542 +/- 5.01e-14]
10      [2.93381472088 +/- 9.20e-12]
20      [4.089760 +/- 5.09e-7]
30      [5.0 +/- 0.0468]
40      [+/- 6.36e+3]
50      -
100     -
1000    -
```

Gaussian elimination in ball arithmetic

Well-conditioned matrix, better ball arithmetic

Solve $Ax = b$, $A =$ size-n DCT matrix, $b = [1, \ldots, 1]^T$

```
n       x_1
----------------------------------------------
1       1.00000000000000
2       [1.41421356237310 +/- 5.53e-15]
3       [1.69270534084004 +/- 6.07e-15]
4       [1.9238795325113 +/- 2.18e-14]
5       [2.1275693661542 +/- 5.01e-14]
10      [2.93381472087850 +/- 4.74e-15]   *
20      [4.08975996439745 +/- 8.09e-15]   *
30      [4.9835836367848 +/- 1.69e-14]    *
40      [5.7396790611281 +/- 3.38e-14]    *
50      [6.4070954725245 +/- 4.13e-14]    *
100     [9.0322673625687 +/- 2.09e-14]    *
1000    [28.479757979501 +/- 3.23e-13]    *
```

* Floating-point solution + *a posteriori* ball certification

Ill-conditioned matrix, floating-point arithmetic

Solve $Ax = b$, $A =$ size-n Hilbert matrix, $b = [1, \ldots, 1]^T$

n	x_1
1	1.0000000000000
2	-2.0000000000000
3	3.0000000000005
4	-4.0000000000134
5	5.0000000002543
10	-9.99995126767237
20	-35.6777214905094
30	6.34155467845874
40	44.5343844893017
50	33.9009376509307
100	52.5690415087492
1000	64.6972177711318

Gaussian elimination in floating-point arithmetic, $p = 53$

Ill-conditioned matrix, ball arithmetic

Solve $Ax = b$, $A =$ size-n Hilbert matrix, $b = [1, \ldots, 1]^T$

```
n       x_1                                 p
---------------------------------------------
1       1.0000000000000000                  64
2       [-2.00000... +/- 1.85e-18]          64
3       [3.00000... +/- 3.14e-35]           128
4       [-4.00000... +/- 1.64e-32]          128
5       [5.00000... +/- 3.56e-29]           128
10      [-10.00000... +/- 7.41e-50]         256
20      [-20.00000... +/- 8.85e-85]         512
30      [-30.00000... +/- 2.82e-33]         256
40      [-40.00000... +/- 1.81e-142]        1024
50      [-50.00000... +/- 1.61e-90]         1024   # 0.1 s
100     [-100.00000... +/- 1.74e-118]       2048   # 0.8 s
1000    [-1000.00000... +/- 4.62e-937]      8192   # 4 hours
```

Ball arithmetic, $p = 64, 128, 256, \ldots$ until error $< 2^{-53}$

Calculus

Consider:

- Differentiation: $f'(x)$
- Integration: $\int_a^b f(x)dx$

How is f represented?

- Symbolic expression
- Black-box functions (computable functions)
- Polynomial approximant
- ...?

Symbolic calculation

Differentiation: the chain rule (easy)

- Efficient implementation: automatic differentiation

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Indefinite integration: the Risch algorithm (complicated)

- Decision procedure for integrating elementary functions in closed form
- Subject to equality testing of constants:
  $f(x) = x + (b - a)e^{x^2}$ is elementary integrable $\iff a = b$

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What symbols?

- Introduce $\mathrm{erf}(x) \implies$ can integrate e^{x^2}
- Introduce $\Gamma(x) \implies$ no closed form for $\Gamma'(x)$ (until we add this as yet another function)

Symbolic definite integration

- Risch algorithm + fundamental theorem of calculus

$$\int_a^b f(x)dx = F(b) - F(a)$$

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$$\int_0^\infty e^{-zx^2} dx = \tfrac{1}{2}(\pi/z)^{1/2}, \quad z > 0$$

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- Other methods: integral transforms, differential equations, residue theorem, lookup tables . . .

Numerical computation: black-box functions

Computable function f: have algorithm which, given p and a computable x, outputs $\tilde{y}$ with $|f(x) - \tilde{y}| < 2^{-p}$

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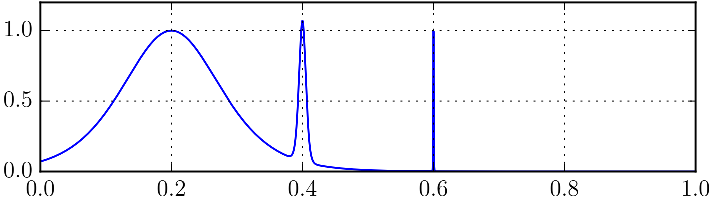
For error bounds, need some knowledge about the regularity of f (typically a bound for the higher derivatives).

Example: the spike integral

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



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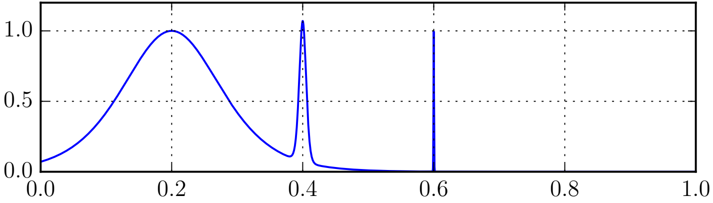

Mathematica `NIntegrate`: 0.209736

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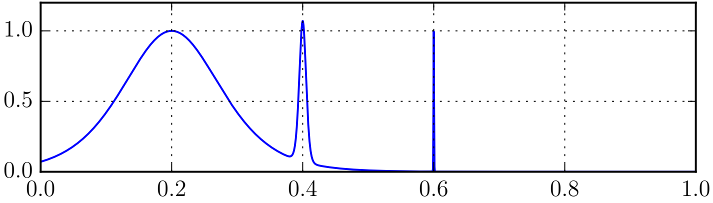

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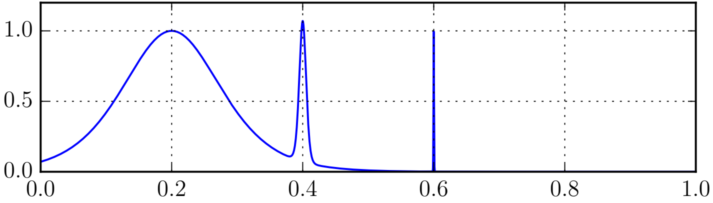

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Sage `numerical_integral`:	0.209736, error estimate 10^{-14}

Example: the spike integral

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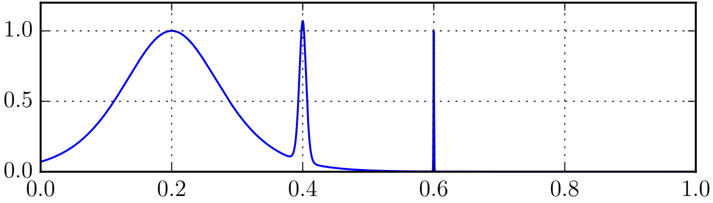

Mathematica `NIntegrate`:	0.209736
Octave `quad`:	0.209736, error estimate 10^{-9}
Sage `numerical_integral`:	0.209736, error estimate 10^{-14}
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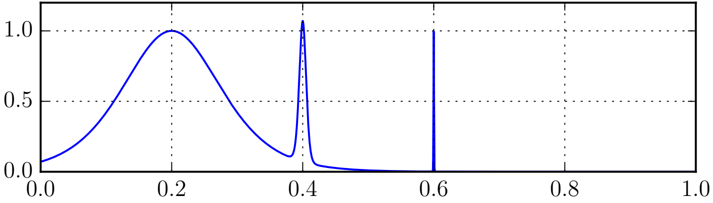

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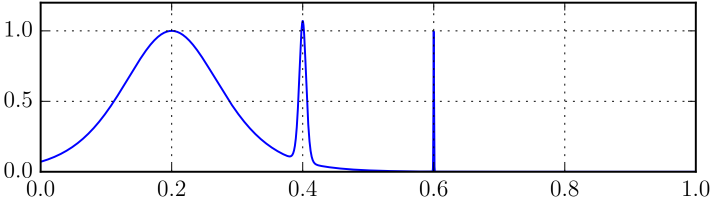

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Pari/GP `intnum`:	0.211316

Example: the spike integral

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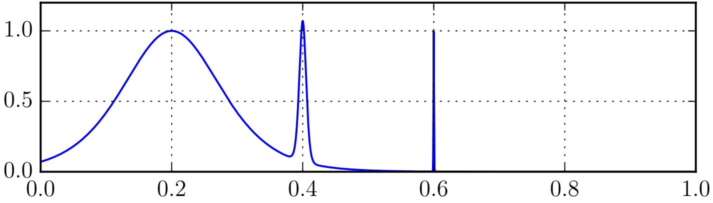

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Actual value:	0.210803

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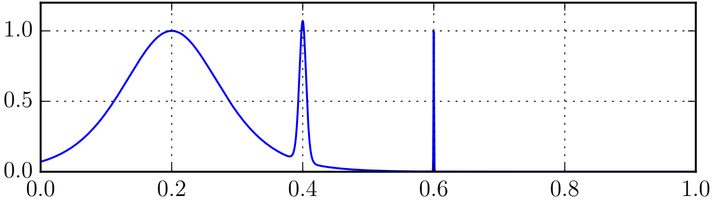

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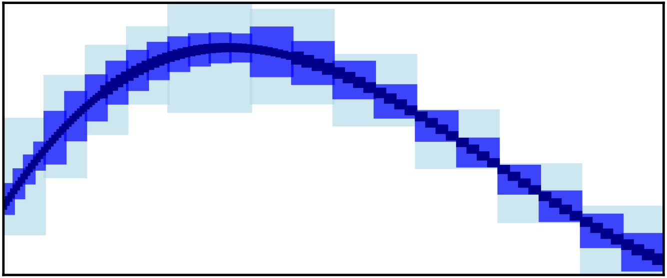
mpmath `quad`:	0.209819
Pari/GP `intnum`:	0.211316
Actual value:	0.210803
Arb:	$[0.21080273550054928 \pm 4.55 \cdot 10^{-18}]$

Integration in interval arithmetic: subdivision

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



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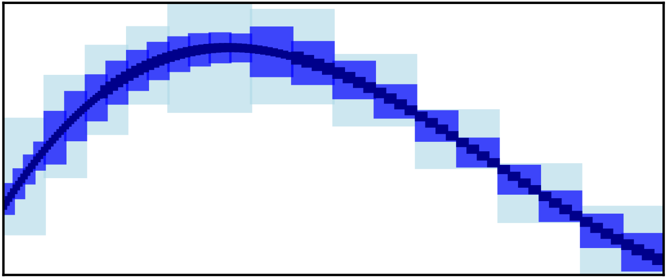
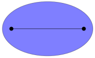


Unfortunately, we need $2^{O(p)}$ evaluations for p-bit accuracy

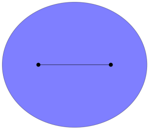
Efficient integration of piecewise holomorphic functions

- Gauss-Legendre quadrature with error bounds

$$\left|\int_a^b f(x)dx - \sum_{k=1}^n w_k f(x_k)\right| \le \frac{M}{\rho^{2n}} \cdot |b-a| C_\rho, \quad |f(z)| \le M$$



$\rho = 2.00$



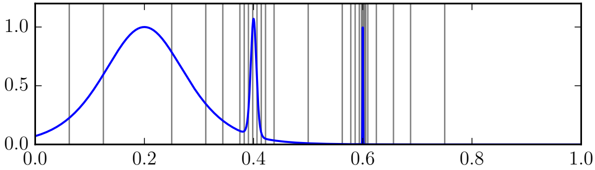
$\rho = 3.73$

- If there are singularities too close to $[a, b]$, bisect (possibly falling back to direct enclosure)

Adaptive subdivision

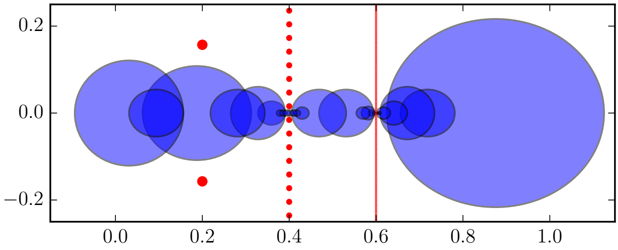
$$\int_0^1 \operatorname{sech}^2(10(x-0.2)) + \operatorname{sech}^4(100(x-0.4)) + \operatorname{sech}^6(1000(x-0.6))\ dx$$

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



Complex ellipses
used for bounds

Red dots = poles



Summary

- High precision needed for some problems
- Interval and ball arithmetic as tools for rigorous computation
- Pessimistic error bounds, slow convergence $\implies$ need numerical analysis!