Floating point accuracy

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Floating World Computation

Revisiting "What Every Computer Scientist Should Know About Floating-point Arithmetic"

- Numbers: real, algebraic, constructibles, decimal, binary, floating point…
- « Primitive » types: `float`, `double`, `long double`, `quad`, `half`…
- When computations don't turn out as expected…(why, how)
  - rounding errors
  - conversion errors
  - propagating errors
  - composing errors
- Heuristics for accuracy:

  how a rough estimate can save epsilons
- Nondimensionalisation and formula entropy reduction
- How to reconcile nondimensionalisation and performance
- How to reconcile abstraction and accuracy: functions of a complex variable
- Why are geometrical computations so hard
- The hidden side of functional programming: towards total functions

Numbers that cost and kill

- Patriot Missiles, first Gulf War, 1991:
  600 m error for interception : 28 killed, a hundred injured
- Vancouver Stock Exchange, 1982 :
  error cumulated over two years on the value of a stock market index
  52 % error : 524.811 $ instead 1098.892 $

`https://doi.org/10.1145/103162.103163`

`https://www.validlab.com/goldberg/paper.pdf` (avec annexe)

"Floating-point arithmetic is considered an esoteric subject by many people"

What Every Computer Scientist Should Know About Floating-Point Arithmetic

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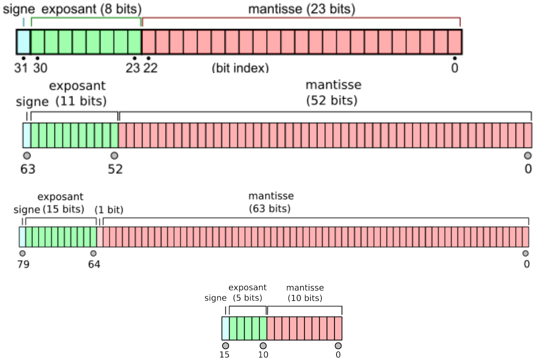
Floating-point arithmetic is considered an esotoric subject by many people. This is rather surprising, because floating-point is ubiquitous in computer systems: Almost every language has a floating-point datatype; computers from PCs to supercomputers have floating-point accelerators; most compilers will be called upon to compile floating-point algorithms from time to time; and virtually every operating system must respond to floating-point exceptions such as overflow This paper presents a tutorial on the aspects of floating-point that have a direct impact on designers of computer systems. It begins with background on floating-point representation and rounding

Formats

« computing is about representation »

Scientific notation:
 significand $\times$ base$^{\text{exponent}}$ significand $\in \mathbb{Z}$, exponent $\in \mathbb{Z}$

Standard form: mantissa, alias *normalized significand*
 mantissa $\times$ base$^{\text{exponent}}$ Trick, for base 2: the most significant digit is always 1...



In the FPU registers, we widen mantissa with three bits: guard bit, round bit, "sticky" bit

Example `float32`

$$\texttt{float} = (-1)^S \times 2^{E-127} \times (1+M), \quad M \in [0,1[$$

31 30 29 28 27 26 25 24 23 22 21 20 19 18 17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0

S	E	M	
			$\texttt{float} = (-1)^S \times 2^{E-127} \times (1+M)$
0	0111 1111	000 0000 0000 0000 0000 0000	$1 = 2^0 \times (1+0)$
0	1000 0000	000 0000 0000 0000 0000 0000	$2 = 2^1 \times (1+0)$
0	1000 0000	100 0000 0000 0000 0000 0000	$3 = 2^1 \times (1+1/2)$
0	1000 0000	110 0000 0000 0000 0000 0000	$3.5 = 2^1 \times (1+1/2+1/4)$
0	1000 0000	111 0000 0000 0000 0000 0000	$3.75 = 2^1 \times (1+1/2+1/4+1/8)$
1	0111 1111	000 0000 0000 0000 0000 0000	$-1 = -2^0 \times (1+0)$
0	0111 1110	000 0000 0000 0000 0000 0000	$1/2 = 2^{-1} \times (1+0)$
0	0111 1100	100 1100 1100 1100 1100 1101	$0.2 = 2^{-3} \times (1+1/2) \times \sum_n 1/16^n$
0	0111 1101	010 1010 1010 1010 1010 1011	$1/3 = 2^{-2} \times (1+1/4) \times \sum_n 1/16^n$
0	0111 1111	011 0101 0000 0100 1111 0011	$\sqrt{2}$
0	1000 0000	100 1001 0000 1111 1101 1011	$\pi \simeq 2^1 \times (1+1/2+1/16+1/128+\cdots)$
0	0000 0000	000 0000 0000 0000 0000 0000	0 special representation
1	0000 0000	000 0000 0000 0000 0000 0000	0_ special representation
0	1111 1110	111 1111 1111 1111 1111 1111	largest float $3.402823466 \times 10^{38}$
0	1111 1111	000 0000 0000 0000 0000 0000	$+\infty$ = `Inf` special representation
0	1111 1111	1xx xxxx xxxx xxxx xxxx xxxx	`NaN` special representation
0	1111 1111	1xx xxxx xxxx xxxx xxxx xxxx	`qNaN` *quiet* special representation
0	1111 1111	01x xxxx xxxx xxxx xxxx xxxx	`sNaN` *signaling* special representation
0	0000 0001	000 0000 0000 0000 0000 0000	smallest positive float $1.17549435 \times 10^{-38}$
0	0000 0000	000 0000 0000 0000 0000 0001	smallest **denormal** positive float 1.401×10^{-45}
0	0000 0000	111 1111 1111 1111 1111 1111	largest **denormal** positive float $1.175\,493\,79 \times 10^{-38}$

⇒ *using the link below, represent your favorite numbers:* *https://www.h-schmidt.net/FloatConverter/IEEE754.html*

Get HexaDecimal displayed C

```c
#include <stdio.h>

int main ()
{
    float x = 1.0f;
    printf ("%f = %a\n", x, x);
    x = 2.0f;
    printf ("%f = %a\n", x, x);
    x = 3.0f;
    printf ("%f = %a\n", x, x);
    x = 3.141592653589793f;
    printf ("%f = %a\n", x, x);
}
```

```
1.000000 = 0x1p+0
2.000000 = 0x1p+1
3.000000 = 0x1.8p+1
3.141593 = 0x1.921fb6p+1
```

Get HexaDecimal displayed C++

```
#include <iostream>

int main ()
{
    float x = 1.0f;
    std::cout << x << " = " << std::hexfloat << x << std::defaultfloat << '\n';
    x = 2.0f;
    std::cout << x << " = " << std::hexfloat << x << std::defaultfloat << '\n';
    x = 3.0f;
    std::cout << x << " = " << std::hexfloat << x << std::defaultfloat << '\n';
    x = 3.141592653589793f;
    std::cout << x << " = " << std::hexfloat << x << std::defaultfloat << '\n';
}
```

```
1 = 0x1p+0
2 = 0x1p+1
3 = 0x1.8p+1
3.14159 = 0x1.921fb6p+1
```

Get HexaDecimal displayed Fortran

```
program hexfloat
  use, intrinsic :: iso_fortran_env, only: real32
  implicit none
  real (real32) :: x

  x = 1
  write (*, '(F10.6,A,Z16)') x, ' = ', x
  x = 2
  write (*, '(F10.6,A,Z16)') x, ' = ', x
  x = 3
  write (*, '(F10.6,A,Z16)') x, ' = ', x
  x = acos (-1.0_real32)
  write (*, '(F10.6,A,Z16)') x, ' = ', x
end program hexfloat
```

```
  1.000000 =         3F800000
  2.000000 =         40000000
  3.000000 =         40400000
  3.141593 =         40490FDB
```

Get HexaDecimal displayed Python

```
#!/usr/bin/python3

x = 1.0
print (x, " = ", float.hex(x))
x = 2.0
print (x, " = ", float.hex(x))
x = 3.0
print (x, " = ", float.hex(x))
x = 3.141592653589793
print (x, " = ", float.hex(x))
```

```
1.0  =  0x1.0000000000000p+0
2.0  =  0x1.0000000000000p+1
3.0  =  0x1.8000000000000p+1
3.141592653589793  =  0x1.921fb54442d18p+1
```

Get HexaDecimal displayed Ada

```
with Ada.Text_Io;

procedure Hexfloat is
    use Ada.Text_Io;
    X : Float := 1.0;
begin
    Put_Line (X'Image & " = 2^" & Float'Exponent (X)'Image & " × " & Float'Fraction (X)'Image);
    X := 2.0;
    Put_Line (X'Image & " = 2^" & Float'Exponent (X)'Image & " × " & Float'Fraction (X)'Image);
    X := 3.0;
    Put_Line (X'Image & " = 2^" & Float'Exponent (X)'Image & " × " & Float'Fraction (X)'Image);
    X := 3.141592653589793;
    Put_Line (X'Image & " = 2^" & Float'Exponent (X)'Image & " × " & Float'Fraction (X)'Image);
end Hexfloat;
```

```
 1.00000E+00 = 2^ 1 ×  5.00000E-01
 2.00000E+00 = 2^ 2 ×  5.00000E-01
 3.00000E+00 = 2^ 2 ×  7.50000E-01
 3.14159E+00 = 2^ 2 ×  7.85398E-01
```

```rust
fn extract_components(x: f32) -> (char, i32, u32) {
    let bits = x.to_bits();
    let sign = if (bits >> 31) & 1 == 0 { '+' } else { '-' };
    let mantissa = (bits & ((1 << 23) - 1)) * 2;
    let exponent = (((bits >> 23) & 0xFF) as i32) - 127;
    (sign, exponent, mantissa)
}

pub fn main() {
    let x: f32 = 1.0;
    let (sign, exponent, mantissa) = extract_components(x);
    println!("{} = {}0x1.{:x}p{}", x, sign, mantissa, exponent);
    let x: f32 = 2.0;
    let (sign, exponent, mantissa) = extract_components(x);
    println!("{} = {}0x1.{:x}p{}", x, sign, mantissa, exponent);
    let x: f32 = 3.0;
    let (sign, exponent, mantissa) = extract_components(x);
    println!("{} = {}0x1.{:x}p{}", x, sign, mantissa, exponent);
    let x: f32 = 3.141592653589793;
    let (sign, exponent, mantissa) = extract_components(x);
    println!("{} = {}0x1.{:x}p{}", x, sign, mantissa, exponent);
    let x: f32 = -0.3141592653589793;
    let (sign, exponent, mantissa) = extract_components(x);
    println!("{} = {}0x1.{:x}p{}", x, sign, mantissa, exponent);
}
```

```
1 = +0x1.0p0
2 = +0x1.0p1
3 = +0x1.800000p1
3.1415927 = +0x1.921fb6p1
-3.1415927 = -0x1.921fb6p1
```

C / C++ (/ Python)	Fortran'90	ieee_arithmetic	Ada
copysign (d x, d y)	sign (x, y)	ieee_copy_sign (x, y)	F'Copy_Sign (value, sign)
frexp (d x, i *exp)	exponent (x) fraction (x)	ieee_logb (x)	F'Exponent (x) F'Fraction (x)
ldexp (d x, i exp) scalbn (d x, i exp)	set_exponent (x, i)	ieee_scalb (x, i)	F'Scaling (x, adjustment)
nextafter(d x, d y)	nearest (x, s)	ieee_next_after (x, y)	F'Adjacent (x, towards)
numeric_limits::radix	radix (x)		F'Machine_Radix
numeric_limits::epsilon ()	epsilon (x)		F'Model_Epsilon
	precision (x)		
numeric_limits::digits	digits (x)		
	range (x)		
			F'Machine_Mantissa
numeric_limits::min_exponent	minexponent (x)		F'Machine_Emin
numeric_limits::max_exponent	maxexponent (x)		F'Machine_Emax
	spacing (x)		
	rrspacing (x)		
nearbyint (d x) rint(d x)	nint (x)	ieee_rint (x)	F'Rounding (x)
floor (d x)	floor (x)		F'Floor (x)
ceil (d x)	ceiling (x)		F'Ceiling (x)
		ieee_rem (x, y)	F'Remainder (x, y)

Unfortunately the C/C++ API doesn't vectorise well.

You might need to extract exponent and mantissa in non standard way for performance

$0.1 + 0.2 \neq 0.3?$

$$\Sigma = a + b \stackrel{?}{=} c \qquad \Delta = a + b - c$$

with

$$a = 0.1 \qquad b = 0.2 \qquad c = 0.3$$

$0.1 + 0.2 \neq 0.3?$

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with

$$a = 0.1 \qquad b = 0.2 \qquad c = 0.3$$

	a	b	c	Σ	Δ
fp32	0.100000001	0.200000003	0.300000012	0.300000012	0
fp64	0.10000000000000001	0.20000000000000001	0.29999999999999999	0.30000000000000004	$5.551 \cdots 10^{-17}$
fp80	0.1000000000000000000001	0.2000000000000000000003	0.3000000000000000000011	0.3000000000000000000011	0
fp16	0.099976	0.19995	0.30005	0.29980	$2.4414 \cdots 10^{-4}$

$0.1 + 0.2 \neq 0.3?$

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$$a = 0.1 \qquad b = 0.2 \qquad c = 0.3$$

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fp80	0.1000000000000000000001	0.2000000000000000000003	0.3000000000000000000011	0.3000000000000000000011	0
fp16	0.099976	0.19995	0.30005	0.29980	$2.4414 \cdots 10^{-4}$

$\Rightarrow \mathbb{D} \not\subset \mathbb{B}$: some decimal are not binary

$\Rightarrow$ binary conversion needs some rounding

$\frac{1}{5} = 0.2_{10} = 0.00\overline{1100}_2 \cdots \ominus 13421773 \times 2^{-26} = 0.2 + 2,98 \times 10^{-9}$

God created the integers, all else is the work of man.

Kronecker

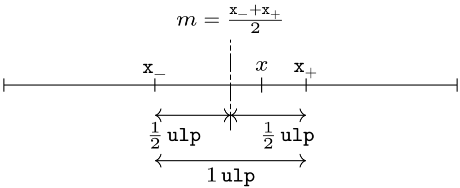
$\mathbb{D} = \left\{ \frac{n}{10^p}, n \in \mathbb{Z}, p \in \mathbb{N} \right\} = \mathbb{Z}[1/10]$ (decimal)
$\mathbb{B} = \left\{ \frac{n}{2^p}, n \in \mathbb{Z}, p \in \mathbb{N} \right\} = \mathbb{Z}[1/2]$ (binary)
$\mathbb{B} \subset \mathbb{D}$ but $\mathbb{D} \not\subset \mathbb{B}$: $\frac{1}{5} \in \mathbb{D}$, $\frac{1}{5} \notin \mathbb{B} \Rightarrow 0.1 + 0.2 \neq 0.3$ $\left(\frac{1}{5} = 0.00\overline{1100}_2\ldots \right)$ $\Rightarrow$ not good for financial computations...

- closure:
  $\forall (x, y) \in \mathbb{B}^2, \quad x + y \in \mathbb{B}$,
  $\forall (x, y) \in \mathbb{B}^2, \quad x \times y \in \mathbb{B}$
- commutativity $\forall (x, y) \in \mathbb{B}^2, \quad x + y = y + x$,
  $\forall (x, y) \in \mathbb{B}^2, \quad x \times y = y \times x$
- associativity:
  $\forall (x, y, z) \in \mathbb{B}^3, \quad x + (y + z) = (x + y) + z$,
  $\forall (x, y, z) \in \mathbb{B}^3, \quad x \times (y \times z) = (x \times y) \times z$
- distributivity:
  $\forall (x, y, z) \in \mathbb{B}^3, \quad x \times (y + z) = x \times y + x \times z$
- total order:
  $\forall (x, y, z) \in \mathbb{B}^3, \quad x \leq y$ and $y \leq z \Rightarrow x \leq z$ (transitivity) ;
  $\forall (x, y) \in \mathbb{B}^2, \quad x \leq y$ and $y \leq x \Rightarrow x = y$ (antisymmetry) ;
  $\forall x \in \mathbb{B}, \quad x \leq x$ (reflexivity) ;
  $\forall (x, y) \in \mathbb{B}^2, \quad x \leq y$ or $y \leq x$ (totality).
- topology:
  $\mathbb{B} \subset \mathbb{D} \subset \mathbb{Q}$ are dense in $\mathbb{R} \Rightarrow$ arbitrarily close approximations to the real numbers

- closure:
  $\forall (x,y) \in \mathbb{F}^2, \quad x+y \notin \mathbb{F},$
  $\forall (x,y) \in \mathbb{F}^2, \quad x \times y \notin \mathbb{F}$
  $\Rightarrow$ rounding and extension $\overline{\mathbb{F}} = \mathbb{F} \cup \{\pm\texttt{Inf}\} \cup \{\texttt{NaN}\} \cup \{0\_\}$ overflow, underflow, inexact
- commutativity $\forall (x,y) \in \mathbb{F}^2, \quad x+y = y+x,$
  $\forall (x,y) \in \mathbb{F}^2, \quad x \times y = y \times x$
- associativity:
  $\forall (x,y,z) \in \mathbb{F}^3, \quad x+(y+z) \neq (x+y)+z,$
  $\forall (x,y,z) \in \mathbb{F}^3, \quad x \times (y \times z) \neq (x \times y) \times z$
- distributivity:
  $\forall (x,y,z) \in \mathbb{F}^3, \quad x \times (y+z) \neq x \times y + x \times z$
- total order:
  $\forall (x,y,z) \in \mathbb{F}^3, \quad x \leq y \wedge y \leq z \Rightarrow x \leq z$ (transitivity) ;
  $\forall (x,y) \in \mathbb{F}^2, \quad x \leq y \wedge y \leq x \Rightarrow x = y$ (antisymmetry) ;
  $\forall x \in \mathbb{F}, \quad x \leq x$ (reflexivity) ;
  $\exists (x,y) \in \overline{\mathbb{F}}^2, \quad x \leq y \wedge y \leq x$ ($\texttt{NaN}$).
- topology:
  $\mathbb{B} \subset \mathbb{D} \subset \mathbb{Q}$ are dense in $\mathbb{R} \Rightarrow$ arbitrarily close approximations to the real numbers
  but
  $\mathbb{F}$: floating point numbers, finite parts of $\mathbb{B}$ (or $\mathbb{D}$) are dense nowhere

Rounding

$\forall x \in \mathbb{R}, \exists(\mathtt{x}_-, \mathtt{x}_+) \in \mathbb{F}^2 \,|\, \mathtt{x}_- \leq x \leq \mathtt{x}_+$ (closest representable neighbours)



⇒ correct rounding requires at least 2 extra bits beyond target accuracy (*cf* guard bit, round bit, "sticky" bit)
or even more (*table maker's dilemma*)
correct rounding, faithful rounding, happy-go-lucky rounding

rounding is non-linear but completely deterministic!

Conversion

- $\mathbb{D} \not\subset \mathbb{B}$: every decimal is not a binary
  $\Rightarrow$ conversion to binary relies on rounding
  $\frac{1}{5} = 0.2_{10} = 0.00\overline{1100}_2 \cdots \ominus 13421773 \times 2^{-26} = 0.2 + 2,98 \times 10^{-9}$

4 byte	`float`	$25.4E0 = 25.399999619 \cdots$
8 byte	`double`	$25.4D0 = 25.399999999999858 \cdots$
10 byte	`long-double`	$25.4T0 = 25.39999999999999999653 \cdots$
16 byte	`quadruple`	$25.4Q0 = 25.39999999999999999999999999999877 \cdots$
2 byte	`half`	$25.4\_2 = 25.406 \cdots$

- $\mathbb{B} \subset \mathbb{D}$: every binary is a decimal
  However, converting a binary, usually from a computation, usually for display or storage, is not toward the exactly corresponding decimal: it would require too many meaningless decimal digits.
  $\frac{1}{8} = 0.001_2 = 0.125_{10} \ominus 0.1_{10} \cdots$
  $\Rightarrow$ conversion to decimal also relies on rounding

Decimal conversion

⇒ use decimal floating points: `_Decimal32`, `_Decimal64`, `_Decimal128` (starting from `C23`)

⇒ program in `SQL` or `COBOL`...

⇒ change scale:
count integer hundredth if you need 2 exact places

⇒ fixed point instead of floating point

pi $\neq \pi$?

	exact	fp32	fp64	fp16*
$\sin\pi$	0	-8.7422777e-8	1.2246467991473532e-16	9.6750e-4
$\cos\pi$	-1	-1.000000	-1.000000000000000	-1.000
$\sin\frac{\pi}{6}$	$\frac{1}{2}$	0.5000000	0.4999999999999999	0.4998
$\cos\frac{\pi}{3}$	$\frac{1}{2}$	0.5000000	0.5000000000000001	0.5005
$\sin\frac{\pi}{3}$	$\frac{\sqrt{3}}{2}$	0.8660254	0.8660254037844386	0.8657
$\cos\frac{\pi}{6}$	$\frac{\sqrt{3}}{2}$	0.8660254	0.8660254037844387	0.8662

$$\sin 0 = 0 \quad \Leftrightarrow \quad \texttt{sin(0.0)} = 0$$

$$\sin\pi = 0 \quad \text{but} \quad \texttt{sin(pi)} \neq 0 \qquad \text{no finite representation...}$$

$$\texttt{pi} = \pi - \eta, \quad \sin\texttt{pi} \quad = \quad \sin\pi - \eta = \sin\eta \underset{0}{\sim} \eta$$

$$|\eta| < \pi\varepsilon/2, \Rightarrow |\sin\texttt{pi}| < \frac{\pi}{2}\varepsilon$$

pi $\neq \pi$?

If it is a problem

- $\Rightarrow$ use half-turn trig functions: `sinpi`, `cospi`,…(starting from `C23`…)
- $\Rightarrow$ use degrees trig functions: `sind`, `cosd`,…(all good `Fortran` compilers…+ `F23`)

Addition

$$\sum_{n=1}^{N} 1/n \sim \ln N + \gamma$$

Table – *Harmonic sum*

fp	N	up sum	down sum	theoretical sum
fp16	250	6.063	6.098	6.098
fp16	500	7.039	6.793	6.793
fp16	1 000	7.086	7.477	7.484
fp16	2 000	7.086	8.188	8.180
fp16	4 000	7.086	8.789	8.875
fp16	8 000	7.086	9.797	9.563
fp16	16 000	7.086	9.797	10.26
fp16	32 000	7.086	9.797	10.95
fp32	32 000	10.95073	10.95072	10.95071
fp32	3 200 000	15.55911	15.55588	15.55588

Addition

```fortran
  program harmonique_fp16
  use, intrinsic :: iso_fortran_env, only: sp => REAL32, dp => REAL64
  implicit none
  integer (8), parameter :: pr = sp   , nbmax = 3200000
  integer (8) :: idx
  real (pr) :: somme_croissante = 0, somme_decroissante = 0
  real (pr), parameter :: euler = 0.57721566, &
       somme_theorique = euler + log (real (nbmax, sp))

  do idx = 1, nbmax
    somme_croissante = somme_croissante + 1.0_pr / real (idx, pr)
  end do

  do idx = nbmax, 1, -1
    somme_decroissante = somme_decroissante + 1.0_pr / real (idx, pr)
  end do

  write (*, *) nbmax, somme_croissante, somme_decroissante, somme_theorique
end program harmonique_fp16
```

Hierarchy of operations

- **arithmetic**: $+$, $-$, $\times$, $/$, integer powers
- **algebraic**: $\sqrt{}$, $\sqrt[n]{}$, fractional powers and roots of polynomials
- **elementary (transcendental) functions**:
  exp, ln, sin, cos, irrational powers, all circular and hyperbolic trigonometry
- **higher transcendental functions *a.k.a.* special functions**:
  Bessel, Airy, Polylogarithm, elliptic integral, Euler Γ function, Riemann ζ function,...

Correct rounding is guaranted by the standard for:

- **arithmetic**
- **square root**

transcendantal functions

- ... costly
- ... **correct rounding** not garanteed

Rounding is **non-linear**

$\Rightarrow$ mixing various scales

$\Rightarrow$ start runoff (butterfly effect)

to get correct rounding with n digits/bits... https://members.loria.fr/PZimmermann/wc/decimal32.html

$$\exp(0.5091077534282133) = \underbrace{1.663806007261509}_{\text{16 digits}}\,\underbrace{5000000000000000}_{\text{16 digits}}\,49\ldots$$

$$\exp(0.7906867968553504) = \underbrace{2.204910231771509}_{\text{16 digits}}\,\underbrace{4999999999999999}_{\text{16 digits}}\ldots$$

Double rounding (rounding from high precision to intermediate precision, then to low precision) can also give worse final rounding than expected.

By way of exception in base 10 (not in binary)! mantissa: 3 decimal digits
For $a = 3.34$ and $b = 3.33$

- $a \ominus b = 0.01 \Rightarrow$ **cancellation** (reducing relative accuracy) but a **benign** one (the floating point result is exact: $a \ominus b = a - b$)
- $\begin{cases} a^2 - b^2 & = 0.0667 = 6.67 \times 10^{-2} \\ a \otimes a \ominus b \otimes b & = 0.1 = 1.00 \times 10^{-1} \end{cases}$ 50% of relative error on the result, or 333 `ulp`, no digit is even correct: **catastrophic cancellation**
- When does this occur?
- How many digits are lost?

Plus, there is an ***overflow*** risk
$\Rightarrow$ Let's **factorize** this!

$$(a \oplus b) \otimes (a \ominus b) = 6.67 \otimes 0.01 = 6.67 \times 10^{-2} \qquad \text{exact}$$

$\Rightarrow$ The Right Way™

Cursed Cancellation

⇒ higher degree polynomials can degrade high resolutions (*cf* Rump)

$$P = 333.75y^6 + x^2(11x^2y^2 - y^6 - 121y^4 - 2) + 5.5y^8 + x/(2y)$$

with $x = 77617$, $y = 33096$ (coprime integers)

[S.M. Rump, 1983, *"How reliable are results of computers"*
`https://www.tuhh.de/ti3/paper/rump/Ru83b.pdf`]

Cursed Cancellation

⇒ higher degree polynomials can degrade high resolutions (*cf* RUMP)

$$P = 333.75y^6 + x^2(11x^2y^2 - y^6 - 121y^4 - 2) + 5.5y^8 + x/(2y)$$

with $x = 77617$, $y = 33096$ (coprime integers)

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`fp16`:	$P =$ `NaN`

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`long double`:	$P = +5.76460752303423489188e + 17$
`quad`:	$P = +1.17260394005317863185883490452018380$
`fp16`:	$P = \texttt{NaN}$
exact:	$P \approx -0.827396059946821368141165095479816292$
	$P = -\frac{54767}{66192}$

How to control rounding errors?

HORNER-RUFFINI

- computational cost of all the exponentiation,
- accuracy loss it represents.

$$\begin{aligned} p(x) &= a_0 + a_1 x + \cdots + a_{n-1} x^{n-1} + a_n x^n \\ &= a_n (x - x_1) \times \cdots \times (x - x_n) \\ &= a_0 + x\Big(a_1 + x(\cdots + x(a_{n-1} + x\, a_n)\cdots)\Big) \end{aligned} \tag{1}$$

- gain in speed, (saving of operations)
- also in accuracy, partly for the same reason,
- guarantee of stability of the result and safety against intermediate overshoots

$\Rightarrow$ "multiply-accumulate" machine instructions (`fma`).

$+$ compensation summation techniques, such as the summation algorithm of W. KAHAN

Variance ... and all statistics

- A difference...
- ...of squares...
- ...of sums...
- ...and sums...
- ...of squares...

- two passes approach
- arbitrary data shift towards some expected average value
- 1-pass online Welford's algorithm (one more division per iteration)

Typical computation

- dot product
- convolution product (“backwards” dot product)
- Fourier transform
- matrix product is a matrix of dot products

turns out to be a sum of simple products (quadratic in essence).
$\Rightarrow$ we expect to encounter problems similar to difference of squares and variance computation.
But here we can’t use the factorisation trick...

- mixed precision
- `fma` (fused multiply accumulate)
- `fma` used to extract exact product
- combined with Kahan or other compensated sums

Quadratic

$$\begin{aligned} ax^2+bx+c &= 0 \qquad (a\neq 0) \\ \Delta &= b^2-4ac \\ x_\pm &= \frac{-b\pm\sqrt{\Delta}}{2a} \end{aligned}$$

2 possible *catastrophic cancelation* (« *compensation calamiteuse* »)

- $-b$ & $\sqrt{\Delta}$

$$\Rightarrow q \quad = \quad -b-\mathrm{sgn}(b)\sqrt{\Delta} = -\mathrm{sgn}(b)\left(|b|+\sqrt{\Delta}\right)$$

$$\begin{cases} x_1 = \frac{q}{2a} \\ x_2 = \frac{2c}{q} = \frac{c}{ax_1} \end{cases}$$

- discriminant $\Delta = b^2-4ac \qquad \Rightarrow$ `fma`

4 possible *overflow*:

- b^2 : *spurious overflow* (if $|b|>10^{19}, \Delta=\texttt{Inf}, |q|=\texttt{Inf}$ while $|q|\sim 2\times 10^{19}$)
- ac
- b/a
- c/b

$$Q = \frac{\sqrt{|ac|}}{b}$$

$$F = \frac{1}{2}\left(1 + \sqrt{1 - 4\sigma Q^2}\right)$$

$$x_1 = -\frac{b}{a}F \qquad x_2 = -\frac{c}{b}\frac{1}{F}$$

si $\sigma = +1$ $\qquad F = \frac{1}{2}\left(1 + \sqrt{(1-2Q)(1+2Q)}\right)$

si $\sigma = -1$ $\qquad F = \frac{1}{2}\left(1 + \sqrt{\texttt{fma}(2Q, 2Q, 1)}\right)$

- Low entropy formula
- Importance of dimensional analysis (dimensionless numbers implementation)

Middlebrook, R.D., *"Methods of Design-Oriented Analysis: The Quadratic Equation Revisited"*,

https://doi.org/10.1109/FIE.1992.683365

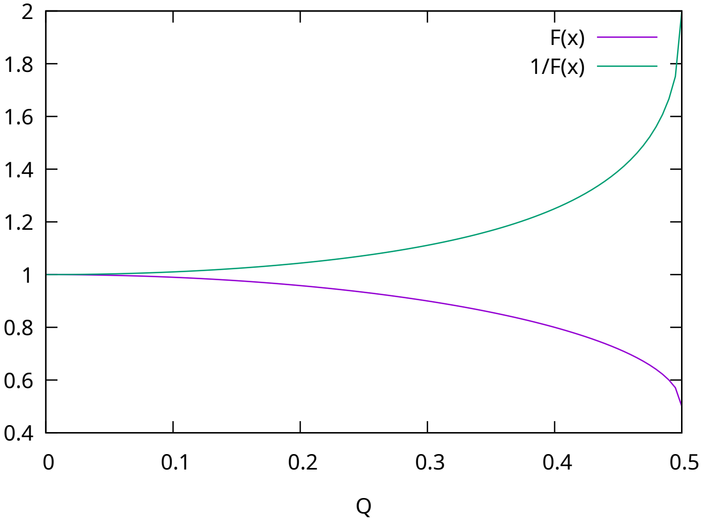

Figure – $F = \frac{1}{2}\left(1 + \sqrt{1 - 4Q^2}\right)\ \forall Q \in [0; 1/4[$.

$$F = \frac{1}{2}\left(1 + \sqrt{1 - 4Q^2}\right) \qquad \forall Q \in [0; 1/4[$$

$$\kappa = \frac{-8Q^2}{\sqrt{1 - 4Q^2}\left(1 + \sqrt{1 - 4Q^2}\right)} \qquad \forall Q \in [0; 1/4[$$

Table – *Quadratic roots*

A	$-B/2$	C	true Δ	true roots	computed Δ	computed roots
10.27 10.28	29.61 29.62	85.37 85.34	0.0022 0.0492	2.88772... 2.87859... 2.90290... 2.86075...	0.1000 0	2.914 2.852 `dec4` 2.881 2.881 `dec4`
10.27 10.28	29.61 29.62	85.37 85.34	0.0022 0.0492	2.88772... 2.87859... 2.90290... 2.86075...	0.1000 0	2.883 `fp16` 2.881 `fp16`
94906265.625	94906267.000	94906268.375	1.89...	1.000000028975958... 1.0	0.0	1.000000014487979 1.000000014487979
94906266.375	94906267.375	94906268.375	1.0	1.000000021073424... 1.0	2.0	1.000000025437873 0.999999995635551

The art of nondimensionalization

Dimensional analysis, split

- scale parameters, or problem's **characteristic scales**
- … **dimensionless** shape parameters (pure numbers)
- lower formulas entropy
- often many ways to do it
  - problem's symmetries,
  - limit computation complexity,
  - limit computation exceptions.
- if the math solution has no float representation, we should allow intermediate results not to be representable as well
- bring values close to unity
  where the floating point density is highest!

COMPTON Scattering

$$\theta = \text{arccos}\left[1 + m_e c^2 \left(\frac{1}{E_1 + E_2} - \frac{1}{E_2}\right)\right]$$

- 2 (same sign) substractions

$$\theta = \text{arccos}\left[1 - m_e c^2 \left(\frac{1}{E_2} - \frac{1}{E_1 + E_2}\right)\right]$$

- basic algebra:

$$\theta = \text{arccos}\left[1 - \frac{m_e c^2 E_1}{E_2 (E_1 + E_2)}\right]$$

- ...one remaining (same sign) substraction
- basic trigonometry: $\cos 2\alpha = 1 - 2\sin^2 \alpha \Leftrightarrow \sin^2 \frac{\theta}{2} = \frac{1 - \cos\theta}{2} = \frac{\text{versin}\,\theta}{2} = \text{haversin}\,\theta$

$$\theta = 2\,\text{arcsin}\sqrt{\frac{m_e c^2 E_1}{2 E_2 (E_1 + E_2)}}$$

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Compound interest

$$A = P\left(1 + \frac{r}{n}\right)^{nt}$$

$$I = P\left(1 + \frac{r}{n}\right)^{nt} - P$$

$$I = P\left[\left(1 + \frac{r}{n}\right)^{nt} - 1\right]$$

$$I = P\left[\mathtt{pow}\left(\left(1 + \frac{r}{n}\right), nt\right) - 1\right]$$

$$I = P\left[\exp\left(nt \ln\left(1 + \frac{r}{n}\right)\right) - 1\right]$$

$$I = P\left[\exp\left(nt\, \mathtt{log1p}\left(\frac{r}{n}\right)\right) - 1\right]$$

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Compound interest

If `log1p` is not available (*cf.* GOLDBERG)

$$\ln(1+x) = \begin{cases} x & \text{if } 1 \oplus x = 1 \\ \frac{x \ln(1+x)}{(1+x)-1} & \text{else.} \end{cases}$$

Area of triangle

area S as a function of lengths a, b and c of edges

$$S = \sqrt{p(p-a)(p-b)(p-c)}$$ (Heron of Alexandria, *Stereometrica*)

$p = \frac{a+b+c}{2}$ half-perimeter

Symmetric, but numericaly unstable, for needle-like triangles (when large and small values meet in the same formula)

Kahan Re-labelling: $a > b > c$

$$\frac{1}{4}\sqrt{[a+(b+c)]\,[c-(a-b)]\,[c+(a-b)]\,[a+(b-c)]}$$

Apparent Symmetry is lost, but the formula is way more robust

Originating from a determinantal expression

$$S = \frac{1}{4}\sqrt{\begin{vmatrix} 0 & a^2 & b^2 & 1 \\ a^2 & 0 & c^2 & 1 \\ b^2 & c^2 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{vmatrix}}$$

⇒ *exercise: code and test data from* `https://people.eecs.berkeley.edu/~wkahan/Triangle.pdf`

Volume of the tetrahedron

$$V = \sqrt{\frac{1}{288}\begin{vmatrix} 0 & a^2 & b^2 & c^2 & 1 \\ a^2 & 0 & C^2 & B^2 & 1 \\ b^2 & C^2 & 0 & A^2 & 1 \\ c^2 & B^2 & A^2 & 0 & 1 \\ 1 & 1 & 1 & 1 & 0 \end{vmatrix}}$$

$$\begin{aligned} X &= (c - A + b)(A + b + c) & x &= (A - b + c)(b - c + A) \\ Y &= (a - B + c)(B + c + a) & y &= (B - c + a)(c - a + B) \\ Z &= (b - C + a)(C + a + b) & z &= (C - a + b)(a - b + C) \end{aligned}$$

$$\xi = \sqrt{xYZ} \qquad \eta = \sqrt{yZX} \qquad \zeta = \sqrt{zXY} \qquad \lambda = \sqrt{xyz}$$

$$V = \frac{1}{192abc}\sqrt{(\xi + \eta + \zeta - \lambda)(\lambda + \xi + \eta - \zeta)(\eta + \zeta + \lambda - \xi)(\zeta + \lambda + \xi - \eta)}$$

```
for (unsigned nbTot = NBITERMIN; nbTot < NBITERMAX; nbTot++) {
  float x = X0;
  for (unsigned nbIter = 0; nbIter < nbTot; nbIter++) x = sqrt (x);
  float bottomRadix = x;
  for (unsigned nbIter = 0; nbIter < nbTot; nbIter++) x = x * x;
  printf ("%d %f %f (%+e) %f (%+e)\n", nbTot, X0, x, x-X0, bottomRadix, bottomRadix-1.0);
}
```

iter	X0	x	x − X0	btmRdx	btmRdx − 1
10	2.000000	1.999958	(−4.184246e−05)	1.000677	(+6.771088e−04)
11	2.000000	2.000196	(+1.962185e−04)	1.000339	(+3.385544e−04)
12	2.000000	2.000196	(+1.962185e−04)	1.000169	(+1.692772e−04)
13	2.000000	2.000196	(+1.962185e−04)	1.000085	(+8.463860e−05)
14	2.000000	2.000196	(+1.962185e−04)	1.000042	(+4.231930e−05)
15	2.000000	1.996286	(−3.713965e−03)	1.000021	(+2.110004e−05)
16	2.000000	1.988545	(−1.145530e−02)	1.000010	(+1.049042e−05)
17	2.000000	1.988545	(−1.145530e−02)	1.000005	(+5.245209e−06)
18	2.000000	1.988545	(−1.145530e−02)	1.000003	(+2.622604e−06)
19	2.000000	1.988545	(−1.145530e−02)	1.000001	(+1.311302e−06)
20	2.000000	1.868132	(−1.318680e−01)	1.000001	(+5.960464e−07)
21	2.000000	1.648514	(−3.514862e−01)	1.000000	(+2.384186e−07)
22	2.000000	1.648514	(−3.514862e−01)	1.000000	(+1.192093e−07)
23	2.000000	1.000000	(−1.000000e+00)	1.000000	(+0.000000e+00)

What is the relative sensitivity of a function with respect to input argument fluctuation?
$\Rightarrow$ *condition number* or absolute value of *elasticity*

$$\kappa(x) = \frac{\left|\frac{f(x_a)-f(x)}{f(x)}\right|}{\left|\frac{x_a-x}{x}\right|} = \frac{\left|\frac{f(x_a)-f(x)}{(x_a-x)}\right|}{\left|\frac{f(x)}{x}\right|} \sim \left|\frac{x f'(x)}{f(x)}\right| = \left|\frac{\mathrm{d}\,(\ln|f(x)|)}{\mathrm{d}\ln|x|}\right| \tag{2}$$

κ is dimensionless, a pure number (*doubly logarithmic derivative*)
Power law $x \to C \times x^n$ (with C and n real constants) are the functions with uniform condition number: $\forall x,\ \kappa(x) = n$.
$\log_2 \kappa$: number of accuracy bits lost *in the best case, with correct rounding*
$f : x \to x^2 \Rightarrow \kappa = \frac{2x \cdot x}{x^2} = 2$: no singularity, relative error doubles on each iteration
$f : x \to \sqrt{x} \Rightarrow \kappa = \frac{1}{2}$: no singularity, relative error is halved on each iteration (but can't really get below $\frac{1}{2}$ `ulp`)
Very few uncertainty caused by iterations of $\sqrt{\ }$, still the last half `ulp` is responsible for losing 100% of accuracy

then iterations of $x \to x^2$ amplify this generaly negligible error to a macroscopic one.

$$\kappa_{f\circ g} = \kappa_f \times \kappa_g$$
$$\kappa_{f\times g} = \kappa_f + \kappa_g$$
$$\kappa_{f^n} = n\kappa_f$$

- $f : x \to x - c \Rightarrow \kappa = \frac{x}{x-c}$: singularity $x = c$ *(catastrophic cancellation)*
- $f : x \to \ln x \Rightarrow \kappa(x) = \frac{1}{\ln x}$: singularity $x = 1,\ f(x = 1 + h) = \ln(1 + h)$

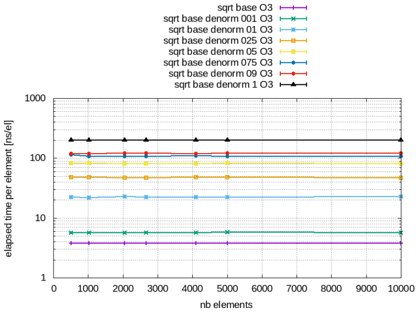
$$\kappa(h) = \frac{h}{(1+h)\ln(1+h)} \underset{h\to 0}{\sim} \frac{1}{(1+h)}$$ hence the importance of `log1p`

- $f : x \to \exp x - 1 \Rightarrow \kappa(x) = \frac{x \exp x}{\exp x - 1}$: indeterminate form $x = 0,\ \kappa(h) \underset{h\to 0}{\sim} 1$
  hence the importance of `expm1`
- $f : x \to \cos x - 1 \Rightarrow \kappa(x) = \frac{-x \sin x}{\cos x - 1}$: indeterminate form $x = 0,\ \kappa(h) = \frac{h \cos \frac{h}{2}}{\sin \frac{h}{2}} \underset{h\to 0}{\sim} 2$
  hence the importance of trigonometry

To bypass cleanly this « tower of roots » problem (even in single precision), one needs to change the naive approach and use `log1p` and `expm1` $\Rightarrow$ *exercise: do it!*

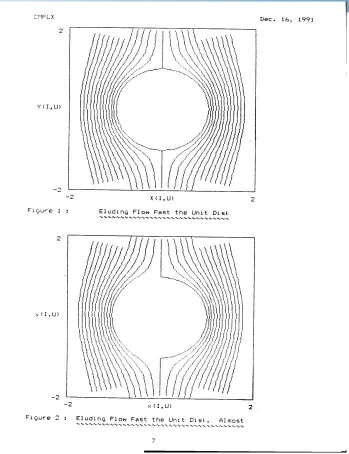
Denormals

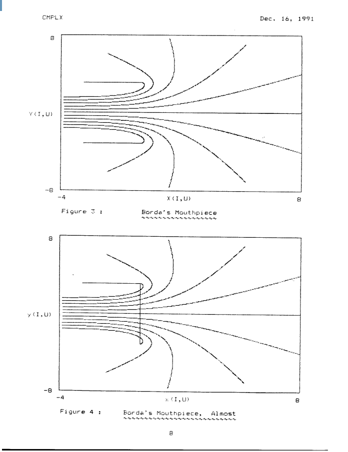
- below 1.17×10^{-38} for `fp32`
- below 2.22×10^{-308} for `fp64`
- below 6.09×10^{-5} for `fp16`
  (up to 5.96×10^{-8})
- Why?
  $\Rightarrow$ alllow for “gradual underflow”
- Why not?
  $\Rightarrow$ $100\times$ slower
  (see Pierre AUBERT)
- How?
  - float difference around the minimum normal threshold
  - decreasing geometric progression



Function of a complex variable

function, but multivalued?

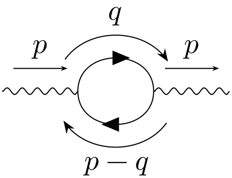




Eluding Flow past a Disk: $f : Z \mapsto (Z - 1/Z)/2$ and $g : W \mapsto W - i\sqrt{iW-1}\sqrt{iW+1}$
Do not "simplify" $g(W)$ to $W - i\sqrt{-W^2-1}$ nor to $W - \sqrt{W^2+1}$ since they behave differently. Though $\forall W,\ f(g(W)) = W,\ \forall |Z| > 1,\ g(f(Z)) = Z$ only, and some $|Z| = 1$; otherwise $g(f(Z)) = -1/Z$.
Deducing where these identities hold is tricky.

Borda's Mouthpiece: $W \mapsto 1 + W^2 + W\sqrt{W^2+1} + \ln(W^2 + W\sqrt{W^2+1})$

as W runs on radial straight lines through 0 in the right half-plane, including the imaginary axis.



$$
\begin{aligned}
B_0(p,m_1,m_2) &= 16\pi^2 Q^{4-n}\int \frac{d^n q}{i\,(2\pi)^n}\,\frac{1}{\left[q^2-m_1^2+i\varepsilon\right]\left[(q-p)^2-m_2^2+i\varepsilon\right]} \\
&= \frac{1}{\hat\epsilon} - \int_0^1 dx\ \ln\frac{(1-x)\ m_1^2 + x\ m_2^2 - x(1-x)\ p^2 - i\varepsilon}{Q^2} \\
&= \frac{1}{\hat\epsilon} - \ln\left(\frac{p^2}{Q^2}\right) - f_B(x_+) - f_B(x_-)
\end{aligned}
$$

$$
s = p^2 - m_2^2 + m_1^2,\ x_\pm = \frac{s \pm \sqrt{s^2 - 4p^2(m_1^2 - i\varepsilon)}}{2p^2}\ ,\quad f_B(x) = \ln(1-x) - x\ln\left(1-x^{-1}\right) - 1
$$

⇒ the (microscopic) difference of ε induces a (macroscopic) difference of 2π on the imaginary part

⇒ the analytic functions[1] of complex analysis are sharply discontinuous at the crossing of their *branch cut*

Discrete Stochastic Arithmetic (DSA) [Vignes'04]

Classic arithmetic

$A \oplus B \longrightarrow R$

$R =$3.14237654356891

DSA

Random rounding

$A_1 \oplus B_1 \longrightarrow R_1$

$A_2 \oplus B_2 \longrightarrow R_2$

$A_3 \oplus B_3 \longrightarrow R_3$

$R_1 =$**3.14**1354786390989
$R_2 =$**3.14**3689456834534
$R_3 =$**3.14**2579087356598

- each operation executed 3 times with a random rounding mode
- number of correct digits in the results estimated using Student's test with the confidence level 95%
- operations executed synchronously
  - ⇒ detection of numerical instabilities
    Ex: `if (A>B)` with `A-B` numerical noise
  - ⇒ optimization of stopping criteria

The CADNA library

- implements stochastic arithmetic for C/C++ or Fortran codes
- few code rewriting
- all operators and mathematical functions overloaded
- support for MPI, OpenMP, GPU, vectorised codes
- supports emulated ou native half precision
- in one CADNA execution: accuracy of any result, complete list of numerical instabilities

CADNA cost

- memory: 4
- run time $\approx$ 10

Executing CADNA

Before modifying the precisions used, we want to explore the current accuracy.

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Before modifying the precisions used, we want to explore the current accuracy.

To execute CADNA, we essentially change the types.

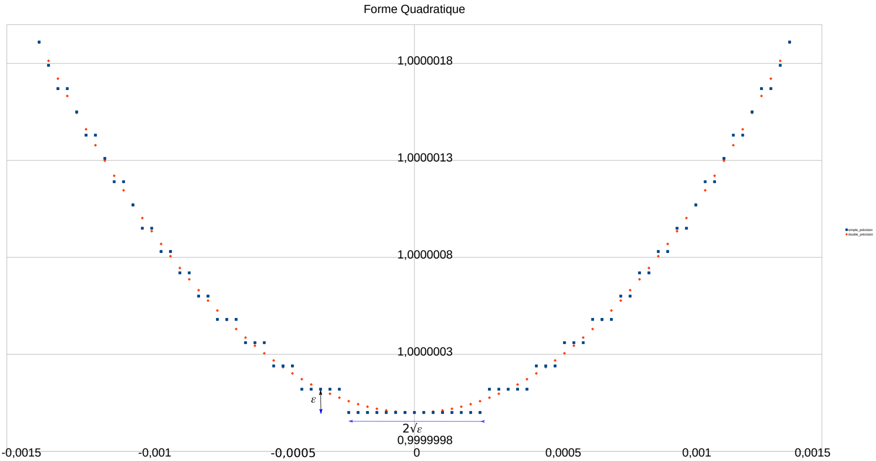
This execution exposed multiple numerical instabilities that hide potential massive loss of accuracy.

```
----------------------------------------------------------------
CADNA_C 3.1.11 software

CRITICAL WARNING: the self-validation detects major problem(s).
The results are NOT guaranteed.

There are 538393974 numerical instabilities
10409 UNSTABLE DIVISION(S)
40122229 UNSTABLE MULTIPLICATION(S)
267297 UNSTABLE BRANCHING(S)
448561143 UNSTABLE INTRINSIC FUNCTION(S)
266 UNSTABLE MATHEMATICAL FUNCTION(S)
49432630 LOSS(ES) OF ACCURACY DUE TO CANCELLATION(S)
----------------------------------------------------------------
```

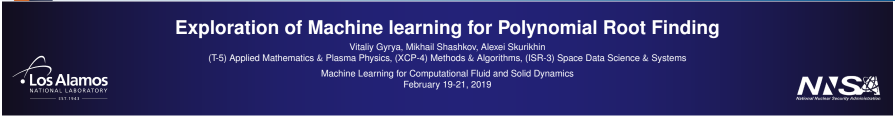
Minimisation

Numerical evaluation of derivatives / gradients / Jacobian / Hessian

$$x \mapsto 1+(x-1)^2 \quad \Rightarrow \quad f(x=x_0+h) = f(x_0) + \underbrace{h\cdot\frac{\partial f}{\partial}}_{=0 \text{ at extremum}} + {}^t h \cdot \frac{\partial^2 f}{\partial\partial}\cdot h + o\left(h^2\right)\cdots \text{TAYLOR}$$



Neural Network



Exploration of Machine learning for Polynomial Root Finding

Vitaliy Gyrya, Mikhail Shashkov, Alexei Skurikhin

(T-5) Applied Mathematics & Plasma Physics, (XCP-4) Methods & Algorithms, (ISR-3) Space Data Science & Systems

Machine Learning for Computational Fluid and Solid Dynamics

February 19-21, 2019

Los Alamos NATIONAL LABORATORY EST.1943

NNSA National Nuclear Security Administration

Motivation

We are interested in application of Machine Learning (ML) for improving numerical methods for solving partial differential equations (PDEs). One example of such an improvement is the optimization of the parameters of artificial viscosity for Lagrangian and arbitrary-Lagrangian-Eulerian methods. Another example is solving the Riemann problem, which is at the core of many numerical methods for computational gas and solid dynamics. To build confidence in ML methods and understand their strengths and weaknesses we decided to start by applying ML to solve simple quadratic equations of one variable.

Problem

Consider a quadratic equation, $ax^2 + bx + c = 0$, whose roots are r_L and r_R. We would like to learn the function

$$(a, b, c) \to (r_L, r_R)$$

without relying on our knowledge of the underlying processes. Instead we will consider a number of observations observations (training set)

$$(a^i, b^i, c^i) \to (r_L^i, r_R^i), \qquad i = 1, \ldots, N.$$

From which we will try to predict

$$(a^j, b^j, c^j) \to (\tilde{r}_L^j, \tilde{r}_R^j) \approx (r_L^j, r_R^j), \qquad j = N+1, \ldots, N+K.$$

The goal is to minimize

$$\text{COST} = \sum_j (r_L^j - \tilde{r}_L^j)^2 + \sum_j (r_R^j - \tilde{r}_R^j)^2.$$

Challenges

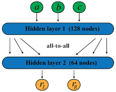
The quadratic equation was selected as a proxy for the following reasons that are relevant to many complex practical problems:

- There are several branches in the solution: if $a = 0$, the quadratic equation becomes a linear equation, which has one root – this is a qualitative change from one regime to a different one; depending on the discriminant the number of roots as well as the nature of the roots changes (real vs. complex).
- Finding solution involves different arithmetic operations some of which can be difficult to model by machine learning techniques. For example, division and square root are a challenge for neural networks to represent as activation functions.
- Probably, the most significant challenge is that for a small range of input parameters for which output values are increasingly large.

Feed-forward Neural Network

NN Architecture:

Input Layer:	3 nodes
Hidden Layer 1:	128 ReLU
Hidden Layer 2:	64 ReLU
Output Layer:	2 Linear
Connectivitys: full.	

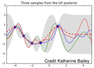


NN Training:

Batch size:	200
Training epochs:	under 500
Oprimizer:	Adam (https://arxiv.org/abs/1412.6980v8)

Gauss Process Regression (GPR)

- Probabilistic Bayesian generalization of linear regression approach.
- Built in model of uncertainty estimator.
- Need to specify a covariance kernel. Our choice of kernel:
  $ConstantKernel() +$
  $Matern(length\_scale = 2, nu = 3/2) +$
  $WhiteKernel(noise_level = 1)$



Test & training sets

We considered a number of distributions for the coefficients (a, b, c). In all these cased we assumed that

$$a \in [\epsilon, 1], \quad b \in [-1, 1], \quad c \in [-1, 1], \quad \epsilon = 1/20$$

and the roots (r_L, r_R) are real, i.e. $D = b^2 - 4ac \geq 0$.

We considered the following distributions for (a, b, c)

- Uniform random distribution.
- Regular distribution for (a, b, c), i.e. distribution on a grid.
- Regular distribution for $(1/a, b, c)$, i.e. distribution on a grid.

The sizes of the training and test sets were approximately equal and were on the order of 40K to 50K data points.

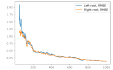
GPR for large datasets

- GPR performance degrades quickly (scaling $\sim N^3$).
- Depending on the machine the threshold of tractable training sets was between 5K and 50K sample points.
- More advanced techniques are needed for larger data sets.
- Ensambles of smaller GPR could be used

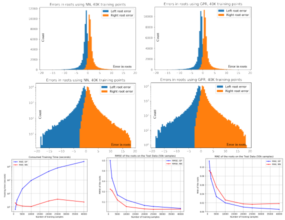
Adaptive sampling with GPR

Adaptation procedure:

- Consider the pool of uniformly distributed parameters $(a^i.b^i.c^i)$.
- Select an initial training set of points (50) at random. Generated GPR based on these points.
- For the given GPR consider the "uncertainty" σ at all of the sample points. Find the triples (a^i, b^i, c^i) with the largest uncertainty and add them to the training set.
- Generate a new GPR for the updated training set.
- Repeat steps 3-4 untill stopping criteria is statisfied, e.g. training set reached predefined size.



Results



Conclusions

- For small data sets (2K points) GPR is more accurate
- GPR can utilize adaptive sampling
- GPR does not scale well to larger data sets (~2K points).
- NN scales well for large data sets and has better accuracy over GPR (more that 5K points) .
- NN produces fewer large errors vs. GPR for large data sets (RMSE

Floating Point Types

`float` and `double` are identified as simple or even primitive types, but they are much richer than it seems.
Object point of view: do these types fit into a hierarchy of classes?
⇒ Violation of the LISKOV's substitution principle (LSP)

if S subtypes T, what holds for T-objects holds for S-objects.

If S is a subtype of T, objects of type T in a program can be replaced by objects of type S without changing any of the desirable properties of that program (e.g. correct results)

A poorly encapsulated abstraction (*leaky*): we can measure the smallest positive non-zero float, the largest one, the machine epsilon, the base: we can access the implementation details

Not metrology: we do not seek "precision for precision's sake"

The **functional** paradigm invites us to write computer function approaching mathematical functions, and we tend to focus on the aspect of **purity**.

But a mathematical function also seeks **totality** (being defined on the largest domain of definition):

the function should be calculable for any argument for which it is defined.

- *removing non-jump and non-essential discontinuity*: $\Rightarrow \left.\frac{\sin x}{x}\right|_{x=0} = 1$ (*naively* `sin (0.0) / 0.0 = NaN`)
- *analytic continuation*: factorial $\Rightarrow \Gamma$, or RIEMANN ζ function

$\Rightarrow$ *maximal extension of function domain*
$\Rightarrow$ piecewise function definition, *casuistry*

Using IEEE-754 exceptional values, we can reach a "weak totality":

- `log (0.0) = -Inf` (mathematically correct)
- `log (-1.0) = NaN` (mathematically correct? more precisely `NaRN`)

Precision limitations lead to a gray zone in this kind of totality:

- `expf (88.72284) = + Inf` (but mathematically it's 2^{128} $\Rightarrow$ `domainException`)
- `expf (-103.972084) = 0.0f` (but mathematically it's just below 2^{-150} $\Rightarrow$ `domainException`)
- `gammaf (35.0401001) = + Inf` (but mathematically it's 2^{128})

OK with `double`, but not with `float`.

Not all `Inf` have the same meaning, not all `NaN` have the same meaning, *cf* `null` in `SQL`

« Why aiming for precision? »

⇒ Implicit **contract**: the fonction will

1. (if the argument is inside the mathematical domain of the mathematical function)
2. (if the type representation of the argument is inside the domain of the function that has a representable image in the return type)
3. return a result
4. this result is relevant(?)
5. (ideally the returned value is the representation of the image of the mathematical function applied on the represented argument)

« Why aiming for precision? »

totality (mathematical) *vs.* representable totality

A representable solution resulting from representable arguments CAN go through a non-representable intermediate calculation.
IEEE-754 exceptional values are not the value of the function, relative error of 100%, as in catastrophic cancelation.

least surprise principle

- we agree to compute erroneous results, because we know that we cannot compute exact results: exact results are rarely (= almost never) representable: π, e, $\sqrt{2}$, $1/3$, $1/5$ in base 2…
- On the other hand, we don't want things to be very wrong: mathematical result 2 but the function returns `NaN`

If the calculation is badly carried out, we can end up with

- infinite roots, where they exist and can be represented
- to an absence of roots, where they exist and are representable
- to a presence of roots, where they do not exist

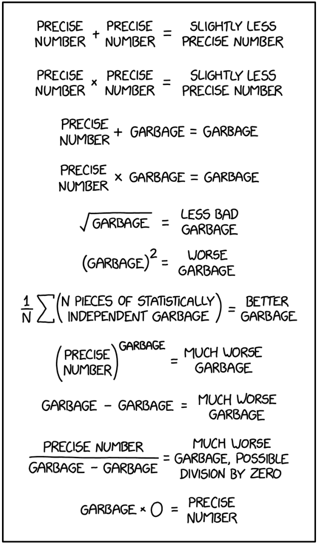
a difference of degree generates a difference of nature (catastrophe theory, bifurcation, chaos)

The relative size of the danger zone in the parameter space will be much larger in low precision.

Annex for a less costly nondimensionalization:

« *You Could Learn a Lot from a Quadratic* » `doi:10.1145/609742.609746`, shows how to nondimensionalize with binary, much less costly in time and accuracy than divisions (and roots) in physicist nondimensionalization. Easy when knowing IEEE-754 API.

« precision? » a take-away



https://xkcd.com/2295/