Floating Point Precision & Accuracy

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Floating World Computation

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

- Numbers: real, decimal, binary, floating point...
- When computations don't turn out as expected...(why, how)
  - global errors
  - local errors
  - composing errors
- Heuristics for accuracy:

  how a rough estimate can save epsilons
- How to reconcile adimensionalisation 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

Formats

« computing is about representation »

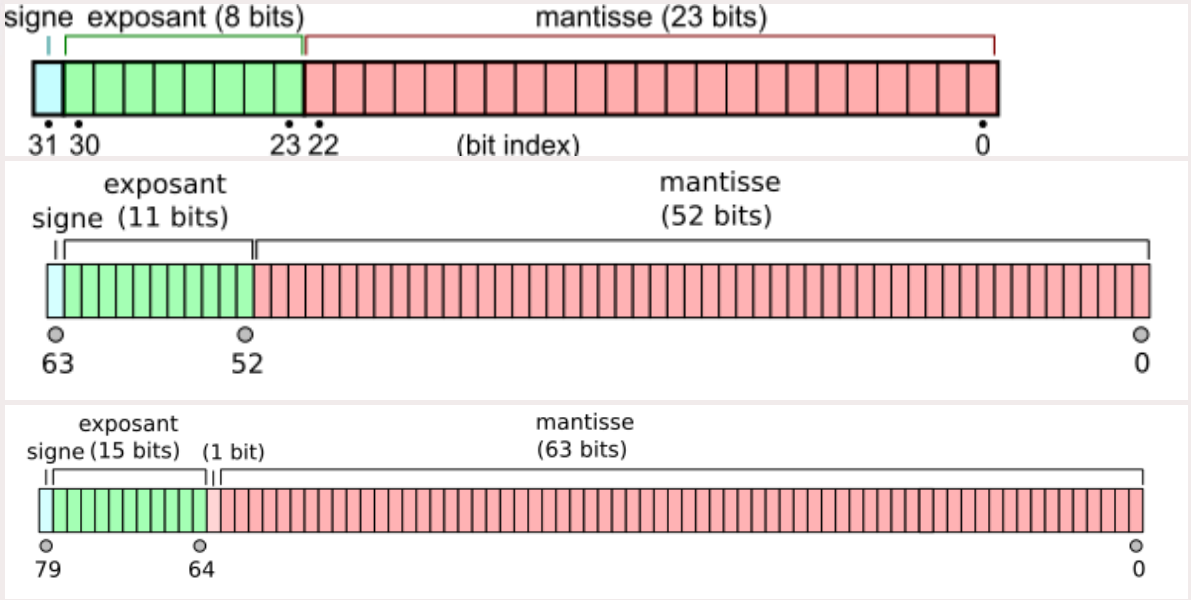
Scientific notation:

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

Standard form: mantissa, alias *normalized significand*

mantissa $\times$ base$^{\text{exponent}}$ mantissa $\in [1; \text{base}[$, exponent $\in \mathbb{Z}$

Trick, for base 2: the most significant digit is always 1...



In the registers, we widen mantissa with three bits:

- guard bit
- round bit
- sticky bit

Problems

- apparent: rounding $\Rightarrow$ catastrophic `cancelation`
- apparent: conversion. Goes unnoticed or perceived as minor.
- apparent: `overflow`. Apparent, but not treated.
- less apparent: `underflow`, gradual `underflow`: denormal numbers

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	
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	$3.75 = 2^1 \times (1+1/2+1/4+1/8)$
0	1000 0000	100 1001 0000 1111 1101 1011	$\pi \simeq 2^1 \times (1+1/2+1/16+1/128+\cdots)$
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	0000 0000	000 0000 0000 0000 0000 0000	0 special representation
1	0000 0000	000 0000 0000 0000 0000 0000	0_-
0	1111 1111	000 0000 0000 0000 0000 0000	$+\infty$ = `Inf` special representation
0	1111 1111	111 1111 1111 1111 1111 1111	`NaN` special representation

$\Rightarrow$ *exercise: using the link below, represent number such as* $\sqrt{2}$, $\frac{1+\sqrt{5}}{2}$, e, $\ln 2$,...

`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 = 3.1415926535897 93f;
    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++

```cpp
#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 = 3.1415926535897 93f;
    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
```

$0.1 + 0.2 \neq 0.3$?

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

with

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

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with

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

a	b	c	Σ	Δ
0.100000001	0.200000003	0.300000012	0.300000012	0
0.10000000000000001	0.20000000000000001	0.29999999999999999	0.30000000000000004	$5.551\cdots10^{-17}$
0.100000000000000000001	0.200000000000000000003	0.300000000000000000011	0.300000000000000000011	0

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with

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a	b	c	Σ	Δ
0.100000001	0.200000003	0.300000012	0.300000012	0
0.10000000000000001	0.20000000000000001	0.29999999999999999	0.30000000000000004	$5.551\cdots10^{-17}$
0.100000000000000000001	0.200000000000000000003	0.300000000000000000011	0.300000000000000000011	0

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

$\Rightarrow$ binary conversion needs some rounding

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

Decimal *vs.* binary ...and binary *vs.* floating

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

Decimal *vs.* binary ...and binary *vs.* floating

- closure:
  $\exists (x, y) \in \mathbb{F}^2, \quad x + y \notin \mathbb{F}$,
  $\exists (x, y) \in \mathbb{F}^2, \quad x \times y \notin \mathbb{F}$
  $\Rightarrow$ rounding and extension $\overline{\mathbb{F}} = \mathbb{F} \cup \{\pm\texttt{Inf}\} \cup \{\texttt{NaN}\} \cup \{\texttt{0\_}\}$ 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:
  $\exists (x, y, z) \in \mathbb{F}^3, \quad x + (y + z) \neq (x + y) + z$,
  $\exists (x, y, z) \in \mathbb{F}^3, \quad x \times (y \times z) \neq (x \times y) \times z$
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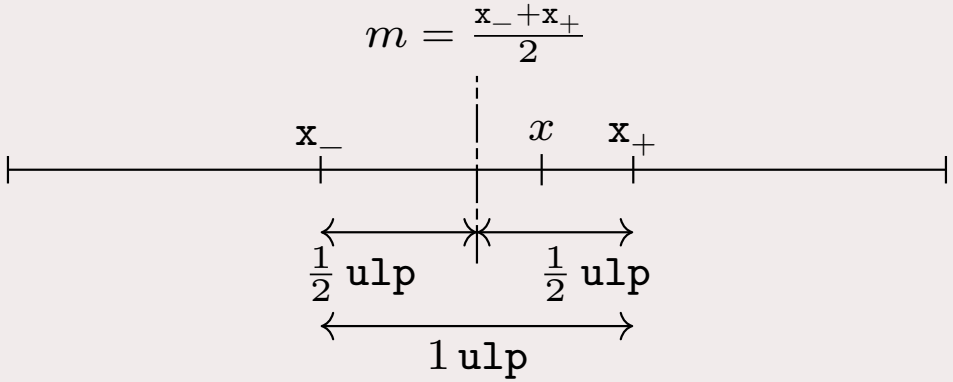
  $\forall (x, y) \in \mathbb{F}^2, \quad x \leq y$ or $y \leq x$ (totality).
  $\exists (x, y) \in \overline{\mathbb{F}}^2, \quad x \leq y$ and $y \leq x$ (NaN).
- topology:
  $\mathbb{B} \subset \mathbb{D} \subset \mathbb{Q}$ are dense in $\mathbb{R} \Rightarrow$ arbitrarily close approximations to the 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)



$\Rightarrow$ correct rounding requires at least 2 extra bits beyond target accuracy
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`	$25.4D0 = 25.3999999999999858\cdots$
10 byte	`long-double`	$25.4T0 = 25.39999999999999999653\cdots$
16 byte	`quadruple`	$25.4Q0 = 25.399999999999999999999999999999877\cdots$

- $\mathbb{B} \subset \mathbb{D}$: 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

Can division by a constant be replaced by multiplication by this constant reciprocal?
This replacement can induce an extra uncertainty.
Counter-example: dividing by 2 (has an exact representation) induces no uncertainty, and the reciprocal of 2 having an exact representation, multiplying by $\frac{1}{2}$ induces no uncertainty either.
Example: dividing by 5 or by 10, or even by 3: one uncertainty coming from division operation, two uncertainties coming from multiplication operation and misrepresentation of operand
Counter-example: dividing by π : the inexact representation of π induces one uncertainty, the inexact representation of its reciprocal also induces one uncertainty (almost the same relative uncertainty: $0,37\,\mathtt{ulp}$ and $0,43\,\mathtt{ulp}$ respectively)

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 roots**

The Table Maker's Dilemma

transcendental functions

- ... costly
- ... **correct rounding** is not guaranted

to get correct rounding with n digits/bits...[1]

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

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

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

[1] `https://members.loria.fr/PZimmermann/wc/decimal32.html`

Catastrophic Cancellation?

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** (réduction de la précision relative)
  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™

Area of triangle

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

$$S = \sqrt{p(p-a)(p-b)(p-c)} \qquad \text{(Heron of Alexandria)}$$

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

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

$\Rightarrow$ *exercise: code and test data from*

https://people.eecs.berkeley.edu/~wkahan/Triangle.pdf

could also apply to cyclic quadrilateral area $S = \sqrt{(p-a)(p-b)(p-c)(p-d)}$ (Brahmagupta's formula) or more likely to Bretschneider's formula for general non crossed quadrilateral than can get needle-like

Volume of the tetrahedron

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

$$X = (c - A + b)(A + b + c) \qquad x = (A - b + c)(b - c + A)$$
$$Y = (a - B + c)(B + c + a) \qquad y = (B - c + a)(c - a + B)$$
$$Z = (b - C + a)(C + a + b) \qquad z = (C - a + b)(a - b + C)$$

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

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

Stable provided relabeling: order pairs of edges so that the 3 smallest among 12 faces differences are among the 9 used.

Testing precision with BASIC'85

```
for (unsigned nbTot = NBITERMIN; nbTot < NBITERMAX; nbTot++) {
  float x = X0;
  for (unsigned nblter = 0; nblter < nbTot; nblter++) x = sqrt (x);
  float bottomRadix = x;
  for (unsigned nblter = 0; nblter < nbTot; nblter++) 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)

Elasticity and condition number

Von Neuman'48

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

$$\kappa(x) = \frac{\left|\frac{f(x_a)-f(x)}{f(x)}\right|}{\left|\frac{x_a-x}{x}\right|} = \frac{\left|\frac{f(x_a)-f(x)}{(x_a-x)}\right|}{\left|\frac{f(x)}{x}\right|} \sim \left|\frac{xf'(x)}{f(x)}\right| = \left|\frac{\mathrm{d}\ (\ln|f(x)|)}{\mathrm{d}\ln|x|}\right| \quad (1)$$

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.

Elasticity and condition number

Von Neuman'48

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

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

$$\kappa_{f^n} = n\kappa_f$$

$f : x \to x + c \Rightarrow \kappa = \frac{x}{x+c}$: 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`

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

Elasticity and condition number

$\Rightarrow$ higher degree polynomials can degrade high resolutions

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

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

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

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`float`: $P = -6.33825300e + 29$

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`float`:	$P = -6.33825300e + 29$
`double`:	$P = -1.1805916207174113e + 021$

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`long double`:	$P = +5.764607523034234891 88e + 17$

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`float`:	$P = -6.33825300e + 29$
`double`:	$P = -1.18059162071741 13e + 021$
`long double`:	$P = +5.76460752303423489188e + 17$
`quad`:	$P = +1.17260394005317863185883490452018380$

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

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

`float`:	$P = -6.33825300e + 29$
`double`:	$P = -1.18059162071741 13e + 021$
`long double`:	$P = +5.76460752303423489188e + 17$
`quad`:	$P = +1.17260394005317863185883490452018380$
exact:	$P \approx -0.82739605994682136814116509547981629 2$
	$P = -\frac{54767}{66192}$

How to control rounding errors?

Variance: Alice '08

- dimuons spectrometer, wire chamber: 10^6 channels
- $\forall$ channel, $\exists$ noise:
  - average noise $\bar{n} = En$
  - noise fluctuation $\sigma = \sqrt{Vn}$
- $\Rightarrow$ 99,7 % noise cut pedestal $p = \bar{n} + 3\sigma = En + 3\sqrt{Vn}$

  to be reevaluated $\forall$ channel, before each run (temperature or hygrometry fluctuations, high voltage, detector getting old)
- 2 ways:

$$\sigma^2 = Vn = \overline{(n - \bar{n})^2} \quad \text{2 passes} \geq 0 \tag{2}$$

$$= \overline{n^2} - (\bar{n})^2 \quad \text{1 pass} \tag{3}$$

BUT

Variance: Alice '08

- n is digitized on 12 bits $[0..4095]$
- n^2 is digitized on 24 bits
- the sample has $N = 500$ measures$\sim 2^9$ (not big data...), $\sum_N n^2$ is digitized on 33 bits

$\Rightarrow$ doesn't fit in a `float` (24 bits mantissa), inexact representation (9 bits loss)
$\Rightarrow$ *catastrophic cancellation*, negative variance[2],
$\Rightarrow$ trivialy avoided with `double` precision!

$\Rightarrow$ doesn't fit in an `unsigned int`, (`overflow`)
$\Rightarrow$ `unsigned long long` allows exact sommations[3]

[2] seen on production launch
[3] ... forgetting calibration

Variance '$_{91}$

- TP solid state physic:
  measuring solid state property transition with temperature
- IBM PC data acquisition with `BASIC`
- display of whisker boxes

$\Rightarrow$ online variance evaluation, 1-pass

It was a time with no `Wikipedia` around to check for other algos...

- 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* »)

- between $-b$ and $\sqrt{\Delta}$

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

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

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

4 possible *overflow*:

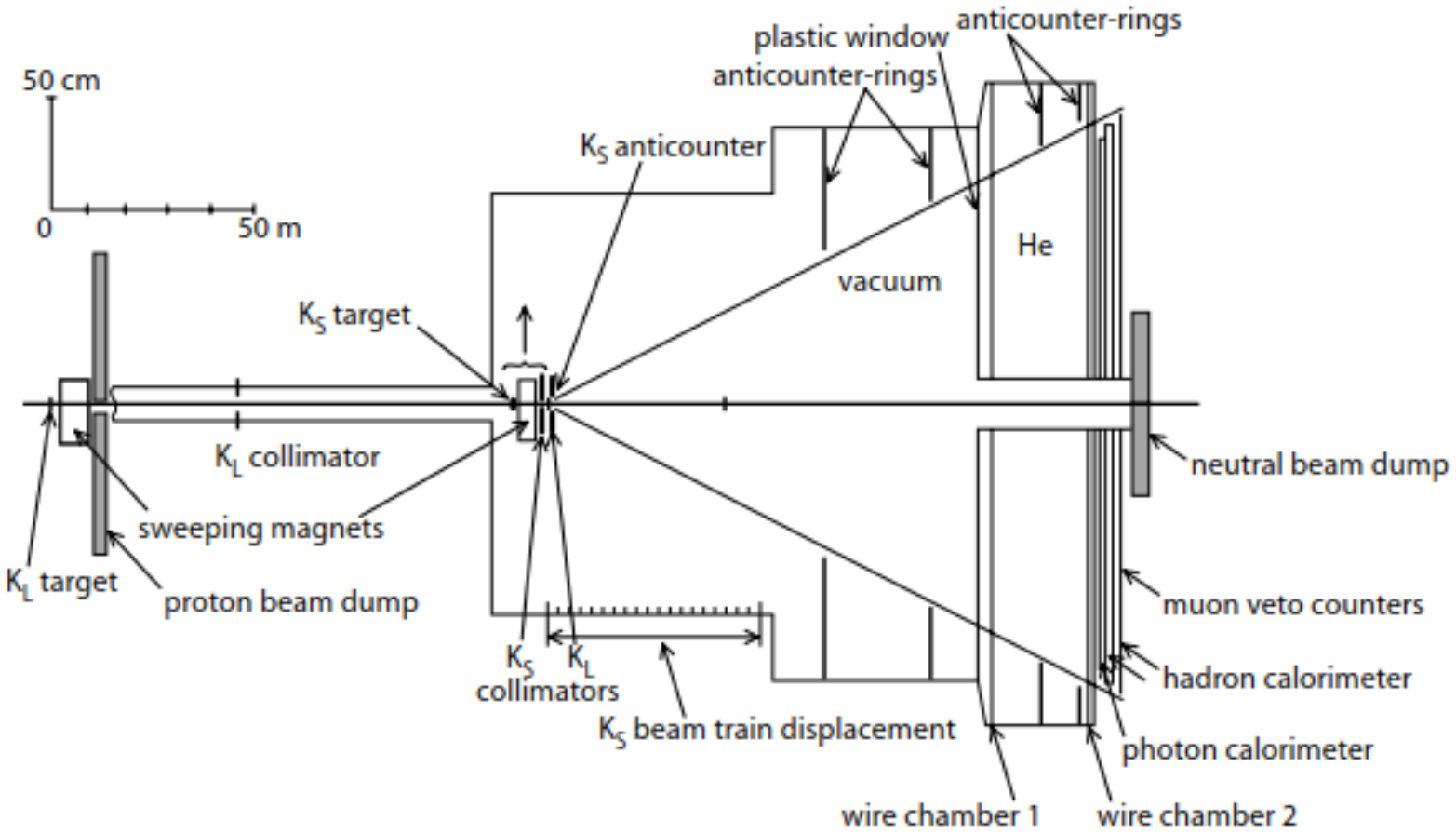
- b^2 : *spurious overflow* (if $|b| > 10^{19}$, $\Delta =$ `Inf`, $|q| =$ `Inf` while $|q| \sim 2 \times 10^{19}$)
- ac
- b/a
- c/b

BAKER, Henry G., *"You Could Learn a Lot from a Quadratic: Overloading Considered Harmful"*,

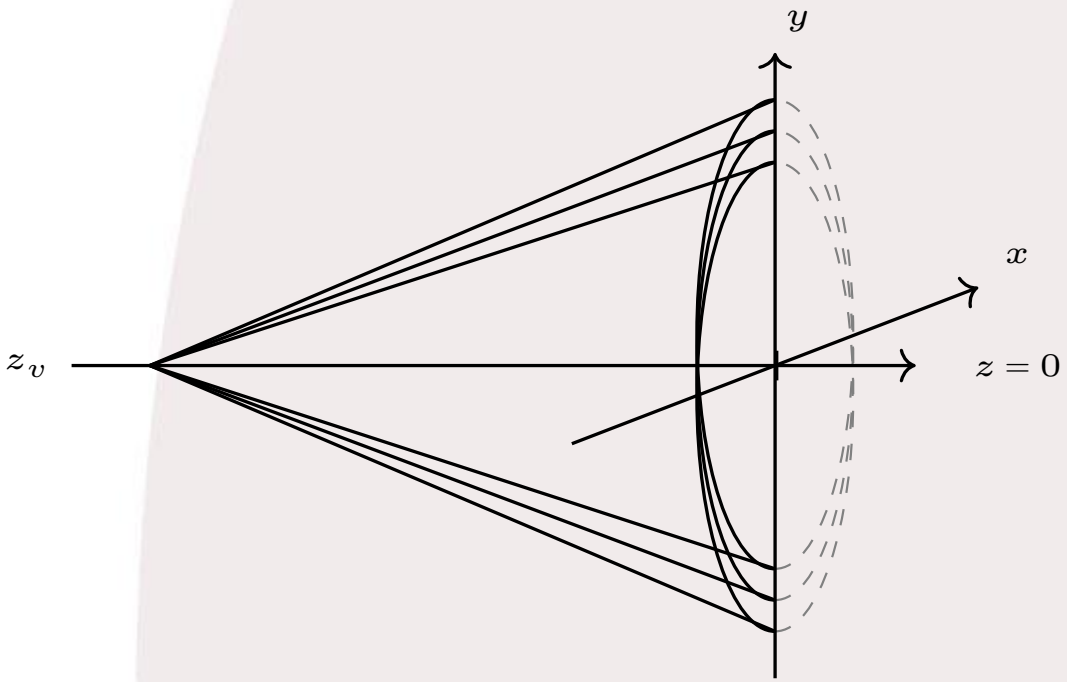
doi:10.1145/609742.609746

Quadratic: NA-31 '92

- neutral kaons precise mass measurement
- $m_{K^0} = 497,611 \pm 0,013 = 497,611 \times (1 \pm 2,6 \times 10^{-5})$ MeV/c²
  $m_{K^0} = 497,671 \pm 0,031 = 497,671 \times (1 \pm 6,2 \times 10^{-5})$ MeV/c² in PDG 1990 & 1992
- $K^0 \to \pi^0\pi^0$ and $\pi^0 \to \gamma\gamma$: $K^0 \to \gamma\gamma\gamma\gamma$



Quadratic: NA-31 '92



Quadratic: NA-31 '$_{92}$

- $\tau_{\pi^0} \ll \tau_{K^0}$ (τ electromagnetic $\ll \tau$ weak)
- $E_{K^0} \sim 100\,\text{GeV}$ $\quad \theta_{K^0\pi^0} \sim 4,18\,\text{mrad}$
  $E_{\pi^0} \sim 50\,\text{GeV}$ $\quad \theta_{\pi^0\gamma} \sim 2,70\,\text{mrad}$
  $\Rightarrow$ $\quad \theta_{K^0\gamma} \in [1,48; 6,88]\,\text{mrad}$
- $\Rightarrow$ small angles approximation $\sin\theta \sim \theta \sim \tan\theta$
- for two photons impacts (w_1, E_1), (w_2, E_2) in the calorimeter, vertex reconstruction on axis $z \sim \frac{|w_1 - w_2|}{\frac{m_{\pi^0}}{\sqrt{E_1 E_2}}} \underset{\eta\to 0}{\sim} \frac{|w_1 - w_2|}{\sqrt{2}\eta}$
- $\frac{\delta \sin}{\sin} \in [0,11; 2,37] \times 10^{-5}$
  $\frac{\delta m}{m} \in [2,61; 6,23] \times 10^{-5}$
- $\sin\theta = \theta - \frac{1}{6}\theta^3 + o(\theta^3) = \theta\left(1 - \frac{1}{6}\theta^2 + o(\theta^2)\right)$
- $\sin\arctan\rho = \rho - \frac{1}{2}\rho^3 + o(\rho^3) = \rho\left(1 - \frac{1}{2}\rho^2 + o(\rho^2)\right)$

Quadratic: NA-31 '$_{92}$

biquadratic equation (quadratic in $\mathcal{Z} = z^2$)

$$\begin{aligned} \eta &= \frac{m_\pi}{\sqrt{2E_1E_2}} \sim 1.9 \times 10^{-3} \sim 2^{-9} \\ \xi &= 1 - \eta^2 \end{aligned}$$

$$\boxed{\left(1-\xi^2\right)\mathcal{Z}^2 + \left[2\Re w_1 w_2^* - \xi^2\left(|w_1|^2 + |w_2|^2\right)\right]\mathcal{Z} + \left[\left(\Re w_1 w_2^*\right)^2 - \xi^2\left(|w_1|^2|w_2|^2\right)\right] = 0}$$

Expanded form

$$\begin{aligned} & \eta^2\left(2-\eta^2\right)\mathcal{Z}^2 \\ -\left[|w_1-w_2|^2 - \eta^2\left(2-\eta^2\right)\left(|w_1|^2+|w_2|^2\right)\right]&\mathcal{Z} \\ -\left[\left(\Im w_1 w_2^*\right)^2 - \eta^2\left(2-\eta^2\right)|w_1|^2|w_2|^2\right] &= 0 \end{aligned}$$

$$\boxed{\Delta = \xi^2\left[|w_1-w_2|^4 - \eta^2\left(2-\eta^2\right)\left(|w_1|^2-|w_2|^2\right)^2\right]}$$

The problem is not in evaluating roots (we compute the cancelation-free one: we can evaluate it the naive way)
the problem is in properly evaluating polynomial coefficients
the correction happens around 15th bit (single precision is enough);
naive evaluation leads to 9th bit discrepancy
the correction always occurs in the same direction.

1. Approximation wrongly evaluated
2. Quadratic solution level wrongly evaluated
3. A good numerical evaluation comes from a good symbolical evaluation

Quadratic: NA-31 '92

$$\eta = \frac{m_\pi}{\sqrt{2E_1E_2}} \sim 1.9\times10^{-3} \sim 2^{-9}$$
$$\xi = 1-\eta^2$$

$$\mathcal{Z} = \frac{|w_1-w_2|^2 - \eta^2(2-\eta^2)\left(|w_1|^2+|w_2|^2\right)}{2\eta^2(2-\eta^2)} + \frac{\left(1-\eta^2\right)\sqrt{|w_1-w_2|^4 - \eta^2(2-\eta^2)\left(|w_1|^2-|w_2|^2\right)^2}}{2\eta^2(2-\eta^2)}$$

$$\mathcal{Z} = \frac{|w_1-w_2|^2}{2\eta^2(2-\eta^2)} - \frac{1}{2}\left(|w_1|^2+|w_2|^2\right) + \frac{\left(1-\eta^2\right)|w_1-w_2|^2\sqrt{1-\eta^2(2-\eta^2)\left(\frac{|w_1|^2-|w_2|^2}{|w_1-w_2|^2}\right)^2}}{2\eta^2(2-\eta^2)}$$

$$\mathcal{Z} = \frac{\left(2-\eta^2\right)|w_1-w_2|^2}{2\eta^2(2-\eta^2)} - \frac{1}{2}\left(|w_1|^2+|w_2|^2\right) + \left(1-\eta^2\right)|w_1-w_2|^2\frac{\sqrt{1-\eta^2(2-\eta^2)\left(\frac{|w_1|^2-|w_2|^2}{|w_1-w_2|^2}\right)^2}}{2\eta^2(2-\eta^2)}$$

$$\mathcal{Z} = \left(\frac{|w_1-w_2|}{\sqrt{2}\eta}\right)^2 - \frac{1}{2}\left(|w_1|^2+|w_2|^2\right) + \left(1-\eta^2\right)|w_1-w_2|^2\frac{\sqrt{1-\eta^2(2-\eta^2)\left(\frac{|w_1|^2-|w_2|^2}{|w_1-w_2|^2}\right)^2}-1}{2\eta^2(2-\eta^2)}$$

$$\mathcal{Z} = \left(\frac{|w_1-w_2|}{\sqrt{2}\eta}\right)^2\left[1-\eta^2\frac{|w_1|^2+|w_2|^2}{|w_1-w_2|^2} + \left(1-\eta^2\right)\frac{\sqrt{1-\eta^2(2-\eta^2)\left(\frac{|w_1|^2-|w_2|^2}{|w_1-w_2|^2}\right)^2}-1}{2-\eta^2}\right]$$

Interlude

Matrix condition number

$$\kappa(A) = \left\|A^{-1}\right\| \|A\| \geq \left\|A^{-1} A\right\| = 1$$

maximum ratio in relative error on x to relative error on b in $Ax = b$

multi variables functions condition number

$$\kappa = \frac{\|J(x)\|}{\|f(x)\|/\|x\|} = \frac{\|x\| \|J(x)\|}{\|f(x)\|} = \frac{\|x_k\| \left\|\frac{\partial f_i}{\partial x_j}\right\|}{\|f(x)\|}$$

dimensional analysis

- scale relativity: *laws of nature shouldn't depend on our arbitrary scale choices*
  (in the same way that there is neither center of the Universe, nor privileged direction, nor reference Ether of the speeds, nor **absolute** reference potential… but centers, directions, reference frame, scales **relevant relatively** to a given problem) invariance of scale, covariance of scale
- Scale effects: Kant: intensive / extensive quantities
  Galileo: size of animals (*Square-Cube Law*); Kleiber: animal metabolism ($3/4$, not $2/3$)
- **dimension**: nature of a quantity (length, surface, volume, mass, duration, speed, force, angle…)
- **homogeneity**: *thou shouldst only add same dimension quantities* (*cf homogeneous function* $f(tx) = t^{\alpha} f(x)$)
- pendulum period (small oscillations): $T = 2\pi\sqrt{\frac{l}{g}}$ $g \sim L \cdot T^{-2}$
- constraint on the arguments of analytic functions: $f(z) = \sum_n a_n z^n \Rightarrow z$ dimensionless argument (and result f)
- fluid mechanics & scaling (models): Mach $\frac{v}{c_s}$, Reynolds $\frac{VL}{\nu}$, Froude, Weber, Prandtl, Nusselt, Grashof, Hersey, Sommerfeld…
- Sommerfeld fine structure constant: $\alpha = \frac{e^2}{4\pi\varepsilon_0\hbar c} = 1/137{,}035\,999\,206\ldots$
- Schwarzschild black hole horizon: $R_s = \frac{2GM}{c^2}$
- Planck relativistic quantum gravity: $l_{\mathrm{P}} = \sqrt{\frac{\hbar G}{c^3}} = 1,6 \times 10^{-35}\,\mathrm{m}$, $t_{\mathrm{P}} = \sqrt{\frac{\hbar G}{c^5}} = 5,4 \times 10^{-44}\,\mathrm{s}$
- Sir Geoffrey Ingram Taylor, 1950: Trinity test atomic bomb energy, starting from photos with radius of action: $R(t, E, \mu) = K t^{\frac{2}{5}} E^{\frac{1}{5}} \mu^{-\frac{1}{5}}$
- Bertrand, 1878: cooling time of the homogeneous sphere
- dimensional equation, (Bertrand-Vaschy-Buckingham) Π théorem *A physically meaningful equation involving a certain number n of physical variables, can be rewritten in terms of a set of $p = n - k$ dimensionless parameters $\pi_1, \pi_2, \cdots, \pi_p$ constructed from the original variables, where k is the number of physical dimensions involved*
- **« zeroth principle of theoretical Physics »** (John A. Wheeler, *Spacetime Physics*, 1966)
  « Never make a calculation until you know the answer. »
  qualitative Physics, heuristic guide, and source of inspiration for the rest of us
  back of a napkin calculations, back-of-the-envelope calculations

The art of nondimensionalization

dimensional analysis equation

Back to our quadratic function equation $y = ax^2 + bx + c$
Let's use the following notations for dimensions of the argument and of the function: $x \sim X$, $y \sim Y$
Then the dimensions of coefficients are

- $c \sim Y$
- $b \sim Y \cdot X^{-1}$
- $a \sim Y \cdot X^{-2}$
- $\Rightarrow \Delta = b^2 - 4ac \sim Y^2 \cdot X^{-2}$

We try to evaluate the possible roots which are homogeneous to X, from the coefficients, of which none is homogeneous to X.

What quantities can be formed as monomials of the data in the problem?

$$G \sim a^n b^m c^l \sim X^{-2n-m} Y^{n+m+l}$$

- $G \sim X \iff \begin{array}{rcrcrcl} n & + & m & + & l & = & 0 \\ -2n & - & m & & & = & 1 \end{array}$ affine equation
- $G \sim Y \iff \begin{array}{rcrcrcl} n & + & m & + & l & = & 1 \\ -2n & - & m & & & = & 0 \end{array}$ affine equation
- $G \sim 1 \iff \begin{array}{rcrcrcl} n & + & m & + & l & = & 0 \\ -2n & - & m & & & = & 0 \end{array}$ linear equation

underspecified system(s) (3 unknowns, 2 equations)...

The art of nondimensionalization

We lack an equation...

- normal for the dimensionless α coefficient:
  $\forall \lambda, \alpha^\lambda \sim 1$ is also dimensionless
- if the linear system was fully specified, it would get a single null solution:
  $G = a^0 b^0 c^0 = 1$ would be the only dimensionless parameter of this problem
- How to plug the holes? $\Rightarrow$ exploit formal symmetry between a and c (associating one of the zeros to its reciprocal): $l = \pm n$

$\alpha = \left|\frac{ac}{b^2}\right|^{\lambda=1}$ is the simplest to evaluate, but is subject to overflow (and underflow)

$\beta = \sqrt{\alpha} = \left|\frac{ac}{b^2}\right|^{\lambda=\frac{1}{2}} = \frac{\sqrt{|a|}\sqrt{|c|}}{|b|}$ is better protected from overflow (and ...)

$\Rightarrow$ exponents are smaller (limits the exposure to overflow),
but not the simplest (roots must be extracted)

- the solutions of affine systems are the linear combination of a particular solution of the affine system and the space of solutions of the linear system

a solution for the scale X is $\frac{|b|}{|a|}$; solutions for the scale X are $\forall \mu$, $\frac{|b|}{|a|}\beta^\mu$

so for example, another solution for X is $\frac{|b|}{|a|}\beta = \frac{\sqrt{|c|}}{\sqrt{|a|}}$

The art of nondimensionalization

$$Y \sim |b|\sqrt{\frac{|c|}{|a|}}$$

What is the interest of Y in finding roots, homogeneous to X?
When we **check that a value** x_0 found as root of the trinomial $y = P(x) = ax^2 + bx + c$ **is valid**, we won't find exactly $P(x_0) = 0$:
the rounding errors mean that we expect to find a value of the order of $\varepsilon_{\texttt{machine}}$.
But $\varepsilon_{\texttt{machine}}$ is dimensionless, and dimensional analysis tells us that $P(x_0) \sim Y$:

$$P(x_0) \approx Y\varepsilon_{\texttt{machine}}$$

So we can find values of $P(x_0)$ which seem to be large but remain small in front of Y, and it is this smallness which makes it a good root.
Similarly, to **evaluate the sign of** Δ the theoretical threshold of 0 will be obtained for
$\varepsilon_{\texttt{machine}} Y^2 \cdot X^{-2} = \varepsilon_{\texttt{machine}}|ac|$
This reflection applies to all **comparisons between floats**: *"float equality considered harmful"*: it is illusory to expect strict equalities, and if the margin associated with rounding can only be proportional to $\varepsilon_{\texttt{machine}}$, it must also have the right dimension.

$$X \sim \frac{|b|}{2|a|} \qquad Y \sim \frac{|b|^2}{4|a|} \qquad \beta' = 2\frac{\sqrt{|a|}\sqrt{|c|}}{|b|} \qquad x = X\xi \qquad y = Y\upsilon$$

$$\upsilon = \frac{P(X\xi)}{Y} = \operatorname{sgn} a\left[\xi^2 + 2\operatorname{sgn} a \operatorname{sgn} b\xi + \operatorname{sgn} a \operatorname{sgn} c\beta'^2\right] = \operatorname{sgn} a\left[\xi^2 + 2\sigma\xi + \tau\beta'^2\right]$$

$$\xi_\pm = -\sigma\left[1 \pm \sqrt{\delta = 1 - \tau\beta'^2}\right] \quad \Rightarrow \quad \xi_1 = -\sigma\left[1 + \sqrt{\delta}\right] \quad ; \quad \xi_2 = \tau\frac{\beta'^2}{\xi_1}$$

$$\delta = 1 - \beta'^2 = (1-\beta')(1+\beta') \quad || \quad \delta = 1 + \beta'^2 = \texttt{fma}(\beta', \beta', 1) \quad ; \quad \beta' > \sqrt{2/\varepsilon} \Rightarrow \sqrt{\delta} := \beta'$$

$$\beta' > 2/\varepsilon \Rightarrow \sqrt{\delta} := \beta' \quad ; \quad \xi_1 = -\sigma\beta' \quad ; \quad \xi_2 = -\sigma\tau\beta'$$

The art of nondimensionalization

$$\begin{array}{rcl} a & = & \sigma_a 2^{\alpha} A \qquad b = \sigma_b 2^{\beta} B \qquad c = \sigma_c 2^{\gamma} C \\ a & = & \sigma_a 2^{2\alpha'} A' \qquad b = \sigma_b 2^{\beta} B \qquad c = \sigma_c 2^{\gamma'} C' \\ A' & \in & [1;4[\qquad B \in [1;2[\qquad C' \in [1;4[\end{array}$$

$$X \sim \frac{|b|}{2|a|} = 2^{\beta-2\alpha'-1}\frac{B}{A'} \qquad Y \sim \frac{|b|^2}{4|a|} = 2^{2(\beta-\alpha'-1)}\frac{B^2}{A'}$$

$$\begin{array}{rcl} \Delta & = & 1 - 4\dfrac{\sigma_a 2^{2\alpha'} A' \times \sigma_c 2^{2\gamma'} C'}{(2^{\beta} B)^2} \\ & = & 1 - 4\sigma_a\sigma_c 2^{2\alpha'+2\gamma'-2\beta}\dfrac{A'C'}{B^2} \\ & = & 1 - \sigma_a\sigma_c 2^{2(\alpha'+\gamma'-\beta+1)}\dfrac{A'C'}{B^2} \end{array}$$

$$\begin{array}{rcl} A'C' & \in & [1;16[\qquad B^2 \in [1;4[\qquad B^{-2} \in]1/4;1] \qquad A'C'B^{-2} \in]1/4;16[\\ \sqrt{A'C'B^{-2}} & = & \sqrt{A'C'}B^{-1} \in]1/2;4[\qquad BA'^{-1} \in]1/4;2[\qquad B^2A'^{-1} \in]1/4;4[\\ \tau & = & 2^{\alpha'+\gamma'-\beta+1}\sqrt{A'C'B^{-2}} = 2^{\alpha'+\gamma'-\beta+1}\sqrt{A'C'}B^{-1} \end{array}$$

The art of nondimensionalization

nondimensionalizing a set of quantities from **dimensional analysis equation**, one can

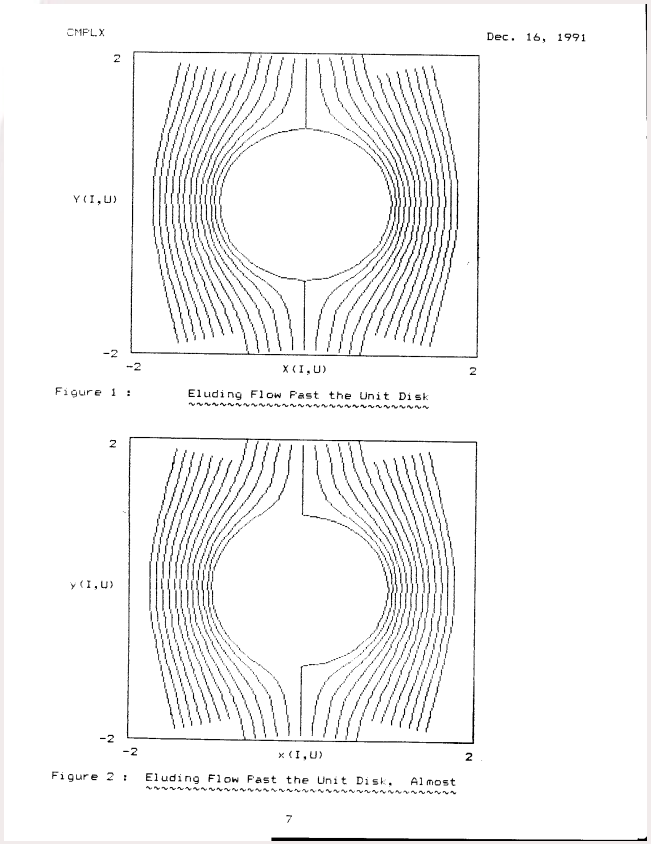
- link together **characteristic scales** of the different quantities
- to make appear a set of **dimensionless parameters** (pure numbers) of the problem
  ("shape parameters" as opposed to "scale parameters")
- for a set of quantities, there are generally *many ways* to scale it
- we need to add other criteria to select one way:
  - symmetries of the problem,
  - limit the complexity of the calculation,
  - limit the exceptions of the calculation.
- this scaling cannot solve all the problems
  if the solution is not representable, the intermediate calculations are allowed not to be representable
- the exceptions on β' do not necessarily propagate correctly to the roots
  the roots thus found are not necessarily relevant ; $\Rightarrow$ asymptotic development (*cf* condition)
- anticipate the overflows
- qualify the asymptotic regimes of the function (x large... but in front of what?)
- evaluate the proximity to 0 (y small... but in front of what?)

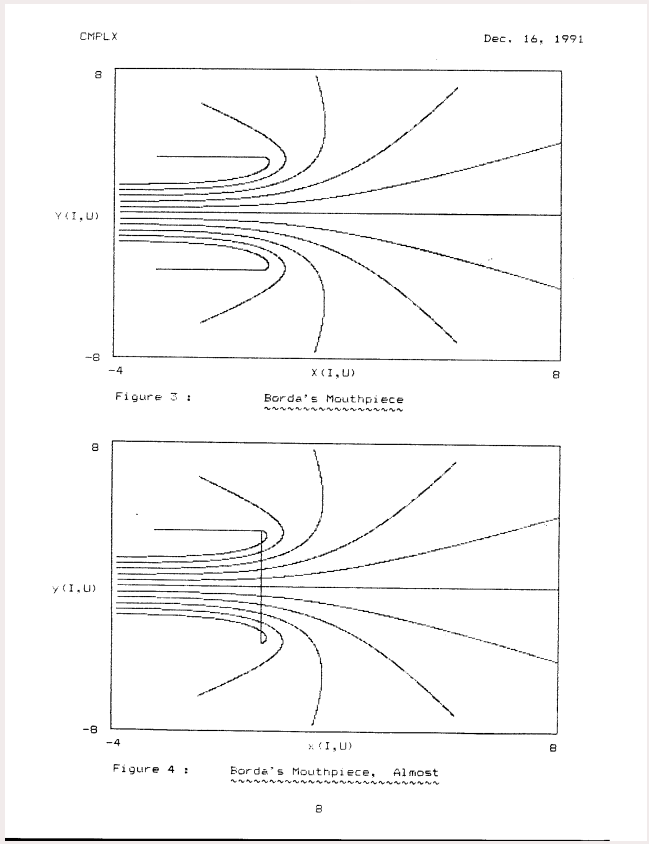
A bit expensive...

- 2 more roots and 2 more divisions
- 3 more branches ( **branchless** paradigm: specific to floating point) (catch exception?)
- naive double precision evaluation would solve it

Function of a complex variable

function, but multivalued?





Eluding Flow past a Disk: $f : Z \mapsto (Z - 1/Z)/2$ and $g : W \mapsto W - i\sqrt{iW - 1}\sqrt{iW + 1}$

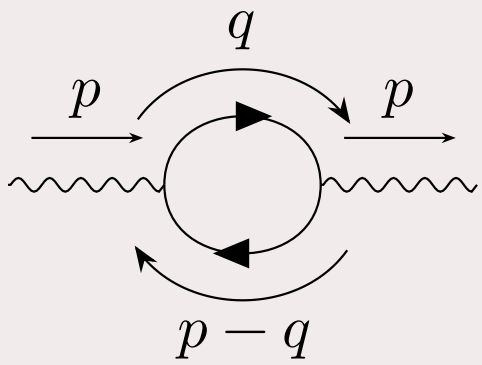
Do not "simplify" $g(W)$ to $W - i\sqrt{-W^2 - 1}$ nor to $W - \sqrt{W^2 + 1}$ since they behave differently. Though $\forall W$, $f(g(W)) = W$, $\forall |Z| > 1$, $g(f(Z)) = Z$ only, and some $|Z| = 1$; otherwise $g(f(Z)) = -1/Z$.
Deducing where these identities hold is tricky.

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.

« Branch Cuts for Complex Elementary Functions, or Much Ado About Nothing's Sign Bit, » ch. 7 in *The State of the Art in Numerical Analysis* (1987) http://http.cs.berkeley.edu/~wkahan/ieee754status/baleful.ps

Function of a complex variable



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

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

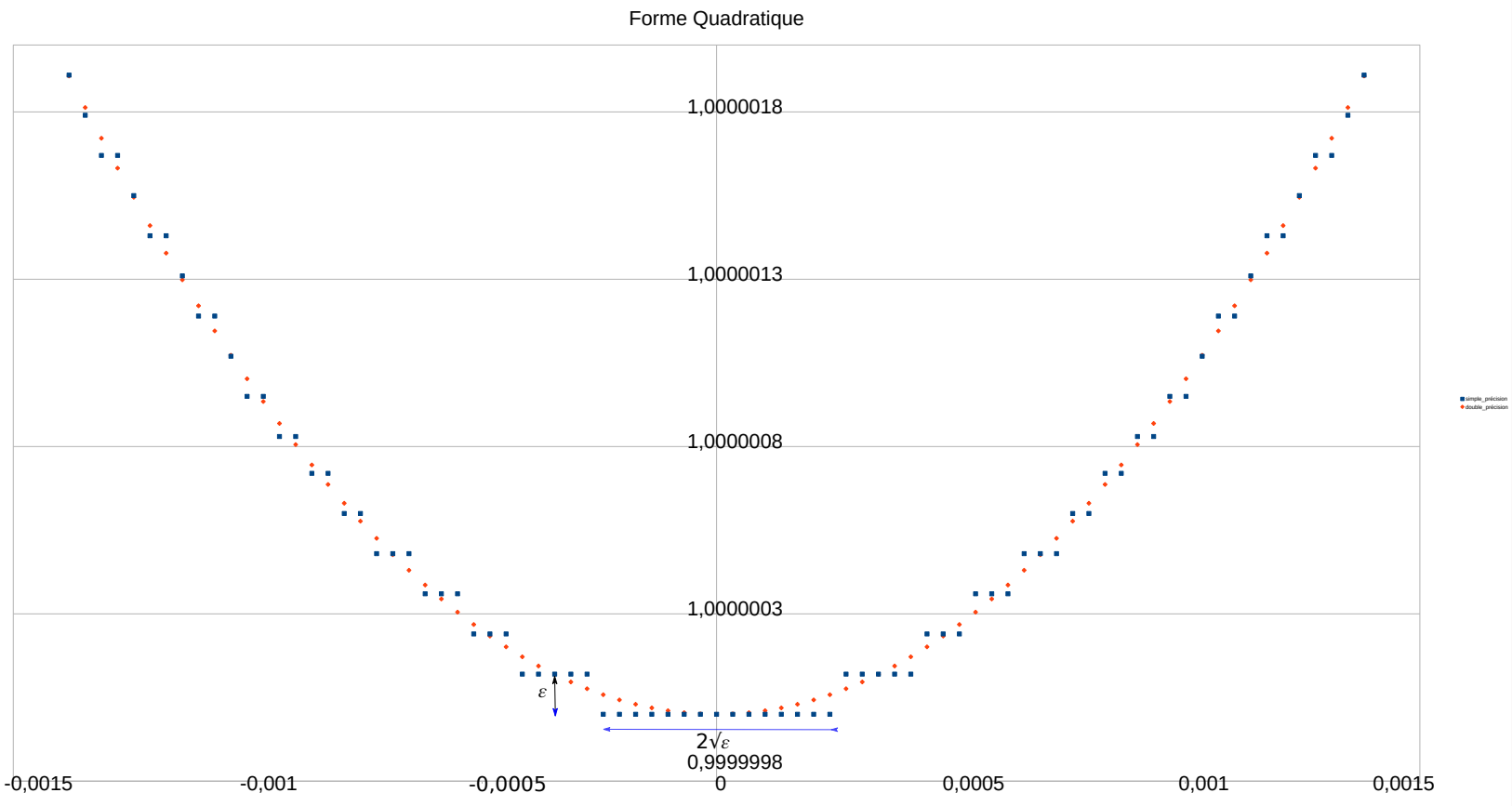
$\Rightarrow$ the (microscopic) difference of ε induces a (macroscopic) difference of 2π on the imaginary part
$\Rightarrow$ the analytic functions[4] of complex analysis are sharply discontinuous at the crossing of their *branch cut*

[4] *a minima* indefinitely continuously differentiable

Minimisation

Numerical evaluation of derivatives / gradients / Jacobian / Hessian

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



5793 distincts `float` in the wok's bottom; $\approx 190 \times 10^6$ distincts `double`

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

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.

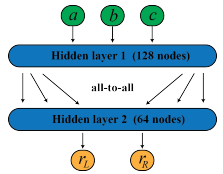
Feed-forward Neural Network

NN Architecture:

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

NN Training:

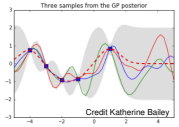
Batch size:	200
Training epochs:	under 500
Oprimizer:	Adam (https://arxiv.org/abs/1412.6980v8)



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.

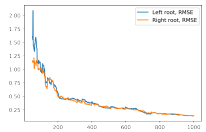
GPR for large datasets

- 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.

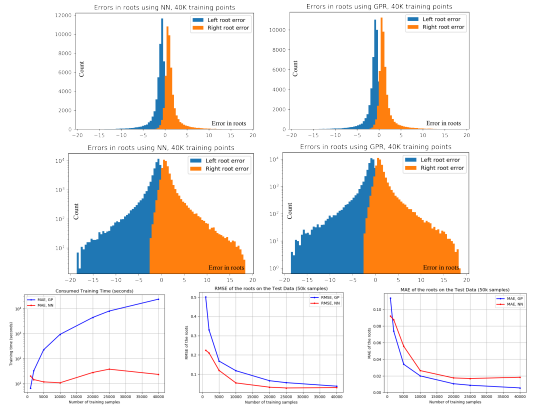
Adaptive sampling with GPR

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 vs MAE).

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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

Interface

Table: *leaky abstraction*: standardize the interface

C / C++	Fortran'90	ieee_arithmetic	Ada
copysign (d x, d y)	sign (x, y)	ieee_copy_sign (x, y)	F'Copy_Sign (value, s
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, adjustm
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) precision (x)		F'Model_Epsilon
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) spacing (x) rrspacing (x)		F'Machine_Emax
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

« Why aiming for precision? »

extension of the field of struggle

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*: $\Rightarrow \left.\frac{\sin x}{x}\right|_{x=0} = 1$
- *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?)

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

- `expf (88.72284) = + Inf` (but mathematically it's 2^{128} $\Rightarrow$ `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? »

$\Rightarrow$ 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? »

$$\text{PRECISE NUMBER} + \text{PRECISE NUMBER} = \text{SLIGHTLY LESS PRECISE NUMBER}$$

$$\text{PRECISE NUMBER} \times \text{PRECISE NUMBER} = \text{SLIGHTLY LESS PRECISE NUMBER}$$

$$\text{PRECISE NUMBER} + \text{GARBAGE} = \text{GARBAGE}$$

$$\text{PRECISE NUMBER} \times \text{GARBAGE} = \text{GARBAGE}$$

$$\sqrt{\text{GARBAGE}} = \text{LESS BAD GARBAGE}$$

$$(\text{GARBAGE})^2 = \text{WORSE GARBAGE}$$

$$\frac{1}{N}\sum(\text{N PIECES OF STATISTICALLY INDEPENDENT GARBAGE}) = \text{BETTER GARBAGE}$$

$$(\text{PRECISE NUMBER})^{\text{GARBAGE}} = \text{MUCH WORSE GARBAGE}$$

$$\text{GARBAGE} - \text{GARBAGE} = \text{MUCH WORSE GARBAGE}$$

$$\frac{\text{PRECISE NUMBER}}{\text{GARBAGE} - \text{GARBAGE}} = \text{MUCH WORSE GARBAGE, POSSIBLE DIVISION BY ZERO}$$

$$\text{GARBAGE} \times 0 = \text{PRECISE NUMBER}$$

https://xkcd.com/2295/