Computer arithmetic

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Justification

This short session will explain the basics of floating point arithmetic, mostly focusing on round-off and its influence on computations.

Numbers in scientific computing

- Integers: $\ldots, -2, -1, 0, 1, 2, \ldots$
- Rational numbers: $1/3, 22/7$: not often encountered
- Real numbers $0, 1, -1.5, 2/3, \sqrt{2}, \log 10, \ldots$
- Complex numbers $1 + 2i, \sqrt{3} - \sqrt{5}i, \ldots$

Computers use a finite number of bits to represent numbers, so only a finite number of numbers can be represented, and no irrational numbers (even some rational numbers).

First we dig into bits

	boolean	bitwise (C)	bitwise (F)	bitwise (Py)
and	`&&`	`&`	`iand`	`&`
or	`||`	`|`	`ior`	`|`
not	`!`			`~`
xor		`^`	`ieor`	

Bit shift operations in C:

left shift	`<<`
right shift	`>>`

Fortran: `mvbits`

Arithmetic with bit ops

- Left-shift is multiplication by 2:

```
i_times_2 = i<<1;
```

- Extract bits:

```
i_mod_8 = i & 7
```

(How does that last one work?)

Exercise 1: Bit operations

Use bit operations to test whether a number is odd or even.
Can you think of more than one way?

Integers

Integers

Scientific computation mostly uses real numbers. Integers are mostly used for array indexing.
We look at

1. integers as supported by the hardware;
2. integers as they exist in programming languages;
3. (and not software-defined integers)

C:

- A short int is at least 16 bits;
- An integer is at least 16 bits, but often 32 bits;
- A long integer is at least 32 bits, but often 64;
- A `long long` integer is at least 64 bits.

Fortran uses kinds, not necessarily equal to number of bytes:

```
integer(2) :: i2
integer(4) :: i4
integer(8) :: i8
```

Specify the number of decimal digits with `selected_int_kind(n)`.

Exercise 2: Powers of two

Print 2^n for $n = 0, \ldots, 31$. There are at least two ways of generating these powers.
Also print the bit pattern. What is unexpected?

Negative integers

Problem:

- How do we represent them?
- How do we do efficient arithmetic on them?

Define

$$\mathrm{rep}\colon \mathcal{Z} \to 2^n$$

'representation of the number $N \in \mathcal{Z}$ as bitstring of length n.'

$$\mathrm{int}\colon 2^n \to \mathcal{Z}$$

'interpretation of the bitstring of length n as number $N \in \mathcal{Z}$'

Negative integers

Use of sign bit: typically first bit

s	$i_1 \ldots i_n$

Simplest solution:

$$\begin{cases} n \geq 0 & \mathrm{rep}(n) = 0, i_1, \ldots i_{31} \\ n < 0 & \mathrm{rep}(-n) = 1, i_1, \ldots i_{31} \end{cases}$$

Sign bit

Interpretation

bitstring	$00\cdots0$	$\ldots$	$01\cdots1$	$10\cdots0$	$\ldots$	$11\cdots1$
as unsigned int	0	$\ldots$	$2^{31}-1$	2^{31}	$\ldots$	$2^{32}-1$
as naive signed	0	$\ldots$	$2^{31}-1$	-0	$\ldots$	$-2^{31}+1$

TACC

Interpret unsigned number n as $n - B$

bitstring	$00\cdots0$	...	$01\cdots1$	$10\cdots0$	...	$11\cdots1$
as unsigned int	0	...	$2^{31}-1$	2^{31}	...	$2^{32}-1$
as shifted int	-2^{31}	...	-1	0	...	$2^{31}-1$

Let m be a signed integer, then the 2's complement 'bit pattern' $\mathrm{rep}(m)$ is a non-negative integer defined as follows:

- If $0 \leq m \leq 2^{31} - 1$, the normal bit pattern for m is used, that is
$$0 \leq m \leq 2^{31} - 1 \Rightarrow \mathrm{rep}(m) = m.$$
- For $-2^{31} \leq n \leq -1$, n is represented by the bit pattern for $2^{32} - |n|$:
$$-2^{31} \leq n \leq -1 \Rightarrow \mathrm{rep}(m) = 2^{32} - |n|.$$

bitstring	$00\cdots0$	$\ldots$	$01\cdots1$	$10\cdots0$	$\ldots$	$11\cdots1$
as unsigned int	0	$\ldots$	$2^{31}-1$	2^{31}	$\ldots$	$2^{32}-1$
as 2's comp. integer	0	$\cdots$	$2^{31}-1$	-2^{31}	$\cdots$	-1

Problem: processor is very good at artithmetic on (unsigned) bit strings.
How does that translate to arithmetic on integers?

$$\mathrm{int}\,(\mathrm{rep}(x) * \mathrm{rep}(y)) \stackrel{?}{=} x * y$$

Add $m+n$, where m,n are representable:

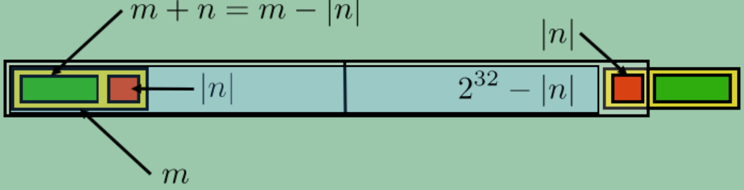
$$0 \leq |m|,|n| < 2^{31}.$$

The easy case is $0 < m,n$, as long as there is no overflow.

Case $m > 0$, $n < 0$, and $m + n > 0$. Then $\mathrm{rep}(m) = m$ and $\mathrm{rep}(n) = 2^{32} - |n|$, so the unsigned addition becomes

$$\mathrm{rep}(m) + \mathrm{rep}(n) = m + (2^{32} - |n|) = 2^{32} + m - |n|.$$

Since $m - |n| > 0$, this result is $> 2^{32}$.



However, this is basically $m + n$ with the overflow bit set.

Subtraction $m-n$:

- Case: $m<n$. Observe that $-n$ has the bit pattern of $2^{32}-n$. Also, $m+(2^{32}-n)=2^{32}-(n-m)$ where $0<n-m<2^{31}-1$, so $2^{32}-(n-m)$ is the 2's complement bit pattern of $m-n$.
- Case: $m>n$. The bit pattern for $-n$ is $2^{32}-n$, so $m+(-n)$ as unsigned is $m+2^{32}-n=2^{32}+(m-n)$. Here $m-n>0$. The 2^{32} is an overflow bit; ignore.

Overflow

There is a limited number of bits, so numbers that are too large in absolute value can not be represented.
Overflow.
This is not a fatal error: your program continues with the wrong result.

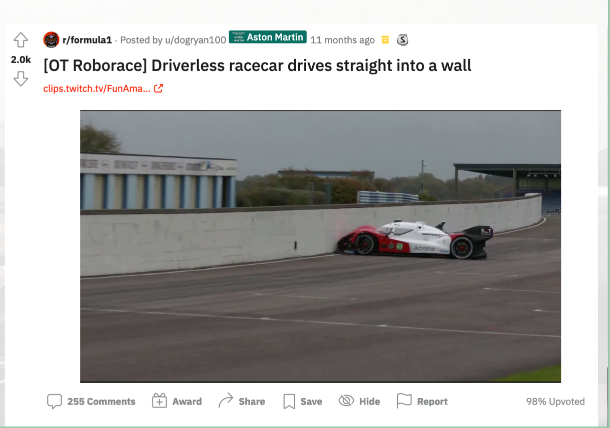
Exercise 3: Integer overflow

Investigate what happens when you perform an integer calculation that leads to overflow. What does your compiler say if you try to write down a nonrepresentible number explicitly, for instance in a declaration or assignment statement?
Language lawyer remark: signed integer overflow is Undefined Behavior in C/C++.

Floating point numbers

Floating point math is hard!

And the consequences if you get it wrong can be considerable.



Analogous to scientific notation $x = 6.022 \cdot 10^{23}$:

$$x = \pm\Sigma_{i=0}^{t-1} d_i \beta^{-i} \beta^e$$

- sign bit
- β is the base of the number system
- $0 \leq d_i \leq \beta - 1$ the digits of the *mantissa*:
  one digit before the *radix point*, so mantissa $< \beta$
- $e \in [L, U]$ exponent, stored with bias: unsigned int where $\mathrm{fl}(L) = 0$

Examples of floating point systems

	β	t	L	U
IEEE single (32 bit)	2	23	-126	127
IEEE double (64 bit)	2	53	-1022	1023
Old Cray 64bit	2	48	-16383	16384
IBM mainframe 32 bit	16	6	-64	63
packed decimal	10	50	-999	999

BCD is tricky: 3 decimal digits in 10 bits

(we will often use $\beta = 10$ in the examples, because it's easier to read for humans, but all practical computers use $\beta = 2$)

Internal processing in 80 bit

Overflow: more than $\beta(1-\beta^{-t+1})\beta^{U}$ or less than $-\beta(1-\beta^{-t+1})\beta^{U}$
Underflow: positive numbers less than β^{L}
Gradual underflow: $\beta^{-t+1}\cdot\beta^{L}$
Overflow leads to `Inf`.

Exercise 4: Floating point overflow

For real numbers x, y, the quantity $g = \sqrt{(x^2 + y^2)/2}$ satisfies

$$g \leq \max\{|x|, |y|\}$$

so it is representable if x and y are. What can go wrong if you compute g using the above formula? Can you think of a better way?

Overflow: `Inf`

`Inf`$-$`Inf`$\rightarrow$`NaN`

also $0/0$ or $\sqrt{-1}$

This does not stop your program in general

sometimes possible

The normalization problem

Do we allow

$$1.100 \cdot 10^0, \quad 0.110 \cdot 10^1, \quad 0.011 \cdot 10^2?$$

This makes testing for equality hard.
Solution: normalized numbers have one nonzero before the radix point.

Normalized floating point numbers

Require first digit in the mantissa to be nonzero.
Equivalent: mantissa part $1 \leq x_m < \beta$
Unique representation for each number,
also: in binary this makes the first digit 1, so we don't need to store that.
(do you see a problem?)
With normalized numbers, underflow threshold is $1 \cdot \beta^L$;
'gradual underflow' possible, but usually not efficient.

sign	exponent	mantissa
p	$e = e_1 \cdots e_8$	$s = s_1 \ldots s_{23}$
31	$30 \cdots 23$	$22 \cdots 0$
$\pm$	2^{e-127} (except $e = 0, 255$)	$s_1 \cdot 2^{-1} + \cdots + s_{23} \cdot 2^{-23}$

IEEE 754, 32-bit, all cases

$(e_1 \cdots e_8)$	numerical value	range
$(0 \cdots 0) = 0$	$\pm 0.s_1 \cdots s_{23} \times 2^{-126}$	$s = 0 \cdots 01 \Rightarrow 2^{-23} \cdot 2^{-126} = 2^{-149} \approx 10^{-45}$ $s = 1 \cdots 11 \Rightarrow (1 - 2^{-23}) \cdot 2^{-126}$
$(0 \cdots 01) = 1$	$\pm 1.s_1 \cdots s_{23} \times 2^{-126}$	$s = 0 \cdots 01 \Rightarrow 1 \cdot 2^{-126} \approx 10^{-37}$
$(0 \cdots 010) = 2$	$\pm 1.s_1 \cdots s_{23} \times 2^{-125}$	
$\cdots$		
$(01111111) = 127$	$\pm 1.s_1 \cdots s_{23} \times 2^{0}$	$s = 0 \cdots 00 \Rightarrow 1 \cdot 2^{0} = 1$ $s = 0 \cdots 01 \Rightarrow 1 + 2^{-23} \cdot 2^{0} = 1 + \varepsilon$ $s = 1 \cdots 11 \Rightarrow (2 - 2^{-23}) \cdot 2^{0} = 2 - \varepsilon$
$(10000000) = 128$	$\pm 1.s_1 \cdots s_{23} \times 2^{1}$	$s = 0 \cdots 00 \Rightarrow 1 \cdot 2^{1} = 2$
$\cdots$		et cetera
$(11111110) = 254$	$\pm 1.s_1 \cdots s_{23} \times 2^{127}$	
$(11111111) = 255$	$s_1 \cdots s_{23} = 0 \Rightarrow \pm\infty$ $s_1 \cdots s_{23} \neq 0 \Rightarrow \mathtt{NaN}$	

Exercise 5: Float vs Int

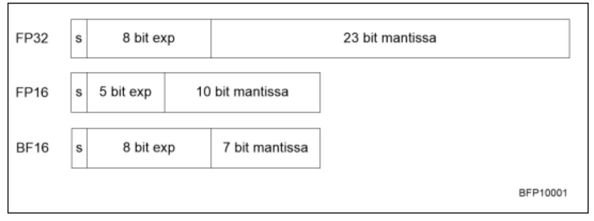
Note that the exponent doesn't come at the end. This has an interesting consequence.
What is the interpretation of

$$0 \cdots 0111$$

as int? What as float?
What is the largest integer that is representible as float?

Other precisions

- There is a 64-bit format, with 53 bits mantissa.
- IEEE envisioned a sliding scale of precisions: see Intel 80-bit registers
- Half precision, and recent invention `bfloat16`



Floating point math

Error between number x and representation $\tilde{x}$:
absolute $x-\tilde{x}$ or $|x-\tilde{x}|$
relative $\frac{x-\tilde{x}}{x}$ or $\left|\frac{x-\tilde{x}}{x}\right|$
Equivalent: $\tilde{x}=x\pm\varepsilon \Leftrightarrow |x-\tilde{x}|\leq\varepsilon \Leftrightarrow \tilde{x}\in[x-\varepsilon,x+\varepsilon]$.
Also: $\tilde{x}=x(1+\varepsilon)$ often shorthand for $\left|\frac{\tilde{x}-x}{x}\right|\leq\varepsilon$

Example

Decimal, $t = 3$ digit mantissa: let $x = 1.256$, $\tilde{x}_{\mathrm{round}} = 1.26$, $\tilde{x}_{\mathrm{truncate}} = 1.25$
Error in the 4th digit.
Different story for decimal vs binary.
How would this story change with a non-zero exponent, for instance $1.256 \cdot 10^{12}$?

Exercise 6: Round-off

The number $e \approx 2.72$, the base for the natural logarithm, has various definitions. One of them is

$$e = \lim_{n\to\infty} (1 + 1/n)^n. \tag{1}$$

Write a single precision program that tries to compute e in this manner. (Do not use the `pow` function: code the power explicitly.) Evaluate the expression for an upper bound $n = 10^k$ for some k. (How far do you let k range?) Explain the output for large n. Comment on the behavior of the error.

Machine precision

Any real number can be represented to a certain precision:
$\tilde{x} = x(1+\varepsilon)$ where
truncation: $\varepsilon = \beta^{-t+1}$
rounding: $\varepsilon = \frac{1}{2}\beta^{-t+1}$
This is called *machine precision*: maximum relative error.
32-bit single precision: $mp \approx 10^{-7}$
64-bit double precision: $mp \approx 10^{-16}$
Maximum attainable accuracy.
Another definition of machine precision: smallest number ε such that $1+\varepsilon > 1$.

Exercise 7: Machine epsilon

Write a small program that computes the machine epsilon for both single and double precision. Does it make any difference if you set the compiler optimization levels low or high?
(For C++ programmers: can you write a templated program that works for single and double precision?)

Addition

1. align exponents
2. add mantissas
3. adjust exponent to normalize

Example: $1.00 + 2.00 \times 10^{-2} = 1.00 + .02 = 1.02$. This is exact, but what happens with $1.00 + 2.55 \times 10^{-2}$?

Example: $5.00 \times 10^{1} + 5.04 = (5.00 + 0.504) \times 10^{1} \to 5.50 \times 10^{1}$

Any error comes from limiting the mantissa: if x is the true sum and $\tilde{x}$ the computed sum, then $\tilde{x} = x(1+\varepsilon)$ with $|\varepsilon| < 10^{-2}$

The ‘correctly rounded arithmetic’ model

Assumption (enforced by IEEE 754):

The numerical result of an operation is the rounding of the exactly computed result.

$$\mathrm{fl}(x_1 \odot x_2) = (x_1 \odot x_2)(1+\varepsilon)$$

where $\odot = +,-,*,/$

Note: this holds only for a single operation!

Guard digits

Correctly rounding is not trivial, especially for subtraction.
Example: $t=2,\beta=10$: $1.0-9.5\times10^{-1}$, exact result $0.05=5.0\times10^{-2}$.

- Simple approach:
  $1.0-9.5\times10^{-1}=1.0-0.9=0.1=1.0\times10^{-1}$
- Using 'guard digit':
  $1.0-9.5\times10^{-1}=1.0-0.95=0.05=5.0\times10^{-2}$, exact.

In general 3 extra bits needed.

Fused Mul-Add instructions

(also ‘fused multiply-accumulate’)

$$c \leftarrow a * b + c$$

- Addition plus multiplication, but not independent
- Processors can have dedicated hardware for FMA (also IEEE 754-2008)
- Internally evaluated in higher precision: 80-bit.
- Very useful for certain linear algebra (which?) Not for other operations (examples?)

Computate $4+6+7$ in one significant digit.
Evaluation left-to-right gives:

$$\begin{array}{lll}
(4\cdot 10^0+6\cdot 10^0)+7\cdot 10^0 & \Rightarrow 10\cdot 10^0+7\cdot 10^0 & \text{addition}\\
& \Rightarrow 1\cdot 10^1+7\cdot 10^0 & \text{rounding}\\
& \Rightarrow 1.0\cdot 10^1+0.7\cdot 10^1 & \text{using guard digit}\\
& \Rightarrow 1.7\cdot 10^1 & \\
& \Rightarrow 2\cdot 10^1 & \text{rounding}
\end{array}$$

On the other hand, evaluation right-to-left gives:

$$\begin{array}{lll}
4\cdot 10^0+(6\cdot 10^0+7\cdot 10^0) & \Rightarrow 4\cdot 10^0+13\cdot 10^0 & \text{addition}\\
& \Rightarrow 4\cdot 10^0+1\cdot 10^1 & \text{rounding}\\
& \Rightarrow 0.4\cdot 10^1+1.0\cdot 10^1 & \text{using guard digit}\\
& \Rightarrow 1.4\cdot 10^1 & \\
& \Rightarrow 1\cdot 10^1 & \text{rounding}
\end{array}$$

Error propagation under addition

Let $s = x_1 + x_2$, and $x = \tilde{s} = \tilde{x}_1 + \tilde{x}_2$ with $\tilde{x}_i = x_i(1+\varepsilon_i)$

$$\begin{aligned}
\tilde{x} &= \tilde{s}(1+\varepsilon_3) \\
&= x_1(1+\varepsilon_1)(1+\varepsilon_3) + x_2(1+\varepsilon_2)(1+\varepsilon_3) \\
&= x_1 + x_2 + x_1(\varepsilon_1+\varepsilon_3) + x_2(\varepsilon_2+\varepsilon_3) \\
\Rightarrow \tilde{x} &= s(1+2\varepsilon)
\end{aligned}$$

$\Rightarrow$ errors are added
Assumptions: all ε_i approximately equal size and small;
$x_i > 0$

1. add exponents
2. multiply mantissas
3. adjust exponent

Example:
$.123 \times .567 \times 10^1 = .069741 \times 10^1 \rightarrow .69741 \times 10^0 \rightarrow .697 \times 10^0$.
What happens with relative errors?

Examples

Correct rounding only applies to a single operation.
Example: $1.24 - 1.23 = 0.01 \rightarrow 1. \times 10^{-2}$:
result is exact, but only one significant digit.
What if $1.24 = \mathrm{fl}(1.244)$ and $1.23 = \mathrm{fl}(1.225)$? Correct result 1.9×10^{-2}; almost 100% error.

- *Cancellation* leads to loss of precision
- subsequent operations with this result are inaccurate
- this can not be fixed with guard digits and such
- $\Rightarrow$ avoid subtracting numbers that are likely close.

ABC-formula

Example: $ax^2 + bx + c = 0 \rightarrow x = \frac{-b\pm\sqrt{b^2-4ac}}{2a}$
suppose $b > 0$ and $b^2 \gg 4ac$ then the '$+$' solution will be inaccurate
Better: compute $x_- = \frac{-b-\sqrt{b^2-4ac}}{2a}$ and use $x_+ \cdot x_- = -c/a$.

Equation

$$f(x) = \varepsilon x^2 - (1+\varepsilon^2)x + \varepsilon,$$

Roots for ε small:

$$x_+ \approx \varepsilon^{-1}, \qquad x_- \approx \varepsilon.$$

Textbook solution for small ε

$$x_- \approx 0, \qquad f(x_-) \approx \varepsilon$$

Accurately:

$$f(x_-) \approx \varepsilon^3$$

	textbook		accurate	
ε	x_-	$f(x_-)$	x_-	$f(x_-)$
10^{-3}	$1.000 \cdot 10^{-03}$	$-2.876 \cdot 10^{-14}$	$1.000 \cdot 10^{-03}$	$-2.168 \cdot 10^{-19}$
10^{-4}	$1.000 \cdot 10^{-04}$	$5.264 \cdot 10^{-14}$	$1.000 \cdot 10^{-04}$	0.000
10^{-5}	$1.000 \cdot 10^{-05}$	$-8.274 \cdot 10^{-13}$	$1.000 \cdot 10^{-05}$	$-1.694 \cdot 10^{-21}$
10^{-6}	$1.000 \cdot 10^{-06}$	$-3.339 \cdot 10^{-11}$	$1.000 \cdot 10^{-06}$	$-2.118 \cdot 10^{-22}$
10^{-7}	$9.992 \cdot 10^{-08}$	$7.993 \cdot 10^{-11}$	$1.000 \cdot 10^{-07}$	$1.323 \cdot 10^{-23}$
10^{-8}	$1.110 \cdot 10^{-08}$	$-1.102 \cdot 10^{-09}$	$1.000 \cdot 10^{-08}$	0.000
10^{-9}	0.000	$1.000 \cdot 10^{-09}$	$1.000 \cdot 10^{-09}$	$-2.068 \cdot 10^{-25}$
10^{-10}	0.000	$1.000 \cdot 10^{-10}$	$1.000 \cdot 10^{-10}$	0.000

(2)

Serious example

Evaluate $\sum_{n=1}^{10000} \frac{1}{n^2} = 1.644834$
in 6 digits: machine precision is 10^{-6} in single precision
First term is 1, so partial sums are ≥ 1, so $1/n^2 < 10^{-6}$ gets ignored, $\Rightarrow$ last 7000 terms (or more) are ignored, $\Rightarrow$ sum is 1.644725: 4 correct digits
Solution: sum in reverse order; exact result in single precision
Why? Consider ratio of two terms:

$$\frac{n^2}{(n-1)^2} = \frac{n^2}{n^2-2n+1} = \frac{1}{1-2/n+1/n^2} \approx 1+\frac{2}{n}$$

with aligned exponents:

$$\begin{array}{rlll} n-1: & .00\cdots0 & 10\cdots00 & \\ n: & .00\cdots0 & 10\cdots01 & 0\cdots0 \\ & & k=\log(n/2) \text{ positions} & \end{array}$$

The last digit in the smaller number is not lost if $n < 2/\varepsilon$

Previous example was due to finite representation; this example is more due to algorithm itself.

Consider $y_n = \int_0^1 \frac{x^n}{x-5} dx = \frac{1}{n} - 5y_{n-1}$ (monotonically decreasing)

$y_0 = \ln 6 - \ln 5$.

In 3 decimal digits:

computation		correct result
$y_0 = \ln 6 - \ln 5 = .182\vert 322 \times 10^1 \ldots$		1.82
$y_1 = .900 \times 10^{-1}$		.884
$y_2 = .500 \times 10^{-1}$		.0580
$y_3 = .830 \times 10^{-1}$	going up?	.0431
$y_4 = -.165$	negative?	.0343

Reason? Define error as $\tilde{y}_n = y_n + \varepsilon_n$, then

$$\tilde{y}_n = 1/n - 5\tilde{y}_{n-1} = 1/n + 5n_{n-1} + 5\varepsilon_{n-1} = y_n + 5\varepsilon_{n-1}$$

so $\varepsilon_n \geq 5\varepsilon_{n-1}$: exponential growth.

Problem: solve $Ax = b$, where b inexact.

$$A(x + \Delta x) = b + \Delta b.$$

Since $Ax = b$, we get $A\Delta x = \Delta b$. From this,

$$\left\{ \begin{array}{ll} Ax & = b \\ \Delta x & = A^{-1}\Delta b \end{array} \right\} \Rightarrow \left\{ \begin{array}{rl} \|A\|\|x\| & \geq \|b\| \\ \|\Delta x\| & \leq \|A^{-1}\|\|\Delta b\| \end{array} \right.$$

$$\Rightarrow \frac{\|\Delta x\|}{\|x\|} \leq \|A\|\|A^{-1}\|\frac{\|\Delta b\|}{\|b\|}$$

'Condition number'. Attainable accuracy depends on matrix properties

Consequences of roundoff

Multiplication and addition are not associative:
problems for parallel computations.

compute $a+b+c+d$	
sequential	parallel
$((a+b)+c)+d$	(a+b)+(c+d)

Operations with “same” outcomes are not equally stable:
matrix inversion is unstable, elimination is stable

Consider the iteration

$$x_{n+1} = f(x_n) = \begin{cases} 2x_n & \text{if } 2x_n < 1 \\ 2x_n - 1 & \text{if } 2x_n \geq 1 \end{cases}$$

Does this function have a fixed point, $x_0 \equiv f(x_0)$, or is there a cycle $x_1 = f(x_0)$, $x_0 \equiv x_2 = f(x_1)$ et cetera?
Now code this function and see what happens with various starting points x_0. Can you explain this?

More

Complex numbers

Two real numbers: real and imaginary part.
Storage:

- Store real/imaginary adjacent: easy to pass address of one number
- Store array of real, then array of imaginary. Better for stride 1 access if only real parts are needed. Other considerations.

Some compilers support higher precisions.
Arbitrary precision: GMPlib
Interval arithmetic
Half precision bfloat16