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

Bit operations

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

Bit string operations:

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

Arithmetic with bit ops

- Right-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.

16/32/64 bit: `short,int,long,long long` in C, size not standardized, use `sizeof(long)` et cetera. (Also `unsigned int` et cetera)

`INTEGER*2/4/8` Fortran, also `KIND`

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

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

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

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

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

Negative integers

Use of sign bit: typically first bit

$$\boxed{s} \boxed{i_1 \ldots i_n}$$

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	$\ldots$	$-2^{31}+1$

Shifting

Interpret unsigned number n as $n - B$

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 shifted int	-2^{31}	$\ldots$	-1	0	$\ldots$	$2^{31}-1$

2's Complement

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 $0 \le m \le 2^{31} - 1$, the normal bit pattern for m is used, that is

$$0 \le m \le 2^{31} - 1 \Rightarrow \mathrm{rep}(m) = m.$$

- For $-2^{31} \le n \le -1$, n is represented by the bit pattern for $2^{32} - |n|$:

$$-2^{31} \le n \le -1 \Rightarrow \mathrm{rep}(m) = 2^{32} - |n|.$$

2's complement visualized

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

Integer arithmetic

Problem: processor is very good at artithmetic on (unsigned) bit strings.

How does that translate to arithmetic on integers?

$$\mathrm{int}\left(\mathrm{rep}(x) * \mathrm{rep}(y)\right) \overset{?}{=} x * y$$

Addition in 2’s complement

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

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

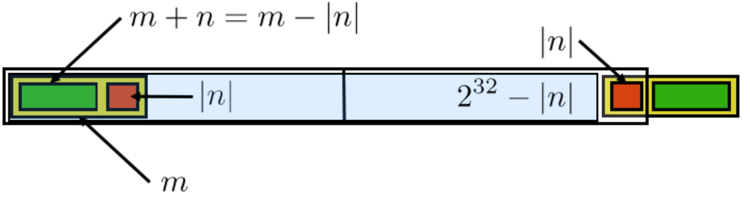
The easy case is $0 < m,n$, as long as there is no overflow.

Addition in 2's complement (cont'd)

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 in 2's complement

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?

Floating point numbers

Floating point numbers

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

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

- 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	24	-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

Limitations

Overflow: more than $\beta(1-\beta^{-t+1})\beta^U$ or less than $\beta(1-\beta^{-t+1})\beta^L$

Underflow: numbers less than $\beta^{-t+1}\cdot\beta^L$

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?

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.

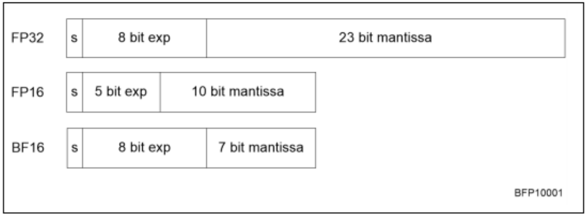
IEEE 754, 32-bit

sign	exponent	mantissa
s	$e_1 \cdots e_8$	$s_1 \ldots s_{23}$
31	$30 \cdots 23$	$22 \cdots 0$

$(e_1 \cdots e_8)$	numerical value
$(0 \cdots 0) = 0$	$\pm 0.s_1 \cdots s_{23} \times 2^{-126}$
$(0 \cdots 01) = 1$	$\pm 1.s_1 \cdots s_{23} \times 2^{-126}$
$(0 \cdots 010) = 2$	$\pm 1.s_1 \cdots s_{23} \times 2^{-125}$
$\cdots$	
$(01111111) = 127$	$\pm 1.s_1 \cdots s_{23} \times 2^{0}$
$(10000000) = 128$	$\pm 1.s_1 \cdots s_{23} \times 2^{1}$
$\cdots$	
$(11111110) = 254$	$\pm 1.s_1 \cdots s_{23} \times 2^{127}$
$(11111111) = 255$	$\pm\infty$ if $s_1 \cdots s_{23} = 0$, otherwise `NaN`

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

Representation error

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 $x = 1.256$, $\tilde{x}_{\text{round}} = 1.26$, $\tilde{x}_{\text{truncate}} = 1.25$

Error in the 4th digit: $|\varepsilon| < \beta^{t-1}$ (this example had no exponent, how about if it does?)

Exercise 5: Round-off

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

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

Write a single precision program that tries to compute e in this manner. Evaluate the expression for an upper bound $n = 10^k$ with $k = 1, \ldots, 10$. Explain the output for large n. Comment on the behavior of the error.

Can you come up with a better way of computing e? How is this number actually computed?

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 6: 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: $5.00 \times 10^1 + 5.04 = (5.00 + 0.504) \times 10^1 \rightarrow 5.50 \times 10^1$

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: $t = 2, \beta = 10$: $1.0 - 9.5 \times 10^{-1}$, exact result $0.05 = 5.0 \times 10^{-2}$.

- Simple approach:
  $1.0 - 9.5 \times 10^{-1} = 1.0 - 0.9 = 0.1 = 1.0 \times 10^{-1}$
- Using 'guard digit':
  $1.0 - 9.5 \times 10^{-1} = 1.0 - 0.95 = 0.05 = 5.0 \times 10^{-2}$, 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?)

Associativity

Computate $4+6+7$ in one significant digit.

Evaluation left-to-right gives:

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

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

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

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;
$x_i > 0$

Multiplication

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

Subtraction

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 $x_+ \cdot x_- = -c/a$.

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:

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

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

Another serious example

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
$y_0 = \ln 6 - \ln 5 = .182\|322 \times 10^1 \ldots$		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.

Stability of linear system solving

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,

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

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

'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

Exercise 7: Fixed-point iteration

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.

Other arithmetic systems

Some compilers support higher precisions.

Arbitrary precision: GMPlib

Interval arithmetic

Half precision bfloat16