

Computer arithmetic

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First we dig into bits
Integers
Floating point numbers
Floating point math
Examples
More

Justification

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

1 Numbers in scientific computing

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

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
Integers
Floating point numbers
Floating point math
Examples
More

First we dig into bits

2 Bit operations

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

Bit string operations:

left shift	<<
right shift	>>

3 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?)

First we dig into bits
Integers
Floating point numbers
Floating point math
Examples
More

Exercise 1: Bit operations

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

First we dig into bits
Integers
Floating point numbers
Floating point math
Examples
More

Integers

4 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)

5 In C and Fortran

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:

```
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 $n = 0, \dots, 31$. There are at least two ways of generating these powers.

Also print the bit pattern. What is unexpected?

6 Negative integers

Problem:

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

Define

$$\text{rep}: \mathbb{Z} \rightarrow 2^n$$

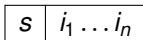
‘representation of the number $N \in \mathbb{Z}$ as bitstring of length n .’

$$\text{int}: 2^n \rightarrow \mathbb{Z}$$

‘interpretation of the bitstring of length n as number $N \in \mathbb{Z}$ ’

7 Negative integers

Use of sign bit: typically first bit



Simplest solution:

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

8 Sign bit

Interpretation

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

9 Shifting

Interpret unsigned number n as $n - B$

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

10 2's Complement

Let m be a signed integer, then the 2's complement 'bit pattern' $\text{rep}(m)$ 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

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

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

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

11 2's complement visualized

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

12 Integer arithmetic

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

How does that translate to arithmetic on integers?

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

13 Addition in 2's complement

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

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

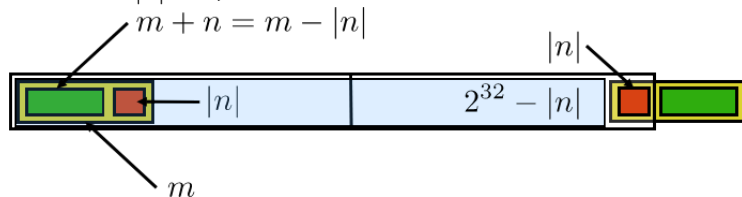
The easy case is $0 < m, n$, as long as there is no overflow.

14 Addition in 2's complement (cont'd)

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

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

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



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

15 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.

16 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 nonrepresentable number explicitly, for instance in a declaration or assignment statement?

Language lawyer remark: signed integer overflow is undefined in C/C++.

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Floating point numbers
Floating point math
Examples
More

Floating point numbers

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Integers
Floating point numbers
Floating point math
Examples
More

17 Floating point math is hard!

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

↑
2.0k
↓
r/formula1 · Posted by u/dogryan100 · **Aston Martin** · 11 months ago · 🇬🇧
[OT Roborace] Driverless racecar drives straight into a wall
clips.twitch.tv/FunAma...



💬 255 Comments 🏆 Award ➦ Share 📌 Save 🙋 Hide 🚩 Report

98% Upvoted

18 Floating point numbers

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

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

- 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 $\text{mantissa} < \beta$
- $e \in [L, U]$ exponent, stored with bias: unsigned int where
 $\text{fl}(L) = 0$

19 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

20 Limitations

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 $\beta^{-t+1} \cdot \beta^L$

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?

21 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.

22 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.

23 IEEE 754, 32-bit pattern

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

24 IEEE 754, 32-bit, all cases

$(e_1 \cdots e_8)$	numerical value	range
$(0 \cdots 0) = 0$	$\pm 0.s_1 \cdots s_{23} \times 2^{-126}$	$s = 0 \cdots 01 \Rightarrow 2^{-23} \cdot 2^{-126} = 2^{-149} \approx 10^{-50}$ $s = 1 \cdots 11 \Rightarrow (1 - 2^{-23}) \cdot 2^{-126}$
$(0 \cdots 01) = 1$	$\pm 1.s_1 \cdots s_{23} \times 2^{-126}$	
$(0 \cdots 010) = 2$	$\pm 1.s_1 \cdots s_{23} \times 2^{-125}$	
...		
$(01111111) = 127$	$\pm 1.s_1 \cdots s_{23} \times 2^0$	$s = 0 \cdots 00 \Rightarrow 1 \cdot 2^0 = 1$ $s = 0 \cdots 01 \Rightarrow 1 + 2^{-23} \cdot 2^0 = 1 + \epsilon$ $s = 1 \cdots 11 \Rightarrow (2 - 2^{-23}) \cdot 2^0 = 2 - \epsilon$
$(10000000) = 128$	$\pm 1.s_1 \cdots s_{23} \times 2^1$	
...		$s = 0 \cdots 00 \Rightarrow 1 \cdot 2^1 = 2$ et cetera
$(11111110) = 254$	$\pm 1.s_1 \cdots s_{23} \times 2^{127}$	
$(11111111) = 255$	$s_1 \cdots s_{23} = 0 \Rightarrow \pm \infty$ $s_1 \cdots s_{23} \neq 0 \Rightarrow \text{NaN}$	

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

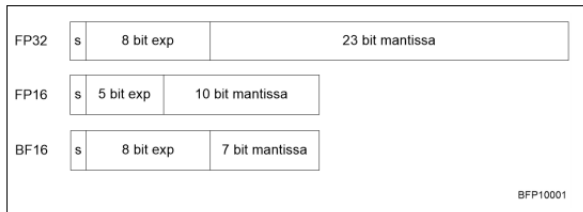
$0 \cdots 0111$

as int? What as float?

What is the largest integer that is representible as float?

25 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`



First we dig into bits
Integers
Floating point numbers
Floating point math
Examples
More

Floating point math

26 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 $|\frac{x - \tilde{x}}{x}|$

Equivalent: $\tilde{x} = x \pm \epsilon \Leftrightarrow |x - \tilde{x}| \leq \epsilon \Leftrightarrow \tilde{x} \in [x - \epsilon, x + \epsilon]$.

Also: $\tilde{x} = x(1 + \epsilon)$ often shorthand for $|\frac{\tilde{x} - x}{x}| \leq \epsilon$

27 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: $|\epsilon| < \beta^{t-1}$ (this example had no exponent, how about if it does?)

Exercise 6: Round-off

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

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

Write a single precision program that tries to compute e in this manner. Evaluate the expression for an upper bound $n = 10^k$ with $k = 1, \dots, 10$. 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?

28 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?)

29 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 $|\varepsilon| < 10^{-2}$

30 The ‘correctly rounded arithmetic’ model

Assumption (enforced by IEEE 754):

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

$$\text{fl}(x_1 \odot x_2) = (x_1 \odot x_2)(1 + \epsilon)$$

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

Note: this holds only for a single operation!

31 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':

$$1.0 - 9.5 \times 10^{-1} = 1.0 - 0.95 = 0.05 = 5.0 \times 10^{-2}, \text{ exact.}$$

In general 3 extra bits needed.

32 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?)

33 Associativity

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

Evaluation left-to-right gives:

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

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

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

34 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;

$x_i > 0$

35 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?

First we dig into bits
Integers
Floating point numbers
Floating point math
Examples
More

Examples

36 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 $1.24 = \text{fl}(1.244)$ and $1.23 = \text{fl}(1.225)$? 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.

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

38 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:

$$\begin{array}{r|l} n-1: & .00\dots0 \quad 10\dots00 \\ n: & .00\dots0 \quad 10\dots01 \quad 0\dots0 \\ & k = \log(n/2) \text{ positions} \end{array}$$

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

39 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
$y_0 = \ln 6 - \ln 5 = .182 322 \times 10^1 \dots$		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 $\tilde{y}_n = y_n + \epsilon_n$, then

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

so $\epsilon_n \geq 5\epsilon_{n-1}$: exponential growth.

40 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,

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

‘Condition number’. Attainable accuracy depends on matrix properties

41 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 8: 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?

First we dig into bits
Integers
Floating point numbers
Floating point math
Examples
More

More

42 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.

43 Other arithmetic systems

Some compilers support higher precisions.

Arbitrary precision: GMPlib

Interval arithmetic

Half precision bfloat16