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Errors in computation; where do they come from?

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objectives

- look at floating point representation in its basic form
- expose errors of a different form: rounding error
- highlight IEEE-754 standard

why this is important:

- Errors come in two forms: truncation error and rounding error
 - we always have them ...
 - case study: Intel
 - our jobs as developers: reduce impact

example: calculating x = x + 0.1

next: floating point numbers

• We're familiar with base 10 representation of numbers:

$$1234 = 4 \times 10^{0} + 3 \times 10^{1} + 2 \times 10^{2} + 1 \times 10^{3}$$

and

$$.1234 = 1 \times 10^{-1} + 2 \times 10^{-2} + 3 \times 10^{-3} + 4 \times 10^{-4}$$

• we write 1234.1234 as an integer part and a fractional part:

$$a_3 a_2 a_1 a_0 . b_1 b_2 b_3 b_4$$

• For some (even simple) numbers, there may be an *infinite* number of digits to the right:

$$\pi = 3.14159...$$
 $1/9 = 0.11111...$
 $\sqrt{2} = 1.41421...$

other bases

- So far, we have just base 10. What about base β ?
- binary ($\beta = 2$), octal ($\beta = 8$), hexadecimal ($\beta = 16$), etc
- ullet In the eta-system we have

$$(a_n \dots a_2 a_1 a_0 . b_1 b_2 b_3 b_4 \dots)_{\beta} = \sum_{k=0}^n a_k \beta^k + \sum_{k=0}^\infty b_k \beta^{-k}$$

integer conversion

An algorithm to compute the base 2 representation of a base 10 integer

$$(N)_{10} = (a_j a_{j-1} \dots a_2 a_0)_2$$

= $a_j \cdot 2^j + \dots + a_1 \cdot 2^1 + a_0 \cdot 2^0$

Compute $(N)_{10}/2 = Q + R/2$:

$$\frac{N}{2} = \underbrace{a_j \cdot 2^{j-1} + \dots + a_1 \cdot 2^0}_{=Q} + \underbrace{\frac{a_0}{2}}_{=R/2}$$

Example

Example: compute $(11)_{10}$ base 2

$$11/2 = 5R1$$
 \Rightarrow $a_0 = 1$
 $5/2 = 2R1$ \Rightarrow $a_1 = 1$
 $2/2 = 1R0$ \Rightarrow $a_2 = 0$
 $1/2 = 0R1$ \Rightarrow $a_3 = 1$

So
$$(11)_{10} = (1011)_2$$

the other way...

Convert a base-2 number to base-10:

$$(11\,000\,101)_2$$
= $1 \times 2^7 + 1 \times 2^6 + 0 \times 2^5 + 0 \times 2^4 + 0 \times 2^3 + 1 \times 2^2 + 0 \times 2^1 + 1 \times 2^0$
= $1 + 2(0 + 2(1 + 2(0 + 2(0 + 2(1 + 2(1)))))))$
= 197

converting fractions

- straight forward way is not easy
- goal: for $x \in [0,1]$ write

$$x = 0.b_1b_2b_3b_4\cdots = \sum_{k=1}^{\infty} c_k\beta^{-k} = (0.c_1c_2c_3\dots)_{\beta}$$

- $\bullet \ \beta(x) = (c_1.c_2c_3c_4...)_{\beta}$
- ullet multiplication by eta in base-eta only shifts the radix

fraction algorithm

An algorithm to compute the binary representation of a fraction x:

$$x = 0.b_1b_2b_3b_4...$$

= $b_1 \cdot 2^{-1} + ...$

Multiply x by 2. The integer part of 2x is b_1

$$2x = b_1 \cdot 2^0 + b_2 \cdot 2^{-1} + b_3 \cdot 2^{-2} + \dots$$

Example

Example: Compute the binary representation of 0.625

$$2 \cdot 0.625 = 1.25$$
 \Rightarrow $b_{-1} = 1$
 $2 \cdot 0.25 = 0.5$ \Rightarrow $b_{-2} = 0$
 $2 \cdot 0.5 = 1.0$ \Rightarrow $b_{-3} = 1$

So
$$(0.625)_{10} = (0.101)_2$$

a problem with precision

```
1 r_0 = x

2 for k = 1, 2, ..., m

3 if r_{k-1} \ge 2^{-k}

4 b_k = 1

5 r_k = r_{k-1} - 2^{-k}

6 else

7 b_k = 0

8 end
```

k	2^{-k}	b_k	$r_k = r_{k-1} - b_k 2^{-k}$
0			0.8125
1	0.5	1	0.3125
2	0.25	1	0.0625
3	0.125	0	0.0625
4	0.0625	1	0.0000

binary fraction example

a problem with precision

For other numbers, such as $\frac{1}{5} = 0.2$, an infinite length is needed.

$$0.2 \quad \rightarrow \quad .0011\,0011\,0011\,\dots$$

So 0.2 is stored just fine in base-10, but needs infinite number of digits in base-2

Ш

This is roundoff error in its basic form...

numerical errors

Roundoff

Roundoff occurs when digits in a decimal point (0.3333...) are lost (0.3333) due to a limit on the memory available for storing one numerical value.

Truncation

Truncation error occurs when discrete values are used to approximate a mathematical expression.

uncertainty: well- or ill-conditioned?

Errors in input data can cause uncertain results

- input data can be experimental or rounded. leads to a certain variation in the results
- well-conditioned: numerical results are insensitive to small variations in the input
- *ill-conditioned*: small variations lead to drastically different numerical calculations (a.k.a. poorly conditioned)

our job

As numerical analysts, we need to

- 1. solve a problem so that the calculation is not susceptible to large roundoff error
- 2. solve a problem so that the approximation has a *tolerable* truncation error

How?

- incorporate roundoff-truncation knowledge into
 - the mathematical model
 - the method
 - the algorithm
 - the software design
- ullet awareness o correct interpretation of results

floating points

Normalized Floating-Point Representation Real numbers are stored as

$$x = \pm (0.d_1d_2d_3\ldots d_m)_{\beta} \times \beta^e$$

- $d_1d_2d_3...d_m$ is the mantissa, e is the exponent
- e is negative, positive or zero
- ullet the general normalized form requires $d_1
 eq 0$

floating point

Example

In base 10

• 1000.12345 can be written as

$$(0.100012345)_{10} \times 10^4$$

0.000812345 can be written as

$$(0.812345)_{10} \times 10^{-3}$$

floating point

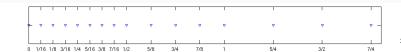
Suppose we have only 3 bits for a mantissa and a 1 bit exponent stored like

$$d_1 \mid d_2 \mid d_3 \mid e_1$$

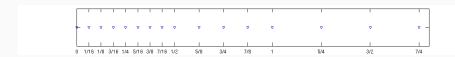
All possible combinations give:

$$000_2 = 0$$
 ... $\times 2^{-1,0,1}$ $111_2 = 7$

So we get $0, \frac{1}{16}, \frac{2}{16}, \dots, \frac{7}{16}, 0, \frac{1}{4}, \frac{2}{4}, \dots, \frac{7}{4}$, and $0, \frac{1}{8}, \frac{2}{8}, \dots, \frac{7}{8}$. On the real line:



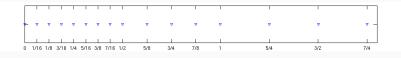
overflow, underflow

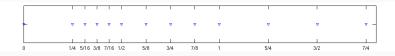


- computations too close to zero may result in underflow
- computations too large may result in overflow
- overflow error is considered more severe
- underflow can just fall back to 0

normalizing

If we use the normalized form in our 4-bit case, we lose $0.001_2 \times 2^{-1,0,1}$ along with other. So we cannot represent $\frac{1}{16}$, $\frac{1}{8}$, and $\frac{3}{16}$.



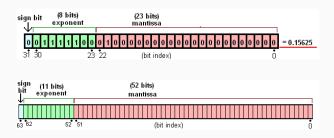


ieee-754 why this is important:

- IEEE-754 is a widely used standard accepted by hardware/software makers
 - defines the floating point distribution for our computation
 - offer several rounding modes which effect accuracy
- Floating point arithmetic emerges in nearly every piece of code
 - even modest mathematical operation yield loss of significant bits
 - · several pitfalls in common mathematical expressions

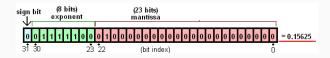
ieee floating point (v. 754)

- How much storage do we actually use in practice?
- 32-bit word lengths are typical
- IEEE Single-precision floating-point numbers use 32 bits
- IEEE Double-precision floating-point numbers use 64 bits
- Goal: use the 32-bits to best represent the normalized floating point number



ieee single precision (marc-32)

$$x = \pm q \times 2^m$$



Notes:

- 1-bit sign
- 8-bit exponent |m|
- 23-bit mantissa q
- The leading one in the mantissa q does not need to be represented: $b_1=1$ is hidden bit
- IEEE 754: put x in 1.f normalized form
- 0 < m + 127 = c < 255
- Largest exponent = 127, Smallest exponent = -126
- Special cases: c = 0.255

ieee single precision

$$x = \pm q \times 2^m$$

Process for x = -52.125:

1. Convert both integer and fractional to binary:

$$x = -(110100.00100000000)_2$$

- 2. Convert to 1.f form: $x = \underbrace{-}_{1} (1.\underbrace{101\,000\,010\,000\,\dots\,0}_{23})_{2} \times 2^{5}$
- 3. Convert exponent $5 = c 127 \Rightarrow c = 132 \Rightarrow c = (\underbrace{10\,000\,100}_{8})_{2}$

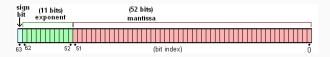
$$\underbrace{1}_{1} \underbrace{\underbrace{10\,000\,100}_{8} \underbrace{101\,000\,010\,000\dots0}_{23}}_{23}$$

ieee single precision

Special Cases:

- denormalized/subnormal numbers: use 1 extra bit in the significant: exponent is now -126 (less precision, more range), indicated by 00000000_2 in the exponent field
- two zeros: +0 and -0 (0 mantissa, 0 exponent)
- two ∞ 's: $+\infty$ and $-\infty$
- ∞ (0 mantissa, 111111111₂ exponenet)
- NaN (any mantissa, 11111111₂ exponent)
- see appendix C.1 in NMC 6th ed.

ieee double precision



- 1-bit sign
- 11-bit exponent
- 52-bit mantissa
- single-precision: about 6 decimal digits of precision
- double-precision: about 15 decimal digits of precision
- m = c 1023

precision vs. range

type	range	approx range
	$-3.40 \times 10^{38} \le x \le -1.18 \times 10^{-38}$	
single	0	$2^{-126} o 2^{128}$
	$1.18 \times 10^{-38} \le x \le 3.40 \times 10^{38}$	
	$-1.80 \times 10^{318} \le x \le -2.23 \times 10^{-308}$	
double	0	$2^{-1022} o 2^{1024}$
	$2.23 \times 10^{-308} \le x \le 1.80 \times 10^{308}$	

small numbers example

plus one example

$$\epsilon_{m}$$

Take x = 1.0 and add $1/2, 1/4, \dots, 2^{-i}$:

Hidden bit

\downarrow	\leftarrow		52 bits								\rightarrow		
1	1	0	0	0	0	0	0	0	0	0	0	е	е
1	0	1	0	0	0	0	0	0	0	0	0	е	е
1	0	0	1	0	0	0	0	0	0	0	0	е	е

.

1	0	0	0	0	0	0	0	0	0	0	1	е	е
1	0	0	0	0	0	0	0	0	0	0	0	е	е

- Ooops!
- use fl(x) to represent the floating point machine number for the real number x

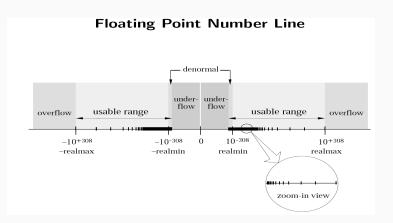
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$$f(1+2^{-52}) \neq 1$$
, but $f(1+2^{-53}) = 1$

ϵ_m : machine epsilon

Machine epsilon ϵ_m is the smallest number such that

$$fl(1+\epsilon_m) \neq 1$$

- The double precision machine epsilon is about 2^{-52} .
- The single precision machine epsilon is about 2^{-23} .



floating point errors

- Not all reals can be exactly represented as a machine floating point number. Then what?
- Round-off error
- IEEE options:
 - Round to next nearest FP (preferred), Round to 0, Round up, and Round down

Let x_+ and x_- be the two floating point machine numbers closest to x

- round to nearest: $round(x) = x_{-}$ or x_{+} , whichever is closest
- round toward 0: $round(x) = x_-$ or x_+ , whichever is between 0 and x
- round toward $-\infty$ (down): $round(x) = x_-$
- round toward $+\infty$ (up): $round(x) = x_+$

floating point errors

How big is this error? Suppose $(x \text{ is closer to } x_{-})$

$$x = (0.1b_2b_3 \dots b_{24}b_{25}b_{26})_2 \times 2^m$$

$$x_- = (0.1b_2b_3 \dots b_{24})_2 \times 2^m$$

$$x_+ = ((0.1b_2b_3 \dots b_{24})_2 + 2^{-24}) \times 2^m$$

$$|x - x_-| \le \frac{|x_+ - x_-|}{2} = 2^{m-25}$$

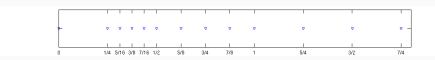
$$\left|\frac{x - x_-}{x}\right| \le \frac{2^{m-25}}{1/2 \times 2^m} \le 2^{-24} = \epsilon_m/2$$

floating point arithmetic

- Problem: The set of representable machine numbers is FINITE.
- So not all math operations are well defined!
- Basic algebra breaks down in floating point arithmetic

Example

$$a + (b+c) \neq (a+b) + c$$



floating point arithmetic

Rule 1.

$$fl(x) = x(1+\epsilon)$$
, where $|\epsilon| \le \epsilon_m$

Rule 2.

For all operations \odot (one of +, -, *, /)

$$f(x \odot y) = (x \odot y)(1 + \epsilon_{\odot}), \text{ where } |\epsilon_{\odot}| \le \epsilon_m$$

Rule 3.

For +, * operations

$$fl(a \odot b) = fl(b \odot a)$$

There were many discussions on what conditions/rules should be satisfied by floating point arithmetic. The IEEE standard is a set of standards adopted by many CPU manufacturers.

floating point arithmetic

Consider the sum of 3 numbers: y = a + b + c.

Done as
$$fl(fl(a+b)+c)$$

 $\eta = fl(a+b) = (a+b)(1+\epsilon_1)$
 $y_1 = fl(\eta+c) = (\eta+c)(1+\epsilon_2)$
 $= [(a+b)(1+\epsilon_1)+c](1+\epsilon_2)$
 $= [(a+b+c)+(a+b)\epsilon_1)](1+\epsilon_2)$
 $= (a+b+c)\left[1+\frac{a+b}{a+b+c}\epsilon_1(1+\epsilon_2)+\epsilon_2\right]$

So disregarding the high order term $\epsilon_1\epsilon_2$

$$f(f(a+b)+c) = (a+b+c)(1+\epsilon_3)$$
 with $\epsilon_3 \approx \frac{a+b}{a+b+c}\epsilon_1 + \epsilon_2$

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floating point arithmetic

If we redid the computation as $y_2 = fl(a + fl(b + c))$ we would find

$$fl(a+fl(b+c)) = (a+b+c)(1+\epsilon_4)$$
 with $\epsilon_4 \approx \frac{b+c}{a+b+c}\epsilon_1 + \epsilon_2$

Main conclusion:

The first error is $\underline{\text{amplified}}$ by the factor (a+b)/y in the first case and (b+c)/y in the second case.

In order to sum n numbers more accurately, it is better to start with the small numbers first. [However, sorting before adding is usually not worth the cost!]

floating point arithmetic

One of the most serious problems in floating point arithmetic is that of cancellation. If two large and close-by numbers are subtracted the result (a small number) carries very few accurate digits (why?). This is fine if the result is not reused. If the result is part of another calculation, then there may be a serious problem

Example

Roots of the equation

$$x^2 + 2px - q = 0$$

Assume we want the root with smallest absolute value:

$$y = -p + \sqrt{p^2 + q} = \frac{q}{p + \sqrt{p^2 + q}}$$

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catastrophic cancellation

Adding c = a + b will result in a large error if

- a ≫ b
- a ≪ b

Let

$$a = x.xxx \cdots \times 10^{0}$$
$$b = y.yyy \cdots \times 10^{-8}$$

Then
$$\begin{array}{c} & \underbrace{x.xxx.xxxx.xxxx.xxxx} \\ + & 0.000\,0000\,yyyy\,yyyy \\ = & x.xxx.xxxx.xxxx.xxxx \\ & \underbrace{?????????}_{\text{lost precision}} \end{array}$$

catastrophic cancellation

Subtracting c = a - b will result in large error if $a \approx b$. For example

$$a = x.xxxx xxxx xxx1 \underbrace{ssss...}_{lost}$$

$$b = x.xxxx xxxx xxxx xxx0 \underbrace{tttt...}_{lost}$$

Then
$$\begin{array}{c} \underbrace{x.xxx.xxxx.xxx1}_{x.xxx.xxxx.xxx1} \\ + x.xxx.xxxx.xxx0 \\ = 0.0000000000001 \underbrace{????????}_{lost precision} \end{array}$$

summary

- addition: c = a + b if $a \gg b$ or $a \ll b$
- subtraction: c = a b if $a \approx b$
- catastrophic: caused by a single operation, not by an accumulation of errors
- can often be fixed by mathematical rearrangement

Example

x = 0.3721448693 and y = 0.3720214371. What is the relative error in x - y in a computer with 5 decimal digits of accuracy?

$$\frac{|x - y - (\bar{x} - \bar{y})|}{|x - y|} = \frac{|0.3721448693 - 0.3720214371 - 0.37214 + 0.37202|}{|0.3721448693 - 0.3720214371|}$$
$$\approx 3 \times 10^{-2}$$

Loss of Precision Theorem

Let x and y be (normalized) floating point machine numbers with x > y > 0.

If $2^{-p} \le 1 - \frac{y}{x} \le 2^{-q}$ for positive integers p and q, the significant binary digits lost in calculating x - y is between q and p.

Example

Consider x = 37.593621 and y = 37.584216.

$$2^{-11} < 1 - \frac{y}{x} = 0.00025\,01754 < 2^{-12}$$

So we lose 11 or 12 bits in the computation of x - y. yikes!

Example

Back to the other example (5 digits): x = 0.37214 and y = 0.37202.

$$10^{-4} < 1 - \frac{y}{x} = 0.00032 < 10^{-5}$$

So we lose 4 or 5 bits in the computation of x - y. Here, x - y = 0.00012

which has only 1 significant digit that we can be sure about

So what to do? Mainly rearrangement.

$$f(x) = \sqrt{x^2 + 1} - 1$$

So what to do? Mainly rearrangement.

$$f(x) = \sqrt{x^2 + 1} - 1$$

Problem at $x \approx 0$.

So what to do? Mainly rearrangement.

$$f(x) = \sqrt{x^2 + 1} - 1$$

Problem at $x \approx 0$.

One type of fix:

$$f(x) = \left(\sqrt{x^2 + 1} - 1\right) \left(\frac{\sqrt{x^2 + 1} + 1}{\sqrt{x^2 + 1} + 1}\right)$$
$$= \frac{x^2}{\sqrt{x^2 + 1} + 1}$$

no subtraction!