Computational Methods

CMSC/AMSC/MAPL 460

Errors in data and computation

Representing numbers in floating point

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Class Outline

- Computations should be as accurate and as error-free as possible
- Sources of error:
- Poor models of a physical situation
- Ill-posed problems
- Errors due to representation of numbers on a computer and successive operations with these
  - Examples from the book
  - Scientific notation and Floating point representation
  - Concepts: sign, mantissa, base, exponent
  - Distribution of floating point numbers

Error

- What we need to know about error:
  - how does error arise
  - how machines do arithmetic
    - fixed point arithmetic
    - floating point arithmetic
  - how errors are propagated in calculations.
  - how to measure error

Typical task that uses scientific computing

- Evaluate safety of a machine part
- Tasks

1. Measure the parts dimensions, shape etc. and discretize it (e.g., via finite elements)
2. Determine the material it is made of
3. Find the mathematical models (equations) that determine how the part will deform according to loads
4. Discretize the equations (e.g., via finite elements)
5. Solve it on the computer

Errors

- Each step is characterized by some error

1. Measurement errors:
2. Errors in properties
3. Inexact mathematical models
4. Discretization errors: something continuous is represented discretely
5. Errors in the solution to discrete representations of numbers

Errors are inevitable

- Everybody did the best they could
- No one made any mistakes, yet answer could be wrong
- Goal of error analysis is to
  - determine when the answer can be relied upon
  - Which algorithms can be trusted for which data
- In particular we will focus on errors in part 5 (finite representation of numbers today)

Job of a Numerical Analyst/Computational Scientitst

- Numerical analyst
  - Designs algorithms and analyzes them
  - Develops mathematical software
  - Can provide some guarantees as to when the software will be accurate and when the final answer can be trusted
- Computational Scientist
  - Knows about mathematical software
  - Knows about the domain
  - Makes an intelligent choice to use the right tools for the job

Modeling

- Original mathematical models may be poorly specified or unavailable
  - E.g. Newton's laws work for non relativistic dynamics
  - Turbulence
  - …
- Computing with a poor model will lead to inevitable errors
- Quantities that are measured may be done so with error and bias
  - Using them in computation will lead to errors
- Approaches to fix these errors are in the domain of statistics
  - Will not be much discussed in this course

Well posed problems

- Hadamard postulated that for a problem to be "well posed"
  1. *Solution must exist*
  2. *It must be unique*
  3. *Small changes to input data should cause small changes to solution*
- Many problems in science result in "ill-posed" problems.
  – Numerically it is common to have condition 3 violated.
- Converting ill-posed problem to well-posed one is called *regularization*.
- Will discuss this later in the course when talking about optimization and Singular Value Decompositon.

Numerical Modeling and Measurement Errors

- Continuous mathematical models have to be represented in discrete form on the computer
  – Finite-difference or finite-element discretization
  – Continuous quantities may be represented using linear interpolants
  – Model may only reach accurate answer in the limit
  – Round-off errors – continuous numbers represented with discrete representations on the computer
- Focus of today's class:
  – What errors are caused by such representations

Fixed point representation

- How can we represent a number in a computer's memory?
- Fixed point is an obvious way:
- Used to represent integers on computers, and real numbers on some DSPs:
- Each **word** (storage location) in a machine contains a fixed number of digits.
- Example: A machine with a 6-digit word might represent 2005 as

0	0	2	0	0	5

- This only allows us to represent integers and uses a decimal system

Binary/Decimal/Octal/Hexadecimal

- Numbers can be represented in different bases
- Usually humans use decimal
  – Perhaps because we have ten fingers
- Computer memory often has two states
  – Assigned to 0 and 1
  – Leads to a binary representation
- Octal and Hexadecimal representations arise by considering 3 or 4 memory locations together
  – Lead to 2^3 and 2^4 numbers

Binary Representation

- Most computers use **binary (base 2)** representation.

  0 1 0 1 1 0

- Each digit has a value 0 or 1.
- If the number above is binary, its value is
- $1 \times 2^4 + 0 \times 2^3 + 1 \times 2^2 + 1 \times 2^1 + 0 \times 2^0$. (or 22 in base 10)
- Adding numbers in binary

	0	0	0	1	1	
+	0	1	0	1	0	
	0	1	1	0	1	

$0 + 0 = 0$
$0 + 1 = 1$
$1 + 0 = 1$
$1 + 1 = 10$ (binary) $= 10_2 = 2$
$1 + 1 + 1 = 11$ (binary)$=11_2 = 3$

Note the "**carry**" here!

Negative numbers

- One way computers represent negative numbers is using the *sign-magnitude representation:*
- **Sign magnitude**: if the first bit is zero, then the number is positive. Otherwise, it is negative.
- 0 0 0 1 1 Denotes +11.
- 1 0 0 1 1 Denotes -11.

Range of fixed point numbers

Largest 5-digit (5 bit) binary number:	0	1	1	1	1	=15
Smallest:	1	1	1	1	1	=-15
Smallest positive:	0	0	0	0	1	=1

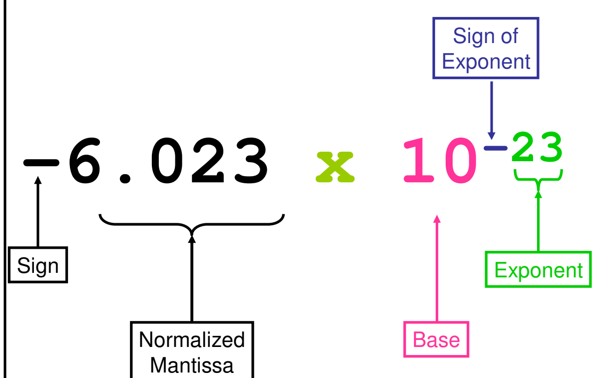
Overflow

If we try to add these numbers:	0	1	1	1	1	=15
+	0	1	0	0	0	= 8
we get	1	0	1	1	1	=-7.

We call this "overflow": the answer is too large to store, since it is Outside the range of this number system.

- Fixed point arithmetic:
  - Easy: always get an integer answer.
  - Either we get exactly the right answer, or we can detect
  - overflow.
  - The numbers that we can store are equally spaced.
  - Disadvantage: **very** limited range of numbers.

Scientific Notation



Floating point on a computer

- Using fixed number of bits represent real numbers on a computer
- Once a base is agreed we store each number as two numbers and two signs
  - Mantissa and exponent
- Mantissa is usually “normalized”
- If we have infinite spaces to store these numbers, we can represent arbitrarily large numbers
- With a fixed number of spaces for the two numbers (mantissa and exponent)

Binary Floating Point Representation

- Same basic idea as scientific notation
- Modifications and improvements based on
  - Hardware architecture
  - Efficiency (Space & Time)
  - Additional requirements
    - Infinity
    - Not a number (NaN)
    - Not normalized
    - etc.

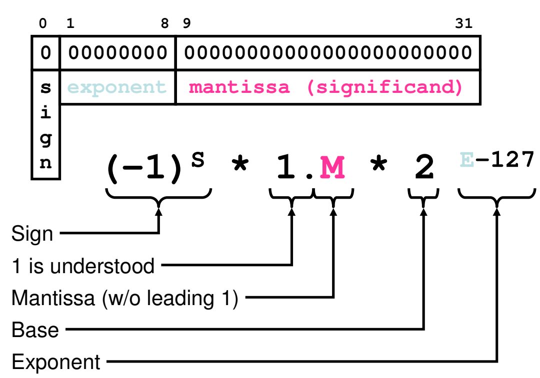
Floating point on a computer

- If we wanted to store 15×2^{11}, we would need 16 bits:

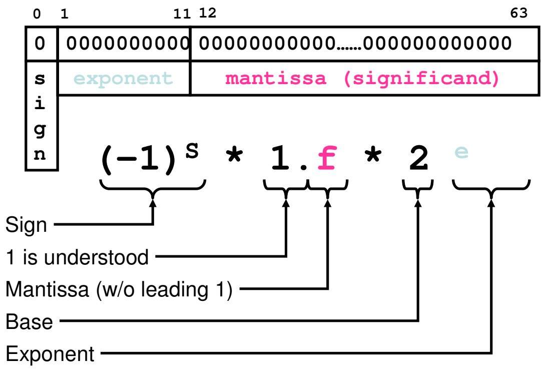
  0 1 1 1 1 0 0 0 0 0 0 0 0 0 0 0
- Instead we store it as three numbers
- $(-1)^S \times F \times 2^E$, with F = 15 saved as 01111 and E = 11 saved as 01011.
- Now we can have fractions/decimals, too:

  binary $.101 = 1 \times 2^{-1} + 0 \times 2^{-2} + 1 \times 2^{-3}$.

IEEE-754 (single precision)



IEEE-754 (double precision)



IEEE - 754

Most nonzero floating-point numbers are normalized. This means they can be expressed as

$$x = \pm(1 + f) \cdot 2^e$$

The quantity f is the fraction or mantissa and e is the exponent. The fraction satisfies

$$0 \leq f < 1$$

and must be representable in binary using at most 52 bits. In other words, $2^{52}f$ is an integer in the interval

$$0 \leq 2^{52}f < 2^{52}$$

The exponent e is an integer in the interval

$$-1022 \leq e \leq 1023$$

The finiteness of f is a limitation on *precision*. The finiteness of e is a limitation on *range*. Any numbers that don't meet these limitations must be approximated by ones that do.

Double-precision floating-point numbers are stored in a 64 bit word, with 52 bits for f, 11 bits for e, and one bit for the sign of the number. The sign of e is accommodated by storing $e + 1023$, which is between 1 and $2^{11} - 2$. The two

Can be written...

	E+1023 == 0	0 < E+1023 < 2047	E+1023 == 2047
f==0	0	Powers of Two	∞
f~=0	Non-normalized typically underflow	Floating point Numbers	Not A Number

- $x = \pm(1+f) \times 2^e$
- $0 \leq f < 1$
- $f = (\text{integer} < 2^{52}) / 2^{52}$

- $-1022 \leq e \leq 1023$
- e = integer

Effects of floating point

Finite f implies finite *precision*.

Finite e implies finite *range*

Floating point numbers have discrete spacing, a maximum and a minimum.

Effects of floating point

- eps *is the distance from* 1 *to the next larger floating-point number.*
- eps = 2^{-52}
- In Matlab

```
         Binary         Decimal
eps      2^(-52)        2.2204e-16
realmin  2^(-1022)      2.2251e-308
realmax  (2-eps)*2^1023 1.7977e+308
```

Rounding vs. Chopping

- **Chopping**: Store x as c, where |c| < |x| and no machine number lies between c and x.
- **Rounding**: Store x as r, where r is the machine number closest to x.
- **IEEE standard arithmetic uses rounding**.

Machine Epsilon

- **Machine epsilon** is defined to be the smallest positive number which, when added to 1, gives a number different from 1.
  - Alternate definition (1/2 this number)
- **Note:** Machine epsilon depends on d and on whether rounding or chopping is done, but does not depend on m or M!

Some numbers cannot be exactly represented

$$\frac{1}{10} = \frac{1}{2^4} + \frac{1}{2^5} + \frac{0}{2^6} + \frac{0}{2^7} + \frac{1}{2^8} + \frac{1}{2^9} + \frac{0}{2^{10}} + \frac{0}{2^{11}} + \frac{1}{2^{12}} + ...$$

$$t = (1 + \frac{9}{16} + \frac{9}{16^2} + \frac{9}{16^3} + ... + \frac{9}{16^{12}} + \frac{10}{16^{13}}) \cdot 2^{-4}$$

Problem 1.34.

```
x = 1; while 1+x > 1, x = x/2, pause(.02), end

x = 1; while x+x > x, x = 2*x, pause(.02), end

x = 1; while x+x > x, x = x/2, pause(.02), end
```