Mathematics Methods for Computer Science

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Reference book: Solomon, Justin. Numerical Algorithms. Published by AK Peters/CRC Press, 2015.

Topics I

1. Numeric
   - Stability and error analysis
   - Floating-point representation
2. Linear algebra
   - Guassian elemination and LU
   - Column space and QR
   - Eigenproblems
   - Applications
3. Root-finding and optimization
   - Single variable
   - Multivariable
   - Constrained optimization
   - Iterative linear solvers; Conjugate gradients

Topics II

4. Interpolation and quadrature
   - Approximating integrals
   - Approximating derivatives
5. Differential equations
   - ODEs: time-stepping, discretization
   - PDEs: Poisson equation, heat equation, waves
   - Techniques: Differencing, finite elements (time-permitting)

Lecture

Numerics And Error Analysis

Prototypical Example

```
double x = 1.0;
double y = x / 3.0;
if (x == y*3.0) cout << "They are equal!";
else cout << "They are NOT equal.";
```

Using Tolerances

```
double x = 1.0;
double y = x / 3.0;
if (fabs(x-y*3.0) <
     numeric_limits<double>::epsilon)
     cout << "They are equal!";
else cout << "They are NOT equal.";
```

A Crucial Point

Mathematically correct
$$\neq$$
Numerically sound

Rarely if ever should the operator $==$ and its equivalents be used on fractional values. Instead, some tolerance should be used to check if they are equal.

Counting in Binary: Integer

$$\begin{aligned} 463 &= 256 + 128 + 64 + 8 + 4 + 2 + 1 \\ &= 2^8 + 2^7 + 2^6 + 2^3 + 2^2 + 2^1 + 2^0 \end{aligned}$$

$$\downarrow$$

1	1	1	0	0	1	1	1	1
2^8	2^7	2^6	2^5	2^4	2^3	2^2	2^1	2^0

Counting in Binary: Fractional

$$
\begin{aligned}
463.25 &= 256 + 128 + 64 + 8 + 4 + 2 + 1 + 1/4 \\
&= 2^8 + 2^7 + 2^6 + 2^3 + 2^2 + 2^1 + 2^0 + 2^{-2}
\end{aligned}
$$

$$\downarrow$$

1	1	1	0	0	1	1	1	1	0	1
2^8	2^7	2^6	2^5	2^4	2^3	2^2	2^1	2^0	2^{-1}	2^{-2}

Familiar Problem

$$\frac{1}{3} = 0.0101010101\ldots_2$$

Finite number of bits

Fixed-Point Arithmetic

1	1	...	0	0	...	1	1
2^{ℓ}	$2^{\ell-1}$	...	2^0	2^{-1}	...	2^{-k+1}	2^{-k}

- Parameters: $k, \ell \in Z$
- $k + \ell + 1$ digits total
- Can reuse integer arithmetic (fast; GPU possibility):

$$a + b = (a \cdot 2^k + b \cdot 2^k) \cdot 2^{-k}$$

Two-Digit Example

$$0.1_2 \times 0.1_2 = 0.01_2 \cong 0.0_2$$

Multiplication and division easily change order of magnitude!

Demand of Scientific Applications

$$9.11 \times 10^{-31} \to 6.022 \times 10^{23}$$

Desired: graceful transition

Observations

- Compactness matters:

$$6.022 \times 10^{23} =$$

602,200,000,000,000,000,000,000

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- Compactness matters:

$$6.022 \times 10^{23} =$$

602,200,000,000,000,000,000,000

- Some operations are unlikely:

$$6.022 \times 10^{23} + 9.11 \times 10^{-31}$$

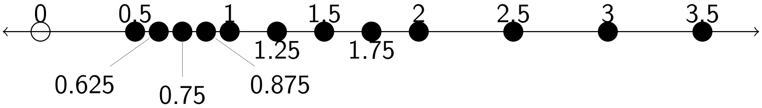
Scientific Notations

Store Significant digits

$$\underbrace{\pm}_{\text{sign}} \underbrace{(d_0 + d_1 \cdot b^{-1} + d_2 \cdot b^{-2} + \cdots + d_{p-1} \cdot b^{1-p}))}_{\text{significand}} \times \underbrace{b^e}_{\text{exponent}}$$

- Base: $b \in N$
- Precision: $p \in N$
- Range of exponents: $e \in [L, U]$

Properties of Floating Point



- Unevenly spaced
  - Machine precision ϵ_m: smallest ϵ_m with $1 + \epsilon_m \not\approx 1$

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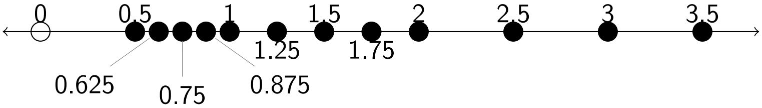

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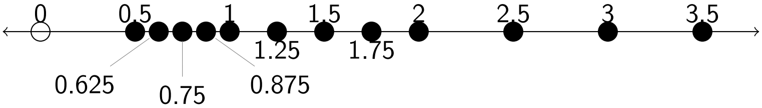

- Unevenly spaced
  - Machine precision ϵ_m: smallest ϵ_m with $1 + \epsilon_m \ncong 1$
- Needs rounding rule (e.g. "round to nearest, ties to even")
- Can remove leading 1

Infinite Precision

$$Q = \{a/b : a, b \in Z\}$$

- Simple rules: $a/b + c/d = (ad + cb)/bd$
- Redundant: $1/2 = 2/4$
- Blowup:

$$\frac{1}{100} + \frac{1}{101} + \frac{1}{102} + \frac{1}{103} + \frac{1}{104} + \frac{1}{105} = \frac{188463347}{3218688200}$$

- Restricted operations: $2 \mapsto \sqrt{2}$

Bracketing

Store range $a \pm \epsilon$

- Keeps track of certainty and rounding decisions
- Easy bounds:

$$(x \pm \epsilon_1) + (y \pm \epsilon_2) = (x + y) \pm (\epsilon_1 + \epsilon_2 + error(x + y))$$

- Implentation via operator overloading

Sources of Error

- Rounding
- Discretization
- Modeling
- Input

Example

What sources of error might affect planets simulation?

Absolute vs. Relative Error

Absolute Error

The difference between the approximate value and the underlying true value.

Absolute vs. Relative Error

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Relative Error

Absolute error divided by the true value.

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Absolute Error

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Relative Error

Absolute error divided by the true value.

$$2\ cm \pm 0.02\ cm$$

$$2\ cm \pm 1\%$$

Relative Error: Difficulty

Problem: Generally not computable

Relative Error: Difficulty

Problem: Generally not computable

Common fix: Be conservative

Computable Measures of Success

Root-finding problem

For $f : \mathbb{R} \to \mathbb{R}$, find x^* such that $f(x^*) = 0$

Actual output: x_{est} with $|f(x_{est})| \ll 1$

Backward Error

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The amount the problem statement would have to change to make the approximate solution exact

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Example 1: $\sqrt{x}$

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Example 1: $\sqrt{x}$

Example 2: $A\vec{x} = \vec{b}$

Conditioning

Well-conditioned:

Small backward error $\Longrightarrow$ small forward error

Poorly conditioned:

Otherwise

Example: Root-finding

Condition Number

Condition number

Ratio of forward to backward error

Condition Number

Condition number

Ratio of forward to backward error

Root-finding example:

$$\frac{1}{|f'(x^*)|}$$

Theme

Extremely careful implementation can be necessary

Example: $||\vec{x}||_2$

```
double normSquared = 0;
for (int i = 0; i < n; i++)
normSquared += x[i]*x[i];
return sqrt(normSquared);
```

Improved $\|\vec{x}\|_2$


```
double maxElement = epsilon;
\\
for (int i = 0; i < n; i++)
maxElement = max(maxElement, fabs(x[i]));
for (int i = 0; i < n; i++) {
double scaled = x[i] / maxElement;
normSquared += scaled*scaled;
}
return sqrt(normSquared) * maxElement;
```

More Involved Example: $\sigma_i x_i$

```
double sum = 0;
for (int i = 0; i < n; i++)
sum += x[i];
```

Motivation for Kahan Algorithm

$$((a+b)-a)-b \stackrel{?}{=} 0$$

Store compensation value !