Elements of Floating-point Arithmetic

Sanzheng Qiao

Department of Computing and Software
McMaster University

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Outline

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Two ways of representing floating-point

On paper we write a floating-point number in the format:

$$\pm d_1.d_2 \cdots d_t \times \beta^e$$

$0 < d_1 < \beta$, $0 \leq d_i < \beta$ $(i > 1)$

- t: precision
- β: base (or radix), almost universally 2, other commonly used bases are 10 and 16
- e: exponent, integer

Two ways of representing floating-point (cont.)

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1.10011×2^{-4}

$t = 6$, $\beta = 2$ (binary), $e = -4$

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$t = 6$, $\beta = 2$ (binary), $e = -4$

The precision t, the base β, and the range of the exponent e determine a floating-point number system.

In memory, a floating-point number is stored in three consecutive fields:

sign (1 bit)
exponent (depends on the range)
fraction (depends on the precision)

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IEEE floating-point standards: single precision and double precision.

Characteristics

A floating-point number system is characterized by four (integer) parameters:

- base β (also called radix)
- precision t
- exponent range $e_{\text{min}} \leq e \leq e_{\text{max}}$

Machine precision

A real number representing the accuracy.

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Thus, $\epsilon_M = \beta^{1-t}$.

Equivalently, the distance between two consecutive floating-point numbers between 1.0 and β. (The floating-point numbers between 1.0 and β are evenly spaced, $1.0...000, 1.0...001, 1.0...010, ..., 1.1...111$.)

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eps = 1.0;
while (1.0 + eps > 1.0)
    eps = eps/2;
end
2*eps,
```

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Examples. ($\beta = 2$)

When $t = 24$, $\epsilon_M = 2^{-23} \approx 1.2 \times 10^{-7}$
When $t = 53$, $\epsilon_M = 2^{-52} \approx 2.2 \times 10^{-16}$

Approximations of real numbers

Since floating-point numbers are discrete, a real number, for example, $\sqrt{2}$, may not be representable in floating-point. Thus real numbers are approximated by floating-point numbers.

We denote

$$\mathrm{fl}(x) \approx x.$$

as a floating-point approximation of a real number x.

Approximations of real numbers (cont.)

Example

The floating-point number $1.10011001100110011001101 \times 2^{-4}$ can be used to approximate 1.0×10^{-1}. The best single precision approximation of decimal 0.1.

1.0×10^{-1} is not representable in binary.

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When approximating, some kind of rounding is involved.

Error measurements: ulp and u

If the nearest rounding is applied and $\mathrm{fl}(x) = d_1.d_2...d_t \times \beta^e$, then the absolute error is bounded by

$$|\mathrm{fl}(x) - x| \leq \frac{1}{2}\beta^{1-t}\beta^e,$$

half of the unit in the last place (ulp);

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the relative error is bounded by

$$\frac{|\mathrm{fl}(x) - x|}{|\mathrm{fl}(x)|} \leq \frac{1}{2}\beta^{1-t}, \text{ since } |\mathrm{fl}(x)| \geq 1.0 \times \beta^e,$$

called the *unit of roundoff* denoted by u.

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The largest number such that $1.0 + u = 1.0$.
Also, when $\beta = 2$, the distance between two consecutive floating-point numbers between 1/2 and 1.0
$(1.0...0 \times 2^{-1}, ..., 1.1...1 \times 2^{-1}, 1.0.)$
$1.0 + 2^{-t} = 1.0$ (Why?)

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```
u = 1.0;
while (1.0 + u > 1.0)
    u = u/2;
end
u,
```

Four parameters

Base $\beta = 2$.

	single	double
precision t	24	53
$e_{\min}$	-126	-1022
$e_{\max}$	127	1023

Formats:

	single	double
Exponent width	8 bits	11 bits
Format width in bits	32 bits	64 bits

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Since $(1/2) \times 2^{23} > (1/3) \times 2^{23}$, there exist $x \neq y \in [3/2, 2)$ such that $1/x = 1/y \in (1/2, 2/3]$.

Hidden bit and biased representation

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Example

Single precision $1.10011001100110011001101 \times 2^{-4}$ is stored as

```
0 01111011 10011001100110011001101
```

Special quantities

The special quantities are encoded with exponents of either $e_{\text{max}} + 1$ or $e_{\text{min}} - 1$. In single precision, `11111111` in the exponent field encodes $e_{\text{max}} + 1$ and `00000000` in the exponent field encodes $e_{\text{min}} - 1$.

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Signed zeros: ± 0

Binary representation:

`X 00000000 00000000000000000000000`

Signed zeros

- When testing for equal, $+0 = -0$, so the simple test `if (x == 0)` is predictable whether x is $+0$ or -0.
- The relation $1/(1/x) = x$ holds when $x = \pm\infty$.
- $\log(+0) = -\infty$ and $\log(-0) = NaN$; $\text{sign}(+0) = 1$ and $\text{sign}(-0) = -1$.

Signed zeros

If $z = -1$, $\sqrt{1/z} = i$, but $1/\sqrt{z} = -i$.

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Why? Square root is multivalued, can't make it continuous in the entire complex plane. However, it is continous for $z = \cos\theta + i\sin\theta$, $-\pi \leq \theta \leq \pi$, if a brabch cut consisting of all negative real numbers is excluded from the consideration.

With signed zeros, for the numbers with negative real part, $-x + i(+0)$, $x > 0$, has a square root of $i\sqrt{x}$; $-x + i(-0)$ has a square root of $-i\sqrt{x}$.

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$z = -1 = -1 + i(+0)$, $1/z = -1 + i(-0)$, then $\sqrt{1/z} = -i = 1/\sqrt{z}$

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With signed zeros, for the numbers with negative real part, $-x + i(+0)$, $x > 0$, has a square root of $i\sqrt{x}$; $-x + i(-0)$ has a square root of $-i\sqrt{x}$.

$z = -1 = -1 + i(+0)$, $1/z = -1 + i(-0)$, then $\sqrt{1/z} = -i = 1/\sqrt{z}$

However, $+0 = -0$, and $1/(+0) \neq 1/(-0)$. (Shortcoming)

Infinities

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- Provide a way to continue when exponent gets too large, $x^2 = \infty$, when x^2 overflows.
- When $c \neq 0$, $c/0 = \pm\infty$.
- Avoid special case checking, $1/(x + 1/x)$, a better formula for $x/(x^2 + 1)$, with infinities, there is no need for checking the special case $x = 0$.

NaN

NaNs (not a number)

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Provide a way to continue in situations like

Operation	NaN Produced By
+	$\infty + (-\infty)$
$*$	$0 * \infty$
/	0/0, ∞/∞
REM	x REM 0, ∞ REM y
sqrt	sqrt(x) when $x < 0$

Example for NaN

The function `zero(f)` returns a zero of a given quadratic polynomial `f`.

If

$$f = x^2 + x + 1,$$

$d = 1 - 4 < 0$, thus $\sqrt{d} = NaN$ and

$$\frac{-b \pm \sqrt{d}}{2a} = NaN,$$

no zeros.

Denormalized numbers

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When $e = e_{\min} - 1$ and the bits in the fraction are $b_2, b_3, ..., b_t$, the number being represented is $0.b_2b_3...b_t \times 2^{e+1}$ (no hidden bit)

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- Guarantee the relation: $x = y \iff x - y = 0$
- Allow gradual underflow. Without denormals, the spacing abruptly changes from $\beta^{-t+1}\beta^{e_{\min}}$ to $\beta^{e_{\min}}$, which is a factor of β^{t-1}.

Example for denormalized numbers

Complex division

$$\frac{a+ib}{c+id} = \frac{ac+bd}{c^2+d^2} + i\frac{bc-ad}{c^2+d^2}.$$

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Underflows when a, b, c, and d are small.

Example for denormalized numbers

Smith's formula

$$\frac{a+b(d/c)}{c+d(d/c)} + i\frac{b-a(d/c)}{c+d(d/c)} \qquad \text{if } |d| < |c|$$

$$\frac{b+a(c/d)}{d+c(c/d)} + i\frac{-a+b(c/d)}{d+c(c/d)} \qquad \text{if } |d| \geq |c|$$

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For $a = 2\beta^{e_{\min}}$, $b = \beta^{e_{\min}}$, $c = 4\beta^{e_{\min}}$, and $d = 2\beta^{e_{\min}}$, the result is 0.5 with denormals ($a + b(d/c) = 2.5\beta^{e_{\min}}$) or 0.4 without denormals ($a + b(d/c) = 2\beta^{e_{\min}}$).

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It is typical for denormalized numbers to guarantee error bounds for arguments all the way down to $\beta^{e_{\min}}$.

IEEE floating-point representations

Exponent	Fraction	Represents
$e = e_{\min} - 1$	$f = 0$	± 0
$e = e_{\min} - 1$	$f \neq 0$	$0.f \times 2^{e_{\min}}$
$e_{\min} \leq e \leq e_{\max}$		$1.f \times 2^{e}$
$e = e_{\max} + 1$	$f = 0$	$\pm\infty$
$e = e_{\max} + 1$	$f \neq 0$	NaN

Examples (IEEE single precision)

- 1 10000001 11100000000000000000000
  represents: $-1.111_2 \times 2^{129-127} = -7.5_{10}$
- 0 00000000 11000000000000000000000
  represents: $0.11_2 \times 2^{-126}$
- 0 11111111 00100000000000000000000
  represents: NaN
- 1 11111111 00000000000000000000000
  represents: $-\infty$.

Underflow

An arithmetic operation produces a number with an exponent that is too small to be represented in the system.

Example.
In single precision,

$$a = 3.0 \times 10^{-30},$$

$a * a$ underflows.
By default, it is set to zero.

Overflow

An arithmetic operation produces a number with an exponent that is too large to be represented in the system.

Example.
In single precision,

$$a = 3.0 \times 10^{30},$$

$a * a$ overflows.
In IEEE standard, the default result is ∞.

Avoiding unnecessary underflow and overflow

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Given $x = (a, b)^T$, $a = 1.0 \times 10^{30}$, $b = 1.0$, compute
$c = \|x\|_2 = \sqrt{a^2 + b^2}$.

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scaling: $s = \max\{|a|, |b|\} = 1.0 \times 10^{30}$

$a \leftarrow a/s$ (1.0),

$b \leftarrow b/s$ (1.0×10^{-30})

$t = \sqrt{a * a + b * b}$ (1.0)

$c \leftarrow t * s$ (1.0×10^{30})

Example: Computing 2-norm of a vector

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Avoid multiple loops:
searching for the largest; Scaling; Summing.

Example: Computing 2-norm of a vector

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$$\sqrt{x_1^2 + x_2^2 + ... + x_n^2}$$

Efficient and robust:

Avoid multiple loops:
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Result: One single loop

Technique: Dynamic scaling

Example: Computing 2-norm of a vector

```
scale = 0.0;
ssq = 1.0;
for i=1 to n
   if (x(i) != 0.0)
      if (scale<abs(x(i))
         tmp = scale/x(i);
         ssq = 1.0 + ssq*tmp*tmp;
         scale = abs(x(i));
      else
         tmp = x(i)/scale;
         ssq = ssq + tmp*tmp;
      end
   end
end
nrm2 = scale*sqrt(ssq);
```

Correctly rounded operations

Correctly rounded means that result must be the same as if it were computed exactly and then rounded, usually to the nearest floating-point number. For example, if $\oplus$ denotes the floating-point addition, then given two floating-point numbers a and b,

$$a \oplus b = \mathrm{fl}(a + b).$$

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Example
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$a = 1.234 \times 10^0$ and $b = 5.678 \times 10^{-3}$

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$\beta = 10$, $t = 4$
$a = 1.234 \times 10^0$ and $b = 5.678 \times 10^{-3}$
Exact: $a + b = 1.239678$
Floating-point: $\mathrm{fl}(a + b) = 1.240 \times 10^0$

Correctly rounded operations

IEEE standards require the following operations are correctly rounded:

- arithmetic operations $+$, $-$, $*$, and $/$
- square root and remainder
- conversions of formats (binary, decimal)

Outline

Rounding error

Due to finite precision arithmetic, a computed result must be rounded to fit storage format.

Example

$\beta = 10, p = 4$ ($u = 0.5 \times 10^{-3}$)

$a = 1.234 \times 10^{0}$, $b = 5.678 \times 10^{-3}$

$x = a + b = 1.239678 \times 10^{0}$ (exact)

$\hat{x} = \mathrm{fl}(a + b) = 1.240 \times 10^{0}$

the result was rounded to the nearest computer number.

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Rounding error: $\mathrm{fl}(a + b) = (a + b)(1 + \epsilon)$, $|\epsilon| \leq u$.

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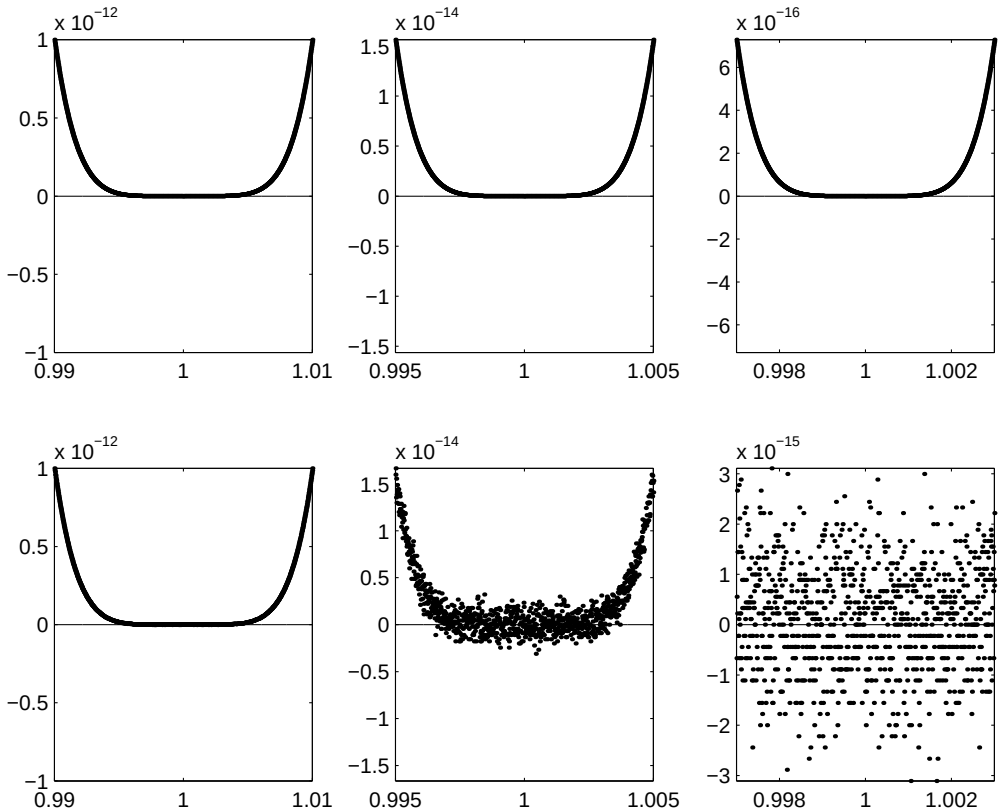
the result was rounded to the nearest computer number.

Rounding error: $\mathrm{fl}(a + b) = (a + b)(1 + \epsilon)$, $|\epsilon| \leq u$.

$1.240 = 1.239678(1 + 2.59... \times 10^{-4})$, $|2.59... \times 10^{-4}| < u$

Effect of rounding errors

Top: $y = (x-1)^6$
Bottom: $y = x^6 - 6x^5 + 15x^4 - 20x^3 + 15x^2 - 6x + 1$



Two ways of evaluating the polynomial $(x-1)^6$

Real to floating-point

```
double x = 0.1;
```

What is the value of x stored?

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What is the value of x stored?

$$1.0 \times 10^{-1} = 1.10011001100110011001\ldots \times 2^{-4}$$

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$$1.0 \times 10^{-1} = 1.10011001100110011001100110011... \times 2^{-4}$$

Decimal 0.1 cannot be exactlly represented in binary. It must be rounded to

$$\begin{aligned} & 1.10011001100...11001101\mathbf{0} \times 2^{-4} \\ > \; & 1.10011001100...11001100110011... \end{aligned}$$

slightly larger than 0.1.

Real to floating-point

```
double x, y, h;
x = 1/2;
h = 0.1;

for i=1 to 5
   x = x + h;
end
y = 1.0 - x;
```

$$y > 0 \quad \text{or} \quad y < 0 \quad \text{or} \quad y = 0?$$

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```

$$y > 0 \quad \text{or} \quad y < 0 \quad \text{or} \quad y = 0?$$

Answer: $y \approx 1.1 \times 10^{-16} > 0$

Real to floating-point (cont.)

Why?

$$\begin{aligned} 0.5 &= 1.00000000...00 \times 2^{-1} \\ h &= 0.00110011...11010 \times 2^{-1} \end{aligned}$$

Real to floating-point (cont.)

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$$\begin{aligned} 0.5 &= 1.00000000...00 \times 2^{-1} \\ h &= 0.00110011...11010 \times 2^{-1} \end{aligned}$$

Rounding errors in floating-point addition.

Integer to floating-point

Fallacy

Java converts an integer into its mathematically equivalent floating-point number.

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long k = 1801439850948199; \\
long d = k - (long)((double) k);
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Note $1801439850948199 = 2^{54} + 1$

$d = 0$?

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$d = 0$?

No, d = 1!

Integer to floating-point

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$$\begin{aligned} k &= 1.00...0001 \times 2^{54} \\ (\texttt{double})\, k &= 1.00...00 \times 2^{54} \end{aligned}$$

Truncation error

When an infinite series is approximated by a finite sum, truncation error is introduced.
Example. If we use

$$1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \cdots + \frac{x^n}{n!}$$

to approximate

$$e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \cdots + \frac{x^n}{n!} + \cdots,$$

then the truncation error is

$$\frac{x^{n+1}}{(n+1)!} + \frac{x^{n+2}}{(n+2)!} + \cdots.$$

Discretization error

When a continuous problem is approximated by a discrete one, discretization error is introduced.
Example. From the expansion

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!}f''(\xi),$$

for some $\xi \in [x, x+h]$, we can use the following approximation:

$$y_h(x) = \frac{f(x+h) - f(x)}{h} \approx f'(x).$$

The discretization error is $E_{\text{dis}} = |f''(\xi)|h/2$.

Example

Let $f(x) = e^x$, compute $y_h(1)$.

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The discretization error is

$$E_{\text{dis}} = \frac{h}{2}|f''(\xi)| \leq \frac{h}{2}e^{1+h} \approx \frac{h}{2}e \quad \text{for small} \quad h.$$

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The computed $y_h(1)$:

$$\widehat{y}_h(1) = \frac{(e^{(1+h)(1+\epsilon_1)}(1+\epsilon_2) - e(1+\epsilon_3))(1+\epsilon_4)}{h}(1+\epsilon_5),$$

$|\epsilon_i| \leq u$.

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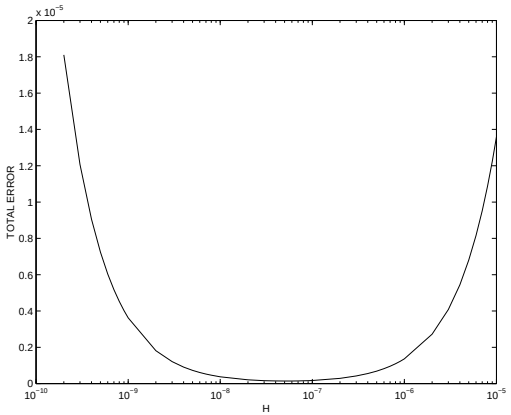
$|\epsilon_i| \leq u$.
The rounding error is

$$E_{\text{round}} = \widehat{y}_h(1) - y_h(1) \approx \frac{7u}{h}e.$$

Example (cont.)

The total error:

$$E_{\text{total}} = E_{\text{dis}} + E_{\text{round}} \approx \left(\frac{h}{2} + \frac{7u}{h} \right) e.$$



Total error in the computed $y_h(1)$.

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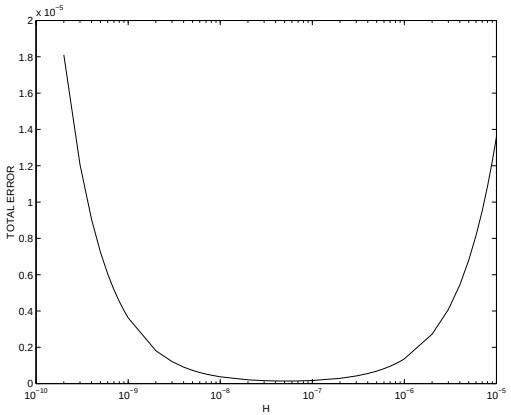

Total error in the computed $y_h(1)$.

The optimal h: $h_{\text{opt}} = \sqrt{12u} \approx \sqrt{u}$.

Outline

Backward errors

Recall that

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The computed sum (result) is the exact sum of slightly different a and b (inputs).

Example

$\beta = 10, p = 4$ $(u = 0.5 \times 10^{-3})$
$a = 1.234 \times 10^{0}, b = 5.678 \times 10^{-3}$
$a \oplus b = 1.240 \times 10^{0}, a + b = 1.239678$

$$1.240 = 1.239678(1 + 2.59... \times 10^{-4}), |2.59... \times 10^{-4}| < u$$

$$1.240 = a(1 + 2.59... \times 10^{-4}) + b(1 + 2.59... \times 10^{-4})$$

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Backward errors (cont.)

A general example

$$s_n = x_1 \oplus x_2 \oplus \cdots \oplus x_n$$

The computed result $(x_1 \oplus \cdots \oplus x_n)$ is the exact result of the problem with slightly perturbed data. $(x_1(1+\eta_1), ..., x_n(1+\eta_n))$.
Backward errors:
$|\eta_1| \leq 1.06(n-1)u$
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If the backward errors are small, then we say that the algorithm is backward stable.

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The result is sensitive to the perturbation in the data.

Perturbation analysis

Example: $a + b$

$$\begin{aligned} & \frac{|a(1+\delta_a) + b(1+\delta_b) - (a+b)|}{|a+b|} \\ \leq \quad & \frac{|a| + |b|}{|a+b|}\,\delta, \quad \delta = \max(\delta_a, \delta_b). \end{aligned}$$

Perturbation analysis

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$$\leq \frac{|a| + |b|}{|a+b|}\,\delta, \quad \delta = \max(\delta_a, \delta_b).$$

Condition number: $(|a| + |b|)/|a+b|$, magnification of the relative error.

$$\frac{\text{relative error in result}}{\text{relative error in data}} \leq \text{cond}$$

Condition number is a measurement (an upper bound) of the sensitivity of the problem to changes in data.

Example

Two methods for calculating $z(x + y)$:

$$z \otimes x \oplus z \otimes y \quad \text{and} \quad z \otimes (x \oplus y)$$

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$x = 1.002, y = -0.9958, z = 3.456$
Exact $z(x+y) = 2.14272 \times 10^{-2}$
$z \otimes (x \oplus y) = \mathrm{fl}(3.456 * 6.200 \times 10^{-3})$
$= 2.143 \times 10^{-2}$
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More than 200 times!

Example (cont.)

Backward error analyses

$$
\begin{aligned}
& z \otimes x \oplus z \otimes y \\
= \; & (zx(1+\epsilon_1) + zy(1+\epsilon_2))(1+\epsilon_3) \\
= \; & z(1+\epsilon_3)(x(1+\epsilon_1) + y(1+\epsilon_2)), \; |\epsilon_i| \leq u
\end{aligned}
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Example (cont.)

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\end{aligned}
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Both methods are backward stable.

Example (cont.)

Perturbation analysis

$$
\begin{aligned}
& z(1+\delta_z)(x(1+\delta_x)+y(1+\delta_y)) \\
\approx\ & zx(1+\delta_z+\delta_x)+zy(1+\delta_z+\delta_y) \\
=\ & z(x+y)+zx(\delta_z+\delta_x)+zy(\delta_z+\delta_y) \\
=\ & z(x+y)(1+(\delta_z+\delta_x)+(\delta_y-\delta_x)/(x/y+1))
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& \frac{|z(1+\delta_z)(x(1+\delta_x)+y(1+\delta_y))-z(x+y)|}{|z(x+y)|} \\
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The condition number can be large if $y \approx -x$ and $\delta_x \neq \delta_y$.

Example (cont.)

Forward error analysis

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$$
\frac{|(z \otimes x \oplus z \otimes y) - z(x+y)|}{|z(x+y)|} \leq \left(2 + \frac{2}{|\frac{x}{y}+1|}\right) u
$$

Example (cont.)

Forward error analysis (cont.)

$$z \otimes (x \oplus y) \approx z(x+y)(1+\epsilon_1+\epsilon_3), \quad |\epsilon_i| \leq u$$

$$\frac{|z \otimes (x \oplus y) - z(x+y)|}{|z(x+y)|} \leq 2u$$

Summary

$$\text{forward error} \leq \text{cond} \cdot \text{backward error}$$

- If we can prove the algorithm is stable, in other words, the backward errors are small, say, no larger than the measurement errors in data, then we know that large forward errors are due to the ill-conditioning of the problem.
- If we know the problem is well-conditioned, then large forward errors must be caused by unstable algorithm.
- Condition number is an upper bound. It is possible that a well-designed stable algorithm can produce good results even the problem is ill-conditioned.

Example revisited

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Exact $z(x + y) = 2.14272 \times 10^{-2}$

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Cancellation in subtracting two computed (contaminated) numbers. (Catastrophic)

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Cancellation in subtracting two original (not contaminated) numbers. (Benign)

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Cancellation in subtracting two original (not contaminated) numbers. (Benign)

Catastrophic cancellation v.s. benign cancellation.

A classic example of avoiding cancellation

Solving quadratic equation

$$ax^2 + bx + c = 0$$

Text book formula:

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

Computational method:

$$x_1 = \frac{2c}{-b - \text{sign}(b)\sqrt{b^2 - 4ac}}, \quad x_2 = \frac{c}{ax_1}$$

Question

Suppose $\beta = 10$ and $t = 8$ (single precision), solve

$$ax^2 + bx + c = 0,$$

where

$$a = 1, \quad b = -10^5, \quad \text{and} \quad c = 1,$$

using the both methods.

Outline

Fallacies

- Cancellation in the subtraction of two nearly equal numbers is always bad.
- The final computed answer from an algorithm cannot be more accurate than any of the intermediate quantities, that is, errors cannot cancel.
- Arithmetic much more precise than the data it operates upon is needless and wasteful.
- Classical formulas taught in school and found in handbooks and software must have passed the Test of Time, not merely withstood it.

Summary

- A computer number system is determined by four parameters: Base, precision, $e_{\min}$, and $e_{\max}$
- IEEE floating-point standards, single precision and double precision. Special quantities: Denormals, $\pm\infty$, NaN, ± 0, and their binary representations.
- Error measurements: Absolute and relative errors, unit of roundoff, unit in the last place (ulp)
- Sources of errors: Rounding error (computational error), truncation error (mathematical error), discretization error (mathematical error). Total error (combination of rounding error and mathematical errors)
- Issues in floating-point computation: Overflow, underflow, cancellations (benign and catastrophic)
- Error analysis: Forward and backward errors, sensitivity of a problem and stability of an algorithm