Elements of Floating-point Arithmetic

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Outline

Representing floating-point numbers

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

Examples

1.00×10^{-1}

$t = 3$ (trailing zeros count), $\beta = 10$, $e = -1$

1.234×10^{2}

$t = 4$, $\beta = 10$, $e = 2$

1.10011×2^{-4}

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

Characteristics

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

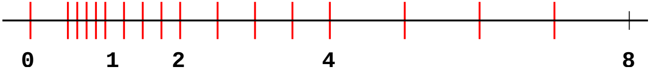
- base β (also called radix)
- precision t
- exponent range $e_{\text{min}} \leq e \leq e_{\text{max}}$

Some properties

A floating-point number system is

- discrete (not continuous)
- not equally spaced throughout
- finite

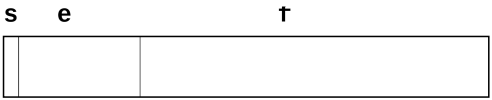
Example. The 33 points in a small system: $\beta = 2$, $t = 3$, $e_{\min} = -1$, and $e_{\max} = 2$. (Negative part not shown.)



In general, how many numbers in a system: β, t, $e_{\min}$, $e_{\max}$?

Storage

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



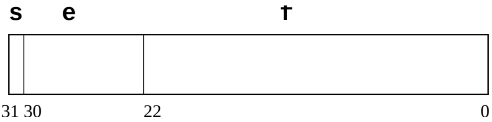
sign (1 bit)
exponent (depends on the range)
fraction (depends on the precision)

Standards

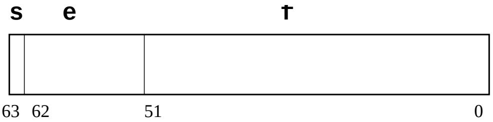
In order for a memory representation to be useful, there must be a standard.

IEEE floating-point standards:

single precision



double precision



Machine precision

A real number representing the accuracy.

Machine precision

Denoted by ϵ_M, defined as the distance between 1.0 and the next larger floating-point number, which is 0.0...01 $\times \beta^0$.

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($= \beta^0$) and β are equally spaced: 1.0...000, 1.0...001, 1.0...010, ..., 1.1...111.)

Machine precision (cont.)

How would you compute the underlying machine precision?

The smallest ϵ such that $1.0 + \epsilon > 1.0$.

For $\beta = 2$:

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

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. (Try to convert decimal 0.1 into binary.)

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);

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.

Unit of roundoff u

When $\beta = 2$, $u = 2^{-t}$.
How would you compute u?

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

```
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

Hidden bit and biased representation

Since the base is 2 (binary), the integer bit is always 1. This bit is not stored and called *hidden bit*.

The exponent is stored using the biased representation. In single precision, the bias is 127. In double precision, the bias is 1023.

Example

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

$$\texttt{0 01111011 10011001100110011001101}$$

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 $e_{\text{min}} - 1$.

Signed zeros

Signed zeros: ± 0

Binary representation:

`X 00000000 00000000000000000000000`

- When testing for equal, $+0 = -0$, so the simple test `if (x == 0)` is predictable whether x is $+0$ or -0.

Infinities

Infinities: $\pm\infty$

Binary Representation:

`X 11111111 00000000000000000000000`

- 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)

Binary representation:

`X 11111111 nonzero fraction`

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

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

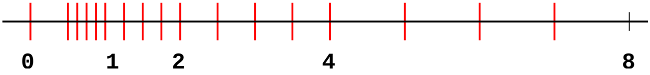
no zeros.

Denormalized numbers

Denormalized Numbers

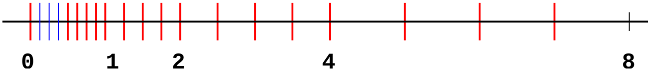
The small system: $\beta = 2$, $t = 3$, $e_{\text{min}} = -1$, $e_{\text{max}} = 2$

Without denormalized numbers (negative part not shown)



With (six) denormalized numbers (negative part not shown)

$$0.01 \times 2^{-1},\ 0.10 \times 2^{-1},\ 0.11 \times 2^{-1}$$



Denormalized numbers

Binary representation:

`X 00000000 nonzero fraction`

When $e = e_{\text{min}} - 1$ 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)

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

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.

Avoiding unnecessary underflow and overflow

Sometimes, underflow and overflow can be avoided by using a technique called scaling.

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

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

Compute

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

Efficient and robust:

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

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,

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

Example
$\beta = 10$, $t = 4$
$a = 1.234 \times 10^0$ 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)

Rounding error

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

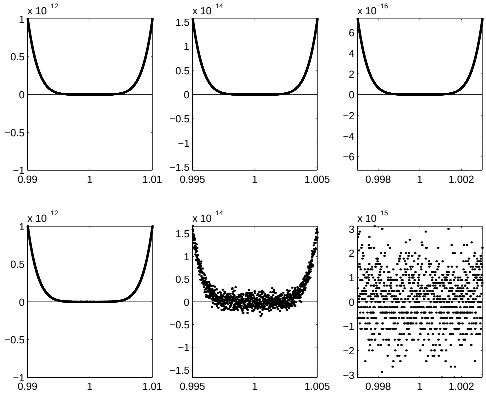
Example
$\beta = 10$, $p = 4$ ($u = 0.5 \times 10^{-3}$)
$a = 1.234 \times 10^0$, $b = 5.678 \times 10^{-3}$
$x = a + b = 1.239678 \times 10^0$ (exact)
$\hat{x} = \mathrm{fl}(a + b) = 1.240 \times 10^0$
the result was rounded to the nearest computer number.

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?

$$1.0 \times 10^{-1} = 1.100110011001100110011... \times 2^{-4}$$

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

$$\begin{array}{ll} & 1.10011001100...1100110\textcolor{red}{10} \times 2^{-4} \\ > & 1.10011001100...110011001100110011... \end{array}$$

slightly larger than 0.1.

Real to floating-point

```
double x, y, h;
x = 0.0;
h = 0.1;

for i=1 to 10
   x = x + h;
end
y = 1.0 - x;
```

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

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

Real to floating-point (cont.)

Why?

$$
\begin{aligned}
&i = 1\\
&x = h = 1.100...110011010 \times 2^{-4} > 1.0 \times 10^{-1}\\
&i = 2\\
&x = 1.100...110011010 \times 2^{-3} > 2.0 \times 10^{-1}\\
&i = 3\\
&x = 1.001...1001100110 \times 2^{-2}\\
&\rightarrow 1.001...10100 \times 2^{-2} > 3.0 \times 10^{-1}\\
&i = 4\\
&x = 1.100...1100110110 \times 2^{-2}\\
&\rightarrow 1.100...110011010 \times 2^{-2} > 4.0 \times 10^{-1}
\end{aligned}
$$

Real to floating-point (cont.)

$$
\begin{aligned}
&i = 5\\
&x = 1.000...0000\color{red}{010} \times 2^{-1}\\
&\rightarrow 1.000...0000 \times 2^{-1} = 5.0 \times 10^{-1}\\
&i = 6\\
&x = 1.001...100110011\color{red}{010} \times 2^{-1}\\
&\rightarrow 1.001...100110011 \times 2^{-1} < 6.0 \times 10^{-1}\\
&\vdots
\end{aligned}
$$

Rounding errors in floating-point addition.

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 $y_h(1)$.
The discretization error is

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

The computed $y_h(1)$:

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

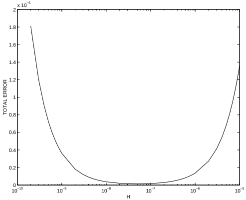
$|\epsilon_i| \leq u$.
The rounding error is

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

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 $y_h(1)$.

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

Backward errors

Recall that

$$a \oplus b = \mathrm{fl}(a+b) = (a+b)(1+\eta), \quad |\eta| \leq u$$

In other words,

$$a \oplus b = \tilde{a} + \tilde{b}$$

where $\tilde{a} = a(1+\eta)$ and $\tilde{b} = b(1+\eta)$, for $|\eta| \leq u$, are slightly different from a and b respectively.

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

Example

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

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

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

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

Example

Example: $a + b$

$a = 1.23$, $b = 0.45$, $s = a + b = 1.68$

Slightly perturbed
$\widehat{a} = a(1 + 0.01)$, $\widehat{b} = b(1 + 0.001)$, $\widehat{s} = \widehat{a} + \widehat{b} = 1.69275$

Relative perturbations in data (a and b) are at most 0.01.
Causing a relative change in the result $|\widehat{s} - s|/|s| \approx 0.0076$, which is about the same as the perturbation 0.01

The result is insensitive to the perturbation in data.

Example (cont.)

$a = 1.23$, $b = -1.21$, $s = a + b = 0.02$

Slightly perturbed
$\widehat{a} = a(1 + 0.01)$, $\widehat{b} = b(1 + 0.001)$, $\widehat{s} = \widehat{a} + \widehat{b} = 0.03109$

Relative perturbations in data (a and b) are at most 0.01.
Causing a relative change in the result $|\widehat{s} - s|/|s| \approx 0.5545$, which is more than 55 times as the perturbation 0.01

The result is sensitive to the perturbation in the data.

Example of stability/sensitivity

Compute the integrals

$$E_n = \int_0^1 x^n e^{x-1} dx, \qquad n = 1, 2, \dots.$$

Using integration by parts,

$$\int_0^1 x^n e^{x-1} dx = x^n e^{x-1}|_0^1 - \int_0^1 n x^{n-1} e^{x-1} dx,$$

or

$$E_n = 1 - nE_{n-1}, \qquad n = 2, \dots,$$

where $E_1 = 1/e$.

Example of stability/sensitivity

$$E_n = 1 - nE_{n-1}$$

Double precision

$$\begin{array}{lll} E_1 \approx 0.3679 & E_7 \approx 0.1124 & E_{13} \approx 0.0669 \\ E_2 \approx 0.2642 & E_8 \approx 0.1009 & E_{14} \approx 0.0627 \\ E_3 \approx 0.2073 & E_9 \approx 0.0916 & E_{15} \approx 0.0590 \\ E_4 \approx 0.1709 & E_{10} \approx 0.0839 & E_{16} \approx 0.0555 \\ E_5 \approx 0.1455 & E_{11} \approx 0.0774 & E_{17} \approx 0.0572 \\ E_6 \approx 0.1268 & E_{12} \approx 0.0718 & E_{18} \approx -0.0295 \end{array}$$

Apparently, $E_{18} > 0$.

Unstable algorithm or ill-conditioned problem?

Example of stability/sensitivity

$E_n = 1 - nE_{n-1}$

Perturbation analysis. Suppose that we perturb E_1:

$$\tilde{E}_1 = E_1 + \epsilon,$$

then $\tilde{E}_2 = 1 - 2\tilde{E}_1 = E_2 - 2\epsilon$.

In general,

$$\tilde{E}_n = E_n - n!\,\epsilon.$$

Thus this problem is ill-conditioned.

We can show that this algorithm is backward stable.

Example of stability/sensitivity

$E_{n-1} = (1 - E_n)/n$
Note that E_n goes to zero as n goes to ∞.
Start with $E_{40} = 0.0$

$E_{35} \approx 0.0270$	$E_{29} \approx 0.0323$	$E_{23} \approx 0.0401$
$E_{34} \approx 0.0278$	$E_{28} \approx 0.0334$	$E_{22} \approx 0.0417$
$E_{33} \approx 0.0286$	$E_{27} \approx 0.0345$	$E_{21} \approx 0.0436$
$E_{32} \approx 0.0294$	$E_{26} \approx 0.0358$	$E_{20} \approx 0.0455$
$E_{31} \approx 0.0303$	$E_{25} \approx 0.0371$	$E_{19} \approx 0.0477$
$E_{30} \approx 0.0313$	$E_{24} \approx 0.0385$	$E_{18} \approx 0.0501$

Example of stability/sensitivity

$E_{n-1} = (1 - E_n)/n$

Perturbation analysis. Suppose that we perturb E_n:

$$\tilde{E}_n = E_n + \epsilon,$$

then $\tilde{E}_{n-1} = E_{n-1} - \epsilon/n$.

In general,

$$\tilde{E}_k = E_k + \epsilon_k, \quad |\epsilon_k| = \frac{\epsilon}{n(n-1)...(k+1)}.$$

Thus this problem is well-conditioned.

Note that we view these two methods as two different problems, since they have different inputs and outputs.

Example `myexp`

Using the Taylor series

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

we write a function `myexp`:

```
oldy = 0.0;
y = 1.0;
term = 1.0;
k = 1;
while (oldy ~= y)
    term = term*(x/k);
    oldy = y;
    y = y + term;
    k = k + 1;
end
```

Example `myexp`

About the stopping criterion

- When x is negative, the terms have alternating signs, then it is guaranteed that the truncation error is smaller then the last term in the program.
- When x is positive, all the terms are positive, then it is not guaranteed that the truncation error is smaller than the last term in the program. For example, when $x = 678.9$, the last two digits of the computed result are inaccurate.

Example myexp

When $x = -7.8$

k	sum	term
1	1.00000000000000E+0	$-$7.80000000000000E+0
$\vdots$		
10	$-$1.32278417462171 5E+2	2.29711635560962E+2
11	9.74332180987908 6E+1	$-$1.62886432488682E+2
12	$-$6.54532143898915 1E+1	1.05876181117643E+2
$\vdots$		

Example myexp

k	sum	term
26	1.092489579672046E−4	3.880079670499995E−04
⋮		
49	4.097349789682480E−4	−8.4826327262 1995E−20
50	4.097349789682479E−4	1.3232907052 9031E−20

The MATLAB result:

$$4.097349789797868\mathrm{E}-4$$

Example `myexp`

An explanation

When $k = 10$, the absolute value of the intermediate sum reaches the maximum, about 10^{+2}, that is, the ulp is about 10^{-13}. After that, cancellation occurs, so the final result is about 10^{-4}. We expect the error in the final result is 10^{-13}, in other words, ten digit accuracy.

Cancellation magnifies the relative error.

An accurate method.

Break x into the integer part m and the fraction part f. Compute e^m using multiplications, then compute e^f when $-1 < f < 0$ or $1/e^{-f}$ when $0 < f < 1$.

Using this method, the computed $e^{-7.8}$ is

$$4.0973497897978643\mathrm{E}-4$$

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:

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

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

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