Mathematical preliminaries and error analysis

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Outline

1. **Round-off errors and computer arithmetic**
   - IEEE standard floating-point format
   - Absolute and Relative Errors
   - Machine Epsilon
   - Loss of Significance

2. **Algorithms and Convergence**
   - Algorithm
   - Stability
   - Rate of convergence

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IEEE standard floating-point format

Example

What is the binary representation of $\frac{2}{3}$?

Solution: To determine the binary representation for $\frac{2}{3}$, we write

$$\frac{2}{3} = (0.a_1a_2a_3\ldots)_2.$$

Multiply by 2 to obtain

$$\frac{4}{3} = (a_1.a_2a_3\ldots)_2.$$

Therefore, we get $a_1 = 1$ by taking the integer part of both sides.

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Subtracting 1, we have

$$\frac{1}{3} = (0.a_2a_3a_4\ldots)_2.$$

Repeating the previous step, we arrive at

$$\frac{2}{3} = (0.101010\ldots)_2.$$

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IEEE standard floating-point format

- In the computational world, each representable number has only a fixed and finite number of digits.
- For any real number x, let

$$x = \pm 1.a_1 a_2 \cdots a_t a_{t+1} a_{t+2} \cdots \times 2^m,$$

denote the normalized scientific binary representation of x.
- In 1985, the IEEE (Institute for Electrical and Electronic Engineers) published a report called *Binary Floating Point Arithmetic Standard 754-1985*. In this report, formats were specified for single, double, and extended precisions, and these standards are generally followed by microcomputer manufactures using floating-point hardware.

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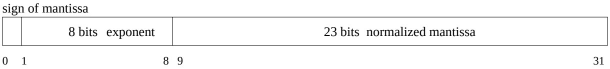
Single precision

- The single precision IEEE standard floating-point format allocates 32 bits for the normalized floating-point number $\pm q \times 2^m$ as shown in the following figure.



- The first bit is a sign indicator, denoted s. This is followed by an 8-bit exponent c and a 23-bit mantissa f.
- The base for the exponent and mantissa is 2, and the actual exponent is $c - 127$. The value of c is restricted by the inequality $0 \leq c \leq 255$.

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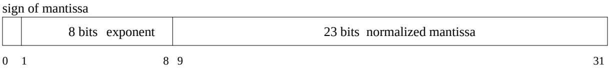

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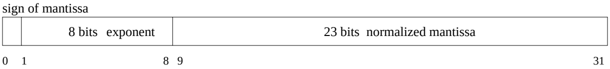

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Example

What is the decimal number of the machine number

$$0\underline{10000001}01000000000000000000000?$$

1. The leftmost bit is zero, which indicates that the number is positive.
2. The next 8 bits, 10000001, are equivalent to
$$c = 1 \cdot 2^7 + 0 \cdot 2^6 + \cdots + 0 \cdot 2^1 + 1 \cdot 2^0 = 129.$$
The exponential part of the number is $2^{129-127} = 2^2$.
3. The final 23 bits specify that the mantissa is
$$f = 0 \cdot (2)^{-1} + 1 \cdot (2)^{-2} + 0 \cdot (2)^{-3} + \cdots + 0 \cdot (2)^{-23} = 0.25.$$
4. Consequently, this machine number precisely represents the decimal number
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$$\begin{aligned} f &= 0\cdot(2)^{-1}+0\cdot(2)^{-2}+1\cdot(2)^{-3}+\cdots+1\cdot(2)^{-23} \\ &= 0.24999998807907105. \end{aligned}$$

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Summary

Above three examples

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0\underline{10000001}00111111111111111111111 & \Rightarrow & 4.99999523162842 \\
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- Only a relatively small subset of the real number system is used for the representation of all the real numbers.
- This subset, which are called the *floating-point numbers*, contains only rational numbers, both positive and negative.
- When a number can not be represented exactly with the fixed finite number of digits in a computer, a near-by floating-point number is chosen for approximate representation.

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The smallest positive number

Let $s = 0$, $c = 1$ and $f = 0$ which is equivalent to

$$2^{-126} \cdot (1 + 0) \approx 1.175 \times 10^{-38}$$

The largest number

Let $s = 0$, $c = 254$ and $f = 1 - 2^{-23}$ which is equivalent to

$$2^{127} \cdot (2 - 2^{-23}) \approx 3.403 \times 10^{38}$$

Definition

If a number x with $|x| < 2^{-126} \cdot (1 + 0)$, then we say that an *underflow* has occurred and is generally set to zero.
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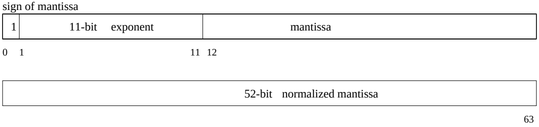
Double precision

- A floating point number in double precision IEEE standard format uses two words (64 bits) to store the number as shown in the following figure.



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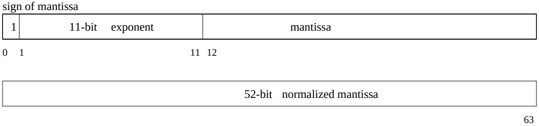

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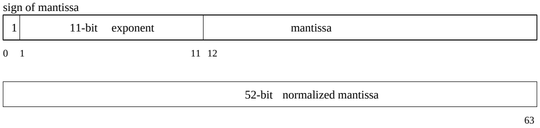

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Format of floating-point number

$$(-1)^s \times (1+f) \times 2^{c-1023}$$

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Let $s=0$, $c=1$ and $f=0$ which is equivalent to

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Let $s=0$, $c=2046$ and $f=1-2^{-52}$ which is equivalent to

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Chopping and rounding

For any real number x, let

$$x = \pm 1.a_1 a_2 \cdots a_t a_{t+1} a_{t+2} \cdots \times 2^m,$$

denote the normalized scientific binary representation of x.

1. **chopping:** simply discard the excess bits $a_{t+1}, a_{t+2}, \ldots$ to obtain

$$fl(x) = \pm 1.a_1 a_2 \cdots a_t \times 2^m.$$

2. **rounding:** add $2^{-(t+1)} \times 2^m$ to x and then chop the excess bits to obtain a number of the form

$$fl(x) = \pm 1.\delta_1 \delta_2 \cdots \delta_t \times 2^m.$$

In this method, if $a_{t+1} = 1$, we add 1 to a_t to obtain $fl(x)$, and if $a_{t+1} = 0$, we merely chop off all but the first t digits.

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The error results from replacing a number with its floating-point form is called *roundoff error* or *rounding error*.

Definition (Absolute Error and Relative Error)

If x is an approximation to the exact value $x^\star$, the absolute error is $|x^\star - x|$ and the relative error is $\frac{|x^\star - x|}{|x^\star|}$, provided that $x^\star \neq 0$.

Example

(a) If $x = 0.3000 \times 10^{-3}$ and $x^* = 0.3100 \times 10^{-3}$, then the absolute error is 0.1×10^{-4} and the relative error is 0.3333×10^{-1}.
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(b) If $x = 0.3000 \times 10^{4}$ and $x^* = 0.3100 \times 10^{4}$, then the absolute error is 0.1×10^{3} and the relative error is 0.3333×10^{-1}.

Definition (Roundoff error)

The error results from replacing a number with its floating-point form is called *roundoff error* or *rounding error*.

Definition (Absolute Error and Relative Error)

If x is an approximation to the exact value $x^\star$, the absolute error is $|x^\star - x|$ and the relative error is $\frac{|x^\star - x|}{|x^\star|}$, provided that $x^\star \neq 0$.

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Remark

As a measure of accuracy, the absolute error may be misleading and the relative error more meaningful.

Definition

The number x^* is said to approximate x to t significant digits if t is the largest nonnegative integer for which

$$\frac{|x - x^*|}{|x|} \leq 5 \times 10^{-t}.$$

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- If the floating-point representation $fl(x)$ for the number x is obtained by using t digits and chopping procedure, then the relative error is

$$\frac{|x - fl(x)|}{|x|} = \frac{|0.00\cdots 0 a_{t+1}a_{t+2}\cdots \times 2^m|}{|1.a_1a_2\cdots a_t a_{t+1}a_{t+2}\cdots \times 2^m|} = \frac{|0.a_{t+1}a_{t+2}\cdots|}{|1.a_1a_2\cdots a_t a_{t+1}a_{t+2}\cdots|} \times 2^{-t}.$$

The minimal value of the denominator is 1. The numerator is bounded above by 1. As a consequence

$$\left|\frac{x - fl(x)}{x}\right| \leq 2^{-t}.$$

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Absolute and Relative Errors

- If t-digit rounding arithmetic is used and
  - $a_{t+1} = 0$, then $fl(x) = \pm 1.a_1 a_2 \cdots a_t \times 2^m$. A bound for the relative error is

$$\frac{|x - fl(x)|}{|x|} = \frac{|0.a_{t+1}a_{t+2}\cdots|}{|1.a_1 a_2 \cdots a_t a_{t+1} a_{t+2} \cdots|} \times 2^{-t} \le 2^{-(t+1)},$$

    since the numerator is bounded above by $\frac{1}{2}$ due to $a_{t+1} = 0$.
  - $a_{t+1} = 1$, then $fl(x) = \pm(1.a_1 a_2 \cdots a_t + 2^{-t}) \times 2^m$. The upper bound for relative error becomes

$$\frac{|x - fl(x)|}{|x|} = \frac{|1 - 0.a_{t+1}a_{t+2}\cdots|}{|1.a_1 a_2 \cdots a_t a_{t+1} a_{t+2} \cdots|} \times 2^{-t} \le 2^{-(t+1)},$$

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Definition (Machine epsilon)

The floating-point representation, $fl(x)$, of x can be expressed as

$$fl(x) = x(1+\delta), \quad |\delta| \le \varepsilon_M, \tag{1}$$

where $\varepsilon_M = 2^{-t}$ is referred to as the *unit roundoff error* or *machine epsilon*.

Single precision IEEE standard floating-point format

The mantissa f corresponds to 23 binary digits (i.e., $t = 23$), the machine epsilon is

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The mantissa f corresponds to 52 binary digits (i.e., $t = 52$), the machine epsilon is

$$\varepsilon_M = 2^{-52} \approx 2.220 \times 10^{-16}.$$

which provides between 15 and 16 decimal digits of accuracy.

Summary of IEEE standard floating-point format

	single precision	double precision
ε_M	1.192×10^{-7}	2.220×10^{-16}
smallest positive number	1.175×10^{-38}	2.225×10^{-308}
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- Whenever two machine numbers x and y are to be combined arithmetically, the computer will produce $fl(x \odot y)$ instead of $x \odot y$.
- Under (1), the relative error of $fl(x \odot y)$ satisfies

$$fl(x \odot y) = (x \odot y)(1 + \delta), \quad \delta \leq \varepsilon_M, \tag{2}$$

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- But if x, y are not machine numbers, then they must first rounded to floating-point format before the arithmetic operation and the resulting relative error becomes

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Example

Let $x = 0.54617$ and $y = 0.54601$. Using rounding and four-digit arithmetic, then

- $x^* = fl(x) = 0.5462$ is accurate to four significant digits since

$$\frac{|x - x^*|}{|x|} = \frac{0.00003}{0.54617} = 5.5 \times 10^{-5} \leq 5 \times 10^{-4}.$$

- $y^* = fl(y) = 0.5460$ is accurate to five significant digits since

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But

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Since

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Loss of Significance

- One of the most common error-producing calculations involves the cancellation of significant digits due to the subtraction of nearly equal numbers or the addition of one very large number and one very small number.
- Sometimes, loss of significance can be avoided by rewriting the mathematical formula.

Example

The quadratic formulas for computing the roots of $ax^2 + bx + c = 0$, when $a \neq 0$, are

$$x_1 = \frac{-b + \sqrt{b^2 - 4ac}}{2a} \quad \text{and} \quad x_2 = \frac{-b - \sqrt{b^2 - 4ac}}{2a}.$$

Consider the quadratic equation $x^2 + 62.10x + 1 = 0$ and discuss the numerical results.

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Consider the quadratic equation $x^2 + 62.10x + 1 = 0$ and discuss the numerical results.

Solution

- Using the quadratic formula and 8-digit rounding arithmetic, one can obtain

$$x_1 = -0.01610723 \qquad \text{and} \qquad x_2 = -62.08390.$$

- Now we perform the calculations with 4-digit rounding arithmetic. First we have

$$\sqrt{b^2 - 4ac} = \sqrt{62.10^2 - 4.000} = \sqrt{3856 - 4.000} = 62.06,$$

and

$$fl(x_1) = \frac{-62.10 + 62.06}{2.000} = \frac{-0.04000}{2.000} = -0.02000.$$

The relative error in computing x_1 is

$$\frac{|fl(x_1) - x_1|}{|x_1|} = \frac{|-0.02000 + 0.01610723|}{|-0.01610723|} \approx 0.2417 \leq 5\times 10$$

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- In calculating x_2,
$$fl(x_2) = \frac{-62.10 - 62.06}{2.000} = \frac{-124.2}{2.000} = -62.10,$$
and the relative error in computing x_2 is
$$\frac{|fl(x_2) - x_2|}{|x_2|} = \frac{|-62.10 + 62.08390|}{|-62.08390|} \approx 0.259 \times 10^{-3} \leq 5 \times 10^{-4}.$$
- In this equation, $b^2 = 62.10^2$ is much larger than $4ac = 4$. Hence b and $\sqrt{b^2 - 4ac}$ become two nearly equal numbers. The calculation of x_1 involves the subtraction of two nearly equal numbers.
- To obtain a more accurate 4-digit rounding approximation for x_1, we change the formulation by rationalizing the numerator, that is,
$$x_1 = \frac{-2c}{b + \sqrt{b^2 - 4ac}}.$$

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Then

$$fl(x_1) = \frac{-2.000}{62.10 + 62.06} = \frac{-2.000}{124.2} = -0.01610.$$

The relative error in computing x_1 is now reduced to 6.2×10^{-4} ∎

Example

Let

$$\begin{aligned} p(x) &= x^3 - 3x^2 + 3x - 1, \\ q(x) &= ((x-3)x + 3)x - 1. \end{aligned}$$

Compare the function values at $x = 2.19$ with using three-digit arithmetic.

Then

$$fl(x_1) = \frac{-2.000}{62.10 + 62.06} = \frac{-2.000}{124.2} = -0.01610.$$

The relative error in computing x_1 is now reduced to 6.2×10^{-4} ■

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Solution

Use 3-digit and rounding for $p(2.19)$ and $q(2.19)$.

$$\begin{aligned}
\hat{p}(2.19) &= ((2.19^3 - 3 \times 2.19^2) + 3 \times 2.19) - 1 \\
&= ((10.5 - 14.4) + 3 \times 2.19) - 1 \\
&= (-3.9 + 6.57) - 1 \\
&= 2.67 - 1 = 1.67
\end{aligned}$$

and

$$\begin{aligned}
\hat{q}(2.19) &= ((2.19 - 3) \times 2.19 + 3) \times 2.19 - 1 \\
&= (-0.81 \times 2.19 + 3) \times 2.19 - 1 \\
&= (-1.77 + 3) \times 2.19 - 1 \\
&= 1.23 \times 2.19 - 1 \\
&= 2.69 - 1 = 1.69.
\end{aligned}$$

With more digits, one can have

$$p(2.19) = g(2.19) = 1.685159$$

Hence the absolute errors are

$$|p(2.19) - \hat{p}(2.19)| = 0.015159$$

and

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Definition (Algorithm)

An algorithm is a procedure that describes a finite sequence of steps to be performed in a specified order.

Example

Give an algorithm to compute $\sum_{i=1}^{n} x_i$, where n and $x_1, x_2, \ldots, x_n$ are given.

Algorithm

INPUT $n, x_1, x_2, \ldots, x_n$.
OUTPUT $SUM = \sum_{i=1}^{n} x_i$.
Step 1. Set $SUM = 0$. (Initialize accumulator.)
Step 2. For $i = 1, 2, \ldots, n$ do
  Set $SUM = SUM + x_i$. (Add the next term.)
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Definition (Stable)

An algorithm is called stable if small changes in the initial data of the algorithm produce correspondingly small changes in the final results.

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An algorithm is unstable if small errors made at one stage of the algorithm are magnified and propagated in subsequent stages and seriously degrade the accuracy of the overall calculation.

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Example

Consider the following recurrence algorithm

$$\begin{cases} x_0 = 1, & x_1 = \frac{1}{3} \\ x_{n+1} = \frac{13}{3}x_n - \frac{4}{3}x_{n-1} \end{cases}$$

for computing the sequence of $\{x_n = (\frac{1}{3})^n\}$. This algorithm is unstable.

A Matlab implementation of the recurrence algorithm gives the following result.

n	x_n	x_n^*	RelErr
8	4.57247371e-04	4.57247371e-04	4.4359e-10
10	5.08052602e-05	5.08052634e-05	6.3878e-08
12	5.64497734e-06	5.64502927e-06	9.1984e-06
14	6.26394672e-07	6.27225474e-07	1.3246e-03
15	2.05751947e-07	2.09075158e-07	1.5895e-02
16	5.63988754e-08	6.96917194e-08	1.9074e-01
17	-2.99408028e-08	2.32305731e-08	2.2889e+00

The error present in x_n is multiplied by $\frac{13}{3}$ in computing x_{n+1}. For example, the error will be propagated with a factor of $\left(\frac{13}{3}\right)^{14}$ in computing x_{15}. Additional roundoff errors in computing $x_2, x_3, \ldots$ may also be propagated and added to that of x_{15}.

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Matlab program

```
n = 30;
x = zeros(n,1);
x(1) = 1;
x(2) = 1/3;
for ii = 3:n
    x(ii) = 13 / 3 * x(ii-1) - 4 / 3 * x(ii-2);
    xn = (1/3)^(ii-1);
    RelErr = abs(xn-x(ii)) / xn;
    fprintf(’x(%2.0f) = %20.8d, x_ast(%2.0f) = %20.8d,’, ...
        ’RelErr(%2.0f) = %14.4d \n’, ii,x(ii),ii,xn,ii,RelErr);
end
```

Definition

Suppose $\{\beta_n\} \to 0$ and $\{x_n\} \to x^*$. If $\exists\ c > 0$ and an integer $N > 0$ such that

$$|x_n - x^*| \le c|\beta_n|, \quad \forall\ n \ge N,$$

then we say $\{x_n\}$ converges to x^* with rate of convergence $O(\beta_n)$, and write $x_n = x^* + O(\beta_n)$.

Example

Compare the convergence behavior of $\{x_n\}$ and $\{y_n\}$, where

$$x_n = \frac{n+1}{n^2}, \quad \text{and} \quad y_n = \frac{n+3}{n^3}.$$

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$$x_n = \frac{n+1}{n^2}, \quad \text{and} \quad y_n = \frac{n+3}{n^3}.$$

Solution:

Note that both

$$\lim_{n\to\infty} x_n = 0 \quad \text{and} \quad \lim_{n\to\infty} y_n = 0.$$

Let $\alpha_n = \frac{1}{n}$ and $\beta_n = \frac{1}{n^2}$. Then

$$\begin{aligned} |x_n - 0| &= \frac{n+1}{n^2} \leq \frac{n+n}{n^2} = \frac{2}{n} = 2\alpha_n, \\ |y_n - 0| &= \frac{n+3}{n^3} \leq \frac{n+3n}{n^3} = \frac{4}{n^2} = 4\beta_n. \end{aligned}$$

Hence

$$x_n = 0 + O(\frac{1}{n}) \quad \text{and} \quad y_n = 0 + O(\frac{1}{n^2}).$$

This shows that $\{y_n\}$ converges to 0 much faster than $\{x_n\}$. ■