MATH 3795 Lecture 2. Floating Point Arithmetic

Dmitriy Leykekhman

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Goals

- Basic understanding of computer representation of numbers
- Basic understanding of floating point arithmetic
- Consequences of floating point arithmetic for numerical computation

In everyday life we use decimal representation of numbers. For example

1234.567

for us means

 $1 * 10^4 + 2 * 10^3 + 3 * 10^2 + 4 * 10^0 + 5 * 10^{-1} + 6 * 10^{-2} + 7 * 10^{-3}.$

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More generally

$$\dots d_j \dots d_1 d_0 \dots d_{-1} \dots d_{-i} \dots$$

represents

 $\cdots d_j * 10^j + \cdots + d_1 * 10^1 + d_0 * 10^0 + d_{-1} * 10^{-1} + \cdots + d_{-i} * 10^{-i} + \cdots$

Let $\beta \geq 2$ be an integer. For every $x \in \mathbb{R}$ there exist integers e and $d_i \in \{0, \ldots, \beta - 1\}$, $i = 0, 1, \ldots$, such that

$$x = sign(x) \left(\sum_{i=0}^{\infty} d_i \beta^{-i}\right) \beta^e.$$
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Example

$$\frac{11}{2} = 5 * 10^{0} + 5 * 10^{-1} = (5.5)_{10},$$

$$\frac{11}{2} = 1 * 2^{2} + 0 * 2^{1} + 1 * 2^{0} + 1 * 2^{-1}$$

$$= (1 * 2^{0} + 0 * 2^{-1} + 1 * 2^{-2} + 1 * 2^{-3}) * 2^{2} = (1.011)_{2} * 2^{2}.$$

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The distance between 1 and the next largest floating pt. number is β^{1-m}. Half this number, ε_{mach} = ½β^{1-m}, is called machine precision or unit roundoff. (We will see later why). The spacing between the floating pt. numbers in [1,β] is β^{-(m-1)}. The spacing between the floating pt. numbers in [β^e, ββ^e] is β^{-(m-1)}β^e.

IEEE Floating Point Numbers

- Almost all every modern computer implements the IEEE binary ($\beta = 2$) floating point standard.
- ▶ IEEE single precision floating point numbers are stored in 32 bits.
- ▶ IEEE double precision floating point numbers are stored in 64 bits.
- How these numbers are stored is quite interesting (clever), but a little too involved to get into here. See the references [G91,O01,SUN] given at the end of this lecture.

	Here	are	some	important	numbers.
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Common Name	(Approximate) Equivalent Value		
	Single Precision	Double Precision	
Unit roundoff	$2^{-24} \approx 6.e - 8$	$2^{-53} \approx 1.1e - 16$	
Maximum normal number	3.4e + 38	1.7e + 308	
Minimum positive normal number	1.2e - 38	2.3e - 308	
Maximum subnormal number	1.1e - 38	2.2e - 308	
Minimum positive subnormal number	1.5e - 45	5.0e - 324	

Rounding

Given a real number x we define

fl(x) = normalized floating point number closest to x.

A floating point number \bar{x} closest to x is obtained by rounding. If

$$x = sign(x) \left(\sum_{i=0}^{\infty} d_i \beta^{-i}\right) \beta^e,$$

then

$$\mathsf{fl}(x) = \begin{cases} sign(x) \left(\sum_{i=0}^{m-1} d_i \beta^{-i}\right) \beta^e, & \text{if } d_m < \frac{1}{2}\beta, \\ sign(x) \left(\sum_{i=0}^{m-1} d_i \beta^{-i} + \beta^{-(m-1)}\right) \beta^e, & \text{if } d_m \ge \frac{1}{2}\beta. \end{cases}$$

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Example Let $\beta = 10$, m = 3. Then

$$\begin{array}{rcl} {\sf fl}(1.234*10^{-1}) & = & 1.23*10^{-1}, \\ {\sf fl}(1.235*10^{-1}) & = & 1.24*10^{-1}, \\ {\sf fl}(1.295*10^{-1}) & = & 1.30*10^{-1}. \end{array}$$

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Note, there may be two floating point numbers closest to x. fl(x) picks one of them. For example, let $\beta = 10$, m = 3. Then 1.235 - 1.24 = 0.005, but also 1.235 - 1.23 = 0.005. See [G91,O01,SUN] for more details on 'breaking' ties.

Rounding Error

Theorem

If x is a number within the range of floating point numbers and $|x| \in [\beta^e, \beta^{e+1})$, then the absolute error between x and the floating point number fl(x) closest to x is given by

$$|\mathsf{fl}(x) - x| \le \frac{1}{2}\beta^{e(1-m)}$$

and, provided $x \neq 0$, the relative error is given by

$$\frac{\mathsf{fl}(x) - x|}{|x|} \le \frac{1}{2}\beta^{1-m}.$$
(2)

The number

$$\epsilon_{\rm mach} \stackrel{\rm \tiny def}{=} \frac{1}{2} \beta^{1-m}$$

is called machine precision or unit roundoff.

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is $\beta^{-(m-1)}\beta^e$. Hence if $x \in [\beta^e, \beta^{e+1})$, then the floating point number \bar{x} closest to x satisfies $|\bar{x} - x| \leq \frac{1}{2}\beta^{-(m-1)}\beta^e$. Since $x \geq \beta^e$,

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 $\mathsf{fl}(x)$ is a floating point number closest to $x = \left(\sum_{i=0}^{\infty} d_i \beta^{-i}\right) \beta^e$, $d_0 > 0$?

$$\begin{split} & \mathsf{Examples} \\ & \mathsf{Let} \ \beta = 10, \ m = 3, \ \mathsf{thus} \ \epsilon_{\mathsf{mach}} = 5 * 10^{-3}. \\ & |\mathsf{fl}(1.234 * 10^{-1}) - 1.234 * 10^{-1}| = 0.0004, \\ & \frac{|\mathsf{fl}(1.234 * 10^{-1}) - 1.234 * 10^{-1}|}{1.234 * 10^{-1}} = \frac{0.0004}{1.234 * 10^{-1}} \approx 3.2 * 10^{-3}, \\ & |\mathsf{fl}(1.295 * 10^{-1}) - 1.295 * 10^{-1}| = 0.0005, \\ & \frac{|\mathsf{fl}(1.295 * 10^{-1}) - 1.295 * 10^{-1}|}{1.295 * 10^{-1}} = \frac{0.0005}{1.295 * 10^{-1}} \approx 3.9 * 10^{-3}. \end{split}$$

Floating Point Arithmetic

Let □ represent one of the elementary operations +, -, *, /. If x̄ and ȳ are floating point numbers, then x̄□ȳ may not be a floating point number.

Example: $\beta = 10$, m = 4: $1.234 + 2.751 * 10^{-1} = 1.5091$. What is the computed value for $\bar{x} \Box \bar{y}$?

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In IEEE floating point arithmetic the result of the computation x̄□ȳ is equal to the floating point number that is nearest to the exact result x̄□ȳ. Therefore we use fl(x̄□ȳ) to denote the result of the computation x̄□ȳ

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- ▶ Model for the computation of $\bar{x}\Box\bar{y}$, where \Box is one of the elementary operations +, -, *, /.
 - 1. Given floating point numbers \bar{x} and \bar{y} .
 - 2. Compute $\bar{x}\Box\bar{y}$ exactly.
 - 3. Round the exact result $\bar{x} \Box \bar{y}$ to the nearest floating point number and normalize the result.

Example cont.: $1.234 + 2.751 * 10^{-1} = 1.5091$. Comp. result: 1.509 The actual implementation of the elementary operations is more sophisticated. For more details see [DG91,O01].

Floating Point Arithmetic (Cont.)

Given two numbers \bar{x}, \bar{y} in *floating point format*, the computed result satisfies

$$\frac{\mathsf{fl}(\bar{x}\Box\bar{y}) - (\bar{x}\Box\bar{y})|}{\bar{x}\Box\bar{y}} \leq \epsilon_{\mathsf{mach}}.$$

Examples

Consider the floating point system $\beta = 10$ and m = 4.

- i. $\bar{x} = 2.552 * 10^3$ and $\bar{y} = 2.551 * 10^3$. $\bar{x} - \bar{y} = 0.001 * 10^3 = 1.000 * 10^0$. In this case $\bar{x} - \bar{y}$ is a floating point number and nothing needs to done; no error occurs in the subtraction of \bar{x} , \bar{y} .
- ii. $\bar{x} = 2.552 * 10^3$ and $\bar{y} = 2.551 * 10^2$. $\bar{x} - \bar{y} = 2.2969 * 10^3$. This is not a floating point number. The floating point number nearest to $\bar{x} - \bar{y}$ is fl $(\bar{x} - \bar{y}) = 2.297 * 10^3$.

$$\frac{|\mathbf{fl}(\bar{x}-\bar{y})-(\bar{x}-\bar{y})|}{|\bar{x}-\bar{y}|} = \frac{|2.297*10^3 - 2.2969*10^3|}{2.2969*10^3} \approx 4.4*10^{-5} \\ < \epsilon_{\mathrm{mach}} = 5*10^{-4}.$$

Floating Point Arithmetic: Cancellation

For the previous result on the error between $\bar{x}\Box\bar{y}$ and the computed $\mathrm{fl}(\bar{x}\Box\bar{y})$ only holds if \bar{x}, \bar{y} in floating point format. What happens when we operate with numbers that are not in floating point format?

Example

Consider the floating point system $\beta = 10$ and m = 4. Subtract the numbers $x = 2.5515052 * 10^3$ and $y = 2.5514911 * 10^3$.

- 1. Compute the floating point numbers \bar{x} and \bar{y} nearest to x and y, respectively: $\bar{x} = 2.552 * 10^3$ and $\bar{y} = 2.551 * 10^3$.
- 2. Compute $\bar{x} \bar{y}$ exactly: $\bar{x} \bar{y} = 0.001 * 10^3$.
- 3. Round the exact result $\bar{x} \bar{y}$ to the nearest floating point number: fl(0.001 * 10³) = 0.001 * 10³. Normalize the number: fl(0.001 * 10³) = 1.000. The last digits are filled with (spurious) zeros.

The exact result is $2.5515052 * 10^3 - 2.5514911 * 10^3 = 1.410 * 10^{-2}$. The relative error between exact and computed solution is

$$\frac{|1.000 - 1.410 * 10^{-2}|}{1.410 * 10^{-2}} \approx 70 \gg \epsilon_{\rm mach} = 5 * 10^{-4}.$$

Note that this large error is not due the computation of $fl(\bar{x} - \bar{y})$. The large error is caused by the rounding of x and y at the beginning.

Floating Point Arithmetic: Cancellation (cont.)

 To analyze the analyze the error incurred by the subtraction of two numbers, the following representation is useful:
 For every x ∈ IR, there exists ε with |ε| ≤ ε_{mach} such that

$$\mathsf{fl}(x) = x(1+\epsilon).$$

Note that if $x \neq 0$, then the previous identity is satisfied for $\epsilon \stackrel{\text{def}}{=} (\mathfrak{fl}(x) - x)/x$. The bound $|\epsilon| \leq \epsilon_{\text{mach}}$ follows from (2).

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$$fl(x) = x(1 + \epsilon_1), \quad fl(y) = y(1 + \epsilon_2).$$

Moreover $fl(fl(x) - fl(y)) = (fl(x) - fl(y))(1 + \epsilon_3)$, with $|\epsilon_3| \le \epsilon_{mach}$.

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Thus,

$$fl(fl(x) - fl(y)) = (fl(x) - fl(y))(1 + \epsilon_3) = [x(1 + \epsilon_1) - y(1 + \epsilon_2)](1 + \epsilon_3) = (x - y)(1 + \epsilon_3) + (x\epsilon_1 - y\epsilon_2)(1 + \epsilon_3)$$

and, if $x - y \neq 0$, then the relative error is given by

$$\frac{\left|\mathsf{fl}(\mathsf{fl}(x) - \mathsf{fl}(y)) - (x - y)\right|}{|x - y|} = \left|\epsilon_3 + \frac{x\epsilon_1 - y\epsilon_2}{x - y}(1 + \epsilon_3)\right| \tag{3}$$

If $\epsilon_1 \epsilon_2 \neq 0$ and x - y is small, the quantity on the rhs could be $\gg \epsilon_{mach}$.

- Similar analysis can be carried out for +, -, *, /.
- ► Catastrophic cancelation can only occur with +, -.
- Catastrophic cancelation can only occur if one subtracts two numbers which are not both in floating point format and which have the same sign and are of approximately the same size, see (3), or if one adds two numbers which are not both in floating point format, which have opposite sign and their absolute values of approximately the same size.

	x	$1 - \cos \theta$
	0.500000	0.122417E + 00
	0.125000	0.780231E - 02
Further of 1 and (a) many a 0	0.312500E - 01	0.488222E - 03
Evaluation of $1 - \cos(x)$ hear $x \equiv 0$.	0.781250E - 02	0.305176E - 04
(All computations were done using single precision Fortran.)	0.195312E - 02	0.190735E - 05
	0.488281E - 03	0.119209E - 06
	0.122070E - 03	0.
	0.305176E - 04	0.
	0.762939E - 05	0.
	0.190735E - 05	0.

Since $\cos(0) = 1$ we expect catastrophic cancelation. If x = 0.122070E - 03, then

$$1 - \cos(x) \approx 1.000000000 - 0.9999999254.....$$

= 0.0000000745..... = 7.45054.....e - 09
$$1 - \mathsf{fl}(\cos(x)) \approx 1.000000 - \mathsf{fl}(\underbrace{9.999999}_{7 \text{ digits}}9254.....*10^{-1})$$

= 1.000000 - 1.000000 = 0.

Two alternatives for small |x|.

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Since
$$\cos^2(x) + \sin^2(x) = 1$$
 it holds that $1 - \cos(x) = \frac{\sin^2(x)}{(1 + \cos(x))}$.

The formula $\sin^2(x)/(1 + \cos(x))$ avoids subtraction of two number that are not in floating point format and are almost the same (recall that we consider the case |x| small).

Two alternatives for small |x|.

- Since cos²(x) + sin²(x) = 1 it holds that 1 − cos(x) = sin²(x)/(1 + cos(x)). The formula sin²(x)/(1 + cos(x)) avoids subtraction of two number that are not in floating point format and are almost the same (recall that we consider the case |x| small).
- ▶ The Leibnitz criterion says that if the series $S = \sum_{i=1}^{\infty} (-1)^i c_i$, $c_i \ge 0$, converges, then $|S \sum_{i=1}^{n} (-1)^i c_i| < c_{n+1}$. If we apply this to the Taylor expansion of cos(x),

$$\cos(x) = 1 - \frac{x^2}{2} + \frac{x^4}{4!} - \frac{x^6}{6!} + \frac{x^8}{8!} \pm \dots,$$

then

$$\cos(x) - \left(1 - \frac{x^2}{2} + \frac{x^4}{4!} - \frac{x^6}{6!}\right) \Big| < \frac{x^8}{8!}$$

After some rearrangements we can use the approximation

$$1 - \cos(x) \approx \frac{x^2}{2} \left(1 - \frac{x^2}{12} + \frac{x^4}{360} \right)$$

and we know that the difference is less than $x^8/(8!)$ which allows us to control the error of the approximation.

x	$1 - \cos$	$\sin^2/(1+\cos)$	Taylor
0.500000	0.122417	0.122417	0.122418
0.125000	0.780231E - 02	0.780233E - 02	0.780233E - 02
0.312500E - 01	0.488222E - 03	0.488241E - 03	0.488242E - 03
0.781250E - 02	0.305176E - 04	0.305174E - 04	0.305174E - 04
0.195312E - 02	0.190735E - 05	0.190735E - 05	0.190735E - 05
0.488281E - 03	0.119209E - 06	0.119209E - 06	0.119209E - 06
0.122070E - 03	0.	0.745058E - 08	0.745058E - 08
0.305176E - 04	0.	0.465661E - 09	0.465661E - 09
0.762939E - 05	0.	0.291038E - 10	0.291038E - 10
0.190735E - 05	0.	0.181899E - 11	0.181899E - 11
0.476837E - 06	0.	0.113687E - 12	0.113687E - 12
0.119209E - 06	0.	0.710543E - 14	0.710543E - 14
0.298023E - 07	0.	0.444089E - 15	0.444089E - 15

Computations were performed using single precision Fortran.

• The roots of the quadratic equation $ax^2 + bx + c = 0$ are given by

$$x_{\pm} = \left(-b \pm \sqrt{b^2 - 4ac}\right) / (2a).$$

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When a = 5 * 10⁻⁴, b = 100, and c = 5 * 10⁻³ the computed (using single precision Fortran) first root is

$$x_{+} = 0.$$

Cannot be exact, since x = 0 is a solution of the quadratic equation if and only if c = 0.

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- A remedy is the following reformulation of the formula for x_+ :

$$\frac{-b + \sqrt{b^2 - 4ac}}{2a} = \frac{1}{2a} \frac{\left(-b + \sqrt{b^2 - 4ac}\right)\left(-b - \sqrt{b^2 - 4ac}\right)}{-b - \sqrt{b^2 - 4ac}} = \frac{2c}{-b - \sqrt{b^2 - 4ac}}$$

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Here the subtraction of two almost equal numbers is avoided and the computation using this formula gives $x_{+} = -0.5E - 04$.

► A 'stable' (see later for a description of stability) formula for both roots $x_1 = \left(-b - \operatorname{sign}(b)\sqrt{b^2 - 4ac}\right)/(2a), \quad x_2 = c/(ax_1).$

Summary

- Introduced how numbers are represented on a computer.
- Only a small set of numbers can be represented on the computer.
- ► The relative error between x ≠ 0 and its nearest floating point number fl(x) is

$$\frac{|\mathsf{fl}(x) - x|}{|x|} \le \epsilon_{\mathsf{mach}} \stackrel{\text{\tiny def}}{=} \frac{1}{2}\beta^{1-m}$$

- Introduced basic properties of floating point arithmetic.
- Catastrophic cancellation can occur if one subtracts [adds] two numbers which are not both in floating point format and which have the same [opposite] sign and [their absolute values] are of approximately the same size.

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