MA579H Scientific Computing

Lectures 2 & 3: Errors and Floating-point Arithmetic

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Lecture outline

- Sources of errors
- Floating-point arithmetic
- Rounding error

Sources of errors

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- Modeling error: Earth is modeled as a sphere, idealizing its true shape.
- Measurement error: Computation of the radius r is based on empirical measurements.
- Truncation error: Computation of π requires truncation of infinite process.
- Rounding error: Input data and results of arithmetic operations are rounded in computer.

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Scientific computing analyzes errors that arise during computation. A small error in the input may be amplified

- by a problem (bad problem)
- by an algorithm (bad algorithm) during computation.

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Relative error is considered for analysis of rounding errors.

Anomalous arithmetic

Arithmetic operations on computers are inexact and can produce surprising results. For example, MATLAB produces

$$
\begin{aligned}
(\frac{4}{3} - 1) * 3 - 1 &= -2.2204 \times 10^{-16} \\
5 \times \frac{(1 + \exp(-50)) - 1}{(1 + \exp(-50)) - 1} &= \textbf{NaN} \\
\frac{\log(\exp(750))}{100} &= \textbf{Inf}
\end{aligned}
$$

Normalized floating-point representation

Let $x \in \mathbb{R}$ be nonzero and $\beta > 1$ be an integer. Then we have the normalized floating-point representation

$$x = \pm(\cdot d_1 d_2 \cdots d_t \cdots)_\beta \times \beta^e, \; 0 \leq d_i < \beta, \;\; d_1 \neq 0, \;\; e \in \mathbb{Z}.$$

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$$f = (\cdot d_1 d_2 \cdots d_t \cdots)_\beta = \sum_{j=1}^{\infty} \frac{d_j}{\beta^j}.$$

Note that $0 < f \leq 1$ and $x = \pm f \times \beta^e$ is a unique representation. The number of digits allowed in f is called precision of the floating-point representation, which in the present case is infinite.

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The fraction $f := (\cdot d_1 d_2 \cdots d_t)_\beta = \sum_{j=1}^{t} \frac{d_j}{\beta^j} \leq 1 - \beta^{-t} < 1.$

Example: $(\cdot 101)_2 \times 2^2 = (1 \times 2^{-1} + 0 \times 2^{-2} + 1 \times 2^{-3}) \times 2^2 = 5/2.$

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Note that $\#F(\beta, t, e_{\min}, e_{\max}) = 2(\beta - 1)\beta^{t-1} \times (e_{\max} - e_{\min} + 1) + 1.$

Floating-Point System

Underflow threshold (smallest positive floating point number):

- $\texttt{realmin} := (\cdot 10\cdots 0)_\beta \times \beta^{e_{\min}} = \beta^{e_{\min}-1}$

Overflow threshold (largest positive floating point number):

- $\texttt{realmax} := (\cdot(\beta-1)\cdots(\beta-1))_\beta \times \beta^{e_{\max}} = (1-\beta^{-t})\beta^{e_{\max}}$

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Machine epsilon/precision: **eps** $:= \beta^{1-t}$.

- **eps** $= (\cdot 10\cdots 01)_\beta \times \beta^1 - (\cdot 10\cdots 0)_\beta \times \beta^1 = \beta^{1-t}$

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For MATLAB we have the following

	Binary	Decimal
eps	2^{-52}	2.2204×10^{-16}
realmin	2^{-1022}	2.2251×10^{-308}
realmax	$(2-\texttt{eps}) \times 2^{1023}$	1.7977×10^{308}

IEEE single precision floating-point representation

IEEE specifies $F(2, t, e_{\min}, e_{\max})$ as follows.

sign (1 bit)	exponent (8 bits)	mantissa (23 bits)

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$\#$ Exponents: $2^8 = 256$ Largest exponent: $2^8 - 1 = 255$
Exponent range: $0 \leq b \leq 255$ and $-127 \leq e \leq 128$

$$x = (-1)^s \times (1 \cdot d_1 \cdots d_{23})_2 \times 2^{b-127} \text{ where } e = b - 127.$$

Effective exponent range: $-126 \leq e \leq 127$ as $e = -127$ is reserved for ± 0 and $e = 128$ for $\pm\texttt{inf}$ and $\texttt{NaN}$

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$\texttt{eps} = 2^{-23} \approx 1.192 \times 10^{-7}$, $\texttt{realmin} = 2^{-126} \approx 1.175 \times 10^{-38}$, $\texttt{realmax} = (2 - \texttt{eps}) \times 2^{127} \approx 3.403 \times 10^{38}$

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Gap between floating-point numbers

Let $x \in F(\beta, t, e_{\min}, e_{\max})$ be given by $x = (\cdot d_1 d_2 \cdots d_t)_\beta \times \beta^e$.

Define $\mathrm{ulp}(x) := \beta^{e-t}$. Then $\mathrm{next}(x) := x + \mathrm{ulp}(x)$ is the next floating point number larger than x, that is, $\mathrm{next}(x)$ is the smallest floating-point number larger than x. Hence x and $\mathrm{next}(x)$ are consecutive floating-point numbers.

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This shows that $\mathrm{next}(x) - x = \mathrm{ulp}(x) = \beta^{e-t}$. So, if x is a large number then e is large which implies large gap between x and $\mathrm{next}(x)$. Hence the gap between consecutive floating-point number is nonuniform.

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Example: Consider $x \in F(10, 4, -30, 30)$ given by $x = 10^{-9} = .1000 \times 10^{-8}$. Then $\mathrm{ulp}(x) = 10^{-8-4} = 10^{-12}$ and $\mathrm{next}(x) - x = 10^{-12}$.

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Next, consider $y = 10^{15} = .1000 \times 10^{16}$. Then $\mathrm{ulp}(y) = 10^{16-4} = 10^{12}$ and $\mathrm{next}(y) - y = 10^{12}$.

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$$\frac{\mathrm{next}(x) - x}{x} = \frac{\beta^{e-t}}{(.d_1 \cdots d_t)_\beta \times \beta^e} \leq \beta^{1-t} = \mathrm{eps}.$$

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$$\text{Define } \mathrm{fl}(x) := \begin{cases} x_L, & \text{round down} \\ x_R, & \text{round up} \\ x_L \text{ or } x_R \text{ whichever is closer to } x, & \text{round to nearest} \end{cases}$$

Rounding error

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Proof: Let $x = (\cdot d_1 d_2 \cdots d_t \cdots)_\beta \times \beta^e$. Set $\delta := \frac{\mathrm{fl}(x)-x}{x}$. Then $\mathrm{fl}(x) = x(1+\delta)$. Note that $|\mathrm{fl}(x) - x| \leq \beta^{e-t}$ for chopping, and $|\mathrm{fl}(x) - x| \leq \beta^{e-t}/2$ for round to nearest. Also $x \geq \beta^{e-1}$.

Rounding error

Unit roundoff: $\mathbf{u} := \begin{cases} \beta^{1-t} & \text{round down,} \\ \frac{1}{2}\beta^{1-t}, & \text{round to nearest} \end{cases}$

Theorem: Let $\mathrm{fl} : \mathbb{R} \to F(\beta, t, L, U),\ x \longmapsto \mathrm{fl}(x)$. Then

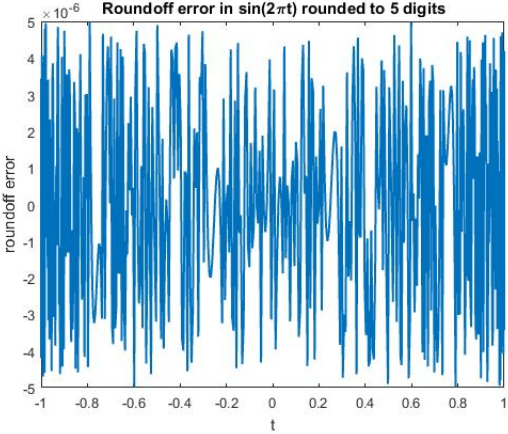
$$\mathrm{fl}(x) = x(1+\delta) \text{ with } |\delta| \leq \mathbf{u}.$$

Proof: Let $x = (\cdot d_1 d_2 \cdots d_t \cdots)_\beta \times \beta^e$. Set $\delta := \frac{\mathrm{fl}(x)-x}{x}$. Then $\mathrm{fl}(x) = x(1+\delta)$. Note that $|\mathrm{fl}(x) - x| \leq \beta^{e-t}$ for chopping, and $|\mathrm{fl}(x) - x| \leq \beta^{e-t}/2$ for round to nearest. Also $x \geq \beta^{e-1}$.
Hence

$$|\delta| \leq \frac{|\mathrm{fl}(x) - x|}{|x|} \leq \begin{cases} \beta^{1-t} & \text{round down,} \\ \frac{1}{2}\beta^{1-t}, & \text{round to nearest.} \end{cases}$$

Rounding error

Let $f(t) := \sin(2\pi t)$ for $t \in [0, 1]$. Consider $F(10, 5, -10, 10)$. Then `t = 0:.001:1; tt = sin(2*pi*t); rt = round(tt, 5);` `roundoff = tt-rt; plot(tt, roundoff, 'LineWidth',1.5)` produces the following



Floating-point arithmetic

Arithmetic model: If $x, y \in F(\beta, t, e_{\min}, e_{\max})$ and $\oplus \in \{+, -, \times, /\}$ and $\mathbf{u}$ is the unit roundoff then

$$\mathrm{fl}(x \oplus y) = (x \oplus y)(1 + \delta), \text{ where } |\delta| \le \mathbf{u}.$$

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Loss of significance (or cancellation): If x and y are not floating-point numbers then we have to start with $\widehat{x} := \mathrm{fl}(x) = x(1+\delta_1)$ and $\widehat{y} := \mathrm{fl}(y) = y(1+\delta_2)$. Then

$$\widehat{x} \pm \widehat{y} = x(1+\delta_1) \pm y(1+\delta_2) = (x \pm y)\left(1 + \frac{x\delta_1 \pm y\delta_2}{x \pm y}\right)$$

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Now, if x and y have the same sign then the relative error $\left|\frac{x\delta_1 + y\delta_2}{x+y}\right| \leq |\delta_1| + |\delta_2| \leq 2\mathbf{u}$ is small but $\left|\frac{x\delta_1 - y\delta_2}{x-y}\right|$ can be arbitrarily large when $x - y$ is very small.

Example

Problem: Solve $ax^2 + bx + c = 0$, where $a, b, c \in \mathbb{R}$

Classical method: Naive use of the formula yields

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

does not avoid subtraction whereas the modified formula

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

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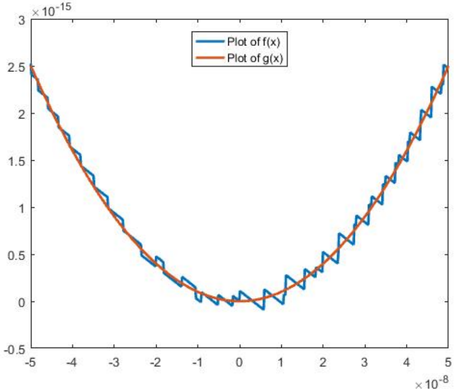
For $10^{-3}x^2 + 10^7 x + 3 = 0$, the classical method in MATLAB yields $x_1 = -10^{10}$ and $x_2 = 0$ whereas the modified method yields the accurate answer $x_1 = -10^{10}$ and $x_2 = -3.0 \times 10^{-7}$.

Example

Evaluate $f(x) := e^x - \cos(x) - x$ for $-5 \times 10^{-8} \leq x \leq 5 \times 10^{-8}$.



Approximation of $f(x)$ using Taylor series avoids cancellation

$$f(x) = 1 + x + \frac{x^2}{2!} + \cdots - (1 - \frac{x^2}{2!} + \frac{x^4}{4!} + \cdots) - x \approx x^2 + x^3/6 = g(x).$$

Cancellation and remedy

Let $f(x) := \dfrac{1-\cos(x)}{\sin(x)}$ for $x \neq 0$. If a is close to 0 then evaluation of $f(x)$ at a causes cancellation as $\cos(a) \approx 1$. The remedy is to rewrite $f(x)$ as

$$f(x) = \frac{1-\cos(x)}{\sin(x)} = \frac{\sin(x)}{1+\cos(x)}$$

which avoids cancellation at $a \approx 0$.

Rounding error of differentiation

Recall that $D_h f(x) := \dfrac{f(x+h) - f(x)}{h}$ approximates $f'(x)$. For small h, $D_h f(x)$ exhibits cancellation error due to rounding, which is magnified by the division of h.

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$$\widehat{D_h f(x)} = \frac{\widehat{f(x+h)} - \widehat{f(x)}}{h} = \frac{f(x+h)(1+\delta(x+h)) - f(x)(1+\delta(x))}{h}$$

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$$
\begin{aligned}
\widehat{D_h f(x)} &= \frac{\widehat{f(x+h)} - \widehat{f(x)}}{h} = \frac{f(x+h)(1+\delta(x+h)) - f(x)(1+\delta(x))}{h} \\
&= D_h f(x) + \frac{\delta(x+h)f(x+h) - \delta(x)f(x)}{h}.
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This shows that the rounding error

$$e_r(x,h) := \frac{|\delta(x+h)f(x+h) - \delta(x)f(x)|}{h} \leq \frac{\mathbf{eps}(|f(x+h)| + |f(x)|)}{h}.$$

Rounding error of differentiation

Recall that $E(x,h) := |f'(x) - D_h f(x)|$. By Taylor theorem

$$f(x+h) = f(x) + f'(x)h + h^2 f''(\xi)/2 \Longrightarrow E(x,h) = h|f''(\xi)|/2.$$

The best accuracy is obtained when $E(x,h) = e_r(x,h)$. Ignoring the constant terms gives

$$h \approx \mathbf{eps}/h \Longrightarrow h \approx \sqrt{\mathbf{eps}}$$

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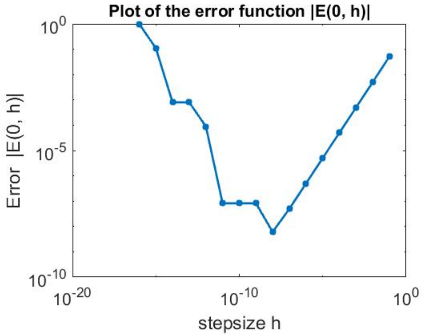
For $f(x) = e^x$, we have



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