# Unavoidable Errors in Computing

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## Overview (1)

- Digital representation of numbers
  - ▷ Size limits
  - ▷ Resolution limits
  - ▷ The floating point number line

- Floating point arithmetic
  - ▷ roundoff
  - ▷ machine precision

## Overview (2)

- Implications for routine computation
  - ▷ Use “close enough” instead of “equals”
  - ▷ loss of significance for addition
  - ▷ catastrophic cancellation for subtraction
- Truncation error
  - ▷ Demonstrate with Taylor series
  - ▷ Order Notation

## What's going on here?

Spontaneous generation of an insignificant digit:

```
>> format long e  % display lots of digits
>> 2.6 + 0.2
ans =
        2.800000000000000e+00
>> ans + 0.2
ans =
        3.000000000000000e+00
>> ans + 0.2
ans =
        3.200000000000001e+00     Why does the least significant digit appear?
>> 2.6 + 0.6
ans =
        3.200000000000000e+00     Why does the small error not show up here?
```

## Bits, Bytes, and Words

| base 10 | conversion | base 2 |
|---|---|---|
| 1 | $1 = 2^0$ | 0000 0001 |
| 2 | $2 = 2^1$ | 0000 0010 |
| 4 | $4 = 2^2$ | 0000 0100 |
| 8 | $8 = 2^3$ | 0000 1000 |
| 9 | $8 + 1 = 2^3 + 2^0$ | 0000 1001 |
| 10 | $8 + 2 = 2^3 + 2^1$ | 0000 1010 |
| 27 | $16 + 8 + 2 + 1 = 2^4 + 2^3 + 2^1 + 2^0$ | $\underbrace{\text{0001 1011}}_{\text{one byte}}$ |

## Digital Storage of Integers (1)

As a prelude to discussing the binary storage of floating point values, first consider the binary storage of integers.

- Integers can be exactly represented by base 2
- Typical size is 16 bits
- $2^{16} = 65536$ is largest 16 bit integer
- $[-32768, 32767]$ is range of 16 bit integers in twos complement notation
- 32 bit and larger integers are available

## Digital Storage of Integers (2)

**Note:** Unless explicitly specified otherwise, all mathematical calculations in MATLAB use double precision floating point numbers.

**Expert's Note:** The built-in `int8`, `int16`, `int32`, `uint8`, `uint16`, and `uint32` classes are used to reduce memory usage for very large data sets.

## Digital Storage of Integers (3)

Let $b$ be a binary digit, i.e. 1 or 0

$$(bbbb)_2 \quad \Longleftrightarrow \quad |2^3|2^2|2^1|2^0|$$

The **rightmost bit** is the **least significant bit** (LSB)

The **leftmost bit** is the **most significant bit** (MSB)

**Example:**

$$\begin{aligned}(1001)_2 &= 1 \times 2^3 \ + \ 0 \times 2^2 \ + \ 0 \times 2^1 \ + \ 1 \times 2^0 \\ &= 8 + 0 + 0 + 1 = 9\end{aligned}$$

## Digital Storage of Integers (4)

**Limitations**:

- A *finite* number of bits are used to store each value in computer memory.
- *Limiting the number of bits limits the size* of integer that can be represented

| | | | |
|---|---|---|---|
| largest 3 bit integer: | $(111)_2$ | $= 4 + 2 + 1 = 7$ | $= 2^3 - 1$ |
| largest 4 bit integer: | $(1111)_2$ | $= 8 + 4 + 2 + 1 = 15$ | $= 2^4 - 1$ |
| largest 5 bit integer: | $(11111)_2$ | $= 16 + 8 + 4 + 2 + 1 = 31$ | $= 2^5 - 1$ |
| largest $n$ bit integer: | | | $= 2^n - 1$ |

## Digital Storage of Floating Point Numbers (1)

Numeric values with non-zero fractional parts are stored as **floating point numbers**.

All floating point values are represented with a normalized scientific notation[1].

**Example:**

$$12.2792 = \underbrace{0.123792}_{\text{Mantissa}} \times 10^{2} \xleftarrow{} \text{Exponent}$$

[1]The IEEE Standard on Floating Point arithmetic defines a normalized *binary* format. Here we use a simplified *decimal* (base ten) format that, while abusing the standard notation, expresses the essential ideas behind the decimal to binary conversion.

## Digital Storage of Floating Point Numbers (2)

Floating point values have a fixed number of bits allocated for storage of the mantissa and a fixed number of bits allocated for storage of the exponent.

Two common precisions are provided in numeric computing languages

| Precision | Bits for mantissa | Bits for exponent |
|---|---|---|
| Single | 23 | 8 |
| Double | 53 | 11 |

## Digital Storage of Floating Point Numbers (3)

A double precision (64 bit) floating point number can be schematically represented as

$$\overbrace{\underbrace{b}_{\text{sign}}\ \ \underbrace{bb\ldots\ldots bbb}_{\substack{\text{52 bit value}\\ \text{of mantissa}}}\,\underbrace{bbbbbbbbbbb}_{\substack{\text{11 bit exponent,}\\ \text{including sign}}}}^{\text{64 bits}}$$

The finite number of bits in the exponent limits the magnitude or *range* of the floating point numbers.

The finite number of bits in the mantissa limits the number of significant digits or the *precision* of the floating point numbers.

## Digital Storage of Floating Point Numbers (4)

The floating point mantissa is expressed in powers of $\frac{1}{2}$

$$\left(\frac{1}{2}\right)^0 = 1 \quad \text{is not used}$$

$$\left(\frac{1}{2}\right)^1 = 0.5 \qquad \left(\frac{1}{2}\right)^2 = 0.25 \qquad \left(\frac{1}{2}\right)^3 = 0.125 \qquad \cdots$$

## Digital Storage of Floating Point Numbers (5)

**Algorithm 5.1 Convert Floating-Point to Binary**

```
$r_0 = \mathsf{x}$
for $k = 1, 2, \ldots, m$
    if $r_{k-1} \geq 2^{-k}$
        $b_k = 1$
        $r_k = r_{k-1} - 2^{-k}$
    else
        $b_k = 0$
        $r_k = r_{k-1}$
    end if
end for
```

## Digital Storage of Floating Point Numbers (6)

**Example:** *Binary mantissa for* $x = 0.8125$ — *Apply Algorithm 5.1*

| $k$ | $2^{-k}$ | $b_k$ | $r_k = r_{k-1} - b_k 2^{-k}$ |
|---|---|---|---|
| 0 | NA | NA | 0.8125 |
| 1 | 0.5 | 1 | 0.3125 |
| 2 | 0.25 | 1 | 0.0625 |
| 3 | 0.125 | 0 | 0.0625 |
| 4 | 0.0625 | 1 | 0.0000 |

Therefore, the binary mantissa for 0.8125 is (exactly) $(1101)_2$

## Digital Storage of Floating Point Numbers (7)

**Example:** *Binary mantissa for* $x = 0.1$ — *Apply Algorithm 5.1*

| $k$ | $2^{-k}$ | $b_k$ | $r_k = r_{k-1} - b_k 2^{-k}$ |
|---|---|---|---|
| 0 | NA | NA | 0.1 |
| 1 | 0.5 | 0 | 0.1 |
| 2 | 0.25 | 0 | 0.1 |
| 3 | 0.125 | 0 | 0.1 |
| 4 | 0.0625 | 1 | 0.1 - 0.0625 = 0.0375 |
| 5 | 0.03125 | 1 | 0.0375 - 0.03125 = 0.00625 |
| 6 | 0.015625 | 0 | 0.00625 |
| 7 | 0.0078125 | 0 | 0.00625 |
| 8 | 0.00390625 | 1 | 0.00625 - 0.00390625 = 0.00234375 |
| 9 | 0.001953125 | 1 | 0.0234375 - 0.001953125 = 0.000390625 |
| 10 | 0.0009765625 | 0 | 0.000390625 |
| $\vdots$ | $\vdots$ | | |

## Digital Storage of Floating Point Numbers $(8)$

Calculations on the preceding slide show that
the binary mantissa for 0.1 is $(00011\,0011\ldots)_2$.

> **The decimal value of 0.1 cannot be represented by a finite number of binary digits.**

## Consequences of Finite Storage (1)

| | | |
|---|---|---|
| Limiting the number of bits allocated for storage of the exponent | $\Longrightarrow$ | Upper and lower limits on the **range** (or magnitude) of floating point numbers |
| Limiting the number of bits allocated for storage of the mantissa | $\Longrightarrow$ | Limit on the **precision** (or number of significant digits) for any floating point number. |

## Consequences of Finite Storage (2)

Most real numbers cannot be stored exactly (they do not exist on the floating point number line)

- Integers less than $2^{52}$ can be stored exactly.

  Try this:

  ```
  >> x = 2^51
  >> s = dec2bin(x)
  >> x2 = bin2dec(s)
  >> x2 - x
  ```

- Numbers with 15 (decimal) digit mantissas that are the exact sum of powers of (1/2) can be stored exactly.

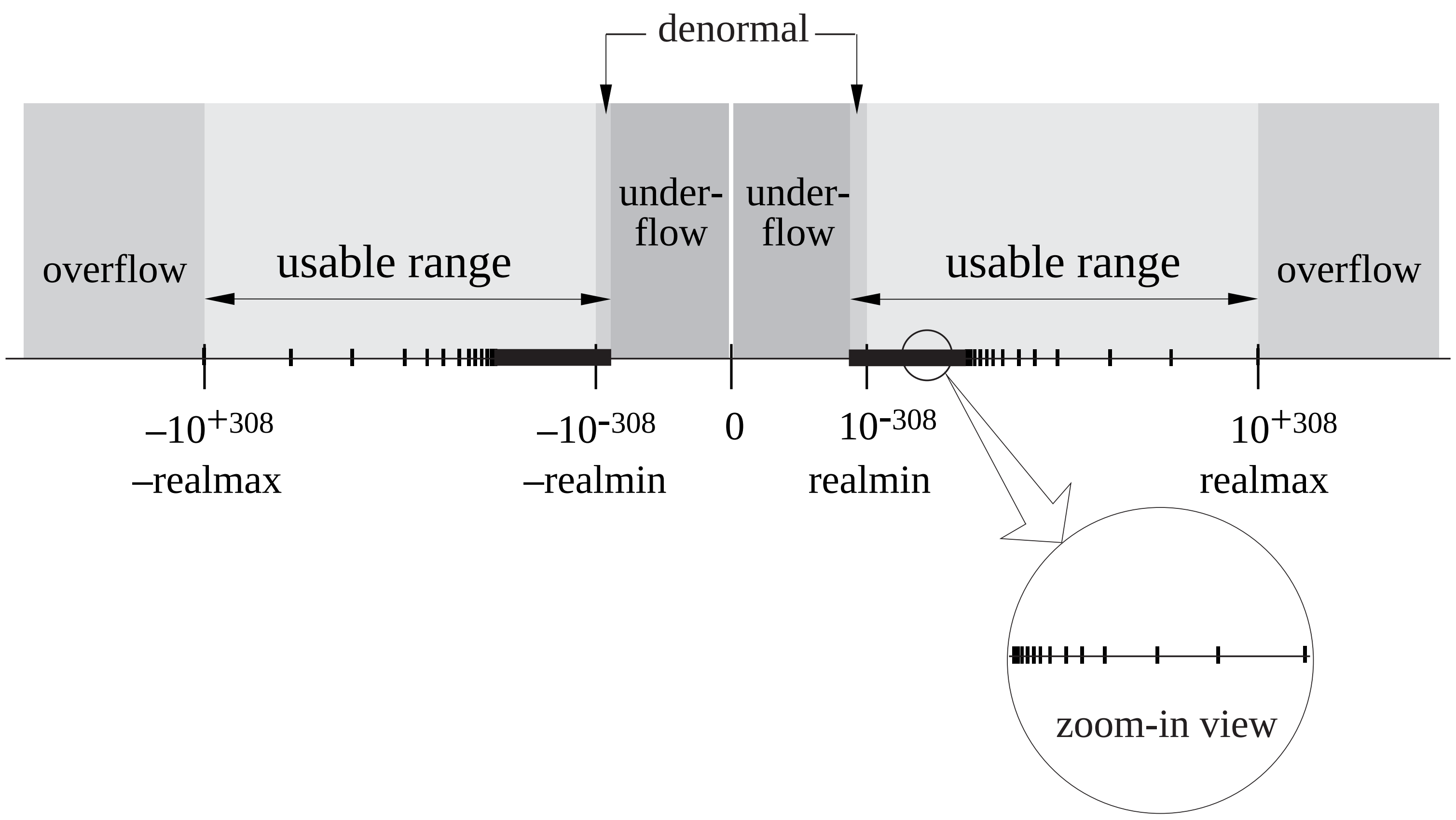
## Floating Point Number Line

Compare floating point numbers to real numbers.

| | Real numbers | Floating point numbers |
|---|---|---|
| **Range** | **Infinite**: arbitrarily large and arbitrarily small real numbers exist. | **Finite**: the number of bits allocated to the exponent limit the magnitude of floating point values. |
| **Precision** | **Infinite**: There is an infinite set of real numbers between any two real numbers. | **Finite**: there is a finite number (perhaps zero) of floating point values between any two floating point values. |

**In other words:** The floating point number line is a subset of the real number line.

## Floating Point Number Line



## Symbolic versus Numeric Calculation (1)

Commercial software for symbolic computation

- Derive$^{\text{TM}}$
- MACSYMA$^{\text{TM}}$
- Maple$^{\text{TM}}$
- Mathematica$^{\text{TM}}$

Symbolic calculations are exact. No rounding occurs because symbols and algebraic relationships are manipulated without storing numerical values.

## Symbolic versus Numeric Calculation (2)

**Example:** Evaluate $f(\theta) = 1 - \sin^2\theta - \cos^2\theta$

```
>> theta = 30*pi/180;
>> f = 1 - sin(theta)^2 - cos(theta)^2
f =
  -1.1102e-16
```

`f` is close to, but not exactly equal to zero because of *roundoff*. Also note that `f` is a single value, not a formula.

## Symbolic versus Numeric Calculation (3)

Symbolic computation using the Symbolic Math Toolbox in MATLAB

```
>> t = sym('t')     %  declare t as a symbolic variable
t =
t

>> f = 1 - sin(t)^2 - cos(t)^2  %  create a symbolic expression
f =
1-sin(t)^2-cos(t)^2

>> simplify(f)    %  ask Maple engine to make algebraic simplifications
f =
0
```

In the symbolic computation, `f` is exactly zero for any value of `t`. There is no roundoff error in symbolic computation.

## Numerical Arithmetic

Numerical values have limited range and precision. Values created by adding, subtracting, multiplying, or dividing floating point values will also have limited range and precision.

Quite often, the result of an arithmetic operation between two floating point values cannot be represented as another floating point value.

## Integer Arithmetic

| Operation | Result |
|---|---|
| $2 + 2 = 4$ | integer |
| $9 \times 7 = 63$ | integer |
| $\dfrac{12}{3} = 4$ | integer |
| $\dfrac{29}{13} = 2$ | exact result is not an integer |
| $\dfrac{29}{1300} = 0$ | exact result is not an integer |

## Floating Point Arithmetic

| Operation | Floating Point Value is . . . |
|---|---|
| $2.0 + 2.0 = 4$ | exact |
| $9.0 \times 7.0 = 63$ | exact |
| $\frac{12.0}{3.0} = 4$ | exact |
| $\frac{29}{13} = 2.230769230769231$ | approximate |
| $\frac{29}{1300} = 2.230769230769231 \times 10^{-2}$ | approximate |

## Floating Point Arithmetic in Matlab (1)

```
>> format long e
>> u = 29/13
u =
     2.230769230769231e+00

>> v = 13*u
v =
    29

>> v-29
ans =
     0
```

Two rounding errors are made: (1) during computation and storage of `u`, and (2) during computation and storage of `v`. Fortuitously, the combination of rounding errors produces the exact result.

## Floating Point Arithmetic in MATLAB (2)

```
>> x = 29/1300
x =
     2.230769230769231e-02
>> y = 29 - 1300*x
y =
    3.552713678800501e-015
```

In exact arithmetic, the value of `y` should be zero.

The roundoff error occurs when `x` is stored. Since $29/1300$ cannot be expressed with a finite sum of the powers of $1/2$, the numerical value stored in `x` is a truncated approximation to $29/1300$.

When `y` is computed, the expression 1300*`x` evaluates to a number slightly different than 29 because the bits lost in the computation and storage of `x` are not recoverable.

## Roundoff in Quadratic Equation (1)

(See **Example 5.3** in the text)

The roots of

$$ax^2 + bx + c = 0 \tag{1}$$

are

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

Consider

$$x^2 + 54.32x + 0.1 = 0 \tag{3}$$

which has the roots (to eleven digits)

$$x_1 = 54.3218158995, \qquad x_2 = 0.0018410049576.$$

Note that $b^2 \gg 4ac$

$$b^2 = 2950.7 \gg 4ac = 0.4$$

## Roundoff in Quadratic Equation (2)

Compute roots with four digit arithmetic

$$\begin{aligned}\sqrt{b^2 - 4ac} &= \sqrt{(-54.32)^2 - 0.4000} \\ &= \sqrt{2951 - 0.4000} \\ &= \sqrt{2951} \\ &= 54.32\end{aligned}$$

The result of each intermediate mathematical operation is rounded to four digits.

## Roundoff in Quadratic Equation $(3)$

Use $x_{1,4}$ to designate the first root computed with four-digit arithmetic:

$$\begin{aligned} x_{1,4} &= \frac{-b + \sqrt{b^2 - 4ac}}{2a} \\ &= \frac{+54.32 + 54.32}{2.000} \\ &= \frac{108.6}{2.000} \\ &= 54.30 \end{aligned}$$

Correct root is $x_1 = 54.3218158995$. Four digit arithmetic leads to $0.4$ percent error in this example.

## Roundoff in Quadratic Equation (4)

Using four-digit arithmetic the second root, $x_{2,4}$, is

$$\begin{aligned} x_{2,4} &= \frac{-b - \sqrt{b^2 - 4ac}}{2a} \\ &= \frac{+54.32 - 54.32}{2.000} && (i) \\ &= \frac{0.000}{2.000} && (ii) \\ &= 0 && (iii) \end{aligned}$$

An error of $100$ percent!

The poor approximation to $x_{2,4}$ is caused by roundoff in the calculation of $\sqrt{b^2 - 4ac}$. This leads to the subtraction of two equal numbers in line $(i)$.

## Roundoff in Quadratic Equation $(5)$

A solution: rationalize the numerators of the expressions for the two roots:

$$x_1 = \frac{-b+\sqrt{b^2-4ac}}{2a}\left(\frac{-b-\sqrt{b^2-4ac}}{-b-\sqrt{b^2-4ac}}\right) = \frac{2c}{-b-\sqrt{b^2-4ac}}, \tag{4}$$

$$x_2 = \frac{-b-\sqrt{b^2-4ac}}{2a}\left(\frac{-b+\sqrt{b^2-4ac}}{-b+\sqrt{b^2-4ac}}\right) = \frac{2c}{-b+\sqrt{b^2-4ac}} \tag{5}$$

## Roundoff in Quadratic Equation (6)

Now use Equation (5) to compute the troublesome second root with four digit arithmetic

$$x_{2,4} = \frac{2c}{-b + \sqrt{b^2 - 4ac}} = \frac{0.2000}{+54.32 + 54.32} = \frac{0.2000}{108.6} = 0.001842.$$

The result is in error by only $0.05$ percent.

## Roundoff in Quadratic Equation (7)

Compare the formulas for $x_2$

$$x_{2,\mathrm{std}} = \frac{-b - \sqrt{b^2 - 4ac}}{2a}$$

$$x_{2,\mathrm{new}} = \frac{2c}{-b + \sqrt{b^2 - 4ac}}$$

The two formulations for $x_2$ are algebraically equivalent. The difference in the computed values of $x_{2,4}$ is due to roundoff alone.

## Roundoff in Quadratic Equation (8)

Repeat the calculation of $x_{1,4}$ with the new formula

$$\begin{aligned} x_{1,4} &= \frac{2c}{-b - \sqrt{b^2 - 4ac}} \\ &= \frac{0.2000}{+54.32 - 54.32} && (i) \\ &= \frac{0.2000}{0} && (ii) \\ &= \infty. \end{aligned}$$

Limited precision in the calculation of $\sqrt{b^2 + 4ac}$ leads to a *catastrophic cancellation error* in step $(i)$

## Roundoff in Quadratic Equation (9)

A robust solution uses a formula that takes the sign of $b$ into account in a way that prevents catastrophic cancellation.

The ultimate quadratic formula:

$$q \equiv -\frac{1}{2}\left[b + \operatorname{sign}(b)\sqrt{b^2 - 4ac}\right]$$

where

$$\operatorname{sign}(b) = \begin{cases} 1 & \text{if } b \geq 0, \\ -1 & \text{otherwise} \end{cases}$$

Then roots to quadratic equation are

$$x_1 = \frac{q}{a} \qquad x_2 = \frac{c}{q}$$

## Roundoff in Quadratic Equation (10)

**Summary**

- Finite-precision causes roundoff in individual calculations
- Effects of roundoff usually accumulate slowly, but . . .
- Subtracting nearly equal numbers leads to severe loss of precision. A similar loss of precision occurs when two numbers of very different magnitude are added.
- Roundoff is inevitable: good algorithms minimize the effect of roundoff.

## Catastrophic Cancellation Errors (1)

The errors in

$$c = a + b \qquad \text{and} \qquad c = a - b$$

will be large when $a \gg b$ or $a \ll b$.

Consider $c = a + b$ with

$$a = x.xxx\ldots \times 10^{0}$$
$$b = y.yyy\ldots \times 10^{-8}$$

where $x$ and $y$ are decimal digits.

## Catastrophic Cancellation Errors (1)

Evaluate $c = a + b$ with $a = x.xxx\ldots \times 10^0$ and $b = y.yyy\ldots \times 10^{-8}$

Assume for convenience of exposition that $z = x + y < 10$.

$$\begin{array}{rl} & \overbrace{\mathrm{x.xxx\;xxxx\;xxxx\;xxxx}}^{\text{available precision}} \\ + & \mathrm{0.000\;0000\;yyyy\;yyyy\;yyyy\;yyyy} \\ \hline = & \mathrm{x.xxx\;xxxx\;zzzz\;zzzz}\;\underbrace{\mathrm{yyyy\;yyyy}}_{\text{lost digits}} \end{array}$$

The most significant digits of $a$ are retained, but the least significant digits of $b$ are lost because of the mismatch in magnitude of $a$ and $b$.

## Catastrophic Cancellation Errors (2)

**For subtraction**: The error in

$$c = a - b$$

will be large when $a \approx b$.

Consider $c = a - b$ with

$$a = x.xxxxxxxxxxx1ssssss$$
$$b = x.xxxxxxxxxxx0tttttt$$

where $x$, $y$, $s$ and $t$ are decimal digits. The digits $sss\ldots$ and $ttt\ldots$ are lost when $a$ and $b$ are stored in double-precision, floating point format.

## Catastrophic Cancellation Errors (3)

Evaluate $a - b$ in double precision floating point arithmetic when $a = x.xxx\,xxxx\,xxxx\,1$ and $b = x.xxx\,xxxx\,xxxx\,0$

$$
\begin{array}{rl}
 & \overbrace{\mathrm{x.xxx\,xxxx\,xxxx\,1}}^{\text{available precision}} \\
- & \mathrm{x.xxx\,xxxx\,xxxx\,0} \\
\hline
= & 0.000\,0000\,0000\,1\ \ \underbrace{\mathrm{uuuu\,uuuu\,uuuu}}_{\text{unassigned digits}} \\
= & 1.\mathrm{uuuu\,uuuu\,uuuu} \times 10^{-12}
\end{array}
$$

The result has only one significant digit. Values for the uuuu digits are not necessarily zero. The *absolute* error in the result is small compared to either $a$ or $b$. The *relative* error in the result is large because $ssssss - tttttt \neq uuuuuu$ (except by chance).

## Catastrophic Cancellation Errors (4)

### Summary

- Occurs in addition $\alpha + \beta$ or subtraction $\alpha - \beta$ when $\alpha \gg \beta$ or $\alpha \ll \beta$
- Occurs in subtraction: $\alpha - \beta$ when $\alpha \approx \beta$
- Error caused by a single operation (hence the term "catastrophic") not a slow accumulation of errors.
- Can often be minimized by algebraic rearrangement of the troublesome formula. (Cf. improved quadratic formula.)

## **Machine Precision** (1)

The magnitude of roundoff errors is quantified by *machine precision* $\varepsilon_m$.

There is a number, $\varepsilon_m > 0$, such that

$$1 + \delta = 1$$

whenever $|\delta| < \varepsilon_m$.

In exact arithmetic $1 + \delta = 1$ only when $\delta = 0$, so in exact arithmetic $\varepsilon_m$ is identically zero.

MATLAB uses double precision (64 bit) arithmetic. The built-in variable **eps** stores the value of $\varepsilon_m$.

$$\texttt{eps} = 2.2204 \times 10^{-16}$$

## Machine Precision (2)

MATLAB code for Computing Machine Precision:

```
epsilon = 1;
it = 0;
maxit = 100;
while it < maxit
    epsilon = epsilon/2;
    b = 1 + epsilon;
    if b == 1
        break;
    end
    it = it + 1;
end
```

## Implications for Routine Calculations

- Floating point comparisons should test for “close enough” instead of exact equality.

- Express “close” in terms of

  absolute difference, $|x - y|$

  or

  relative difference, $\dfrac{|x - y|}{|x|}$

## Floating Point Comparison

Don’t ask “is $x$ equal to $y$”.

```
if x==y       %  Don’t do this
   ...
end
```

Instead ask, “are $x$ and $y$ ‘close enough’ in value”

```
if abs(x-y) < tol
   ...
end
```

## Absolute and Relative Error (1)

"Close enough" can be measured with either absolute difference or relative difference, or both

Let

$$\begin{aligned} \alpha &= \text{some exact or reference value} \\ \widehat{\alpha} &= \text{some computed value} \end{aligned}$$

*Absolute error*

$$E_{\text{abs}}(\widehat{\alpha}) = \left|\widehat{\alpha} - \alpha\right|$$

## Absolute and Relative Error (1)

*Relative error*

$$E_{\mathrm{rel}}(\widehat{\alpha}) = \frac{\left|\widehat{\alpha} - \alpha\right|}{\left|\alpha_{\mathrm{ref}}\right|}$$

Often we choose $\alpha_{\mathrm{ref}} = \alpha$ so that

$$E_{\mathrm{rel}}(\widehat{\alpha}) = \frac{\left|\widehat{\alpha} - \alpha\right|}{\left|\alpha\right|}$$

## Absolute and Relative Error (2)

**Example:** *Approximating* $\sin(x)$ *for small* $x$

Since

$$\sin(x) = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \ldots$$

we can approximate $\sin(x)$ with

$$\sin(x) \approx x$$

for small enough $|x| < 1$

## Absolute and Relative Error (3)

The absolute error in approximating $\sin(x) \approx x$ for small $x$ is

$$E_{\rm abs} = x - \sin(x) = \frac{x^3}{3!} - \frac{x^5}{5!} + \ldots$$

And the relative error is

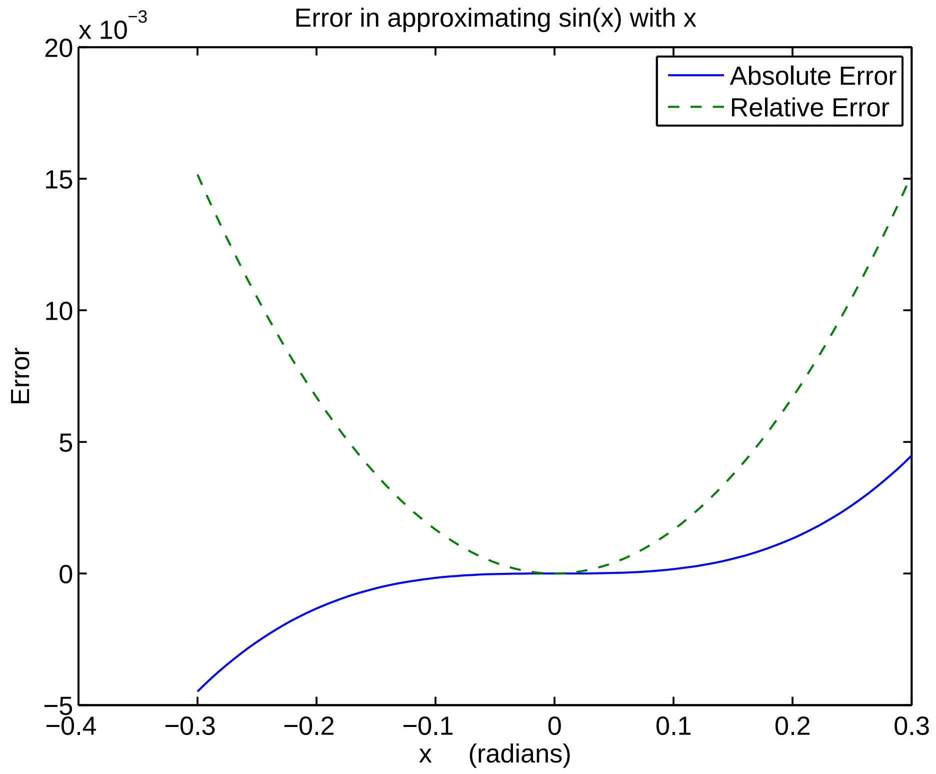
$$E_{\rm abs} = \frac{x - \sin(x)}{\sin(x)} = \frac{x}{\sin(x)} - 1$$

## Absolute and Relative Error (4)

Plot relative and absolute error in approximating $\sin(x)$ with $x$.

Although the absolute error is relatively flat around $x = 0$, the relative error grows more quickly.

The relative error grows quickly because the absolute value of $\sin(x)$ is small near $x = 0$.



## Iteration termination (1)

An iteration generates a sequence of scalar values $x_k, \; k = 1, 2, 3, \ldots$. The sequence converges to a limit $\xi$ if

$$|x_k - \xi| < \delta, \qquad \text{for all } k > N,$$

where $\delta$ is a small.

In practice, the test is usually expressed as

$$|x_{k+1} - x_k| < \delta, \quad \text{when } k > N.$$

## Iteration termination (2)

**Absolute** convergence criterion

Iterate until $|x - x_{\mathrm{old}}| < \Delta_a$ where $\Delta_a$ is the absolute convergence tolerance.

In MATLAB:

```
x = ...                  %  initialize
xold = ...

while abs(x-xold) > deltaa
      xold = x;
      update x
end
```

## Iteration termination (3)

**Relative** convergence criterion

Iterate until $\left|\dfrac{x - x_{\text{old}}}{x_{\text{old}}}\right| < \delta_r$, where $\delta_r$ is the absolute convergence tolerance.

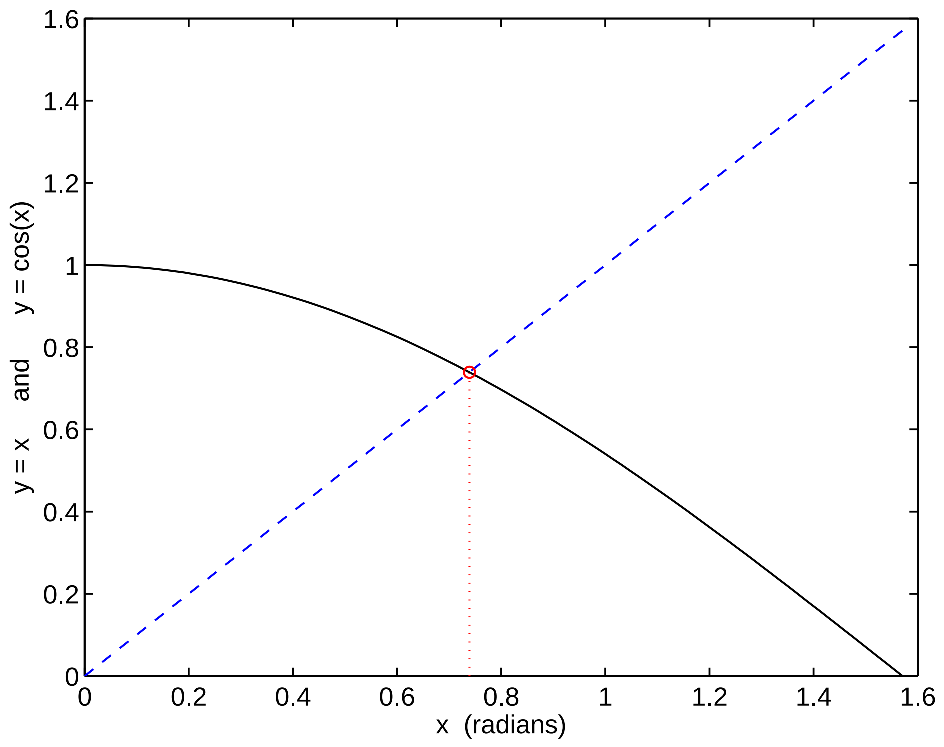
In MATLAB:

```
x = ...                 %  initialize
xold = ...

while abs((x-xold)/xold) > deltar
      xold = x;
      update x
end
```

## Example: Solve $\cos(x) = x$ (1)

Find the value of $x$ that satisfies $\cos(x) = x$.



## Example: Solve $\cos(x) = x$ (2)

The fixed point iteration as a method for obtaining a numerical approximation to the solution of a scalar equation. For now, trust that the follow algorithm will eventually give the solution.

1. Guess $x_0$
2. Set $x_{old} = x_0$
3. Update guess
$$x_{new} = \cos(x_{old})$$
4. If $x_{\text{new}} \approx x_{\text{old}}$ stop; otherwise set $x_{\text{old}} = x_{\text{new}}$ and return to step 3

## **Solve** $\cos(x) = x \qquad (3)$

MATLAB implementation

```
x0 = ...      %  initial guess
k = 0;
xnew = x0;
while NOT_CONVERGED & k < maxit
    xold = xnew;
    xnew = cos(xold);
    it = it + 1;
end
```

Let's examine someways of defining the logical value `NOT_CONVERGED`.

## **Solve** $\cos(x) = x$ (4)

Bad test # 1

```
while xnew ~= xold
```

This test will be true unless `xnew` and `xold` are *exactly* equal. In other words, `xnew` and `xold` are equal only when their bit patterns are identical. This is bad because

- Test may never be met because of oscillatory bit patterns
- Even if test is eventually met, the iterations will probably do more work than needed

## **Solve** $\cos(x) = x \qquad (5)$

Bad test # 2

```
while (xnew-xold) > delta
```

This test evaluates to false whenever `(xnew-xold)` is negative, even if $|(\texttt{xnew} - \texttt{xold})| \gg \texttt{delta}$.

**Example:**

```
>> xold = 100;  xnew = 1;  delta = 5e-9;
>> (xnew-xold) > delta
ans =
     0
```

These values of `xnew` and `xold` are not close, but the erroneous convergence criterion would cause the iterations to stop.

## **Solve** $\cos(x) = x \qquad (6)$

Workable test # 1: **Absolute tolerance**

```
while abs(xnew-xold) > delta
```

An absolute tolerance is useful when the iterative sequence converges to a value with magnitude much less than one.

What value of `delta` to use?

## **Solve** $\cos(x) = x$ (7)

Workable test # 2: **Relative tolerance**

```
while abs( (xnew-xold)/xref ) > delta
```

The user supplies appropriate value of `xref`. For this particular iteration we could use `xref` = `xold`.

```
while abs( (xnew-xold)/xold ) > delta
```

**Note:** For the problem of solving $\cos(x) = x$, the solution is $\mathcal{O}(1)$ so the absolute and relative convergence tolerance will terminate the calculations at roughly the same iteration.

## **Solve** $\cos(x) = x$ (8)

Using the relative convergence tolerance, the code becomes

```
x0 = ...       %  initial guess
k = 0;
xnew = x0;
while ( abs( (xnew-xold)/xold ) > delta )  &  k < maxit
    xold = xnew;
    xnew = cos(xold);
    it = it + 1;
end
```

**Note:** Parentheses around `abs( (xnew-xold)/xold ) > delta` are not needed for correct MATLAB implementation. The parenthesis are added to make the meaning of the clear to humans reading the code.

## Truncation Error

Consider the series for $\sin(x)$

$$\sin(x) = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \cdots$$

For small $x$, only a few terms are needed to get a good approximation to $\sin(x)$. The $\cdots$ terms are "truncated"

$$f_{\mathrm{true}} = f_{\mathrm{sum}} + \text{truncation error}$$

The size of the truncation error depends on $x$ *and* the number of terms included in $f_{\mathrm{sum}}$.

## Truncation of series for $\sin(x)$ (1)

```
function ssum = sinser(x,tol,n)
% sinser  Evaluate the series representation of the sine function
%
% Input:    x   = argument of the sine function, i.e., compute sin(x)
%           tol = tolerance on accumulated sum. Default:  tol = 5e-9
%           n   = maximum number of terms. Default: n = 15
%
% Output:   ssum = value of series sum after nterms or tolerance is met

term = x;  ssum = term;         %  Initialize series
fprintf('Series approximation to sin(%f)\n\n  k      term         ssum\n',x);
fprintf('%3d  %11.3e  %12.8f\n',1,term,ssum);
for k=3:2:(2*n-1)
  term = -term * x*x/(k*(k-1));                  %  Next term in the series
  ssum = ssum + term;
  fprintf('%3d  %11.3e  %12.8f\n',k,term,ssum);
  if abs(term/ssum)<tol, break;  end             %  True at convergence
end
fprintf('\nTruncation error after %d terms is %g\n\n',(k+1)/2,abs(ssum-sin(x)));
```

## Truncation of series for $\sin(x)$ (2)

For small $x$, the series for $\sin(x)$ converges in a few terms

```
>> s = sinser(pi/6,5e-9,15);
Series approximation to sin(0.523599)

  k      term          ssum
  1   5.236e-001    0.52359878
  3  -2.392e-002    0.49967418
  5   3.280e-004    0.50000213
  7  -2.141e-006    0.49999999
  9   8.151e-009    0.50000000
 11  -2.032e-011    0.50000000

Truncation error after 6 terms is 3.56382e-014
```

## Truncation of series for $\sin(x)$ (3)

The truncation error in the series is small relative to the true value of $\sin(\pi/6)$

```
>> s = sinser(pi/6,5e-9,15);
    ⋮
>> err = (s-sin(pi/6))/sin(pi/6)
err =
 -7.1276e-014
```

## Truncation of series for $\sin(x)$ (4)

For larger $x$, the series for $\sin(x)$ converges more slowly

```
>> s = sinser(15*pi/6,5e-9,15);
Series approximation to sin(7.853982)

   k      term          ssum
   1   7.854e+000    7.85398163
   3  -8.075e+001  -72.89153055
   5   2.490e+002  176.14792646
   ⋮       ⋮             ⋮
  25   1.537e-003    1.00012542
  27  -1.350e-004    0.99999038
  29   1.026e-005    1.00000064

Truncation error after 15 terms is 6.42624e-007
```

Increasing the number of terms will allow the series to converge with the tolerance of $5 \times 10^{-9}$. A better solution to the slow convergence of the series are explored in Exercise 23.

## Taylor Series (1)

For a sufficiently continuous function $f(x)$ defined on the interval $x \in [a, b]$ we define the $n^{th}$ order Taylor Series approximation $P_n(x)$

$$P_n(x) = f(x_0) + (x - x_0)\left.\frac{df}{dx}\right|_{x=x_0} + \frac{(x-x_0)^2}{2}\left.\frac{d^2 f}{dx^2}\right|_{x=x_0} + \cdots + \frac{(x-x_0)^n}{n!}\left.\frac{d^n f}{dx^n}\right|_{x=x_0}$$

Then there exists $\xi$ with $x_0 \le \xi \le x$ such that

$$f(x) = P_n(x) + R_n(x)$$

where

$$R_n(x) = \frac{(x-x_0)^{(n+1)}}{(n+1)!}\left.\frac{d^{(n+1)} f}{dx^{(n+1)}}\right|_{x=\xi}$$

## Taylor Series (2)

Big "$\mathcal{O}$" notation

$$f(x) = P_n(x) + \mathcal{O}\left(\frac{(x-x_0)^{(n+1)}}{(n+1)!}\right)$$

or, for $x - x_0 = h$ we say

$$f(x) = P_n(x) + \mathcal{O}\left(h^{(n+1)}\right)$$

## Taylor Series Example

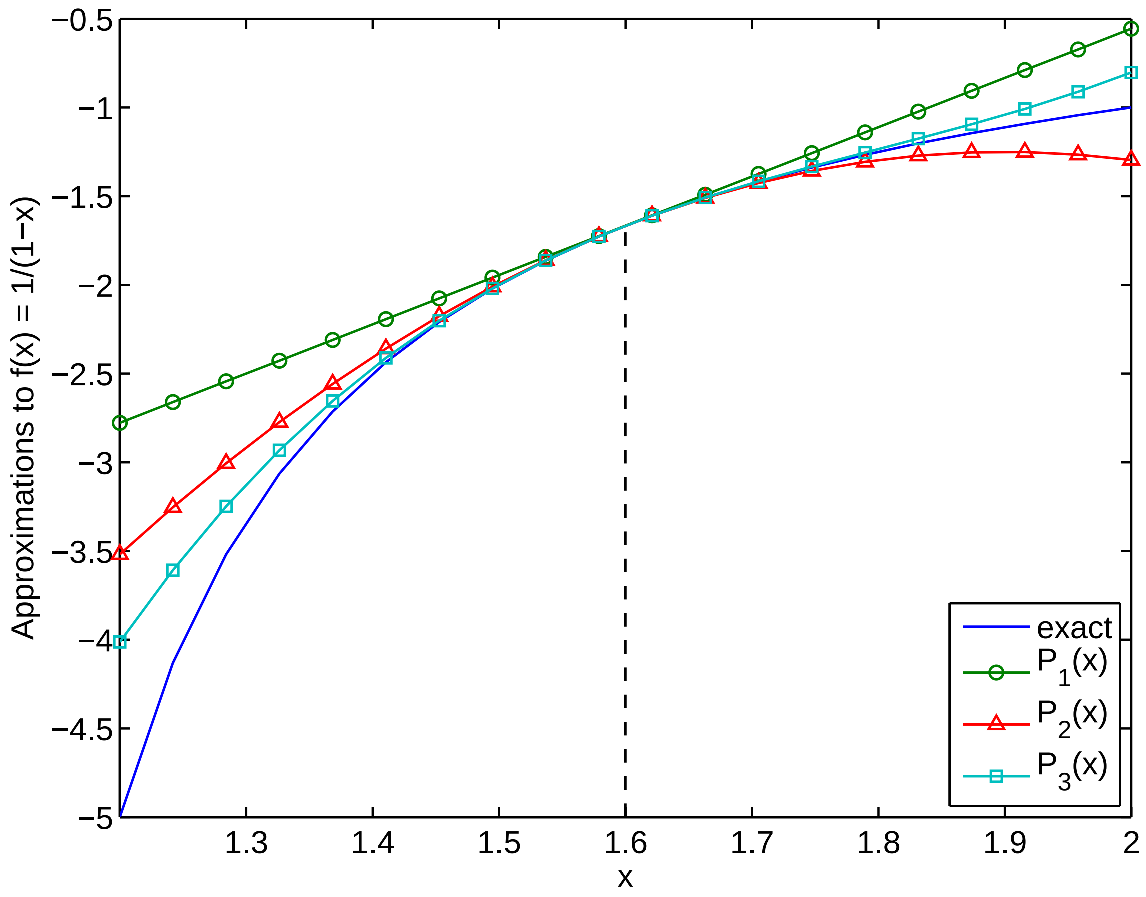
Consider the function

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

The Taylor Series approximations to $f(x)$ of order 1, 2 and 3 are

$$\begin{aligned}
P_1(x) &= \frac{1}{1-x_0} + \frac{x-x_0}{(1-x_0)^2} \\
P_2(x) &= \frac{1}{1-x_0} + \frac{x-x_0}{(1-x_0)^2} + \frac{(x-x_0)^2}{(1-x_0)^3} \\
P_3(x) &= \frac{1}{1-x_0} + \frac{x-x_0}{(1-x_0)^2} + \frac{(x-x_0)^2}{(1-x_0)^3} + \frac{(x-x_0)^3}{(1-x_0)^4}
\end{aligned}$$

## Taylor Series: $P_i(x)$ near $x = 1.6$ (3)



## Roundoff and Truncation Errors $(1)$

Roundoff and truncation errors occur in numerical computation.

**Example:**

Finite difference approximation to $f'(x) = df/dx$

$$f'(x) = \frac{f(x+h) - f(x)}{h} - \frac{h}{2}f''(x) + \ldots$$

This approximation is said to be first order because the leading term in the truncation error is linear in $h$. Dropping the truncation error terms we obtain

$$f'_{fd}(x) = \frac{f(x+h) - f(x)}{h} \qquad \text{or} \qquad f'_{fd}(x) = f'(x) + \mathcal{O}(h)$$

## Roundoff and Truncation Errors (2)

To study the roles of roundoff and truncation errors, compute the finite difference[2] approximation to $f'(x)$ when $f(x) = e^x$.

The relative error in the $f'_{fd}(x)$ approximation to $\dfrac{d}{dx}e^x$ is

$$E_{\text{rel}} = \frac{f'_{fd}(x) - f'(x)}{f'(x)} = \frac{f'_{fd}(x) - e^x}{e^x}$$

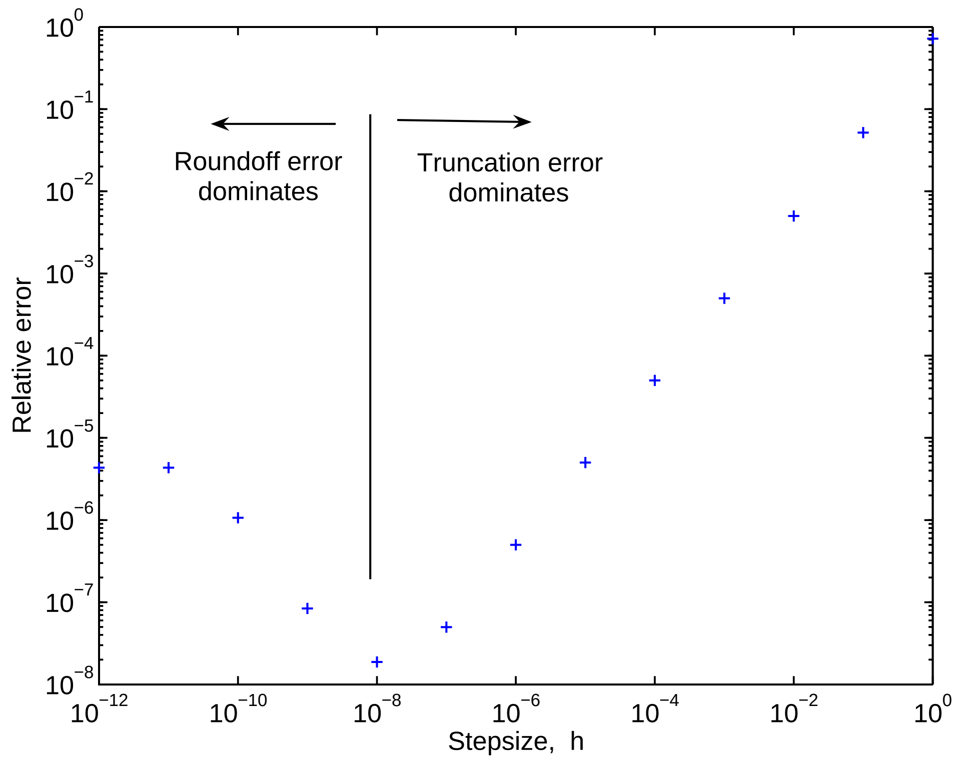
[2]The finite difference approximation is used to obtain numerical solutions to ordinary and partial differentials equations where $f(x)$ and hence $f'(x)$ is *unknown*.

## Roundoff and Truncation Errors (3)

Evaluate $E_{\mathrm{rel}}$ at $x = 1$ for a range of $h$.

Truncation error dominates at large $h$.

Roundoff error in $f(x + h) - f(h)$ dominates as $h \to 0$.


Roundoff error dominates
Truncation error dominates
Relative error
Stepsize, h