Preliminaries to Numerical Analysis

- Numerical linear algebra
  - square linear systems : $A\vec{x} = \vec{b}$
  - overdetermined linear systems : $A\vec{x}$ "=" $\vec{b}$
  - spectral theory : $A\vec{x} = \lambda\vec{x}$
    (eigenvalues, singular values)
- Nonlinear
  - root finding
  - piecewise polynom interp.
  - num. calculus (diff, integ. ODE theory)

Contents

Main Sources of errors.

1. Floating-Point Numbers (how #'s are represented / stored on computer)

2. Conditioning (inherent property of a problem)

3. Stability (algorithm)

Absolute and Relative Errors

In numerical analysis, we use an **algorithm** to *approximate* some quantity of interest.

- We estimate of the accuracy of the computed value via an **absolute error** or a **relative error**:

$$e_{\mathrm{abs}} = A_{\mathrm{approx}} - A_{\mathrm{exact}} \qquad \text{(absolute error)}$$

$$e_{\mathrm{rel}} = \frac{A_{\mathrm{approx}} - A_{\mathrm{exact}}}{A_{\mathrm{exact}}} = \frac{A_{\mathrm{approx}}}{A_{\mathrm{exact}}} - 1\,, \qquad \text{(relative error)}$$

"percentage"

"dimensionless"

  where A_{exact} is the exact, analytical answer and A_{approx} is the approximate, numerical answer.

- If e_{abs} or e_{rel} is small, we say that the approximate answer is **accurate**.

Example: Stirling's Formula

Stirling's formula provides a "good" approximation to $n!$ for large n:

$$n! \approx \sqrt{2\pi n}\left(\frac{n}{e}\right)^n. \qquad (\star)$$

Try in MATLAB:

```
n = ...;
err_abs = sqrt(2*pi*n)*(n/exp(1))^n - factorial(n);
err_rel = err_abs/factorial(n);
disp(err_abs)
disp(err_rel)
```

When $n = 10$:

Abs. err. $= -30104.\cdots$

Rel. err. $= -0.008296$ (0.8%)

When $n = 100$:

Abs. err. $= -7.77\ldots \times 10^{154}$

Rel. err. $= -0.00083298$ (0.08%)

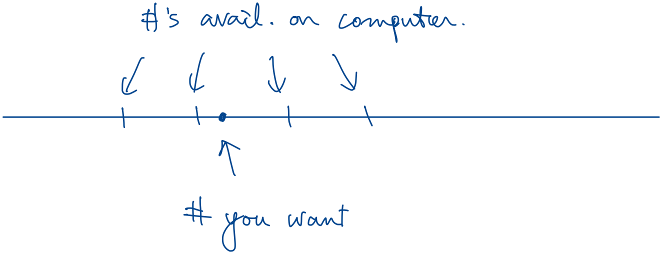
Floating-Point Numbers

Limitations of Digital Representations

A digital computer uses a finite number of bits to represent a real number and so it cannot represent all real numbers.

- The represented numbers cannot be arbitrarily large or small;
- There must be gaps between them.

So for all operations involving real numbers, it uses a subset of $\mathbb{R}$ called the **floating-point numbers**, $\mathbb{F}$.



Scientific notation (base 10)

one digit before dec. pt. ; no zero here.

$$\boxed{3}.14 \times 10^{2} = 314$$

$$3.14 \times 10^{-3} = 0.00314$$

$$3.14 \times 10^{2}$$

$$= (3\times 10^{0} + 1\times 10^{-1} + 4\times 10^{-2}) \times 10^{2}$$

$$= 3\times 10^{2} + 1\times 10^{1} + 4\times 10^{0}$$

$$= 314.$$

Scientific notation (base 2) → 0, 1

one bit here ; not zero.

$$\boxed{1}.101_{(2)} \times 2^{\boxed{10_{(2)}}} \qquad 10_{(2)} \rightarrow 2$$

$$= (1\times 2^{0} + 1\times 2^{-1} + 0\times 2^{-2} + 1\times 2^{-3}) \times 2^{2}$$

$$= 1\times 2^{2} + 1\times 2^{1} + 0\times 2^{0} + 1\times 2^{-1}$$

$$(= 110.1_{(2)})$$

$$= 4 + 2 + 0 + 1/2 = 6.5$$

Rough idea (4 bits)

$$\underbrace{\_\ \ \_}_{\text{bits after } 1.}\ \Big|\ \underbrace{\_\ \ \_}_{\text{exponent}}$$

Ex

$$\underbrace{1\ \ 0}\ \Big|\ \underbrace{1\ \ 1}$$

$$\rightarrow\ 1.\boxed{10}_{(2)} \times 2^{\boxed{11_{(2)}}}$$

*

$$00|00 : 1.00_{(2)} \times 2^{0_{(2)}} = 1$$

$$01|00 : 1.01_{(2)} \times 2^{0_{(2)}} = 1 + 1/4$$

$$10|00 : 1.10_{(2)} \times 2^{0_{(2)}} = 1 + 1/2$$

$$11|00 : 1.11_{(2)} \times 2^{0_{(2)}} = 1 + 1/2 + 1/4$$

$$= 1 + 3/4.$$

*

$$00|11 : 1.00_{(2)} \times 2^{11_{(2)}}$$

$$= 1 \times 2^3 = 8.$$

$$11|11 : 1.11_{(2)} \times 2^{11_{(2)}}$$

$$= (1 + 3/4) \times 8 = 8 + 6$$

$$= 14$$

Floating-Point Numbers

base - 2 Scientific notation.

A *floating-point number* is written in the form $\pm(1+F)2^E$ where

fractional part

- E, the *exponent*, is an integer;
- F, the *mantissa*, is a number $F = \sum_{i=1}^{d} b_i 2^{-i}$, with $b_i = 0$ or $b_i = 1$.

d : # of bits after 1. ____

$= b_1/2 + b_2/2^2 + \cdots + b_d/2^d$

Note that F can be rewritten as

$$F = 2^{-d} \underbrace{\sum_{k=0}^{d-1} b_{d-k} 2^k}_{=:M},$$

where M is an integer in $\mathbb{N}[0, 2^d - 1]$. $= \{0, 1, 2, \cdots, 2^d - 1\}$

Consequently, there are 2^d evenly-spaced numbers between 2^E and 2^{E+1} in the floating-point number system.

Floating-Point Numbers – IEEE 754 Standard

- MATLAB, by default, uses *double precision* floating-point numbers, stored in memory in 64 bits (or 8 bytes):

offset

$$\pm \underbrace{1.\mathrm{xxxxxxxxx}\cdots\mathrm{xxxxxxxxx}_{(2)}}_{\text{mantissa (base 2): 52+1 bits}} \times 2^{\overbrace{\mathrm{xxxx}\cdots\mathrm{xxxx}_{(2)}-1023}^{}}.$$

exponent: 11 bits

Sign bit (s)   s = 0 for (+) ; s = 1 for (−)

$(-1)^s$

0

0

- Predefined variables:
  - `eps` = the distance from 1.0 to the next largest double-precision number:

$$\texttt{eps} = 2^{-52} \approx 2.2204 \times 10^{-16}.$$

  - `realmin` = the smallest positive floating-point number that is stroed to full accuracy; the actual smallest is `realmin/2^52`.
  - `realmax` = the largest positive floating-point number

Machine Epsilon and Relative Errors

The IEEE standard guarantees that the *relative representation error* and the *relative computational error* have sizes smaller than $\boxed{\text{eps}}$, the *machine epsilon*:

- **Representation**: The floating-point representation, $\hat{x} \in \mathbb{F}$, of $x \in \mathbb{R}$ satisfies

$$\hat{x} = x(1 + \epsilon_1), \qquad \text{for some } |\epsilon_1| \leqslant \frac{1}{2}\boxed{\text{eps}}.$$

- **Arithmetic**: The floating-point representation, $\hat{x} \oplus \hat{y}$, of the result of $\hat{x} + \hat{y}$ with $\hat{x}, \hat{y} \in \mathbb{F}$ satisfies

$$\hat{x} \oplus \hat{y} = (\hat{x} + \hat{y})(1 + \epsilon_2), \qquad \text{for some } |\epsilon_2| \leqslant \frac{1}{2}\boxed{\text{eps}}.$$

Similarly with $\ominus, \otimes, \oplus\!\!\!\!\div$ corresponding to $-, \times, \div$, respectively.

Round-Off Errors

Computers CANNOT usually

- represent a number correctly;
- add, subtract, multiply, or divide correctly!!

Run the following and examine the answers:

```
format long
1.234567890123456789 0
12345678901234567890
(1 + eps) - 1
(1 + .5*eps) - 1
(1 + .51*eps) - 1
n = input(' n = '); ( n^(1/3) )^3 - n
```

Catastrophic Cancellation

In finite precision storage, two numbers that are close to each other are indistinguishable. So subtraction of two nearly equal numbers on a computer can result in loss of many significant digits.

Catastrophic Cancellation

Consider two real numbers stored with 10 digits of precision:

$$e = 2.7182818284,$$
$$b = 2.7182818272.$$

- Suppose the actual numbers e and b have additional digits that are not stored.
- The stored numbers are good approximations of the true values.
- However, if we compute $e - b$ based on the stored numbers, we obtain $0.0000000012 = 1.2 \times 10^{-9}$, a number with only two significant digits.

Example 1: Cancellation for Large Values of x

Question

Compute $f(x) = e^x(\cosh x - \sinh x)$ at $x = 1, 10, 100$, and 1000.

Numerically:

```
format long
x = input(' x = ');
y = exp(x) * ( cosh(x) - sinh(x) );
disp([x, y])
```

Example 2: Cancellation for Small Values of x

Question

Compute $f(x) = \dfrac{\sqrt{1+x} - 1}{x}$ at $x = 10^{-12}$.

Numerically:

```
x = 1e-12;
fx = (sqrt(1+x) - 1)/x;
disp( fx )
```

To Avoid Such Cancellations . . .

- Unfortunately, there is no universal way to avoid loss of precision.
- One way to avoid catastrophic cancellation is to remove the source of cancellation by simplifying the given expression before computing numerically.
- For Example 1, rewrite the given expression recalling that

$$\cosh x = (e^x + e^{-x})/2 \qquad \sinh x = (e^x - e^{-x})/2.$$

- For Example 2, try again after rewriting $f(x)$ as

$$f(x) = \frac{\sqrt{1+x} - 1}{x} \cdot \frac{\sqrt{1+x} + 1}{\sqrt{1+x} + 1} = \frac{1}{\sqrt{1+x} + 1}.$$

- Do you now have an improved accuracy?

Conditioning

Problems and Conditioning

- A mathematical *problem* can be viewed as a function $f : X \to Y$ from a data/input space X to a solution/output space Y.
- We are interested in changes in $f(x)$ caused by small perturbations of x.
- A *well-conditioned* problem is one with the property that all small perturbations of x lead to only small changes in $f(x)$

Condition Number

Let $f : \mathbb{R} \to \mathbb{R}$ and $\hat{x} = x(1+\epsilon)$ be the representation of $x \in \mathbb{R}$.

- The ratio of the relative error in f due to the change in x to the relative error in x simplifies to

$$\frac{\left|f(x) - f(x(1+\epsilon))\right|}{\left|\epsilon f(x)\right|}.$$

- In the limit of small error (ideal computer), we obtain

$$\begin{aligned}\kappa_f(x) &:= \lim_{\epsilon \to 0} \frac{\left|f(x) - f(x(1+\epsilon))\right|}{\left|\epsilon f(x)\right|} \\ &= \left|\lim_{\epsilon \to 0} \frac{f(x+\epsilon x) - f(x)}{\epsilon x} \cdot \frac{x}{f(x)}\right| = \left|\frac{x f'(x)}{f(x)}\right|, \qquad (\star)\end{aligned}$$

which is called the **(relative) condition number**.

Example: Conditioning of Subtraction

Consider $f(x) = x - c$ where c is some constant. Using the formula ($\star$), we find that the associated condition number is

$$\kappa(x) = \left| \frac{x f'(x)}{f(x)} \right| = \left| \frac{x}{x - c} \right|.$$

- It is large when $x \approx c$.

Example: Conditioning of Multiplication

The condition number of $f(x) = cx$ is

$$\kappa(x) = \left|\frac{xf'(x)}{f(x)}\right| = \left|\frac{x \cdot c}{cx}\right| = 1.$$

- No magnification of error.

Example: Conditioning of Function Evaluation

The condition number of $f(x) = \cos(x)$ is

$$\kappa(x) = \left|\frac{x f'(x)}{f(x)}\right| = \left|\frac{-x \sin x}{\cos x}\right| = |x \tan x| \, .$$

- The condition number is large when $x = (n + 1/2)\pi$, where $n \in \mathbb{Z}$.

Example: Conditioning of Root-Finding

Let $r = f(a; b, c)$ be a root of $ax^2 + bx + c = 0$. Instead of direct differentiation, use implicit differentiation

$$r^2 + 2ar\frac{dr}{da} + b\frac{dr}{da} = 0.$$

Solve for the derivative,

$$f'(a) = \frac{dr}{da} = -\frac{r^2}{2ar + b} = -\frac{r^2}{\pm\sqrt{b^2 - 4ac}},$$

then compute the condition number using the formula ($\star$) to get

$$\kappa(a) = \left|\frac{a f'(a)}{f(a)}\right| = \left|\frac{ar^2}{\pm r\sqrt{b^2 - 4ac}}\right| = \left|\frac{ar}{\sqrt{b^2 - 4ac}}\right|.$$

- Conditioning is poor for small discriminant, *i.e.*, near repeated roots.

Stability

Algorithms

- Recall that we defined a *problem* as a function $f : X \to Y$.
- An *algorithm* can be viewed as another map $\tilde{f} : X \to Y$ between the same two spaces, which involves errors arising in
  - representing the actual input x as $\hat{x}$;
  - implementing the function f numerically on a computer.

Example: Horner's Method

Consider evaluating a polynomial

$$p(x) = c_n x^{n-1} + c_{n-1} x^{n-2} + \cdots + c_2 x + c_1.$$

Can rewrite it as

$$p(x) = (\cdots((c_n x + c_{n-1})x + c_{n-2})x + \cdots + c_2)x + c_1,$$

```
function p = horner(c, x)
% HORNER evaluates polynomial using Horner's method.
    n = length(c);
    p = c(n);
    for k = n-1:-1:1
        p = p*x + c(k);
    end
end
```

Analysis: General Framework

The relative error of our interest is

$$\left|\frac{\tilde{f}(\hat{x})-f(x)}{f(x)}\right| \leqslant \left|\frac{\tilde{f}(\hat{x})-f(\hat{x})}{f(x)}\right| + \left|\frac{f(\hat{x})-f(x)}{f(x)}\right|$$

$$\lessapprox \underbrace{\left|\frac{\tilde{f}(\hat{x})-f(\hat{x})}{f(\hat{x})}\right|}_{\text{numerical error}} + \underbrace{\left|\frac{f(\hat{x})-f(x)}{f(x)}\right|}_{\text{perturbation error}} \leqslant (\hat{\kappa}_{\text{num}}+\kappa_f)\,\boxed{\text{eps}}.$$

where $\kappa = \kappa_f$ be the (relative) condition number of the exact problem f and

$$\hat{\kappa}_{\text{num}} = \max \left|\frac{\tilde{f}(\hat{x})-f(\hat{x})}{f(\hat{x})}\right| \Bigg/ \left|\frac{\hat{x}-x}{x}\right|.$$

Example: Root-Finding Revisited

Consider again solving the quadratic problem $ar^2 + br + c = 0$.

- Taking $a = c = 1$ and $b = -(10^6 + 10^{-6})$, the roots can be computed exactly by hand: $r_1 = 10^6$ and $r_2 = 10^{-6}$.
- If numerically computed in MATLAB using the quadratic equation formula, r_1 is correct but r_2 has only 5 correct digits.
- Fix it using $r_2 = (c/a)/r_1$.