16. Algorithm stability

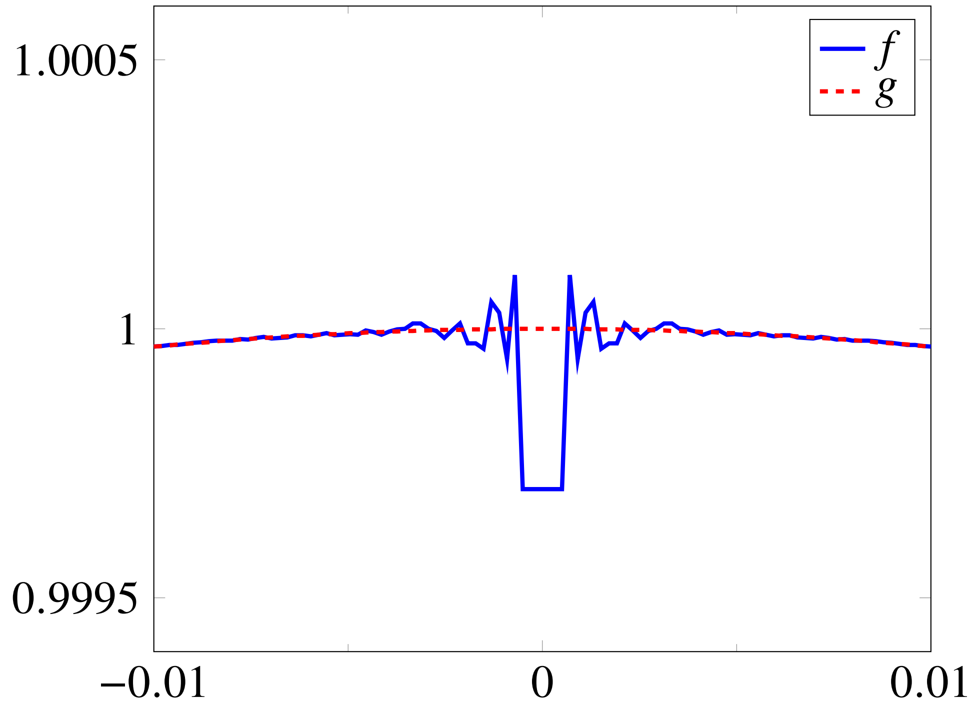
- cancellation
- numerical stability

Example

two expressions for the same function

$$f(x) = \frac{1 - (\cos x)^2}{x^2}$$

$$g(x) = \frac{(\sin x)^2}{x^2}$$



- results of $\cos x$ and $\sin x$ were rounded to 10 significant digits
- other calculations are exact
- plot shows function at 100 equally spaced points between -0.01 and 0.01

Evaluation of f

evaluate $f(x)$ at $x = 5 \cdot 10^{-5}$

- calculate $\cos x$ and round result to 10 digits

$$\begin{aligned} \cos x &= 0.99999999875000\ldots \\ &\rightsquigarrow 0.9999999988 \end{aligned}$$

- evaluate $f(x) = (1 - \cos(x)^2)/x^2$ using rounded value of $\cos x$

$$\frac{1 - (0.9999999988)^2}{(5 \cdot 10^{-5})^2} = 0.9599\ldots$$

has only one correct significant digit (correct value is $0.9999\ldots$)

Evaluation of g

evaluate $g(x)$ at $x = 5 \cdot 10^{-5}$

- calculate $\sin x$ and round result to 10 digits

$$\begin{aligned} \sin x &= 0.499999999791667\ldots \cdot 10^{-5} \\ &\rightsquigarrow 0.4999999998 \cdot 10^{-5} \end{aligned}$$

- evaluate $f(x) = \sin(x)^2/x^2$ using rounded value of $\cos x$

$$\frac{(\sin x)^2}{x^2} \approx \frac{(0.4999999998 \cdot 10^{-5})^2}{(5 \cdot 10^{-5})^2} = 0.9999\ldots$$

has about ten correct significant digits

Conclusion: f and g are equivalent mathematically, but not numerically

Cancellation

$$\hat{a} = a(1 + \Delta a), \qquad \hat{b} = b(1 + \Delta b)$$

- a, b: exact values
- $\hat{a}$, $\hat{b}$: approximations with unknown relative errors Δa, Δb
- relative error in $\hat{x} = \hat{a} - \hat{b} = (a - b) + (a\Delta a - b\Delta b)$ is

$$\frac{|\hat{x} - x|}{|x|} = \frac{|a\Delta a - b\Delta b|}{|a - b|}$$

  if $a \simeq b$, small Δa and Δb can lead to very large relative errors in x

this is called **cancellation**; cancellation occurs when:

- we subtract two numbers that are almost equal
- one or both numbers are subject to error

Example

cancellation occurs in the example when we evaluate the numerator of

$$f(x) = \frac{1 - (\cos x)^2}{x^2}$$

- $1 \simeq (\cos x)^2$ when x is small
- there is a rounding error in $\cos x$

Numerical stability

refers to the accuracy of an algorithm in the presence of rounding errors

- an algorithm is *unstable* if rounding errors cause large errors in the result
- rigorous definition depends on what 'accurate' and 'large error' mean
- instability is often, but not always, caused by cancellation

Examples from earlier lectures

- solving linear equations by LU factorization without pivoting
- Cholesky factorization method for least squares

Roots of a quadratic equation

$$ax^2 + bx + c = 0 \qquad (a \neq 0)$$

Algorithm 1: use the formulas

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

unstable if $b^2 \gg |4ac|$

- if $b^2 \gg |4ac|$ and $b \leq 0$, cancellation occurs in x_2 ($-b \simeq \sqrt{b^2 - 4ac}$)
- if $b^2 \gg |4ac|$ and $b \geq 0$, cancellation occurs in x_1 ($b \simeq \sqrt{b^2 - 4ac}$)
- in both cases b may be exact, but the squareroot introduces small errors

Roots of a quadratic equation

$$ax^2 + bx + c = 0 \qquad (a \neq 0)$$

Algorithm 2: use fact that roots x_1, x_2 satisfy $x_1 x_2 = c/a$

- if $b \leq 0$, calculate

$$x_1 = \frac{-b + \sqrt{b^2 - 4ac}}{2a}, \qquad x_2 = \frac{c}{ax_1}$$

- if $b > 0$, calculate

$$x_2 = \frac{-b - \sqrt{b^2 - 4ac}}{2a}, \qquad x_1 = \frac{c}{ax_2}$$

no cancellation when $b^2 \gg |4ac|$

Exercises

- `chop(x,n)` rounds x to n significant decimal digits
- for example `chop(pi,4)` returns 3.14200000000000

Exercise 1: cancellation occurs in $(1 - \cos x)/\sin x$ when $x \approx 0$

```
>> x = 1e-2;
>> (1 - chop(cos(x), 4)) / chop(sin(x), 4)

ans =

     0
```

(exact value is about 0.005)

give a stable alternative method

Exercise 2: Euler proved that $\sum_{k=1}^{\infty} k^{-2} = \pi^2/6 = 1.644934\cdots$

the sum of the first 3000 terms is

$$\sum_{k=1}^{3000} k^{-2} = 1.6446$$

we compute this sum rounding all intermediate results to 4 digits:

```
>> sum = 0;
>> for k = 1:3000
       sum = chop(sum + 1/k^2, 4);
   end
>> sum
sum =
   1.6240
```

- result has only two correct digits
- not caused by cancellation (there are no subtractions)

explain and propose a better method

Exercise 3: the number $e = 2.7182818\cdots$ can be defined as

$$e = \lim_{n\to\infty} (1 + 1/n)^n$$

this suggests an algorithm for calculating e: take a large n and evaluate

$$\hat{e} = (1 + 1/n)^n$$

results:

n	$\hat{e}$	Number of correct digits
10^4	2.718145926	4
10^8	2.718281798	7
10^{12}	2.718523496	4
10^{16}	1.000000000	0

explain

Exercise 4: on page 2.11 we showed that for an n-vector x,

$$\mathbf{std}(x)^2 = \frac{1}{n}\|x - \mathbf{avg}(x)\mathbf{1}\|^2 = \frac{1}{n}\left(\|x\|^2 - \frac{(\mathbf{1}^T x)^2}{n}\right)$$

we evaluate the second expression for $n = 10$ and

$$x = (1002,\ 1000,\ 1003,\ 1001,\ 1002,\ 1002,\ 1001,\ 1004,\ 1002,\ 1001)$$

```
>> sum1 = 0.0;  sum2 = 0.0;
>> for i = 1:n
       sum1 = chop( sum1 + x(i), 6 );
       sum2 = chop( sum2 + x(i)^2, 6 );
>> end
>> s = chop( ( sum2 - sum1^2 / n ) / n, 6)
s =
    -3.2400
```

a negative number! explain and suggest a better method