16. Algorithm stability

- cancellation
- numerical stability
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

\[
\cos x = 0.99999999875000\ldots \\
\sim 0.9999999988
\]

- 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

\[
\sin x = 0.499999999791667 \ldots \cdot 10^{-5}
\approx 0.4999999998 \cdot 10^{-5}
\]

- 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

\[ \hat{a} = a(1 + \Delta a), \quad \hat{b} = b(1 + \Delta b) \]

- \( a, b \): exact values
- \( \hat{a}, \hat{b} \): approximations with unknown relative errors \( \Delta a, \Delta b \)
- 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 \( a \approx b \), small \( \Delta a \) and \( \Delta b \) 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

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

- \(1 \approx (\cos x)^2\) 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

\[ ax^2 + bx + c = 0 \quad (a \neq 0) \]

**Algorithm 1:** use the formulas

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

unstable if \( b^2 \gg |4ac| \)

- if \( b^2 \gg |4ac| \) and \( b \leq 0 \), cancellation occurs in \( x_2 \) (\( -b \approx \sqrt{b^2 - 4ac} \))

- if \( b^2 \gg |4ac| \) and \( b \geq 0 \), cancellation occurs in \( x_1 \) (\( b \approx \sqrt{b^2 - 4ac} \))

- in both cases \( b \) may be exact, but the squareroot introduces small errors
Roots of a quadratic equation

\[ ax^2 + bx + c = 0 \quad (a \neq 0) \]

**Algorithm 2:** use fact that roots \( x_1, x_2 \) satisfy \( x_1x_2 = c/a \)

- if \( b \leq 0 \), calculate

\[
x_1 = \frac{-b + \sqrt{b^2 - 4ac}}{2a}, \quad x_2 = \frac{c}{ax_1}
\]

- if \( b > 0 \), calculate

\[
x_2 = \frac{-b - \sqrt{b^2 - 4ac}}{2a}, \quad x_1 = \frac{c}{ax_2}
\]

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 \(x \approx 0\)

```matlab
>> 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 \[ \sum_{k=1}^{\infty} k^{-2} = \frac{\pi^2}{6} = 1.644934 \ldots \]

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:

```matlab
>> 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:

<table>
<thead>
<tr>
<th>( n )</th>
<th>( \hat{e} )</th>
<th>Number of correct digits</th>
</tr>
</thead>
<tbody>
<tr>
<td>( 10^4 )</td>
<td>2.718145926</td>
<td>4</td>
</tr>
<tr>
<td>( 10^8 )</td>
<td>2.718281798</td>
<td>7</td>
</tr>
<tr>
<td>( 10^{12} )</td>
<td>2.718523496</td>
<td>4</td>
</tr>
<tr>
<td>( 10^{16} )</td>
<td>1.0000000000</td>
<td>0</td>
</tr>
</tbody>
</table>

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

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

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

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

```matlab
>> 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