Numerical errors in computer simulations

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Today's outline

1 Introduction

2 Roundoff and truncation errors

3 Break errors

4 Loss of digits

5 (Un)stable methods

6 Symbolic math

7 Summary

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Cell	Value
A1	2
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What's happening?

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Give this a thought!

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Significant digits

A numerical result $\tilde{x}$ is an approximation of the real value x.

- Absolute error

  $\delta = |\tilde{x} - x|, x \neq 0$

- Relative error

  $\frac{\delta}{\tilde{x}} = |\frac{\tilde{x} - x}{\tilde{x}}|$

- Error margin

  $\tilde{x} - \delta \leq x \leq \tilde{x} + \delta$

  $x = \tilde{x} \pm \delta$

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Significant digits

- $\tilde{x}$ has m significant digits if the absolute error in x is smaller or equal to 5 at the $(m+1)$-th position:

  $$10^{q-1} \le |\tilde{x}| \le 10^q$$

  $$|x - \tilde{x}| = 0.5 \times 10^{q-m}$$

- For example:

  $$x = \frac{1}{3}, \tilde{x} = 0.333 \Rightarrow \delta = 0.00033333\ldots$$

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Representation of numbers

- Computers represent a number with a finite number of digits: each number is therefore an approximation due to roundoff and truncation errors.
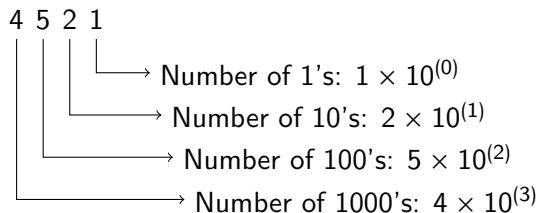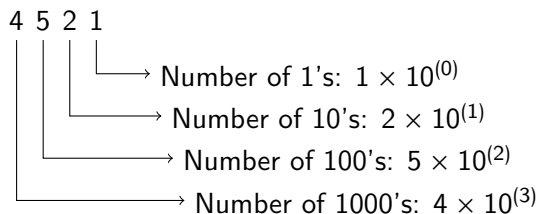
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4 5 2 1

$\longrightarrow$ Number of 1's: $1 \times 10^{(0)}$

$\longrightarrow$ Number of 10's: $2 \times 10^{(1)}$

$\longrightarrow$ Number of 100's: $5 \times 10^{(2)}$

$\longrightarrow$ Number of 1000's: $4 \times 10^{(3)}$

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$(4521)_{10} = 4 \times 10^3 + 5 \times 10^2 + 2 \times 10^1 + 1 \times 10^0$

Representation of numbers

- You could use another basis, computers often use the basis 2:

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$=($

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- In general:

$$(c_m \ldots c_1 c_0)_q = c_0 q^0 + c_1 q^1 + \ldots + c_m q^m, c \in \{0, 1, 2, \ldots, q - 1\}$$

Representation of numbers

- Numbers are stored in binary in the memory of a computer, in segments of a specific length (called a *word*).
- We distinguish multiple types of numbers:
  - Integers: $-301, -1, 0, 1, 96, 2293, \ldots$
  - Floating points: $-301.01, 0.01, 3.14159265, 14498.2$
- A binary integer representation looks like the following bit sequence:

$$z = \sigma \left(c_0 2^0 + c_1 2^1 + \ldots + c_{\lambda-1} 2^{\lambda-1} \right)$$

  σ is the sign of z (+ or -), and λ is the length of the word
- Endianness: the order of bits stored by a computer

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- Excel:
  - Decimal: `=DEC2BIN(214)`
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  - Hexadecimal: `=DEC2HEX(214)`

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    - Hexadecimal: =DEC2HEX(214)

- Matlab:
    - Decimal: dec2bin(214)
    - Other base: dec2base(214,<base>)

Arithmetic operations with binary numbers

Addition:

$0 + 0 = 0$
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$1 + 0 = 1$
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- Multiplication and division are more expensive, and more elaborate

Excercise

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Command	Result
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`format long e`	

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`f`	
`fprintf("%0.16f",f)`	0.1000000000000000

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`f`	
`fprintf("%0.16f",f)`	0.1000000000000000
`fprintf("%0.20f",f)`	0.10000000000000000555

Representation of integer numbers

- In Matlab, integers of the type `int32` are represented by 32-bit words ($\lambda = 31$).

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[1]Matlab does not perform actual integer overflows, it just stops at the maximum.

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- If, during a calculation, an integer number becomes larger than $2^{\lambda} - 1$, the computer reports an overflow[1]

_____

[1]Matlab does not perform actual integer overflows, it just stops at the maximum.

Representation of integer numbers

- In Matlab, integers of the type `int32` are represented by 32-bit words ($\lambda = 31$).

- The set of numbers that an `int32` z can represent is:

$$-2^{31} \leq z \leq 2^{31} - 1 \approx 2 \times 10^9$$

- If, during a calculation, an integer number becomes larger than $2^{\lambda} - 1$, the computer reports an overflow[1]

- How can a computer identify an overflow?

---

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Representation of real (floating point) numbers

- Formally, a real number is represented by the following bit sequence

$$x = \sigma \left(2^{-1} + c_2 2^{-2} + \ldots + c_m 2^{-m} \right) 2^{e-1023}$$

Here, σ is the sign of x and e is an integer value.

- A floating point number hence contains sections that contain the sign, the exponent and the mantissa
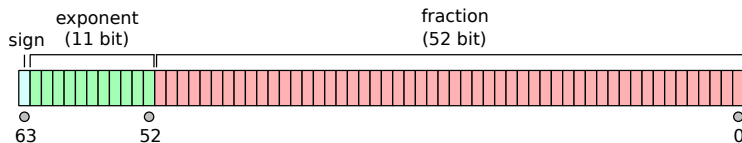
Image: Wikimedia Commons CC by-SA

Representation of real (floating point) numbers

- Example: $\lambda = 3$, $m = 2$, $x = \frac{2}{3}$

$$x = \pm \left(2^{-1} + c_2 2^{-2} \right) 2^e$$

  - $c_0 \in \{0, 1\}$
  - $e = \pm a_0 2^0$
  - $a_0 \in \{0, 1\}$

- Truncation: $fl(x) = 2^{-1} = 0.5$
- Round off: $fl(x) = 2^{-1} + 2^{-2} = 0.75$

Today's outline

① Introduction

② Roundoff and truncation errors

③ Break errors

④ Loss of digits

⑤ (Un)stable methods

⑥ Symbolic math

⑦ Summary

Trigonometric, Logarithmic, and Exponential computations

- Processors can do logic and arithmetic instructions

- Trigonometric, logarithmic and exponential calculations are "higher-level" functions:
  exp, sin, cos, tan, sec, arcsin, arccos, arctan, log, ln, . . .

- Such functions can be performed using these "low level" instructions, for instance using a Taylor series:

$$\sin(x) = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)!} x^{2n+1} = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} + \dots$$

$$e^x = \sum_{n=0}^{\infty} \frac{x^n}{x!} = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \frac{x^4}{4!} + \dots$$

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- These operations involve many multiplications and additions, and are therefore *expensive*
- Computations can only take finite time, for infinite series, calculations are interrupted at N

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- This results in a *break error*

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A computer may use a clever algorithm to limit the number of operations required to perform a higher-level function. A (fictional!) example for the computation of $\sin(x)$:
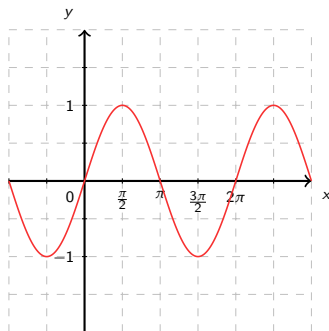
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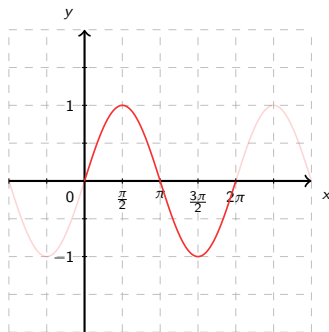3. Use lookup tables for known values
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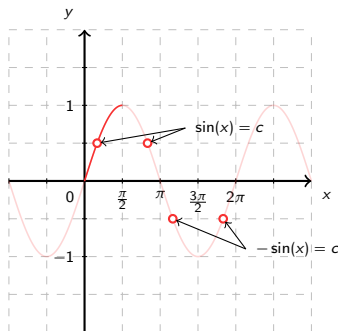
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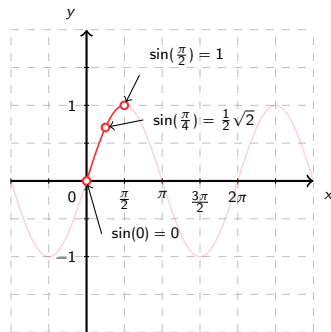
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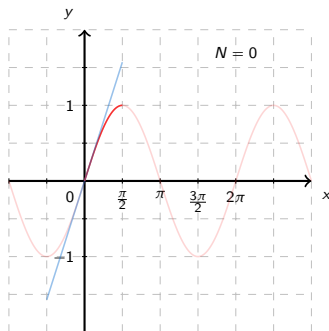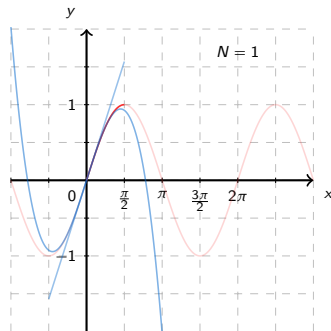
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Today's outline

Loss of digits

- During operations such as $+$, $-$, $\times$, $\div$, an error can add up
- Consider the summation of x and y

$$\tilde{x} - \delta \leq x \leq \tilde{x} + \delta \quad \text{and} \quad \tilde{y} - \varepsilon \leq y \leq \tilde{y} + \varepsilon$$

$$(\tilde{x} + \tilde{y}) - (\delta + \varepsilon) \leq x + y \leq (\tilde{x} + \tilde{y}) + (\delta + \varepsilon)$$

Loss of digits: Example 1

$x = \pi, \tilde{x} = 3.1416$

$y = 22/7, \tilde{y} = 3.1429$

Loss of digits: Example 1

$$\left.\begin{array}{l} x = \pi, \tilde{x} = 3.1416 \\ y = 22/7, \tilde{y} = 3.1429 \end{array}\right\} \;\Rightarrow\; \left.\begin{array}{l} \delta = \tilde{x} - x = 7.35 \times 10^{-6} \\ \varepsilon = \tilde{y} - y = 4.29 \times 10^{-5} \end{array}\right\}$$

Loss of digits: Example 1

$$\left. \begin{array}{l} x = \pi, \tilde{x} = 3.1416 \\ y = 22/7, \tilde{y} = 3.1429 \end{array} \right\} \Rightarrow \left. \begin{array}{l} \delta = \tilde{x} - x = 7.35 \times 10^{-6} \\ \varepsilon = \tilde{y} - y = 4.29 \times 10^{-5} \end{array} \right\}$$

$$x + y = \tilde{x} + \tilde{y} \pm (\delta + \varepsilon) \approx 6.2845 - 5.025 \times 10^{-5}$$

$$x - y = \tilde{x} - \tilde{y} \pm (\delta + \varepsilon) \approx -0.0013 + 3.55 \times 10^{-5}$$

- The absolute error is small ($\approx 10^{-5}$), but the relative error is much bigger (0.028).
- Adding up the errors results in a loss of significant digits!

Loss of digits: Example 2

- Calculate e^{-5}
  - Use the Taylor series
  - Calculate the first 26 terms ($N = 26$)

- Now repeat the calculation, but use for each calculation only 4 digits. What do you find?

- Without errors you would find: $e^{-5} = 0.006738$
- If you only use 4 digits in the calculations, you'll find 0.00998

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Badly (ill) conditioned problems

We consider a system $F(x, y)$ that computes a solution from input data. The input data may have errors:

$$\xrightarrow{\quad x \quad} \boxed{F(x, y) \;=\; 0} \xrightarrow{\quad y \quad} \text{(Without errors)}$$

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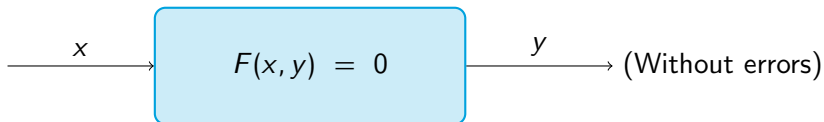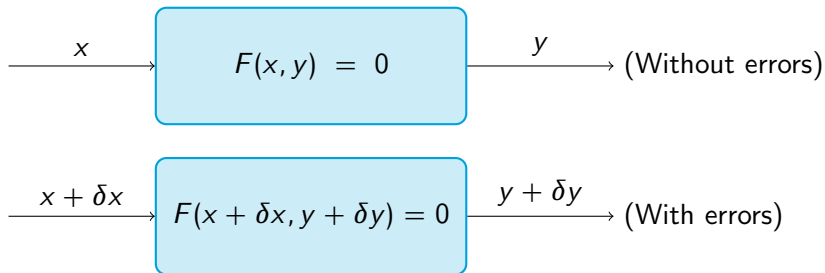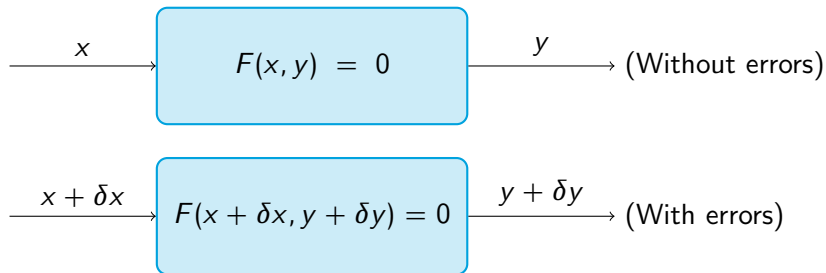
$$y(x + \delta x) - y(x) \approx y'(x)\delta x \qquad\qquad C = \max_{\delta x} \left(\left| \frac{\delta y / y}{\delta x / x} \right| \right)$$

Propagated error on the basis of Taylor expansion

Condition criterion, $C < 10$ error development small

Badly (ill) conditioned problems: Example

Solve the following linear system in Matlab using double and single precision:

$$A = \begin{bmatrix} 1.2969 & 0.8648 \\ 0.2161 & 0.1441 \end{bmatrix}, \quad x = \begin{bmatrix} 0.8642 \\ 0.1440 \end{bmatrix}$$

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Double precision

```
>> clear ; clc ; format long e ;
>> A = [[1.2969 0.8648];
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>> x = [0.8642; 0.1440];
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```

Single precision

```
>> clear;clc;format long e;
>> A = single(
   [[1.2969 0.8648];
   [0.2161 0.1441]] );
>> x = single(
   [0.8642; 0.1440] );
>> y = A\x
y =
   1.3331791e+00
  -1.0000000e+00
```

Badly (ill) conditioned problems: Example

- Matlab already warned us about the bad condition number:
  Warning: Matrix is close to singular or badly scaled.
  Results may be inaccurate. RCOND = 1.148983e-08.

- The RCOND is the reciprocal condition number

- A small error in x results in a big error in y. This is called an ill conditioned problem.

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(Un)stable methods

- The condition criterion does not tell you anything about the quality of a numerical solution method!
- It is very well possible that a certain solution method is more sensitive for one problem than another
- If the method propagates the error, we call it an *unstable method*. Let's look at an example.

The Golden mean

- Let's evaluate the following recurrent relationship:

$$y_{n+1} = y_{n-1} - y_n$$

$$y_0 = 1, \quad y_1 = \frac{2}{1 + \sqrt{5}}$$

- You can prove (by substitution) that:

$$y_n = x^{-n}, \quad n = 0, 1, 2, \ldots, \quad x = \frac{1 + \sqrt{5}}{2}$$

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The Golden mean

Recurrent version

```
% initialise
y(1) = 1;
y(2) = 2 / (1 + sqrt(5));

% Perform recurrent
    approach
for n = 2:39
    y(n+1) = y(n-1)-y(n);
end
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end
```

Powerlaw version

```
% initialise
x = (1 + sqrt(5))/2;
y2(1) = x^0; % n = 1

% Perform powerlaw apprach
for n = 0:39
    y2(n+1) = x^-n
end
```

The Golden mean

n	Recurrent	Powerlaw
1	1.0000	1.0000
1	0.6180	0.6180
2	0.3820	0.3820
3	0.2361	0.2361
. . .	. . .	. . .
37	$3.080 \cdot 10^{-08}$	$2.995 \cdot 10^{-08}$
38	$1.714 \cdot 10^{-08}$	$1.851 \cdot 10^{-08}$
39	$1.366 \cdot 10^{-08}$	$1.144 \cdot 10^{-08}$
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- The recurrent approach enlarges errors from earlier calculations!

The Golden mean

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Start your calculation program of choice (Excel, Matlab, ...)

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Calculate the result of y:

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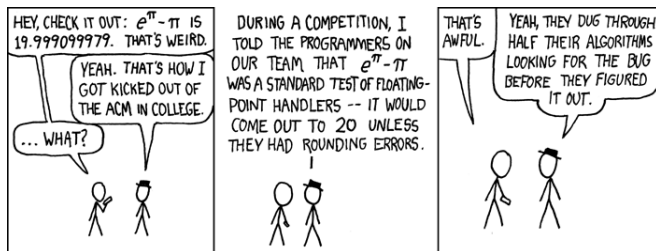
Image: xkcd

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Symbolic math packages

Definition

The use of computers to manipulate mathematical equations and expressions in symbolic form, as opposed to manipulating the numerical quantities represented by those symbols.

- Symbolic integration or differentiation, substitution of one expression into another
- Simplification of an expression, change of subject etc.
- Packages and toolboxes:

Symbolic math packages

Mathematica   Well known software package, license available
               via TU/e

Maple   Well known, license available via TU/e

Wolfram|Alpha Web-based interface by Mathematica developer.
               Less powerful in mathematical respect, but
               more accessible and has a broad application
               range (unit conversion, semantic commands).

Sage   Open-source alternative to Maple,
               Mathematica, Magma, and MATLAB.

Matlab   Symbolic math toolbox

Symbolic math: simplify

$$f(x) = (x-1)(x+1)(x^2+1) + 1$$

Symbolic math: simplify

$$f(x) = (x - 1)(x + 1)(x^2 + 1) + 1$$

```
>> syms x
>> f = (x - 1)*(x + 1)*(x^2 + 1) + 1

f =

(x^2 + 1)*(x - 1)*(x + 1) + 1

>> f2 = simplify(f)

f2 =

x^4
```

Symbolic math: integration and differentiation

$$f(x) = \frac{1}{x^3 + 1}$$

Symbolic math: integration and differentiation

$$f(x) = \frac{1}{x^3 + 1}$$

```
>> syms x
>> f = 1/(x^3+1);
>> my_f_int = int(f)

my_f_int = log(x + 1)/3 - log((x - 1/2)^2 + 3/4)/6 +
    (3^(1/2)*atan((2*3^(1/2)*(x - 1/2))/3))/3

>> my_f_diff = diff(my_f_int)

my_f_diff = 1/(3*(x + 1)) + 2/(3*((4*(x - 1/2)^2)/3 +
    1)) - (2*x - 1)/(6*((x - 1/2)^2 + 3/4))

>> simplify(my_f_diff)

ans = 1/(x^3 + 1)
```

Symbolic math: exercises

Exercise 1

Simplify the following expression:

$$f(x) = \frac{2 \tan x}{(1 + \tan^2 x)}$$

Symbolic math: exercises

Exercise 1

Simplify the following expression:

$$f(x) = \frac{2 \tan x}{(1 + \tan^2 x)} = \sin 2x$$

```
>> simplify(2*tan(x)/(1 + tan(x)^2))
```

Symbolic math: exercises

Exercise 1

Simplify the following expression:

$$f(x) = \frac{2\tan x}{(1 + \tan^2 x)} = \sin 2x$$

```
>> simplify(2*tan(x)/(1 + tan(x)^2))
```

Exercise 2

Calculate the *value* of p:

$$p = \int_0^{10} \frac{e^x - e^{-x}}{\sinh x} dx$$

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Exercise 2

Calculate the *value* of p:

$$p = \int_0^{10} \frac{e^x - e^{-x}}{\sinh x} dx$$

```
>> f = ((exp(x)- exp(-x))/sinh(x));
>> p = int(f,0,10)
p = 20
```

Symbolic math: root finding

A root finding method searches for the values where a function reaches zero. We will cover the numerical methods later, here we show how to use root finding with symbolic math in Matlab.

Symbolic math function

$$f(x) = \frac{3}{x^2 + 3x} - 2$$

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```
>> syms x
>> f = 3 / (x^2 + 3*x) - 2;
>> solve(f)
ans =
    15^(1/2)/2 - 3/2
  - 15^(1/2)/2 - 3/2
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Function as a string

$$f(x) = x^2 - 4x + 2$$

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```

Function as a string

$$f(x) = x^2 - 4x + 2$$

```
>> solve('x^2 - 4*x + 2')
ans =
 2^(1/2) + 2
 2 - 2^(1/2)
```

Symbolic math toolbox: variable precision arithmetic

Variable precision can be used to specify the number of significant digits.

```
>> p = vpa (1/3 ,16)
p = 0.3333333333333333
>> p = vpa (1/3 ,4)
p = 0.3333
>> a = vpa (0.1 , 30)
a = 0.1
>> b = vpa (0.1 , 5);
b = 0.1
>> a-b

ans = 0.00000000000000005684341886080801486968993846751
```

Today's outline

1 Introduction

2 Roundoff and truncation errors

3 Break errors

4 Loss of digits

5 (Un)stable methods

6 Symbolic math

7 Summary

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- Numerical errors mar arise due to truncation, roundoff and break errors, which may seriously affect the accuracy of your solution

- Errors may propagate and accumulate, leading to smaller accuracy

- Ill-conditioned problems and unstable methods have to be identified so that proper measures can be taken

- Symbolic math computations may be performed to solve certain equations algebraically, bypassing numerical errors, but this is not always possible.

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