Matlab and Programming 1 Programming basics and algorithms

Ivo Roghair, Martin van Sint Annaland

Chemical Process Intensification Eindhoven University of Technology

Today's outline

- Introduction
- Variables
- 3 Creating algorithms
- 4 Functions
- Conclusions

Programming

"Everybody in this country should learn to program a computer, because it teaches you to think.."

—Steve Jobs



Why?

- Scientific techniques depend in an increasing fashion upon computer programs and simulation methods
- Knowledge of programming allows you to automate routine tasks
- Ability to understand algorithms by inspection of the code
- Learn to think by dissecting a problem into smaller bits









> Start Matlab, and enter the following commands on the command line. Evaluate the output.

```
>> 2 + 3
                % Some simple calculations
>> 2*3
>> 2*3^2
                % Powers are done with ^
>> a = 2
                % Storing values into the workspace
>> b = 3
>> c = (2*3)^2 % Parentheses set priority
>> 8/a-b
>> sin(a)
                % Mathematical functions can be used
>> \sin(0.5*pi)
                % pi is an internal Matlab variable
>> 1/0
                % Infinity is a thing ...
>> sqrt(-1)
                % ... as are imaginary numbers
```

Introduction to programming

What is a program?

Introduction 000000000000

> A program is a sequence of instructions that is written to perform a certain task on a computer.

- The computation might be something mathematical, such as solving a system of equations or finding the roots of a polynomial
- It can also be a symbolic computation, such as searching and replacing text in a document
- A program may even be used to compile another program
- A program consists of one or more algorithms

- Use an integrated development environment
 - Matlab
 - MS Visual Studio/Code
 - Eclipse
 - Dev C++
 - IDLE, Canopy (express)
- Create a simple program:
 - Hello world
 - Find the roots of a parabola
 - Find the greatest common divisor of two numbers

Some often used programming languages

Python

- Many functionalities available
- Smooth learning curve
- Slow compared to compiled languages
- Many freely available editors

Pascal

- Limited number of libraries available
- Steep learning curve
- Compiled language, may be fast
- Some free compilers (fpc)

C / C++ / C#

- Many functionalities available
- Steeper learning curve
- Needs compilation, very fast (HPC)
- Freely available (gcc, MSVC)

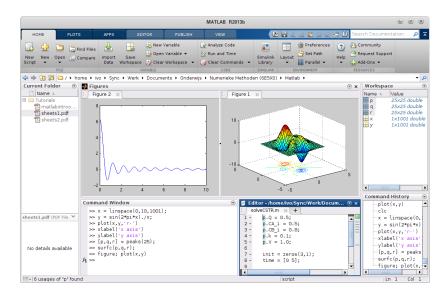
Spreadsheet (Excel, Google Docs, ...)

- High availability
- Low learning curve
- Very limited for larger problems, unbeatable for quick calculations
- Not always free

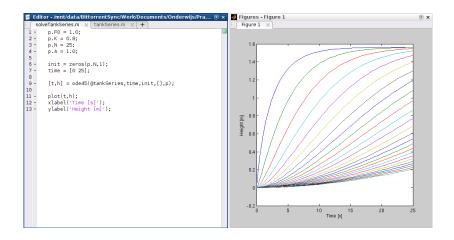
Matlab

- Many functionalities built-in (80+ toolkits!)
- Slow compared to compiled languages

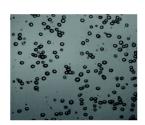
- Fairly smooth learning curve
- Needs a license (alternatives: SciLab, GNU Octave)

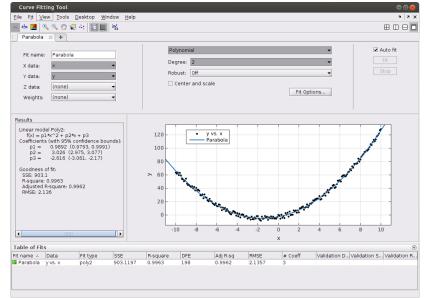


Versatility of Matlab: ODE solver



```
I = imread('bubbles.png');
BW = rgb2gray(I);
E = edge(BW, 'canny');
F = imfill(E, 'holes');
result = regionprops(F);
```





- Matlab documentation: doc or help function
 - Canvas page
 - Introduction to Numerical Methods and Matlab Programming for Engineers. T. Young and M.J. Mohlenkamp (2015).
 GNU-licensed document, online
 - Search the web!



- Variables
- 3 Creating algorithms
- 4 Functions
- G Conclusions

Terminology

Variable Piece of data stored in the computer memory, to be referenced and/or manipulated Function Piece of code that performs a certain operation/sequence of operations on given input Operators Mathematical operators (e.g. + - * or /), relational (e.g. < >or ==, and logical operators (&&, ||) Script Piece of code that performs a certain sequence of operations without specified input/output Expression A command that combines variables, functions, operators and/or values to produce a result.

Variables in Matlab

- Matlab stores variables in the workspace
- You should recognize the difference between the identifier of a variable (its name, e.g. x, setpoint_p), and the data that it actually stores (e.g. 0.5)
- Matlab also defines a number of variables by default, e.g. eps, pi or i.
- You can assign a variable by the = sign:

```
>> x = 4*3
x = 12
```

- If you don't assign a variable, it will be stored in ans
- Clearing the workspace is done with clear.

Vectors in Matlab (1)

A row vector:

$$>> v = [0 1 2 3]$$

A column vector by separating elements with semi-colons:

Access (i.e. read) an entry in a vector:

Manipulate the value of that entry:

Get a slice of a vector:

>>
$$u([2 \ 3 \ 4]) \%$$
 With colon operator: $u(2:4)$

Transposing vectors:

$$>> W = V$$
,

Manual definition may be cumbersome. A colon (:) generates a list:

```
>> a = 1:10 % Default stride is 1
>> x = -1:.1:1 % start:stride:stop specifies list
```

Or, when you prefer to set the *number of elements* instead of the step size:

```
>> y = linspace(0,10,11)
>> p = logspace(2,6,5)
```

Manipulating multiple components:

```
>> y([1 4:7]) = 1
```

Or (by supplying a vector instead of a scalar):

```
>> y([1 4:7]) = 16:20 % equivalent to y([1 4 5 6 7]) = [16 17 18 19 20]
```

Practice

Given a vector

$$x = [2 \ 4 \ 6 \ 8 \ 10 \ 12 \ 14 \ 16 \ 18 \ 20 \ 30 \ 40 \ 50 \ 60 \ 70 \ 80]$$

- Find a way to define the vector without typing all individual elements
- Investigate the meaning of the following commands:

```
>> y = x(5:end)
>> y(4)
>> y(4) = []
>> sum(x)
>> mean(x)
>> std(x)
>> max(x)
>> fliplr(x)
>> diff(x)
```

Operations on vectors (1)

```
>> e = 1:5
>> f = 2*e
>> g = 4*f + 20
>> h = e^2
```

... wait ... what's that?

```
Error using ^
Inputs must be a scalar and a square matrix.
To compute elementwise POWER, use POWER (.^) instead.
```

Matlab uses matrix operations by default, we should use a dot operator to make operations element-wise for *, / and $^{\circ}$.

```
>> e.^2
```

Operations on vectors (2)

To demonstrate the matrix product:

```
>> p = [1; 1; 1]
>> q = [1 2 3]
>> p*q % which is not equal to q*p
```

All kinds of mathematical functions on vectors typically operate on elements:

```
>> x = linspace(0,2*pi,100);
>> s = sin(x)
>> e = exp(x)
```

Building blocks: Mathematics and number manipulation

Programming languages usually support the use of various mathematical functions (sometimes via a specialized library). Some examples of the most elementary functions in Matlab:

Command	Explanation
cos(x), $sin(x)$, $tan(x)$	Cosine, sine or tangens of x
mean(x), std(x)	Mean, st. deviation of vector x
exp(x)	Value of the exponential function e^x
log10(x), log(x)	Base- $10/N$ atural logarithm of x
floor(x)	Largest integer smaller than x
ceil(x)	Smallest integer that exceeds x
abs(x)	Absolute value of x
size(x)	Size of a vector x
length(x)	Number of elements in a vector x
rem(x,y)	Remainder of division of x by y

Printing results

You can prevent displaying the outcome of a command by adding a semi-colon at the end of a line:

```
>> c = linspace(0,10,11);
>> length(c)
>> c
>> size(c)
```

Altering the display format can be done using the format command:

```
>> format compact % loose
>> format long % short
```

Make a plot of the following table

T (°C) | 5 20 30 50 55
$$\mu$$
 (Pa·s) | 0.08 0.015 0.009 0.006 0.0055

```
>> x = [5 20 30 50 55]
y = [0.08 \ 0.015 \ 0.009 \ 0.006 \ 0.0055]
>> plot(x,y)
>> plot(x,y,'*')
>> plot(x,y,'r--')
>> plot(x,y,'ko-','LineWidth',2)
>> xlabel('Temperature [^\circC]')
>> ylabel('Viscosity [Pa s]')
>> title('Experiment 1')
```

Practice

Create plots of the following functions in a single figure for $x \in \{0, 2\pi\}$:

$$y_1 = \cos x$$

$$y_2 = \arctan x$$

$$y_3 = \frac{\sin x}{x}$$

Strategies to draw multiple graphs in 1 figure:

```
>> plot(x,y1,x,y2,x,y3)
```

```
>> plot(x,y1)
>> hold on; % Maintain drawn plots in current figure
>> plot(x,y2)
>> plot(x,y3) % The 'hold-property' was already set
```

Matrices in Matlab

Matrix A is defined as:

In Matlab:

$$A = \begin{bmatrix} 8 & 1 & 6 \\ 3 & 5 & 7 \\ 4 & 9 & 2 \end{bmatrix}$$

Elements can be accessed/manipulated by the following syntax:

- >> A(3,1) % Third row, first column, also A(3)
- >> A(3,:) = [2 4 8] % Set entire third row
- >> A(:,3) % Print third column
- \Rightarrow A(A>5) = 2 % Set elements by condition

There are a few functions that help creating matrices:

- >> A = zeros(4) % A 4x4 matrix with zeros
- \rightarrow A = ones(4,1) % A 4-element vector with ones
- \Rightarrow A = eye(3) % Identity matrix of 3x3
- >> A = rand(3,4) % A 3x4 matrix with random numbers

Find a short Matlab expression to create the following matrix:

$$A = \begin{bmatrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 \\ 9 & 7 & 5 & 3 & 1 & -1 & -3 \\ 4 & 8 & 16 & 32 & 64 & 128 & 256 \end{bmatrix}$$

- Investigate the command max(A). What does it give?
- How to obtain the maximum for each row?
- Use a vector multiplication to compute the following matrix:

$$A = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 2 & 2 & 2 & 2 \\ 3 & 3 & 3 & 3 \\ 4 & 4 & 4 & 4 \end{bmatrix}$$

Matlab uses different types of variables:

Datatype	Example
string	'Wednesday'
integer	15
float	0.15
vector	[0.0; 0.1; 0.2]
matrix	[0.0 0.1 0.2; 0.3 0.4 0.5]
struct	<pre>sct.name = 'MyDataName'</pre>
logical	<pre>sct.number = 13 0 (false) 1 (true)</pre>

About variables

 Matlab variables can change their type as the program proceeds (this is not common for other programming languages!):

```
>> s = 'This is a string'
s =
This is a string
>> s = 10
s =
10
```

- Vectors and matrices are essentially *arrays* of another data type. A vector of struct is therefore possible.
- Variables are *local* to a function (more on this later).

Today's outline

- Introduction
- Variables
- 3 Creating algorithms
- 4 Functions
- 6 Conclusions

Building blocks: conditional statements

if-statement: Check whether a (set of) condition(s) is met.

```
num = floor (10 * rand + 1);
guess = input ('Your guess please : ');
if ( guess ~= num )
  disp (['Wrong, it was ',num2str(num),'. Kbye.']);
else
    disp ('Correct !');
end
```

Other relational operators

==	is equal to
<=	is less than or equal to
>=	is greater than or equal to
<	is less than
>	is greater than

Combining conditional statements

&&	and
11	or
xor	exclusive or

Building blocks: loops

for-loop: Performs a block of code a certain number of times.

```
>> p(1) = 1;
>> p(2) = 1;
>> for i = 2:10
p(i+1) = p(i)+p(i-1);
end
>> p
p =
                   5
       1
                          13 21
                                  34 55
                                           89
```

while-loop: Performs and repeats a block of code until a certain condition.

```
num = floor (10* rand +1);
guess = input ('Your guess please : ');
while ( guess ~= num )
    guess = input ('That is wrong. Try again ... ');
end
if (isempty(guess))
    disp('No number supplied - exit');
else
    disp ('Correct!');
end
```

Example algorithm

Compute the factorial of N: $N! = N \cdot (N-1) \cdot (N-2) \cdot \cdot \cdot 2 \cdot 1$

How to deal with this?

Naive approach

```
Z = 1;
Z = Z*2;
Z = Z*3;
Z = Z*4;
... etc ...
```

For-loop

```
Z = 1;
for i = 1:N
    Z = Z*i;
end
```

While-loop

```
Z = 1;
i = 1;
while (i<=N)
    Z = Z*i;
    i = i+1:
end
```

Note: N must be set beforehand!

Note: Pay attention to the relational operators!

Building blocks: case selection

switch-statement: Selects and runs a block of code.

```
[dnum,dnam] = weekday(now);
switch dnum
    case {1,7}
        disp('Yay! It is weekend!');
    case 6
        disp('Hooray! It is Friday!');
    case {2,3,4,5}
        disp(['Today is ' dnam]);
    otherwise
        disp('Today is not a good day...');
end
```

Many programs require some input to function correctly. A combination of the following is common:

- Input may be given in a parameters file ("hard-coded")
- Input may be entered via the keyboard

```
>> a = input('Please enter the number ');
```

Input may be read from a file, e.g.

```
>> data = getfield(importdata('myData.txt, ' ', 4)
        , 'data');
>> numdata = xlsread('myExcelDataFile.xls');
```

• There are many more advanced functions, e.g. fread, fgets, ...

Input and output

Output of results to screen, storing arrays to a file or exporting a graphic are the most common ways of getting data out of Matlab:

- Results of each expression are automatically shown on screen as long as the line is not ended with a semi-colon;
- Output may be stored via the GUI:
 - Use the 'Export Setup' function
 - Save figure (use .fig, .eps or .png, not .jpg or .pcx)
 - Save variables (right click, save as)
- Save variables automatically (scripted):

```
>> savefile = 'test.mat';
>> p = rand(1,10);
>> q = ones(10);
>> save(savefile,'p','q')
```

More advanced functions can be found in e.g. fwrite, fprintf,

. . .

•00000000

Today's outline

- Introduction
- Variables
- 3 Creating algorithms
- **4** Functions
- Conclusions

Functions - general

A function in a programming language is a program fragment that performs a certain task. Creating functions keeps your code clean, re-usable and structured.

- You can use functions supplied by the programming language, and define functions yourself
- Functions take one or more input parameters (arguments), and return an output (result).
 - If functions do not return a result, it is called a procedure
- In Matlab, functions are defined as follows (2 output variables) and 3 input arguments):

```
function [out1, out2] = myFunction(in1, in2, in3)
```

Functions - locality and arguments

- You are supplying arguments to a function because it does not have acces to previously defined variables. This is called locality.
 - This does not include global variables but they're evil!
 - Local variables created in a function are not accessible to other functions unless they are returned or supplied as an argument!

Exercise: write a function that takes 3 variables, and returns the average:

Approach 1

```
function res = avg1(a,b,c)
    mySum = a + b + c;
    res = mySum / 3;
end
```

Approach 2

```
function res = avg2(a,b,c)
    data = [a; b; c];
    res = mean(data);
end
```

Exercise: create a function

Compute
$$N! = N \cdot (N-1) \cdot (N-2) \cdot \cdot \cdot 2 \cdot 1$$

Create a function of our while-loop approach with N the argument:

```
Original script

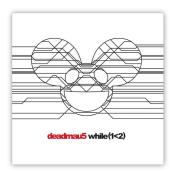
Z = 1;
i = 1;
while (i<=N)
    Z = Z*i;
    i = i+1;
end</pre>
```

```
Function
function Z = fact_while(N)
Z = 1;
i = 1:
while (i<=N)
    Z = Z*i;
    i = i+1:
end
end
```

Functions - checking input

The function we created computes the factorial correctly!

- When the supplied argument is positive and
- When the supplied argument is a natural number...



 In this case, we should check the user input to prevent an infinite loop:

```
if (fix(N)~=N) | (N<O)</pre>
    disp 'Provide a positive
         integer number!'
    return;
end
```

 If no check can be done before a while-loop, you may want to stop after x loops

Functions - checking input

The whole factorial function, including comments:

```
function Z = fact_while(N)
%% This function computes a factorial of input value N
% Usage : fact_while(N)
% N : value of which the factorial is computed
% returns: factorial of N
% Catch non-integer case
if (fix(N)~=N) | (N<O)</pre>
    disp 'Provide a positive integer number!'
    return;
end
Z = 1;
i = 1;
while (i<=N)
    Z = Z*i:
    i = i+1;
end
```

Recursion

- In order to understand recursion, one must first understand recursion
- A recursive function is called by itself (a function within a function)
 - This could lead to infinite calls:
 - A base case is required so that recursion is stopped;
 - Base case does not call itself, simply returns.



Recursion: example

```
function out = mystery(a,b)
if (b == 1)
    % Base case
    out = a;
else
    % Recursive function call
    out = a + mystery(a,b-1);
end
```

- What does this function do?
- Can you spot the error?
- How deep can you go? Which values of b don't work anymore?

Recursion: exercise

Create a function computing the factorial of N, based on recursion.

```
function res = fact_recursive(x)
% Catch non-integer case
if (fix(x)^=x) | (x<0)
    disp 'You should provide a positive integer number
         only'
    return;
end
if (x > 1)
    res = x*fact_recursive(x-1);
else
    res = 1;
end
end
```

Today's outline

- Introduction
- Variables
- 3 Creating algorithms
- 4 Functions
- 6 Conclusions

- Matlab: A versatile development environment, with excellent vector and matrix computations
- Programming basics: variables, operators and functions, locality of variables, recursive operations
- Next lecture: advanced practices (prepare, read instructions) on Canvas)
- For now: exercises 1-4 (basics), 5+6 (advanced).