Octave at BFH-TI Biel

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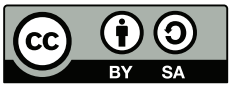
Foreword

These lecture notes were used at my school to familiarize students with *Octave*, to be used to solve engineering problems. A first version was based on MATLAB and you will still find sections to be adapted to *Octave*. Wherever possible I attempted to provide code working with both *Octave* and MATLAB .

The notes consist of two chapters.

- The first chapter is an introduction to the basic *Octave* commands and data structures. The goal is to provide simple example for often used commands and point out some important aspects of programming in *Octave* or MATLAB. The students are expected to work through all of those sections. Then they should be prepared to use *Octave* and MATLAB for their projects.
- The second chapter consists of applications of *Octave*. In each section the question or problem is formulated and then solved with the help of *Octave*. This small set of applications with solutions shall help you to use *Octave* to solve **your** engineering problems. In class I choose a few of those topics and present them to the students.



Contents

Chapter 1

Introduction to *Octave*

The first chapter, consisting of five sections, gives a very brief introduction into programming with *Octave*. This part is by no measure complete and the standard documentation and other references will have to be used. Here are some keywords presented in the sections of this chapter:

- Remarks on `MATLAB` and pointers to documentation.
- Starting up an *Octave* work environment.
- Installing additional packages.
- How to get help.
- Vectors, matrices and vectorized code.
- Script files and function files.
- Data types, functions, control statements, conditions.
- Data files, reading and writing information.
- Solving equations of different type.
- Create basic graphics and manipulate images.
- Solve ordinary differential equations. Include C++ code in *Octave*.

1.1 Starting up *Octave* and First Steps

The goal of this section is to get the students stated using *Octave*, i.e. launching *Octave*, available documentation and information. Some of the information is adapted to the local setup at this school and will have to be modified if used in a different context. program *Octave*[1] is very similar to MATLAB. If you master *Octave* then MATLAB is easy too. *Octave* is developed and maintained on Unix systems. There is a number of excellent additional packages for *Octave* available on the internet[2].

> For most tasks MATLAB and *Octave* are equivalent

The home page of this author[3] [www:sha] gives more information and also a binary package to be installed on Win* systems.

References

- David Griffiths from the University of Dundee prepared an excellent set of notes on MATLAB [Grif01]. These notes are available on the local system as `MatlabNotes.pdf` .

  > Have a copy of these notes ready when working with MATLAB or *Octave*

- The *Octave* manual is available in the form of HTML files and provides basic documentation of all *Octave*–commands. Read the files with a browser. Almost all of the commands apply to MATLAB too. On the local Linux installation of *Octave* find this documentation currently at `/usr/share/doc/octave3.2-htmldoc/interpreter/index.html` .
  On the web site [www:sha] find these files as HTML, PDF or as one compressed file. You are free to copy these files and use them on your computer, even without an internet connection.

  > You **need** access to this information when working with *Octave*

- The book [Hans11] by Jesper Hansen is an elementary and short introduction to *Octave*.
- A good reference for engineers is the book by Biran and Breiner [BiraBrei99].
- Another useful reference is the book by Hanselman and Littlefield ([HansLitt98]). Newer Versions of this book are available.
- On the *Octave* web page there is Frequently Asked Question (FAQ) page:
  `http://www.gnu.org/software/octave/FAQ.html`
- There are active mailing list for *Octave*, currently at
  `https://mailman.cae.wisc.edu/pipermail/help-octave/`. For specific questions I very often use the search engine `Nabble` to be found at
  `http://octave.1599824.n4.nabble.com/` .
- The book [Quat10] is considerably more advanced and shows how to use *Octave* and MATLAB for scientific computing projects.

Since *Octave* and MATLAB are very similar you can also use MATLAB documentation and books.

[1] `http://www.octave.org`
[2] `http://sourceforge.net/projects/octave`
[3] `http://staff.ti.bfh.ch/sha1/`

- The on-line help system of MATLAB allows to find precise description of commands and also to search for commands by name, category or keywords. Learning how to use this help system is an essential step towards getting the most out of MATLAB.
- As part of the help system in MATLAB two files might be handy for beginners:
  - GettingStarted.pdf as a short (138 pages) introduction to MATLAB.
  - UsingMatlab.pdf is a considerably larger, thorough and complete documentation of commands in MATLAB.

  The above documents are also available on the web site of Mathworks at
  http://www.mathworks.com/access/helpdesk/help/techdoc/matlab.shtml

> One of the most important points when using advanced software is how to take advantage of the available documentation.

Notations

In these notes we show most *Octave* or MATLAB code in a block, separated by horizontal lines. If input (commands) and results are shown in the same block, they are separated by a line containing the string `-->` .

Octave

```
code
-->
results
```

Individual commands may be shown within regular text, e.g as `plot(x,sin(x))` .

1.1.1 Starting up *Octave* or MATLAB

Starting up *Octave*

A working environment for *Octave* consists of

1. a command line shell with *Octave* to launch the commands
2. an editor to write the code. Your are free to choose your favorite editor, but editors providing an *Octave* or MATLAB mode simplify coding.
   - This author has a clear preference for the editor EMACS, available for many operations system. On Linux systems ou might want to try gedit.
   - for WIN* systems the editor notepad++ might be a good choice
   - MATLAB has a built in editor.
3. possibly a browser to access the documentation
4. possilbly one or more graphics windows

Thus a working screen might look like Figure 1.1. Your windows manager (e.g. Xfce, KDE or GNOME) will allow you to work with multiple, virtual screens. This is very handy to avoid window cluttering.

To start up *Octave* on a Unix system at our school you may proceed as follows:

- Open a shell. Change to the directory in which you want to work, use cd .

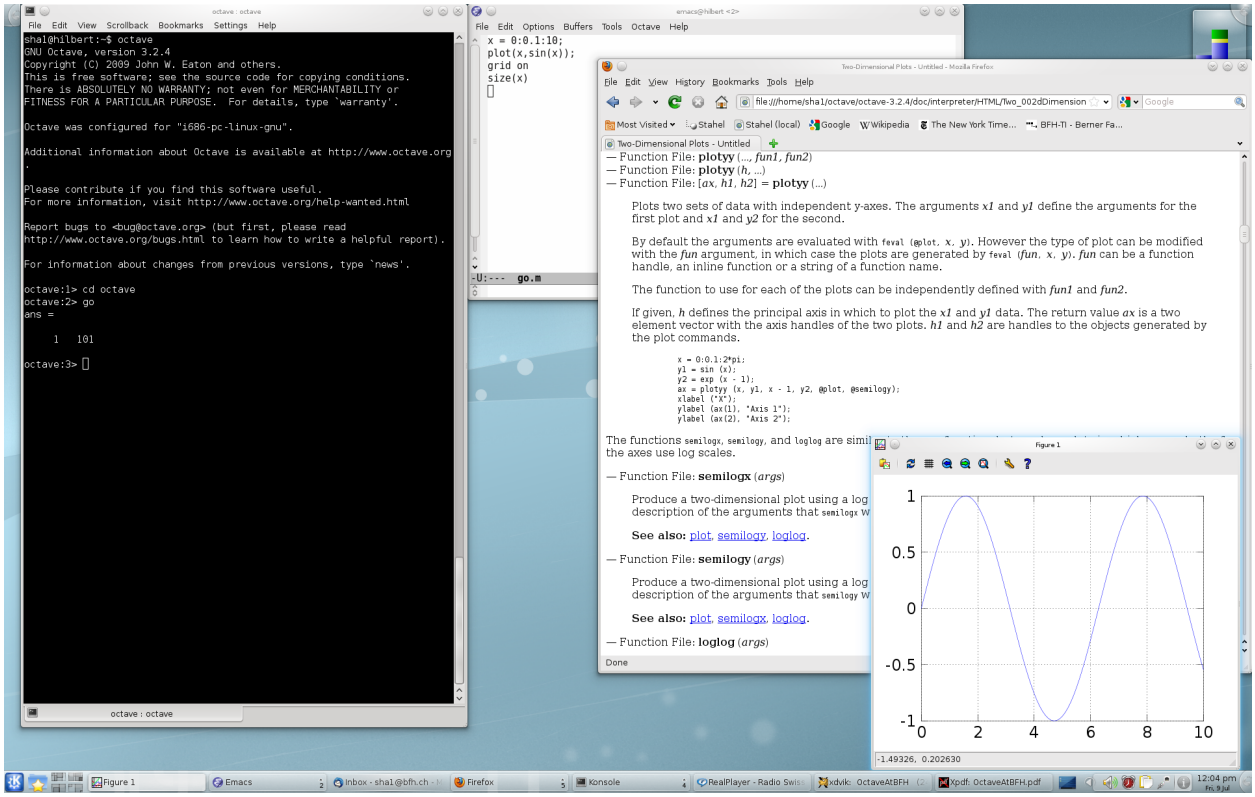


Figure 1.1: Screenshot of an *Octave* work setup

- Type `octave`
- If you prefer a GUI similar to `MATLAB` you may give **qtoctave** a try.
- You may also use the **Xfce or KDE** user interface, locate the menu for *Octave*, click on it and the program will start. You will have to set the working directory with a `cd` command.
- Use your favorite editor to work on your *Octave* files. The standard extension for *Octave* code files is `.m`.
- On startup *Octave* will read a file `.octaverc` in the current users home directory. In this file the user can give commands to *Octave* to be applied at each startup. The file below will set values for the variables `is_matlab` and `is_octave` to decide at runtime which program is currently used. Additionally *Octave* will search in the given directory and all its subdirectories for commands. Thus the user can place his script and function files in this directory and *Octave* will find these commands, independent of the current directory.
  - For versions 3.6.1 of *Octave* I use

.octaverc

```
pkg prefix ~/octave/forge;       # set the prefix to load packages
addpath (genpath ("~/octave/site")); # add this path to the search path
graphics_toolkit fltk            # use the OpenGL based graphics engine
#graphics_toolkit gnuplot        # use gnuplot as graphics engine
is_octave = 1; is_matlab = 0;    # for tests if octave is running
more off  # no paging of output
set(0,'DefaultAxesXGrid','on')   # turn on grids for graphics
set(0,'DefaultAxesYGrid','on')
set(0,'DefaultAxesZGrid','on')
```

	Unix	*Octave*
show current directory	`pwd`	`pwd`
change into directory `MyDir`	`cd MyDir`	`cd MyDir`
change one directory level up	`cd ..`	`cd ..`
list all files in current directory	`ls`	`ls`
list more information about files	`ls -al`	`ls -al`
remove the file `go.m`	`rm go.m`	`delete go.m`
create a directory `newDir`	`mkdir NewDir`	`mkdir NewDir`
remove the directory `newDir`	`rmdir NewDir`	`rmdir NewDir`

Table 1.1: Basic system commands

Using basic Unix commands

When working on a computer system some basic command might be handy. Table 1.1 shows a few useful Unix commands. Some of the commands also work on the *Octave* command line. The behaviour on a Win* system might be different.

How to install a package from OctaveForge

As an essential addition to *Octave* a large set of additional packages is available at `http://octave.sourceforge.net/`. An extensive documentation is given by the option `Function Reference` on the web page. If you find a command in those packages and want to make it available to you installation you have to proceed as follows:

- To be done once:
  - Decide where you want to store your packages. As an example consider the sub directory `octave` in your home directory. Create this directory, launch *Octave* and tell it to store packages there with the command

    Octave
    ```
    pkg prefix ~/octave
    ```

    Since the tilde character ~ replaced by the current users (in this case `sha1`) home directory the packages will be setup in the directory `/home/sha1/octave/` and its sub-directories. This command can ans should be integrated in your **.octaverc** file.
- To be done for each package:
  We examine an example with a plot package, aiming for the command `quiver()`. There are different options to install the plot package, containing this command:
  - It might already be installed, try `help quiver`
  - On a Linux installation use your favorite package manager to install the plot package of *Octave*, e.g. Synaptic or `apt-get ...`
  - Let *Octave* try to download, compile and install the package.

    Octave
    ```
    pkg install -forge plot
    ```
  - You can download, compile and install step by step, as outlined below.

  - Go to the web page `http://octave.sourceforge.net/` and choose the option `packages`. Then search for the package `Plot` and download it to your local disk and store it in the above directory.
  - Launch *Octave* and change in the directory with the package. Then install the package with the command

    Octave
    ```
    pkg install plot-1.0.7.tar.gz
    ```

    From now on the commands provided by the package are available.
  - You may also locate the source for the command `quiver.m` by

    Octave
    ```
    which quiver
    -->
    quiver is the user-defined function from the file
    /home/sha1/octave/plot-1.0.7/quiver.m
    ```

    Having the source code may allow you to adapt the code to you personal needs.

- Commands to maintain the packages:
  - To show a list of all packages use

    Octave
    ```
    pkg list all
    ```
  - To make the additional commands unavailable you may unload a package, e.g.

    Octave
    ```
    pkg unload plot
    ```
  - You can load an already installed package, e.g.

    Octave
    ```
    pkg load plot
    ```

Information about the operating system and the version of *Octave*

When working with *Octave* you can obtain information about the current system with a few commands. Obviously your results may differ from the results below.

- The command `computer()` shows the operating system and the maximal number of elements an array may contain.

  Octave
  ```
  [C, MAXSIZE, ENDIAN] = computer()
  -->
  C = i686-pc-linux-gnu
  MAXSIZE =  2.1475e+09
  ENDIAN = L
  ```

  The result of $2.1475 \cdot 10^9 \approx 2^{31}$ shows that arrays are indexed by 32-bit integers.

- With `uname()` some more information about the computer and the operating system is displayed.

  Octave

```
nn = uname()
—>  scalar structure containing the fields:

    sysname = Linux
    nodename = hilbert
    release = 3.2.0-33-generic
    version = #52-Ubuntu SMP Thu Oct 18 16:29:15 UTC 2012
    machine = x86_64
```

With `version()` the used version of *Octave* is displayed, e.g. 3.6.1. With the command `ver()` the versions of all packages are displayed.

Octave

```
octave:1> ver()
-------------------------------------------------------------------------
GNU Octave Version 3.6.3
GNU Octave License: GNU General Public License
Operating System: Linux 3.2.0-33-generic #52-Ubuntu SMP
                  Thu Oct 18 16:29:15 UTC 2012 x86_64
-------------------------------------------------------------------------
Package Name    | Version | Installation directory
----------------+---------+-----------------------
      control *|   2.4.1 | /home/sha1/octave/control-2.4.1
      general  |   1.3.2 | /home/sha1/octave/general-1.3.2
        image  |   2.0.0 | /home/sha1/octave/image-2.0.0
      mapping  |   1.0.7 | /home/sha1/octave/mapping-1.0.7
miscellaneous  |   1.2.0 | /home/sha1/octave/miscellaneous-1.2.0
       odepkg *|   0.8.2 | /home/sha1/octave/odepkg-0.8.2
        optim  |   1.2.2 | /home/sha1/octave/optim-1.2.2
         plot *|   1.1.0 | /home/sha1/octave/plot-1.1.0
       signal  |   1.2.0 | /home/sha1/octave/signal-1.2.0
      specfun  |   1.1.0 | /home/sha1/octave/specfun-1.1.0
       struct  |  1.0.10 | /home/sha1/octave/struct-1.0.10
```

- With the command `ispc()`, `isunix()` and `ismac()` you can find out what operating system is currently used. These commands are useful for code depending on the OS, e.g. the exact form of file and directory names.

Octave

```
[ispc(), isunix(), ismac()]
—>    0    1    0
```

The results shows that currenly a Unix system is running, in this case Linux. With

Octave

```
octave:16> isieee()
—>  1
```

verify that your system conforms to the IEEE standard for floating point calculations.

- With the command `getrusage()` you can extract information about the current *Octave* process, e.g. memory usage and CPU usage.

Starting up MATLAB

A working environment for MATLAB consists of

1. a command line shell with MATLAB to launch the commands
2. an editor to write the code
3. possibly a browser to access the documentation
4. possilbly one or more graphics windows

To start up MATLAB on a Unix system at our school you may proceed as follows:

- Open a shell.
- Change to the directory in which you want to work, use `cd` .
- Type `matlab -nojvm` to launch MATLAB. The option `-nojvm` launches MATLAB without the splashy Java interface and thus uses a lot less memory, which might be precious resource your system.
- If you type `matlab&` then MATLAB will launch with the flashy Java interface. Using the ampersand `&` allows you to launch other commands in the same shell. Do not combine the option `-nojvm` and MATLAB as a background process, since you need the shell for input and output when no Java inteface is started.
- You may also use the **KDE** user interface, locate the menu for MATLAB click on it and the program will start.
  - After a short wait a flashy interface should appear on the screen.
  - On the right you find the command line for MATLAB. Elementary commands may be entered on this line.
  - On the left you find a history of the previously applied commands
  - On the top you can choose the working directory and a few menus
  - When you launch MATLAB with the interface you will use considerably more memory for the interface (Java) and Greek characters will not show on the screen. You will have to set the working directory with a `cd` command.
- When typing the command `edit` an elementary editor should show up. It might be useful to type longer codes and store them in a regular text file with the extension `.m` , the standard for any MATLAB file. You are free to use your favorite editor to work on your codes.
- On startup MATLAB will read a file `startup.m` in a subdirectory `matlab` of the users home directory. In this file the user can give commands to MATLAB to be applied at each startup. The file below will set values for the variables `is_matlab` and `is_octave` to decide at runtime which program is currently used.

startup.m

```
is_octave = 0;  is_matlab = 1;
```

1.1.2 Where and how to get help

There are different situations when help is useful and important

- You know the command and need to know more details. As an example we use the command `plot()`.
  - Typing `help plot` will display information about the command `help`. You will find a list of all possible arguments of this function.

  - Typing `doc plot` will put you in an on-line version of the *Octave* manual with the documentation on `plot()`. You can use this as a starting points to browse for similar commands. `doc` works with *Octave* only.
  - Typing `lookfor plot` will search in all of the on-line documentation and display a list of all the commands. Type `help lookfor` to find out more.

- Some commands have demos and example codes built in. Examine the command `quiver()`. With `example quiver` find a listing of working examples.

Octave

```
example quiver
—>
quiver example 1:
 clf
 [x,y] = meshgrid (1:2:20);
 h = quiver (x,y, sin (2*pi*x/10), sin (2*pi*y/10));
 set (h, "maxheadsize", 0.33);

quiver example 2:
 clf
 axis ("equal");
 x = linspace (0,3,80);
 y = sin (2*pi*x);
 theta = 2*pi*x + pi/2;
 quiver (x, y, sin (theta)/10, cos (theta)/10);
 hold on; plot(x,y,"r"); hold off;
```

  By calling `demo quiver` the examples will be run online and you can examine the results.

- Most of the *Octave* code is given as script file. You can look at the source and modify if you desire to do so. To locate the source code for `quiver()` use

Octave

```
which quiver
—> 'quiver' is a function from the
      file /usr/local/share/octave/3.6.3/m/plot/quiver.m
```

- If you only know the topic for which you need help, but not the exact command (yet), use the *Octave* manual.
  - Both are available on the net at `http://www.gnu.org/software/octave/` and go to `Support`. You can browse in the HTML files or download the PDF file.
  - Both should be installed on your computer in HTML and PDF form.
    * Search your local disk for the file `octave.html`. It should be a directory and then the file `index.html` is the starting point into the HTML manual.
    * Search your local disk for the file `octave.pdf` with the PDF manual.
  - The manual for *Octave* 3.6.3 is also available on my web site at `staff.ti.bfh.ch/sha1/Octave.html` , as HTML (in compressed form, first download, then uncompress) and as PDF file.

- The references given on page 7 might also be useful, and of hopefully these notes too.

1.1.3 Vectors and matrices

The basic data type in MATLAB (**MAT**rix **LAB**oratory) is a **matrix** of numbers.

- a matrix is enclosed in square brackets (`[ ]`) and is a rectangular set or numbers (real or complex)
- different rows are separated by columns (`;`)
- with each row the entries are separated by commas (`,`) or spaces

Creation of Vectors and Matrices

Vectors are special matrices: a column vector is a $n \times 1$-matrix and a row vector a $1 \times n$-matrix. MATLAB does distinguish between row and column vectors. There are different methods to create vectors:

- To create a row vector with known numbers we may just type them in, separated by commas or spaces.

Octave
```
x = [1 2 3 4 5]
```

To create the same vector as a column vector we may either use the transpose sign or separate the entries by columns.

Octave
```
x = [1 2 3 4 5]'
x = [1; 2; 3; 4; 5]
```

- To create a matrix we use rows and columns, e.g. to create a 3×3 matrix with the numbers 1 through 9 as entries use:

Octave
```
A = [1 2 3;4 5 6;7 8 9]
```

- If the differences between subsequent values are know we can generate the vector more efficiently using double columns (`:`). Examine the results of the elementary code below.

Octave
```
x  = begin:step:end
x2 = 1:10
x1 = 1:0.5:10
```

- With the command `linspace()` we can specify the first and last value, and the total number of points. To generate a vector with 30 points between 0 and 10 we may use

Octave
```
x = linspace(0,10,30)
```

With the command `logspace(a,b,n)` we generate n values between 10^a and 10^b, logarithmically spaced.

Octave
```
x = logspace(0,2,11)
```

- To create a matrix or vector to be filled with zeros or ones *Octave* provides special commands.

Octave

```
x0 = zeros(2,3)
x1 = zeros(5,1)
y1 = ones(10,6)
```

Octave has many built-in functions to generate vectors and matrices of special types. The code below first generates a row vector with 10 elements, all of the values are set to zero. Then the squares of the numbers 1 through 10 are filled in by a simple loop. Finally the result is displayed.

Octave

```
n = 10;
a = zeros(1,n);
for i = 1:n
  a(i) = i^2;
end
a
```

Vector operations

Addition and multiplication of matrices and vectors follows strictly the operational rules of matrix operations.

Octave

```
clear *
a = [1 2 3]  % create a row vector
b = [4;5;6]  % create a column vector

a+b      % not permitted
a+b'     % permitted
a*a      % not permitted
a*a'     % permitted, leading to the scalar product
a'*a     % permitted, leading to a 3x3 matrix
a.*a     % permitted, leading to element wise multiplication
[a b']   % permitted, leading to a concatenation of the two vectors
```

The code below will generate a plot of the function of the function $y = |\cos(x)|$ for $-10 \leq x \leq 10$.

Octave

```
clear
n = 1000;
x = linspace(-10,10,n);
for k = 1:n
  y(k) = abs(cos(x(k)));
end
plot(x,y);
```

But this code does **not** use some of the best features of MATLAB and *Octave*. Many of the built-in functions apply directly to vectors. This is illustrated by the next implementation of the above calculations. A vector of 1000 numbers, ranging from -10 to 10 is generated, then the values of the cos-function is stored in the new vector y . The result is then element-wise multiplied with the sign of the cos-values and then plotted, leading to Figure 1.2.

Octave

```
clear
n = 1000;
x = linspace(-10,10,n);
y = cos(x);    s = sign(y);
plot(x,s.*y);
```

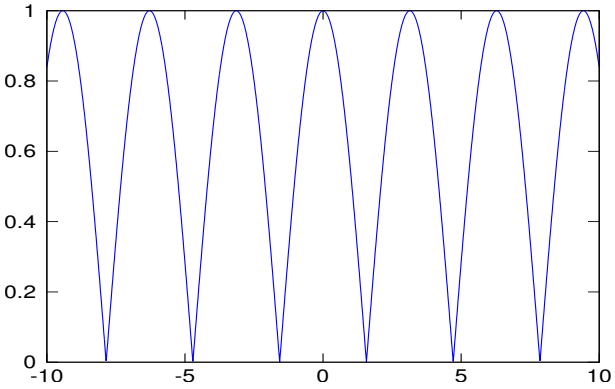


Figure 1.2: Graph of the function $|\cos(x)|$

1 Example : Speed of vectorized code
The three section of code blow compute the values of $\sin(n)$ for $n = 1, 2, 3, \ldots, 100000$. One might expect similar computation times.

Octave

```
clear
N = 100000;

tic();
for n = 1:N
  x(n) = sin(n);
endfor
timer1 = toc()

tic();
x = zeros(N,1);
for n = 1:N
  x(n) = sin(n);
endfor
timer2 = toc()

tic();
x = sin([1:N]);
timer3 = toc()
```

On a sample run we found

timer1 = 48 sec timer2 = 2.4 sec timer3 = 0.013 sec

and thus a drastic difference in performance. There are two major contributions to this drastic effect:

- **preallocation of vectors**[4]
  For the second and third code the resulting vector x was first created with the correct size and then the values of $\sin(n)$ were computed and then filled into the preallocated array. In the first code segment the size of the vector x had to be increased for each computation. Thus the system uses most of the time to allocate new vectors and then copy old values. This is the main difference between the computation time for the first and second code.

- **vectorized code**
  In the third code segment the sin-function was called with a vector as argument and *Octave* could

[4]Newer version of *Octave* use an improved memory allocation scheme and thus the first loop will be considerably faster.

compute all values at once. The penalty for a function call had to be paid only once. This is the main difference between the computation time of the second and third code.

This example clearly illustrates that we should preallocate vectors and matrices and use vectorized code whenever possible. ♢

Since vectorization is important newer versions of *Octave* provide a tool to generate vectorized code. A function $F(x) = x \cdot \cos(x) \cdot e^{x^2}$ is defined first and then the command `vectorize()` is used to generate a vectorized version. More and applied examples of vectorized codes are shown in Section 1.5.

Octave

```
F = inline("x*cos(x)*exp(x^2)")
F(2)
Fv = vectorize(F)
Fv([2,3])
```

2 Example : If the integral of the function in Figure 1.2 is to be computed we may use the trapezoidal rule

$$\int_a^b f(x)\,dx \approx \sum_{k=1}^{n-1} \frac{f(x_k) + f(x_{k+1})}{2}\,(x_{k+1} - x_k)$$

A straightforward implementation of these formula, using a loop, is shown below.

Octave

```
n = 1000;  # number of grid points
x = linspace(-10,10,n);
y = abs(cos(x));
plot(x,y);
integral = 0;
for k = 1:(n-1)
   integral = integral+0.5*(y(k)+y(k+1))*(x(k+1)-x(k));
endfor
integral
```

But this code does again **not** use some of the best features of `MATLAB` and *Octave*. The summation can be written as scalar product of two vectors.

$$\langle \vec{x}\,,\, \vec{y} \rangle = \sum_{k=1}^{n} x_k\, y_k$$

or if the row vectors are regarded as $1 \times n$ matrices, as `MATLAB` does, we find

$$\mathbf{x} \cdot \mathbf{y}' = \sum_{k=1}^{n} x_k\, y_k$$

With the help of $dx_k = x_{k+1} - x_k$ the summation will run considerably faster.

Octave

```
y = cos(x);
y = sign(y).*y;

dx = diff(x);
ynew = (y(2:n)+y(1:n-1))/2;
nintegral = ynew*dx'
```

The built-in function `trapz` uses exactly the above idea to perform a numerical integration. ♢

It is usually much faster to use the built in vectorization of *Octave* than to code simple loops. This vectorization is one of the main speed advantages of *Octave* over other programs. It should be used whenever possible. The command `tic()` starts a stopwatch and the `toc()` displays the passed time. Thus we can determine the time necessary to run through a piece of code.

Octave

```
clear % fast version
x = linspace(-10,10,10000);
tic();
for k = 1:10
  y = exp(sin(x.*x));
endfor
toc()
```

Octave

```
clear % slow version
x = linspace(-10,10,10000);
tic();
for k = 1:10
  for i = 1:10000
    y(i) = exp(sin(x(i)*x(i)));
  end
endfor
toc()
```

Since vectorization is important *Octave* provides support for this. Some of the basic operations (e.g. +-*/) can be performed element-wise on vectors or matrices, i.e. each entry will be computed separately. *Octave* will ignore the vector or matrix structure of the variable. Some books use the key word **point wise** operations instead of element wise operations. As a consequence *Octave* uses a preceding point to indicate element wise operations. As an example to compute $x(n) = n \cdot \sin(n)$ for $n = 1, 2, \ldots, 10$ we can use a loop

Octave

```
for n = 1:10
  x(n) = n*sin(n);
endfor
```

or the faster vectorized code

Octave

```
n = 1:10;
x = n.*sin(n)
```

Timing of code

In the above code we used `tic()` and `toc()` to determine the runtime of the loops. The resolution of this timeer is not very good and it displays the actual time, and not the computation time used by the code. We may use a higher resolution timer based on the function `cputime()`. Examine the example below.

Octave

```
t0 = cputime();
x = sin([1:100000]);
timer = cputime()-t0
```

- The pair `tic`, `toc` is based on the wall clock, i.e. if you wait 10 seconds before typing `toc` those 10 seconds will be taken into account.
- `cputime()` is measuring the CPU time consumed by the current job. Thus just waiting will not increase `cputime()`.

Matrices

Most of the above observations also apply to matrices. This is best illustrated by a few examples.

Octave

```
clear     % clear all previously defined variables and functions
a = [1 2 3; 4 5 6; 7 8 10]
det(a)    % compute the determinant of the matrix
inv(a)    % compute the inverse matrix
a^2       % compute the square of the matrix, using the matrix product
a.^2      % compute the square of each entry in the matrix
(a+a')/2  % compute the symmetric part of the matrix
a*inv(a)  % should yield the identity MATRIX
a.*inv(a) % multiply each entry in the matrix with the corresponding
          % entry in the inverse matrix
```

Systems of linear equations

Obviously `MATLAB` should be capable of solving systems of linear equations. To solve a system $\mathbf{A}\,\vec{x} = \vec{b}$ of 3 linear equations for 3 unknowns we best use the command `x=A\b` , i.e. we 'divide' the vector `b` from the left by the matrix `A`. Of course the inverse matrix could be used, but the computation is not done as efficiently and the results are not as reliable. As an example we consider the linear system

$$\begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 10 \end{bmatrix} \cdot \vec{x} = \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}$$

to be solved with the code below.

Octave

```
clear
A = [1 2 3; 4 5 6; 7 8 10];
b = [1;2;3];
x = inv(A)*b
x = A\b
```

Computing the inverse matrix is rarely a reasonable way to solve a numerical problem. The other method is also more reliable as shown by the example below.

$$\begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{bmatrix} \cdot \vec{x} = \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}$$

Matlab

```
clear
A = [1 2 3 ; 4 5 6; 7 8 9];
b = [1;2;3];
x1 = inv(A)*b;
control = A*x1
x2 = A\b
control2 = A*x2
```

Since this matrix `A` is not invertible the command `null(A)` will give more information about the solvability.

One special 'feature' of *Octave* and `MATLAB` is that also systems with more equations than unknowns lead to a solution. The example considers 4 equations for 3 unknowns (`A` is a 4×3 matrix)

$$\begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 10 \\ 1 & 2 & 4 \end{bmatrix} \cdot \vec{x} = \begin{pmatrix} 1 \\ 2 \\ 3 \\ 2 \end{pmatrix}$$

and is clearly **not** solvable, but consider the result

Matlab

```
clear
A = [1 2 3 ; 4 5 6; 7 8 10;1 2 4 ];
b = [1;2;3;2];
x = A\b
A*x
```

Octave and `MATLAB` return the solution vector `x` with residual vector `r` of smallest length, i.e. the best possible solution

$$\text{Find vector } \vec{x} \text{ such that} \quad \|\vec{r}\| = \|\mathbf{A}\,\vec{x} - \vec{b}\| \quad \text{is minimal}$$

This can be a rather useful feature, but also create a problems of the user is not aware of what `MATLAB` or *Octave* are computing.

1.1.4 Command line, script files and function files

With *Octave* different methods can be used to write code and then test the results.

- Use the **command line** in the interface
  This is useful only for very small sections of code or for debugging.
- Write a **script file**
  Longer pieces of code can be written with your favorite editor and stored in a file with the extension `.m`, e.g. `foobar.m`. Then the code can be run from the command line by typing `foobar`.
- Write a **function file**
  Functions to be used repeatedly can be write with an editor of your choice and then stored. A function can have one or multiple arguments and can also return one or multiple results.

Script files

Script files are used to write code to be run repeatedly, often with slight modifications. This is the most often used method to work with *Octave*.

If the code below is stored in the file `foobar.m`, then a circle with radius 3 in the complex plane will be generated by calling `foobar`.

foobar.m

```
t = linspace(0,2*pi,200);  % generate 200 points, equally spaced from 0 to 2Pi
z = 3*exp(i*t);            % compute the values in the complex plane
plot(z)                    % generate the plot
grid on;                   % add a grid
axis equal                 % equal scaling on both axis
title('Circle, radius 3')  % set a title
```

Observe that on the *Octave* command line you type `foobar` without the trailing extension `.m`.

Function files

Function files can be used to define functions. As a first example we consider a statistical function to compute the mean value and the standard deviation of a vector of values. For a vector $\vec{x}$ with n values we use

$$\begin{aligned} \text{mean} = \mu &= \frac{1}{n}\sum_{k=1}^{n} x_k \\ \text{stdev}^2 = \sigma^2 &= \frac{1}{n-1}\sum_{k=1}^{n}(x_k-\mu)^2 \end{aligned}$$

stat.m

```
function [mean,stdev] = stat(x)
% STAT Interesting statistics.
 n = length(x);
 mean = sum(x)/n;
 stdev = sqrt(sum((x-mean).^2)/(n-1));
```

This code has to be stored in a file `stat.m` and then can be used repeatedly, with one or two return arguments.

Octave

```
mymean = stat([1,2,3,4,5])
[mymean,mydev] = stat([1,2,3,4,5])
```

- `MATLAB` does not allow for definitions of functions within script files. Thus each function has to be given in a file of its own. This often leads to a large number of function files in a directory.
- In *Octave* the definition of a function may also be given within a script file and thus collections of functions in one file are possible. The end of the function has to be indicated by the keyword `endfunction`. `MATLAB` will not recognize this keyword.

1.1.5 Local and global of variables

Octave

```
a = 17    % set the value of a in the global workspace

function res = modify_a(x)
         % the variable a from the global workspace is not visible
  a = 2;  % here a is a new variable in the local context
  res = a*x;
endfunction

a2 = modify_a(a)
```

```
a          % will return the first value in the global context
-->
a  =  17
a2 =  34
a  =  17
```

Octave

```
global a = 17    % set the value of a in the global workspace

function res = modify_a(x)
  global a  % the variable a is global and its valu taken from the workspace
  res = a*x;
  a = 2;  % now the global variable is modified
endfunction

a2 = modify_a(a)
a
-->
a  =  17
a2 =  289
a  =  2
```

Persistent variables

1.1.6 Elementary graphics

Find more information on graphics commands in Section 1.4. To generate a two–dimensional plot use the command `plot()` with the vector of the x and y values as arguments. The code below generates a plot of the function $v = \sin(x)$ with 21 values of x evenly distributed in the interval $0 \leq x \leq 9$. Find the result in Figure 1.3.

Octave

```
x = linspace(0,9,21);
y = sin(x);
plot(x,y)
```

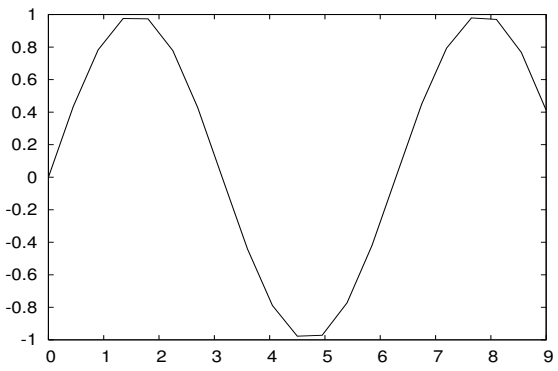


Figure 1.3: Elementary plot of a function

Multiple plots can be generated just as easily by calling `plot()` with more than one set of x and y values.

Octave

```
x = linspace(0,10,50);
plot(x,sin(x), x,cos(x))
```

1.1.7 A breaking needle ploblem

The question

Assume that medical needles will penetrate skin if the applied force is larger than F_p and the same type of needles will break if the applied force is beyond a limiting breaking force F_b. The values of F_p is given by a normal distribution with mean value μ_p and standard deviation σ_p. The values of F_b is given by a normal distribution with mean value μ_b and standard deviation σ_b. To illustrate the method we work with hypothetical values for the parameters.

$$\mu_p = 2.0\ [\mathrm{N}] \quad , \quad \sigma_p = 0.5\ [\mathrm{N}] \quad , \quad \mu_b = 4.5\ [\mathrm{N}] \quad , \quad \sigma_p = 0.635\ [\mathrm{N}]$$

The theory and the code

Since the normal distribution is given by the probability density function

$$p(x) = \frac{1}{\sigma\sqrt{2\,\pi}}\ \exp\left(-\frac{(x-\mu)^2}{2\,\sigma^2}\right)$$

we define as function script to compute the value of this function for a vector of arguments.

Octave

```
mup = 2.0; sigmap = 0.5; mub = 4.5; sigmap = 0.635;

function p = normal_dist(x,mu,sigma)
  p = 1/(sigma*sqrt(2*pi))*exp(-(x-mu).^2/(2*sigma*sigma));
endfunction
```

The above two distributions can then be visualized in Figure 1.4.

Octave

```
df = 0.01;
f  = 0:df:8;   % generate values of forces from 0 to 8 N, stepsize df
pp = normal_dist(f,mup,sigmap);
pb = normal_dist(f,mub,sigmab);
plot(f,pp,f,pb);
```

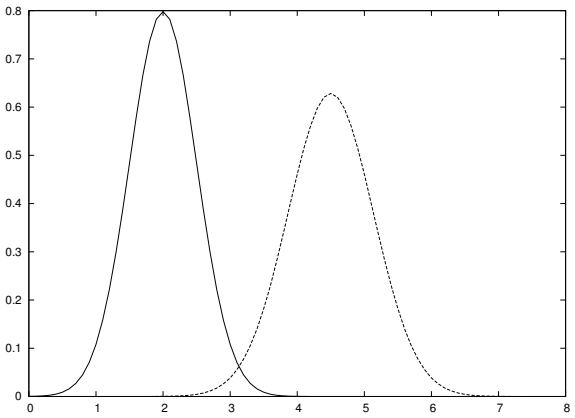


Figure 1.4: Probability of needles to penetrate, or to break

To be determined is the probability at which a given needle will break before it penetrates the skin. To determine this value we examine the following facts for very small values of Δf:

- With probability $p_p(f)\,\Delta f$ a needle does penetrate at a force between f and $f + \Delta f$.
- For this needle to break the breaking force has to be smaller than f. This occurs with probability

$$p_2(f) = \int_{x=-\infty}^{f} p_b(x)\; dx$$

  Since for our example we find $p_b(x) \approx 0$ for $x < 0$ and thus

$$p_2(f) \approx \int_{x=0}^{f} p_b(x)\; dx$$

- The probability for a needle to break before penetration is thus

$$p(f) = p_2(f) \cdot p_p(f)$$

  and the total probability to fail is given by

$$P_{fail} = \int_{f=-\infty}^{\infty} p_2(f) \cdot p_p(f)\; df \approx \int_{f=0}^{8} p_2(f) \cdot p_p(f)\; df$$

The above can be implemented in *Octave*, leading to Figure 1.5 of the probability distribution for failing and total probability of $P_{fail} \approx 0.00101 \approx 1/1000$.

Octave

```
p2 = pb; p2(1) = 0;  # integration
for k = 2:length(pb)
    p2(k) = p2(k-1)+pb(k)*df;
endfor

pfail = pp.*p2;
plot(f,pfail);

trapz(f,pfail)
```

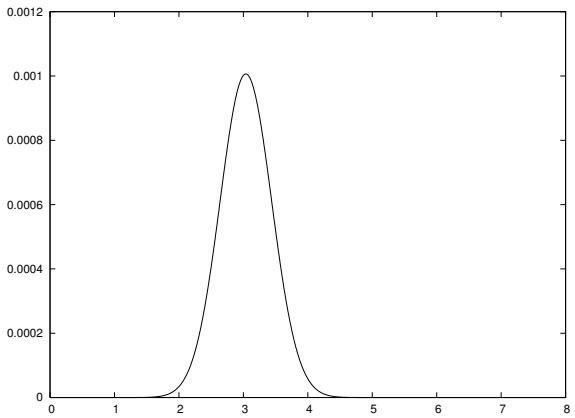


Figure 1.5: Probability distribution of needles to break before penetration

In the above code the function $p_2(f)$ was computed with the help of an integral, but is not the best approach if the underlying distribution is normal. A better approach is to use the **error function** `erf(z)`, defined by

$$\mathrm{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z \exp(-t^2)\, dt$$

Using the definition of the normal distribution

$$p(x) = \frac{1}{\sigma\sqrt{2\,\pi}} \exp\left(-\frac{(x-\mu)^2}{2\,\sigma^2}\right)$$

and basic calculus we find

$$\begin{aligned} g(f) &= \int_{x=-\infty}^{f} p(x)\, dx = \int_{x=-\infty}^{\mu} p(x)\, dx + \int_{x=\mu}^{f} p(x)\, dx \\ &= \frac{1}{2} + \frac{1}{\sigma\sqrt{2\,\pi}} \int_{x=\mu}^{f} \exp\left(-\frac{(x-\mu)^2}{2\,\sigma^2}\right)\, dx \\ &\quad \text{substitution} \qquad t = \frac{x-\mu}{\sqrt{2}\,\sigma} \qquad , \qquad dx = \sqrt{2}\,\sigma\, dt \\ &= \frac{1}{2} + \frac{\sqrt{2}\,\sigma}{\sigma\sqrt{2\,\pi}} \int_{t=0}^{\frac{f-\mu}{\sqrt{2}\,\sigma}} \exp\left(-t^2\right)\, dt \\ &= \frac{1}{2}\left(1 + \mathrm{erf}\left(\frac{f-\mu}{\sqrt{2}\,\sigma}\right)\right) \end{aligned}$$

Thus for the above problem we may equivalently write

$$P_{fail} = \frac{1}{2} \int_{f=\infty}^{\infty} \left(1 + \mathrm{erf}\left(\frac{f-\mu_b}{\sqrt{2}\,\sigma_b}\right)\right)\, p_p(f)\, df$$

This eliminates the need for ignoring extreme values for the forces. In the above code the loop to compute the probability density function p_2 is replaced by a function call.

Octave

```
p2 = 0.5*(1+erf((f-mub)/(sqrt(2)*sigmab)));
```

A simple simulation

To verify the above computation we can run a simulation. The command `randn(1,NN)` creates NN random data with mean 0 and standard deviation 1 . To obtain mean μ and standard deviation σ we have to multiply these values by σ and then add μ . With this type of simulated data for breaking and penetration forces we count the number of pairs where the breaking force is smaller than the penetration force. This number of breaking needles is to be divided by the total number of needles. To understand the behavior of comparison operator consider the following example.

Octave

```
res = [1 2 3 4 5 9]< [0 5 9 1 1 10]

res =  0  1  1  0  0  1
```

Thus to examine, by a simulation, one million needles we may use the code below. The results will vary slightly from one run to the other, but should always be close to the above integration result.

Octave

```
NN = 1e6;                    % one milion samples to be simulated
fpsimul = randn(NN,1)*sigmap+mup;
fbsimul = randn(NN,1)*sigmab+mub;
simulation = sum(fbsimul<fpsimul)/NN
```

1.1.8 Exercises

The exercises

Exercise 1.1–1 Explain why the code

Octave

```
x = -2:0.1:3;
y = exp(-x^2/2);
plot(x,y)
```

will not show a graph of a Gauss $y(x) = e^{x^2/2}$ curve.

Exercise 1.1–2 The breaking needle problem
A different approach to the problem is based on the following argument.

- With probability $p_b(f)\,\Delta f$ a needle does break at a force between f and $f + \Delta f$.
- For this needle to penetrate at a larger force we find a probability

$$p_3(f) = \int_{x=f}^{\infty} p_p(x)\,dx \approx \int_{x=f}^{8} p_p(x)\,dx$$

- The probability for a needle to break before penetration is thus

$$p(f) = p_3(f) \cdot p_b(f)$$

  and the total probability to fail is given by

$$P_{fail} = \int_{f=-\infty}^{\infty} p_3(f) \cdot p_b(f)\,df \approx \int_{f=0}^{8} p_3(f) \cdot p_b(f)\,df$$

The final result has to be the same as for the first approach.

The answers

Exercise 1.1–1 We either have to use a loop or vectorize the code with a point wise multiplication.

Octave

```
x = -2:0.1:3;
y = exp(-x.^2/2);
plot(x,y)
```

Exercise 1.1–2 The breaking needle problem

Octave

```
p3 = pb; p3(length(pp)) = 0;
for k = fliplr(1:(length(pp)-1));
    p3(k) = p3(k+1) + pp(k)*df;
endfor

pfail = pb.*p3;
plot(f,pfail);
trapz(f,pfail)
```

1.2 Programming with *Octave*

This short section can and will not cover all aspect of programing with MATLAB or *Octave*. You certainly have to consult the online documentation and other references, e.g.[Grif01] or [BiraBrei99]. The amount available literature is enormous, free and nonfree.

It is the goal of this section to get you started and point out some important aspects. It is assumed that you are familiar with a prcedural prorgamming language, e.g. C, C++, Java, ...

1.2.1 Commenting code

An essential feature of good code is a readable documentation. In *Octave* you may use the characters % or # to start a comment, i.e. any text after those signs will not be examined by the *Octave* parser. In MATLAB only % can be used.

```
a = 1+2; % this is a comment in Octave and Matlab
b = 2-1; # this is a comment in Octave, but will lead to an error in Matlab
```

1.2.2 Basic data types

Octave provides a few basic data types and a few methods to combine the basic data types. For a defined variable var *Octave* will display its data type with the command typeinfo(var).

Numerical data types

The by far most important data type in *Octave* is a **double precision floating point number**. For most numerical operations this is the default data type and you **have to ask for** other data types. On systems that use the IEEE floating point format, values in the range of approximately 2.2251e-308 to 1.7977e+308 can be stored, and the relative precision is approximately 2.2204e-16, i.e you can at best 15 decimal digits to be correct. The exact values are given by the variables 'realmin', 'realmax', and 'eps', respectively. This is confirmed by the code below.

Octave

```
[realmin, realmax, eps]
-->
ans =   2.2251e-308   1.7977e+308   2.2204e-16
```

Based on floating point numbers we may built vectors and matrices of with real or complex entries.[5] Complex number are described by their real and imaginary parts. All arithmetic operations and most mathematical function can be applied to real or complex numbers.

Octave

```
a = 1.0+2i; b = 3*i;
[a+b, a*b, a/b]
[cos(a), exp(b), log(a+b)]
-->
ans =   1.00000 + 5.00000i   -6.00000 + 3.00000i   0.66667 - 0.33333i
ans =   2.03272 - 3.05190i   -0.98999 + 0.14112i   1.62905 + 1.37340i
```

In recent version *Octave* introduce the data type of **single**, i.e. single precision floating point numbers. It main advantage is to use less memory, the disadantage is a smaller range and resolution.

Octave

[5] For many years a matrix of floating point numbers was the **only** data type in MATLAB.

```
[realmin('single'), realmax('single'), eps('single')]
-->
ans =  1.1755e-38   3.4028e+38   1.1921e-07
```

You can convert between singe and double with the commands `single()` and `double()`.

Octave

```
clear *
a = rand(3);
aSingle = single(a);
whos
-->
Variables in the current scope:

  Attr Name        Size                     Bytes  Class
  ==== ====        ====                     =====  =====
       a           3x3                         72  double
       aSingle     3x3                         36  single

Total is 18 elements using 108 bytes
```

As a special feature *Octave* has a **integer data types** with fixed ranges. We find signed and unsigned integers with 8, 16, 32 or 64 bit resolution. In Table 1.2 find the types and their corresponding ranges. On 32-bit CPU the default integer data type is signed 32 bit, as expected.

type	int8	uint8	int16	uint16	int32	uint32	int64	uint64
intmin	-128	0	-32'768	0	-2'147'483'648	0	-9.2e+18	0
intmax	+127	255	+32'767	65'535	+2'147'483'647	4'294'967'295	+9.2e+18	1.8e+19

Table 1.2: Integer data types and their ranges

The basic arithmetic operations (+-*/) are available for these types, with the usual results, as ilustrated by an elementary example.

Octave

```
a = int16(100); b = int16(111);
[a+b, a-b, 3*b]
-->
ans =  211  -11  333
```

One has to watch out for the range of these types and the consequences on the results.

Octave

```
a = uint8(100); b = uint8(111);
[a+b, a-b, 3*b]
-->
ans = [211 0 255]
```

On newer versions of *Octave* the commands `int8()`, `int16()`, ... do not return the integer part, but use rounding.

Integer data type with a prescribed resolution may be used to develop code for micro controllers, as shown in Section 2.4, starting on page 176.

Characters

Individual letters can be given as characters, internally they are represented by integers and conversions are possible, see Section 1.2.4. The internal representation leads to some surprising results.

Octave

```
char1 = 'a';  char2 = 'b'; char3 = 'A';
b_minus_a = char2-char1
a_minus_A = char1-char3
a97 = (char1==97)
-->
b_minus_a =  1
a_minus_A = 32
a97 =  1
```

1.2.3 Structured data types and arrays of matrices

Strings

Octave also works with strings, consisting of a sequence of characters, enclosed in either singe-quotes or double-quotes. With MATLAB only single quotes are allowed, thus one might consider using those exclusively. Internally strings are represented as vectors of single characters and thus they can be combined to longer strings.

Octave

```
name1 = 'John'  % a string in Octave and Matlab
name2 = "Joe"   % a string in Octave only
combined = [name1,' ',name2]
-->
name1 = John
name2 = Joe
combined = John Joe
```

One may also create a vector of strings, but it will be stored as a matrix of characters. As a consequence each string in the vector of strings will have the same length. Missing characters are replaced by spaces.[6]

Octave

```
combinedMat = [name1;name2]
size(combinedMat)
size(combinedMat(2,:))
-->
combinedMat=
John
Joe
ans = 2 4
ans = 1 4
```

Structures

One of the major disadvantages of matrices is, that all entries have to be of the same type, most often scalars. *Octave* supports structures, whose entries may be of different types. This feature is not yet use in many codes. Consider the trivial example below.

Octave

[6] In MATLAB you will have to use the function `str2mat()`.

```
Customer1.name = 'John';
Customer1.age = 23;
Customer1.address = 'Empty Street'
-->
Customer1 =
{
  address = Empty Street
  age = 23
  name = John
}
```

Lists and cell arrays

Instead of structures we may use cell arrays. To access and create cell arrays curly brackets (i.e. {}) have to be used. As illustration consider the example below.

Octave

```
c = {1, 'name', rand(2,2)}
-->
c =
{
  [1,1] =  1
  [1,2] = name
  [1,3] =
     0.17267   0.87506
     0.73041   0.85009
}
```

Each entry in a cell array may be used independently.

Octave

```
c{2}
-->
ans = name
```

Octave

```
m = c{3}
-->
m =  0.17267   0.87506
     0.73041   0.85009
```

or as a subset of the cell array.

Octave

```
c{2:3}
-->
ans = name
ans = 0.17267   0.87506
      0.73041   0.85009
```

Using cell array we can construct multidimensional matrices. With the code below we store the matrices

$$\begin{bmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix}$$

in two different layers of the $2 \times 3 \times 3$ matrix `mat3` and then we compute

$$\begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix} - \begin{bmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{bmatrix}$$

Octave

```
mat3 = cell(2,1);
mat3{1} = 2*eye(3);
mat3{2} = ones(3);
mat3{2}-mat3{1}
-->
ans =
  -1   1   1
   1  -1   1
   1   1  -1
```

One has to observe that no standard computational rules for 3-d matrices are defined.

Cell arrays can even be used as a counter in a loop.

Octave

```
disp("Loop over a cell array")
for i = {1,"two","three",4}
  i
endfor
```

Arrays of Matrices or N-d Matrices

With *Octave* we may also work with matrices of higher dimensions, i.e. arrays of matrices. The command below constructs 5 matrices of size 3×2 and fills it with random numbers. You may visualize this by stacking the 5 matrices on top of each other and thus obtain a 5 story building with one 3×2 matrix on each floor. Or consider it a matrix with three dimensions of size $3 \times 2 \times 5$. To acces individual entries use thre indices, e.g. `A(2,1,4)`. As an example we compute for each position the average along the height, leading to e 3×2 matrix. The average is computed along the third dimension of the matrix.

Octave

```
A = rand(3,2,5);
Amean = mean(A,3)
-->
Amean =  0.79681   0.70946
         0.60815   0.48610
         0.38403   0.47336
```

To extract the "second floor" matrix you may use `A2=A(:,:,2)`, but the result will be a 3 dimensional object of size $3 \times 2 \times 1$. To convert this into a classical 3×2 matrix use the command `squeeze()`. As an example multiply the transpose of the second floor with the fifth floor, leading to a 2×2 matrix.

Octave

```
squeeze(A(:,:,2))'*squeeze(A(:,:,5))
-->  1.06241   1.05124
     0.84722   1.03028
```

Arrays of matrices can be very convenient and many *Octave*/`MATLAB` command are directly applicable to these N-d matrices, but not all commands.

1.2.4 Built-in functions

Octave contains a large number of built-in functions. Most of them can be applied to scalar arguments, real or complex. This leads to a few surprises.

Functions with scalar arguments

- **trigonometric functions**: `sin()`, `cos()`, `tan()`, `tan()`, `asin()`, `acos()`, `atan()`, `atan2()` Observe that all trigonometric function compute in radians, and not degree. There are a few special version of function using degree, e.g. `sind()`, `cosd()`. This author does not use those.

Octave

```
r1 = cos(pi)
r2 = acos(-1)
r3 = cos(i)
r4 = acos(-1.01)
r5 = acos(-1.01+i*1e-15)
r6 = tan(0.5)
r7 = atan(0.5)
r8 = atan2(-0.5,-1)
```

The function `atan2()` above is very useful to convert cartesian to polar coordinates. For given x and y we find the radius r and angle ϕ by solving

$$x = r\,\cos(\phi) \quad \text{and} \quad y = r\,\sin(\phi)$$

Octave will compute the values by

Octave

```
r   = sqrt(x^2 + y^2)
phi = atan2(y,x)
```

Observe that `atan((-y)/(-x))` will lead to the same rsults as `atan(y/x)`, while `atan2(-x,-y)` and `atan2(x,y)` yield different results.

- **exponential functions**: `exp()`, `cosh()`, `sinh()`, `tanh()`, `pow2()`. For most of the exponential function the corresponding inverse functions are also available: `log()`, `log2()`, `log10()`, `acosh()`, `asinh()`, `atanh()`. The only possible surpise is that the functions can be used with complex arguments. The code below verifies the Euler formula $e^{i\,\alpha} = \cos(\alpha) + i\,\sin(\alpha)$ for $\alpha = 0.2$.

Octave

```
al = 0.2;
[exp(i*al), cos(al), sin(al)]
-->
ans =   0.98007 + 0.19867i   0.98007 + 0.00000i   0.19867 + 0.00000i
```

- **random numbers**: for simulations it is often necessary to generate random numbers with a given probability distribution. The command `rand(3)` will generate a 3×3 matrix of random numbers, uniformly distributed in the interval $[0\,,\,1]$.

Octave

```
r = rand(3)
-->
r =  0.694482   0.747556   0.266156
     0.609030   0.713823   0.054658
     0.461212   0.695820   0.769618
```

As an example we create a vector of 1000 random numbers, with mean 2 and standard deviation 0.5, then we generate a histogram.

Octave

```
N = 1000;
x = 2 + 0.5*randn(N,1);
hist(x)
```

Octave provides a few more distributions of random numbers.

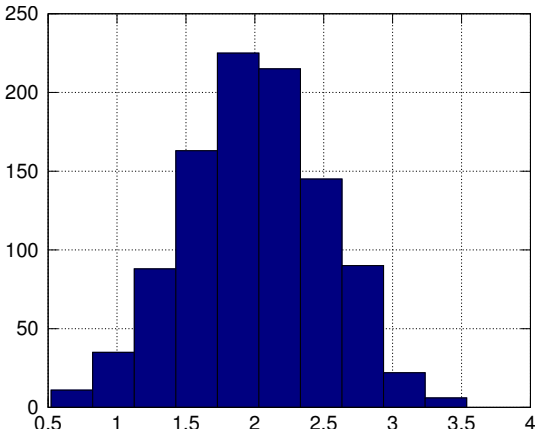


Figure 1.6: Histogram of random numbers with mean 2 and standard deviation 0.5

- `rand()` : uniformly distributed in $[0\,,\,1]$.
- `randn()` : normal distribution with mean 0 and variance 1.
- `rande()` : exponetially distributed.
- `randp()` : Poisson distribution.
- `randg()` : gamma distribution.

- **special functions**: many special functions are directly implemented in *Octave*, e.g. most of the Bessel functions `bessel()`, `besselh()`, `besseli()`, `besselj()`, `besselk()`, `bessely()`. One of the many applications of Bessel functions is radially symmetric vibrating drums, the zeros of the Bessel function $J_0(x)$ lead to the frequencies of the drum. The code below generates the plot of the function $f(x) = J_0(x)$ and its derivative $f'(x) = -J_1(x)$, find the result in Figure 1.7. There are many other special function, e.g `airy()`, `beta()`, `bincoeff()`, `erf()`, `erfc()`, `erfinv()`, `gamma()`, `legendre()`. A good reference for special functions and their basic properties is [AbraSteg].

Octave

```
x = 0:0.01:14;
plot(x, besselj(0,x),';BesselJ0;',...
     x,-besselj(1,x),';derivative;')
```

Functions with matrix and vector arguments

A large number of numerical function can be applied to vectors or matrices as arguments. The corresponding function will be computetd for each of the values. As a simple example for vectors consider

Octave

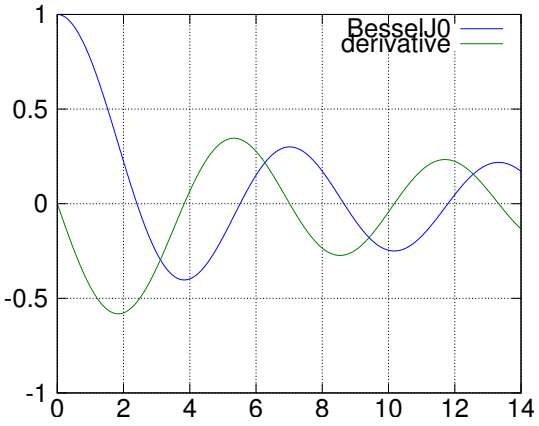


Figure 1.7: Graph of the Bessel function $J_0(x)$ and its derivative

```
x = [-1, 0, 1,3]
exp(x)
cos(x)
sqrt(x)
-->
x =  -1   0   1   3
exp(x) =    0.36788   1.00000   2.71828  20.08554
cos(x) =    0.54030   1.00000   0.54030  -0.98999
sqrt(x)=    0 + 1i    0+ 0i     1 + 0i   1.73205 + 0i
```

or for matrices

Octave

```
A = [ 0 pi 1; -1 -pi 2];
r1 = cos(A)
r2 = exp(A)
r3 = sqrt(A)
-->
r1 =
   1.00000  -1.00000   0.54030
   0.54030  -1.00000  -0.41615

r2 =
    1.000000   23.140693    2.718282
    0.367879    0.043214    7.389056

r3 =
   0.00000 + 0.00000i   1.77245 + 0.00000i   1.00000 + 0.00000i
   0.00000 + 1.00000i   0.00000 + 1.77245i   1.41421 + 0.00000i
```

3 Example : Elementwise operations

Assume that for a vector of x values you want to compute $y = \sin(x)/x$. The obvious code

Octave

```
x = linspace(-1,1);
y1 = sin(x)/x
-->
y1 =  0.90164
```

produces certainly not the desired result. To compute $y_2 = \sin(x) \cdot x^2$ the code below yelds not the expected

vector either.

Octave

```
x = linspace(-1,1);
y2 = sin(x)*x^2
-->
error: for A^b, A must be square
```

In both cases *Octave* (and MATLAB) use matrix operations, instead of applying the above operations to each of the components in the corresponding vector. To obtain the desired result the **dot operations** have to be used, as shown below.

Octave

```
x = linspace(-1,1);
y1 = sin(x)./x ;
y2 = sin(x).*x.^2;
plot(x,y1,x,y2)
```

Leaving out the dot (at first) is the most common syntax problem in MATLAB and *Octave*.

- `x.*y` will multiply each component of x with the corresponding component of y. Thus x and y have to be vectors or matrices of the same size. The result is of the same size too.
- `x./y` will divide each component of x by the corresponding component of y. Thus x and y have to be vectors or matrices of the same size. The result is of the same size too.
- `x.^2` will square each component of x and return the result as a vector or matrix.

♢

4 Example : A few possble implementation of the norm function of a vector

$$\|\vec{x}\| = \sqrt{\sum_{i=1}^{n} x_i^2}$$

are given by

Octave

```
normX1 = sqrt(sum(x.^2))
normX2 = sqrt(sum(x.*x))
normX3 = sqrt(sum(x.*conj(x)))
```

All three return the correct result if the vector is real valued, i.e. $\vec{x} \in \mathbb{R}^n$. The last formula also generates the correct result for complex vectors. ♢

5 Example : Matrix exponential

There are also functions that behave differently. The solution of the linear sysytem of differential equation

$$\frac{d}{dt}\,\vec{x}(t) = \mathbf{A}\,\vec{x}(t) \quad \text{with} \quad \vec{x}(0) = \vec{x}_0$$

can formally be written as

$$\vec{x}(t) = \exp(t\,\mathbf{A})\,\vec{x}_0$$

Theoretically this matrix could be computed with a Taylor series

$$\exp(t\,\mathbf{A}) = \sum_{k=0}^{\infty} \frac{1}{k!}\,t^n\,\mathbf{A}^n = \mathbb{I} + t\,\mathbf{A} + \frac{1}{2}\,t^2\,\mathbf{A}^2 + \frac{1}{6}\,t^3\,\mathbf{A}^3 + \frac{1}{24}\,t^4\,\mathbf{A}^4 + \ldots$$

Unfortunately this neither fast nor reliable, as are many other simple ideas, see [MoleVanLoan03]. *Octave* can compute this matrix $\exp(t\mathbf{A})$ reliably with the command `expm()` (**m**atrix **exp**onential). As example consider

Octave

```
expm([1,2;3,4])
-->
   51.969   74.737
  112.105  164.074
```

Observe that the result is different from `exp([1,2;3,4])`. There also exists a similar function `logm()`, i.e. `A = logm(B)` will compute a matrix $\mathbf{A}$ such that $\mathbf{B} = \exp(\mathbf{A})$. There is also a function to compute the square root of a matrix, as illustrated below.

Octave

```
B = [1,2;3,-4]
sB = sqrtm(B)
sB*sB
-->
B =
   1   2
   3  -4

sB =
   1.21218 + 0.31944i   0.40406 - 0.63888i
   0.60609 - 0.95831i   0.20203 + 1.91663i

sB*sB =
   1.00000 - 0.00000i   2.00000 - 0.00000i
   3.00000 + 0.00000i  -4.00000 + 0.00000i
```

And again is the result different from `sqrt(B)`. ♢

Formatted input and output functions

When reading or writing data one often has to insist in specific formats, e.g. the number of digits displayed. This can be done with the functions in Table 1.3 with the format templates listed in Table 1.4.

`printf()`	formatted output to `stdout`
`sprintf()`	formatted output to a string
`fprintf()`	formatted output to a stream (file)
`sscanf()`	formatted input from a string
`fscanf()`	formatted input from a stream (file)
`disp()`	display a string on the terminal

Table 1.3: Formatted output and input commands

As an example we display the number π in different formats.

Octave

```
printf("this is pi: %6.3f \n",pi)
printf("this is pi: %10.3e \n",pi)
printf("this is pi: %3i \n",pi)
-->
this is pi:  3.142
```

```
this is pi:  3.142e+00
this is pi:   3
```

%i or %d	signed integer
%u	unsigned integer
%f	normal floating point number
%8.3f	in field of width 8 with precision 3
%e	floating point number with exponential notation
%10.5e	in field of width 10 with precision 5
%g	floating point number in normal or exponential format
%s	string
%c	one or multiple characters

Table 1.4: Some output and input conversion templates

6 Example : Formatted Scanning
Formatted scanning has to be used when information is to be extracted from strings, as shown in this example. Within a string `s` a few digits of a number are displayed. First read the correct number of characters, then scan for the scalar number and finally store the remainder of the string. For subsequent calculation the scalar number `piApprox` can be used.

- The format string `%10c%e%s` consists of three contributions.
- `%10c` : read a vector consisting of 10 characters
- `%e` : read one floating point number
- `%s` : read the remainder as a string
- The last parameter `"C"` indicates that we use a C style formatting.

Octave

```
s = 'pi equals 3.14 approximately';
[head, piApprox, tail] = sscanf(s,'%10c%e%s','C')
-->
head = pi equals
piApprox = 3.1400
tail = approximately
```

Codes of the above type have to be used when reading data from a file. MATLAB's version of `scanf()` behaves differently. The function `textscan()` serves as a replacement of `sscanf()`, as shown by the example.

Matlab

```
A = textscan(s,'%10c%f%s')
piApprox = A{2}
```

Another possibility for problems of the above type is to use the function `regexp()`. ♢

Conversion functions

If you need to translate one data type into another *Octave* provides a few functions.

- `char()` : will convert an integer to the corresponding character. The function can be applied to integers, vectors or matrices of integers. You hay also use the function with cell arrays, see `help char`.

Octave
```
c1 = char(65)
c2 = char(65:90)
c3 = char([65:75;97:107])
-->
c1 = A
c2 = ABCDEFGHIJKLMNOPQRSTUVWXYZ
c3 = ABCDEFGHIJK
     abcdefghijk
```

- `toascii()` : will convert a character to the corresponding ASCII code, an integer. The function can be applied to strings or vectors of strings.

Octave
```
oneLetter = toascii('A')
name = toascii('BFH-TI')
mat = toascii(['1 2 3';'abcde'])
-->
oneLetter =  65
name =  66   70   72   45   84   73
mat  =  49   32   50   32   51
        97   98   99  100  101
```

- `int2str` : this function converts integers to strings, e.g.

Octave
```
s = int2str(4711)
-->
s = 4711
```

Observe that in the above code the variable `s` is of type string and not a number, e.g. you can not add 1 to `s` . The functions `num2str()` and `mat2str()` may be useful for similar tasks.

Octave
```
s2 = num2str(10*pi)
s3 = mat2str(rand(2),[4,3])
s4 = s3([1:4])
-->
s2 = 31.416
s3 = [0.6087,0.1361;0.6818,0.5794]
s4 = [0.6
```

- *Octave* provides a few more conversion functions: `str2double()`, `str2num()`, `hex2num()`, `num2hex()`, `num2cell()`,...
- To convert strings to numbers the formatted scanning and printing functions above can to be used, i.e see Section 1.2.4.

The above function can be used when reading data from a file or writing to a file, as examined in Section 1.2.8.

1.2.5 Working with source code

One of the big advantages of open source code projects is that you have access to the source and can thus examine and even modify it to meet your needs.

- Locate the source code. With the command `which` you can find the location of the source code for a given function.

  Octave
  ```
  which logspace
  -->
  'logspace' is a function from the file
      /usr/local/share/octave/3.6.3/m/general/logspace.m
  ```

  Using the location of the source you can copy it into a directory of yours and adapt the code. This is a veru useful feature if a given function does almost what you need. Then take the source as a (usually) good starting point. Not all function are written with *Octave*, but C++ and FORTRAN are used, e.g.

  Octave
  ```
  which cosh
  -->
  'cosh' is a built-in function
  ```

- To just look at the code you can also use `type logspace` and *Octave* will display the source code of the function.

- The source to many functions have built in tests and you can call those with the command `test` .

  Octave
  ```
  test logspace
  -->
  PASSES 6 out of 6 tests
  ```

- The source for many functions have built in demos, try

  Octave
  ```
  demo delaunay
  ```

1.2.6 Loops and control statements

Within *Octave* the standard loops and controls statements are available We illustrate them with elementary examples.[7]

Loops generated by `for`

The general form is given by

Octave
```
for VAR = EXPRESSION
   BODY
endfor
```

We use this example to list all square number from 1 to 9.

Octave

[7] If `MATLAB` is used instead of *Octave* then `endfor` has to be replaced by `end`, `endwhile` by `end` and a few more minor changes of the same type.

```
for k = 1:9
  printf('the square of %i is given by %i \n', k, k^2)
endfor
```

It is not necessary to use subsequent numbering. As an example we use all odd number from 1 through 20, or a given list of 3 numbers (4, 7 , 11).

Octave

```
for k = 1:2:20
  printf('the square of %i is given by %i \n', k, k^2)
endfor

for k = [4 7 11]
  printf('the square of %i is given by %i \n', k, k^2)
endfor
```

Loops generated by `while` or `until`

The general form is given by

Octave

```
while (CONDITION)
  BODY
endwhile
```

As sample code generate the first 10 numbers of the Fibonacci sequence,

Octave

```
fib = ones (1, 10);
i = 3;
while (i <= 10)
  fib (i) = fib (i-1) + fib (i-2);
  i++;
endwhile
fib
```

With the while command the condition is tested first. If the body of the loop has to be executed first, and then the test performed we may use the `until` command whose general form is

Octave

```
do
  BODY
until (CONDITION)
```

The Fibonacci sequence is generated by

Octave

```
fib = ones (1, 10);
i = 2;
do
  i++;
  fib (i) = fib (i-1) + fib (i-2);
until (i == 10)
fib
```

`MATLAB` does not provide a `do--until` loop. One may simulate this with the help of an extra flag.

Matlab

```
flag = true;
while flag
   BODY;
    flag = CONDITION;
end
```

The `if` statements

If a body of code is to be used when a certain condition is satisfied we may use the `if` statement, whose general form is given by

Octave

```
if (CONDITION)
  THEN-BODY
endif
```

The code below will first generate a list of random integers between 0 and 100. Then from all numbers larger than 50 we will subtract 50.

Octave

```
vec = round(rand(1,10)*100)  % generate random numbers between 0 and 100
for k = 1:10
  if (vec(k) >= 50)          % subtract 50, if number larger than 50
    vec(k) += -50;
  endif
endfor
vec
-->
vec =  46  71  18  26  58   3  80  69  92   8
vec =  46  21  18  26   8   3  30  19  42   8
```

If we want to either subtract or add 50, depending of the size of the number we can use the `else` statement whose general form is

Octave

```
if (CONDITION)
   THEN-BODY
else
   ELSE-BODY
endif
```

From the random vector of number we subtract or add 50, depending whether the number is smaller or larger that 50.

Octave

```
vec = round(rand(1,10)*100)
for k = 1:10
  if (vec(k) >= 50)
    vec(k) += -50;
  else
    vec(k) += +50;
  endif
endfor
vec
-->
vec =  54  36  39   3  16  92  63  61  58   5
vec =   4  86  89  53  66  42  13  11   8  55
```

The third and most general form of the 'if' statement allows multiple decisions to be combined in a single statement. Its general form is given by

Octave

```
if (CONDITION)
    THEN-BODY
  elseif (CONDITION)
    ELSEIF-BODY
  else
    ELSE-BODY
endif
```

Jumping out of loops with `continue` and `break`

If the command `continue` appears withn the body of a loop (`for`, `until` or `while`) the rest of the body will be jumped over and the loop restarted with the next value. The example below prints only the even numbers of a selection of 10 random numbers between 0 and 100.

Octave

```
vec = round(rand(1,10)*100)
for x = vec
  if (rem(x,2) != 0)
    continue
  endif
  fprintf("%d ",x)
endfor
fprintf("\n") % generate a new line
-->
vec = 67  68  33   3  69  74  16  62  76  52
68 74 16 62 76 52
```

Observe the we do **not** leave the loop completely, but only ignore the remaining command for the current run through the loop. It is the statement `break` that will leave to loop completely. The code below will display the numbers, until the first value is larger than 70. Then no further number will be displayed.

Octave

```
vec = round(rand(1,10)*100)
for x = vec
  if (x >= 70)
    break
  endif
  fprintf("%d ",x)
endfor
fprintf("\n") % generate a new line
-->
vec =  10   7  14  72   5  71  15  67  96   5
10 7 14
```

The `switch` statment

If a number of different cases have to be considerd we may use multiple, nested `if` statments of the `switch` command.

Octave

```
switch EXPRESSION
  case LABEL
    COMMAND_LIST
  case LABEL
    COMMAND_LIST
    ...
  otherwise
        COMMAND_LIST
endswitch
```

A rather useless example of code is shown below. For a list of 10 random numbers the code prints a statement, depending on the remainder of a division by 5 .

Octave

```
vec = round(rand(1,10)*100)
for k = 1:10
  switch rem(vec(k),5)   % remainder of a division by 5
    case (0)
      fprintf("%i is a multiple of 5\n",vec(k))
    case (1)
      fprintf("A division of %i by of 5 leaves a remainder of 1\n",vec(k))
    case (3)
      fprintf("A division of %i by of 5 leaves a remainder of 3\n",vec(k))
    otherwise
      fprintf("A division of %i by of 5 leaves a remainder of 2 or 4\n",vec(k))
  endswitch
endfor
```

1.2.7 Conditions and selecting elements

When selecting elements in a vector satisfying a given condition you have two options:

- Use the condition directly to obtain a vector of 0 and 1. A number 0 indicates that the condition is not satisfied. A number 1 indicates that the condition is satisfied.
- Use the command `find()` to obtain a list of the indices for which the condition is satisfied.

Both operations are apply directly to vectors, which might have a large influence on computation time.

Octave

```
x = rand(1,10);        % create 10 random numbers with uniform distribution
ans1 = x < 0.5         % indicate the elements larger than 0.5
ans2 = find(x<0.5)     % return indicies of elements satisfying the condition
—>
ans1 =   0   1   1   1   0   1   0   1   0   1
ans2 =   2   3   4   6   8   10
```

7 Example : Selecting elements
We generate a large vector of random numbers with a normal distribution with mean value 0 and standard deviation 1. Then count the numbers between -1 and 1, expecting approximately 69% hits. The results very clearly illustrated the speed advantage of **vectorized code**.

Octave

```
n = 1000000;
x = randn(n,1);     % create the random numbers

time0 = cputime(); % use a for loop with an if condition
```

```
counter = 0;
for i = 1:n
   if abs(x(i))<1 counter +=1; endif
endfor
percentage1 = counter/n
time1 = cputime-time0

time0 = cputime();
percentage2 = sum( abs(x)<1 )/n
time2 = cputime-time0
-->
percentage1 =  0.68374
time1 =  26.038
percentage2 =  0.68374
time2 =  0.032002
```

Assume you want to know the average values of the above random numbers, but only the ones larger than 1. To be able to use vectorized code proceed in three steps:

1. Use the command `find()` to generate the indices `ind` of the numbers satisfying the condition.
2. Generate a new vector with only those numbers, `x(ind)` .
3. Use the command `mean()` to compute the average value.

Octave

```
ind = find(x>1);
result = mean(x(ind))
-->
result =  1.5249
```

♢

1.2.8 Reading and writing data in files

With *Octave* you have different option to read information from a file or write to a file:

- Loading and saving variables with `load()` and `save()`.
- Reading and writing delimited files with `dlmread()` and `dlmwrite()`.
- Read data from files with complicated structures of the data by scanning line by line.

Loading and saving *Octave* variables

With the command `save` you can save some, or all, variable in a file. This allows for later loading of the information with the command `load`. You can load and save information in different formats, including `MATLAB` formats. Use `help save` and `help load` for more information. In the example below a random matrix is created and saved in a file. Then all variables in *Octave* are cleared and the matrix is reloaded.

Octave

`load()`	load *Octave* variables
`save()`	save *Octave* variables
`dlmread()`	read all data from a file
`dlmwrite()`	write data to a file
`fopen()`	open a steam (file)
`fclose()`	close a stream
`fgetl()`	read one line from the file
`sscanf()`	scan a string for formated data

Table 1.5: Exchange information in files

```
clear *
aMat = rand(2);      % create a random matrix
save data.mat aMat   % save this matrix to a file
clear                % clear the valiables
aMat                 % try to access the matrix, should fail
load data.mat        % load the variable
-->
'aMat' undefined near line 5 column 1
aMat =   0.54174   0.83863
         0.17270   0.76162
```

The above commands work with files adhering to *Octave* and `MATLAB` standards only. Using options for the command one can read and write variables for many different versions on `MATLAB` and *Octave*.

When data is generated by other programs or instruments then the format is usually not in the above format and thus we need more flexible commands.

Delimited reading and writing, `dlmread()` and `dlmwrite()`

If your file contains data with known delimiters between the numbers the command `dlmread()` is very handy. As an example consider the file

SampleSimple.txt

```
1   1.2
2   1.2
3  1e-3
4  -3E+3
5  0
```

to be read with a single command

Octave

```
x = dlmread("SampleSimple.txt")
-->
x =
     1.0000e+00    1.2000e+00
     2.0000e+00    1.2000e+00
     3.0000e+00    1.0000e-03
     4.0000e+00   -3.0000e+03
     5.0000e+00    0.0000e+00
```

It is also possible to read only selected columns and rows in a larger set of data. The delimiter used most often are spaces or commas, leading to CSV files, i.e. **C**omma **S**eparated **V**alues. Use `help dlmread` to find

out how the delimiters (e.g. space, TAB, comma, ...) can be set. With `dlmwrite()` you can create files with data, to be read by other programs. These two commands replace `csvread()` and `csvwrite()`.

An application of the above approach is shown in Sections 2.6.2 and 2.2.10.

Scanning each line

There are many files with data in a nonstandard format or with a few header lines. As an example consider the file `Sample.txt` shown below. When reading information from a file (or another data stream) the following steps have to be taken:

- open the file for reading
- read the information, item by item or line by line
- scan the result to convert into the desired format
- close the file

The commands in Table 1.5 are useful for this task and examine Section 1.2.4 for the scanning command `fscanf()`.

Sample.txt

```
this is a header line
the file was generated on Sept 25, 2007

a 4.03   5
b -5.8   4
c 1.0e3  3
d -4.7E-6 2
e 0 1
```

We seek code to read the information on the last lines of the file. The schema of the code is shown above. The formatted scanning has to be done carefully, since three different types of data are given on one line.

Octave

```
filename = "Sample.txt";
infile = fopen(filename,'rt');          % open the file for reading, in text mode
c = blanks(20); x = zeros(1,20); n = x; % prealocate the memory

for k = 1:3                  % read and dump the three header lines
  tline = fgetl(infile);
endfor

k = 1;                       % initialize the data counter
tline = fgetl(infile);
while (!isscalar(tline))     % if tline=-1, then we reached the end of the file
                             % scan the string in the format: character float integer
  [ct,xt,nt] = sscanf(tline,"%1c%g%i","C");
  c(k) = ct; x(k) = xt;n(k) = nt; % store the data in the allocated vectors
  tline = fgetl(infile);     % read the next line
  k++;                       % increment the counter
endwhile

fclose(infile);                          % close the file
c = c(1:k-1); x = x(1:k-1); n = n(1:k-1);  % use only the effectively read data
```

As a result we obtain the string `c` with content `abcde`, the vector `x` with the floating point numbers in the middle column of `Sample.txt` and the vector `n` with the numbers 5 through 1 .

Some examples of the above approach are shown in Sections 2.7.1, 2.8.1 and 2.5.

1.3 Solving equations

In this subsection we show a few examples on how to solve different types of equations with the help of *Octave*. The examples are for instructional purposes only. We will examine:

- systems of linear equations
- zeros of polynomials
- zeros of single nonlinear functions
- zeros of systems of nonlinear functions
- optimization, maxima and minima

Obviously the above list is by no means complete, but may serve as a starting point. There are many other types of very important problems to be solve and ignored in this section:

- Ordinary differential equations: to be examined in Section 1.6, with a few examples.
- Numerical integration : to be examined in Section 2.1, with the magnetic fields as application.
- Linear Regression : to be examined carefully in Section 2.2, with real world, nontrivial examples.
- Nonlinear regression : to be examined carefully in Section 2.2.11, with real world, nontrivial examples.
- Fourier series, FFT : to be examined in Section 2.8, with a vibrating beam example.

solving equations and optimization	
`\`	backslash operator to solve systems of linear equations
`lu()`	LU factorization of matrix, to solve linear systems
`chol()`	Cholesky factorization of matrix, to solve linear systems
`roots()`	find zeros of polynomials
`fzero()`	solve one nonlinear equation
`fsolve()`	solve nonlinear equations and systems
`fsolveNewton()`	Newtons algorithm, naive implementation
`fminbnd()`	mimimization with respect to one variable
`fmins()`	mimimization, one or multiple variables
`fminsearch()`	mimimization, one or multiple variables

Table 1.6: Commands to solve equations and optimization

1.3.1 Systems of linear equations

Since the first main goal of `MATLAB` was to simplify matrix computations it should not come as a surprise that `MATLAB` and *Octave* provide many commands to work with linear systems. We illustrate some of the commands with elementary examples.

Using the backslash \ operator and `lu()` to solve linear equations

8 Example : A linear system with a unique solution
The linear system of three equations

$$\begin{aligned} 1x &+ 2y &+ 3z &= 1 \\ 4x &+ 5y &+ 6z &= 2 \\ 7x &+ 8y &+ 10z &= 3 \end{aligned}$$

should be rewritten using a matrix notation

$$\begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 10 \end{bmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}$$

A linear system is solve by "dividing" by the matrix from the correct side

$$\mathbf{A} \cdot \vec{x} = \vec{b} \qquad \Longleftrightarrow \qquad \vec{x} = \mathbf{A} \backslash \mathbf{A} \cdot \vec{x} = \mathbf{A} \backslash \vec{b}$$

In *Octave* this is implemented by

Octave

```
A = [1 2 3; 4 5 6; 7 8 10]; b = [1;2;3]; % create matrix and vector
x = A\b            % solve the system and display the result
-->
x =  -3.3333e-01
      6.6667e-01
      3.1713e-17
```

This confirms the exact solution $(\frac{-1}{3}, \frac{2}{3}, 0)^T$. This approach is clearly better than computing the inverse matrix $\mathbf{A}^{-1}$ and then computing $\mathbf{A}^{-1}\vec{b}$. For performance and stability reasons it is (almost) never a good idea to compute the inverse matrix.

If many linear systems have to be solved with the same matrix $\mathbf{A}$ then one shall not call the operator \ many times. On may either use a matrix for the right hand sides or use the LU factorization presented below. Find two examples below. If you want the above system and also

$$\begin{aligned} 1x &+ 2y &+ 3z &= -1 \\ 4x &+ 5y &+ 6z &= 0 \\ 7x &+ 8y &+ 10z &= 11 \end{aligned}$$

then use the same matrix as above, but replace the vector with a 3×2 matrix.

Octave

```
b = [1, -1;
     2,  0;
     3, 11];
x = A\b
-->
x =  -3.3333e-01   1.1667e+01
      6.6667e-01  -2.1333e+01
      3.1713e-17   1.0000e+01
```

Octave uses the Gauss algorithm with partial pivoting to solve the system. This can be written as a matrix factorization.

$$\mathbf{L} \cdot \mathbf{U} = \mathbf{P} \cdot \mathbf{A}$$

- **L** is an lower triangular matrix
- **U** is an upper triangular matrix
- **P** is a permutation matrix

Octave

```
[L,U,P] = lu(A)
-->
L =  1.00000   0.00000   0.00000
     0.14286   1.00000   0.00000
     0.57143   0.50000   1.00000

U =  7.00000   8.00000  10.00000
     0.00000   0.85714   1.57143
     0.00000   0.00000  -0.50000

P =  0  0  1
     1  0  0
     0  1  0
```

Then we use

$$\mathbf{A}\,\vec{x} = \vec{b} \quad \Longleftrightarrow \quad \mathbf{L}\,\mathbf{U}\vec{x} = \mathbf{P}\mathbf{A}\,\vec{x} = \mathbf{P}\vec{b} \quad \Longleftrightarrow \quad \begin{cases} \mathbf{L}\,\vec{y} &= \mathbf{P}\,\vec{b} \\ \mathbf{U}\,\vec{x} &= \vec{y} \end{cases}$$

i.e. we first solve the lower triangular system $\mathbf{L}\,\vec{y} = \mathbf{P}\,\vec{b}$ and then the upper triangular system $\mathbf{U}\,\vec{x} = \vec{y}$.

Octave

```
x =  U\(L\(P*b))
-->
x =  -3.3333e-01
      6.6667e-01
      3.1713e-17
```

If many more linear system with different right hand sides $\vec{b}$ have to be solved, only the last step has to be repeated. Thus computing the LU factorization is equivalent to determining the inverse matrix, but with better numerical stability. ♢

9 Example : Solving linear systems is a n^3 process
According to results you have seen in your class on linear algebra to computational effort to solve linear systems is proportional to n^3, the number of equations and unknowns. We want to verify this result with a simulation.

- First generate a list of sizes n of matrices to be examined.
- For each value of n generate a random matrix of size $n \times n$ and add a diagonal matrix to assure that the system is uniquely solvable.
- Measure the CPU time it takes to solve the linear system.

Then generate a plot of the CPU time a function of the size n. We expect

$$\texttt{CPU} \approx c\,n^3$$
$$\log(\texttt{CPU}) \approx \log(c) + 3\,\log(n)$$

On a doubly logarithmic scale we expect a straight line with slope 3. This is confirmed by the code below and the resulting Figure 1.8[8].

Octave

[8] Most of the time for this simulation is used up for generating the random numbers. But only the solving time is measured.

```
nlist = floor(logspace(2.3,3.8,20));
timer = zeros(size(nlist));
for k = 1:length(nlist)
  n = nlist(k);
  A = rand(n)-0.5 + eye(n);
  f = rand(n,1);
  t0 = cputime();
  x = A\f;
  timer(k) = cputime() - t0;
endfor

MFlops = 1/3*nlist.^3./timer/1e6

figure(1)
plot(nlist,timer,'+')
xlabel('n'); ylabel('time');  grid on

figure(2)
plot(log10(nlist),log10(timer))
xlabel('log(n)'); ylabel('log(time)');  grid on
```

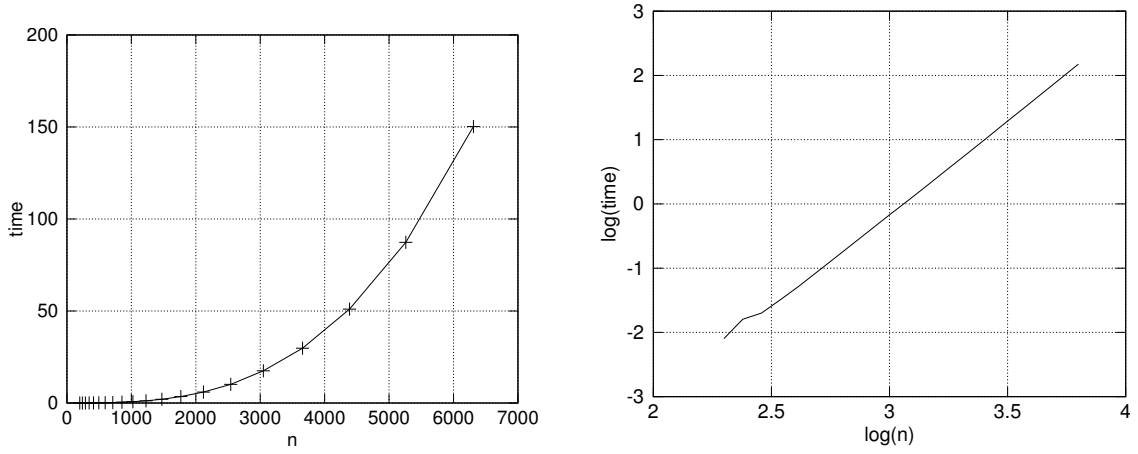


Figure 1.8: Performance of linear system solver

One has to be a bit careful when choosing large values of n. A matrix of size $n \times n$ needs to store n^2 real numbers, requiring approximately $8\,n^2$ bit of memory. For $n = 1024$ this leads to 8 MB of memory, but for $n = 10'240$ we need 800 MB of memory. ♢

Linear systems without solution, over- and under-determined systems

Even if a linear system is over-determined and has no solution, *Octave* and MATLAB will give an answer. If the system is under-determined and has infinitely many solutions, the backslash operator \ will give one answer. You have to use linear algebra to be able to use these answers.

10 Example : A linear system without solution
This will be even more usefull if there are no unique solutions. The system

$$\begin{aligned} 1\,x &+ 2\,y &+ 3\,z &= 1 \\ 4\,x &+ 5\,y &+ 6\,z &= 2 \\ 7\,x &+ 8\,y &+ 9\,z &= 4 \end{aligned}$$

does **not** have a unique solution. We find

Octave

```
A = [1 2 3; 4 5 6; 7 8 9]; b = [1;2;4];
[L,U,P] = lu(A)
-->
L =   1.00000   0.00000   0.00000
      0.14286   1.00000   0.00000
      0.57143   0.50000   1.00000

U =   7.00000   8.00000   9.00000
      0.00000   0.85714   1.71429
      0.00000   0.00000  -0.00000

P =  0   0   1
     1   0   0
     0   1   0
```

The solving $\mathbf{L}\vec{y} = \mathbf{P}\vec{b}$ leads to

Octave

```
y = L\(P*b)
-->
y =  4.00000
     0.42857
    -0.50000
```

and thus the sytem $\mathbf{U}\,\vec{x} = \vec{y}$ turns into

$$\begin{aligned} 7\,x_1 \;+\; 8\,x_2 \;+\; 9\,x_3 &= 4 \\ 0.85714\,x_2 \;+\; 1.71429\,x_3 &= 0.42857 \\ 0\,x_3 &= -0.5 \end{aligned}$$

Obviously the last equation does **not** have a solution. Using the inverse matrix to solve this system with `inv(A)*b` will return a solution, accompanied by a warning message.

```
xInv = inv(A)*b
-->
arning: inverse: matrix singular to machine precision, rcond = 2.20304e-18

xInv =   3.1522e+15
        -6.3044e+15
         3.1522e+15
```

The backslash operator \ leads to a similar result.

```
xBack = A\b
warning: matrix singular to machine precision, rcond = 2.20304e-18
warning: attempting to find minimum norm solution
warning: dgelsd: rank deficient 3x3 matrix, rank = 2

xBack =   0.250000
          0.166667
          0.083333
```

Keep this example in mind and **do not ignore warning messages**.

Since the determinant of the above 3×3 matrix $\mathbf{A}$ vanishes the linear system has only solutions for vector $\vec{b}$ of a special form. Consult you linear algebra book for details. Only if the right hand side $\vec{b}$ of the equation is in the range of the matrix $\mathbf{A}$. Obtain a basis for this space with `orth()`.

Octave

```
RangeSpace = orth(A)
⟶
RangeSpace =  0.21484  −0.88723
              0.52059  −0.24964
              0.82634   0.38794
```

This implies that for vectors

$$\vec{b} = \lambda_1 \begin{pmatrix} 0.21484 \\ 0.52059 \\ 0.82634 \end{pmatrix} + \lambda_2 \begin{pmatrix} -0.88723 \\ -0.24964 \\ 0.38794 \end{pmatrix}$$

the system has a solution $\vec{x}$ of $\mathbf{A}\,\vec{x} = \vec{b}$. This solution is not unique, but we can add a multiple of a vector in the null-space or kernel of the matrix $\mathbf{A}$. The command `null()` computes a basis for the null-space.

Octave

```
ns = null(A)
⟶
ns =  −0.40825
      +0.81650
      −0.40825
```

The result implies that for vectors $\vec{c} = \alpha\,(1\,,\,-2\,,\,1)^T$ we have $\mathbf{A}\vec{c} = \vec{0}$ and any vector $\vec{x} + \mu\,\vec{c}$ is another solution of $\mathbf{A}\,\vec{x} = \vec{b}$. ♢

11 Example : Solving an overdetermined system of linear equations
In the system of four equations

$$\begin{aligned} 1\,x_1 &+ 2\,x_2 &= 1 \\ 4\,x_1 &+ 5\,x_2 &= 2 \\ 9\,x_1 &+ 8\,x_2 &= 4 \\ 3\,x_1 &+ 6\,x_2 &= 0 \end{aligned}$$

we only have two unknowns. The system is **overdetermined**. Surprisingly *Octave* and `MATLAB` give a solution without any warning.

Octave

```
A = [1 2; 4 5; 9 8; 3 6]; b = [1;2;3;0];
x = A\b
⟶
x =   0.48610
     −0.14297
```

A quick test shows that this is **not** a solution.

Octave

```
A∗x − b
⟶
  −0.79984
  −0.77045
   0.23114
   0.60048
```

At first sight this might be surprising and can lead to problems for uninformed users. In fact *Octave* and MATLAB solve an optimization problem. *Octave* returns the vector x such that the norm of the residual $\vec{r} = \mathbf{A}\,\vec{x} - \vec{b}$ is minimized. Thus we might say that *Octave* returns the best possible solution. For many applications this is the desired solution, e.g. for linear regression problems (see Section 2.2). Internally *Octave* is using a QR factorization to solve this problem, i.e the matrix is factored in the form $\mathbf{A} = \mathbf{Q}\,\mathbf{R}$. Some details are spelled out in Section 2.2.5. ♢

12 Example : Solving an underdetermined system of linear equations
The linear system of 2 equations

$$\begin{array}{rcrcrcr} 1\,x & + & 2\,y & + & 3\,z & = & 7 \\ 4\,x & + & 5\,y & + & 6\,z & = & -5 \end{array}$$

must have infinitely many solutions. You find a description of all solutions by finding one particular solution $\vec{x}_p \in \mathbb{R}^3$ and the vector $\vec{n} \in \mathbb{R}^2$ generating the null space. Then all solutions are of the form $\vec{x} = \vec{x}_p + \lambda\,\vec{n}$, where $\lambda \in \mathbb{R}$. *Octave* can generate those vectors.

```
A = [1 2 3; 4 5 6]; b = [7; -5];
xp = A\b
n = null(A)
-->
xp =  -8.8333
      -1.3333
       6.1667

n =    0.40825
      -0.81650
       0.40825
```

The particular solution found by *Octave* is the one with the smallest possible norm, as can be verified by the orthogonality $\langle \vec{x}_p\,,\,\vec{n} \rangle = 0$. ♢

Commands to solve special linear systems

For matrices with special properties *Octave* can take advantage of these properties and find the solution with better reliability of faster.

13 Example : Cholesky factorization for symmetric, positive definite matrices
If the matrix $\mathbf{A}$ is known to be symmetric and positive definite we can use a more efficient and reliable algorithm, based on the Cholesky factorization of the matrix.

$$\mathbf{A} = \mathbf{R}^T \cdot \mathbf{R}$$

where $\mathbf{R}$ is an upper triangular matrix. A linear system of equations can then be solved as a seqence of systems with triangular matrix.

$$\mathbf{A}\,\vec{x} = \vec{b} \quad \Longleftrightarrow \quad \mathbf{R}^T\,\mathbf{R}\,\vec{x} = \vec{b} \quad \Longleftrightarrow \quad \left\{ \begin{array}{rcl} \mathbf{R}^T\,\vec{y} & = & \vec{b} \\ \mathbf{R}\,\vec{x} & = & \vec{y} \end{array} \right.$$

To examine the system

$$\begin{array}{rcrcrcr} 3\,x & + & 0\,y & + & 1\,z & = & 1 \\ 0\,x & + & 3\,y & + & 2\,z & = & 2 \\ 1\,x & + & 2\,y & + & 9\,z & = & 3 \end{array}$$

we use the code below, verifying that we have the same solution with both solution methods.

Octave

```
A = [3,0,1; 0,3,2; 1,2,9];
R = chol(A)
b = [1;2;3];
x1 = A\b;
xChol = R\(R'\b)
MaxError = max(abs(x1-xChol))
-->
R =   1.73205   0.00000   0.57735
      0.00000   1.73205   1.15470
      0.00000   0.00000   2.70801

xChol =   0.27273
          0.54545
          0.18182

MaxError = 0
```

A second output argument of `chol()` indicates whether the matrix was positive definite or not. ♢

14 Example : Sparse matrices

There are many applications where the matrix $\mathbf{A}$ consists mostly of zero entries and thus the standard algorithms will waste a lot of effort dealing with zeros. To avoid this **sparse matrices** were introduced. As an example we consider the $n \times n$ matrix $\mathbf{A}$ given by

$$\mathbf{A} = \frac{1}{(n+1)^2} \begin{bmatrix} 2 & -1 & & & & & \\ -1 & 2 & -1 & & & & \\ & -1 & 2 & -1 & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & -1 & 2 & -1 & \\ & & & & -1 & 2 & \end{bmatrix}$$

This type of matrix appears very often when using the finite difference method to solve differential equations, e.g. heat equations.

Using the command `spdiags()` we create a sparse matrix where *Octave* only stores the nonzero values and their position in the matrix.

Octave

```
n = 10;
A = spdiags([-ones(n,1),2*ones(n,1),-ones(n,1)],[ -1,0,1],n,n)/(n+1)^2
-->
A = Compressed Column Sparse (rows = 10, cols = 10, nnz = 28 [28%])
   (1, 1) -> 0.016529
   (2, 1) -> -0.0082645
   (1, 2) -> -0.0082645
   (2, 2) -> 0.016529
   (3, 2) -> -0.0082645
   (2, 3) -> -0.0082645
   (3, 3) -> 0.016529
   ...
```

Then a system of linear equations can be solved as before, but *Octave* will automatically take advantage of the sparseness of the matrix.

Octave

```
b = ones(n,1);
x = A\b;  % solve the sparse system
x'        % diplay as row vector
-->
605.0   1089.0   1452.0   1694.0   1815.0   1815.0   1694.0  1452.0   1089.0     605.0
```

By changing the size n of the matrix you can solve a large number of linear equations, e.g. $n = 100000$. Working with full matrices you would run out of memory. ♢

15 Example : Sparse Cholesky factorization
The matrix in the previous example is symmetric and positive definite, thus we may use the Cholesky factorization $\mathbf{A} = \mathbf{R}^T\mathbf{R}$. *Octave* returns $\mathbf{R}$ as a sparse matrix.

Octave
```
R = chol(A);
xChol = R\(R'\b)
```

If the matrix $\mathbf{A}$ is known to be sparse we can call the function `chol()` with three output arguments and find a sparsity preserving permutation matrix $\mathbf{Q}$ such that

$$\mathbf{Q}^T \cdot \mathbf{A} \cdot \mathbf{Q} = \mathbf{R}^T \cdot \mathbf{R}$$

The permutation matrix $\mathbf{Q}$ is best returned as a permutation vector. This allows to save large amounts of memory for some applications. To solve the system we have to take the permutation matrices into account. Use the fact that $\mathbf{Q}^{-1} = \mathbf{Q}^T$ to examine the system $\mathbf{A}\,\vec{x} = \vec{b}$ with the help of

$$\mathbf{Q}^T\mathbf{A}\,\mathbf{Q}\mathbf{Q}^T\vec{x} = \mathbf{Q}^T\vec{b} \quad \Longleftrightarrow \quad \mathbf{R}^T\,\mathbf{R}\mathbf{Q}^T\vec{x} = \mathbf{Q}^T\vec{b} \quad \Longleftrightarrow \quad \begin{cases} \mathbf{R}^T\,\vec{y} &= \mathbf{Q}^T\vec{b} \\ \mathbf{R}\,\mathbf{Q}^T\vec{x} &= \vec{y} \end{cases}$$

and thus

$$\vec{x} = \mathbf{Q}\mathbf{R}^{-1}(\mathbf{R}^T)^{-1}\mathbf{Q}^T\vec{b}$$

In *Octave* this is implemented by

Octave
```
[R, P, Q] = chol(A);
x3 = Q*(R\(R'\(Q'*b)));
```

This code is longer than just `x = A\b`, but there are cases where it is considerably faster and saves memory. ♢

1.3.2 Zeros of polynomials

Real or complex polynomials of degree n have exactly n zeros, maybe complex and/or multiple. Thus *Octave* provides a special command to determine those zeros, often called roots, of polynomials. To determine the zeros of

$$p(z) = 1 + 2\,z + 3\,z^3$$

we use

Octave
```
roots([3  0  2  1])
-->
   0.20116 + 0.88773i
   0.20116 - 0.88773i
  -0.40232 + 0.00000i
```

Thus we find one real root at $x \approx -0.4$ and two complex conjugate roots. This is confirmed by the graph of the polynomial $p(x)$ in Figure 1.9.

Octave

```
x = -1:0.01:2;              % choose values between -1 and 2
y = polyval([3 0 2 1],x) % evaluate the polynomial at those points
plot(x,y)                   % generate the plot
```

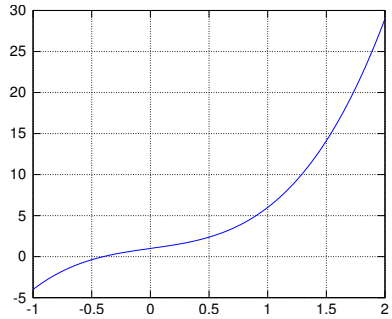


Figure 1.9: Graph of the polynomial $1 + 2\,x + 3\,x^3$

1.3.3 Nonlinear equations

Not all equations are linear equations and solving nonlinear equations, or systems, can be very difficult. *Octave* provides a few algorithms to help solving nonlinear equations.

Single equations

With the commands `fzero()` or `fsolve()` we can solve single equations or systems of equations. Given a good initial guess for a solution of $f(x) = 0$. To determine the obvious solution $x = \pi$ of $\sin(x) = 0$ we can use

Octave

```
x0 = fsolve(@(x)sin(x),3)
-->
x0 =  3.1416
```

16 Example : Zero of a Bessel function
Examine Figure 1.7 (page 35) to see that the function $f(x) = J_0(x)$ has a zero close to $x_0 = 6$. Since the value of x and y are displayed for each evaluation of the function we can observe the iterations and its convergence. With the help of options we are asking for 12 correct digits.

Octave

```
x0 = 6.0;

clear options
options.TolFun = 1e-12;
options.TolX   = 1e-12;

function y = f(x)
  y = besselj(0,x);
  [x y]
endfunction

[x, fval, info] = fsolve(@f,x0,options)
-->
   6.00000   0.15065
   6.00004   0.15066
```

```
    5.99996    0.15064
    5.455533   -0.022077
    5.455566   -0.022065
    5.455500   -0.022088
    5.5198e+00   -9.8715e-05
    5.5201e+00   -9.3923e-07
    5.5201e+00   -8.9600e-09
    5.5201e+00   -8.5477e-11
    5.5201e+00   -8.1499e-13

x =  5.5201
fval = -8.1499e-13
info =  1
```

The algorithm seems to lead to a linear convergence, i.e. the number of correct digits increases at a constant rate. We needed 11 iterations to arrive at the desired accuracy. The return value of `info` contains information on whether the solution converged or not. Find information on the interpretation of the values of info by

Octave

```
perror ("fsolve", 1)
perror ("fsolve", 3)
-->
solution converged to requested tolerance
iteration is not making good progress
```

♢

17 Example : Using a user provided Jacobian

The algorithm used in `fsolve()` may use a Newton like iteration

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$$

to determine an approximate solution. This algorithm should converge quadratically, i.e. the number of correct digits is doubled at each step. The documentation of *Octave* states[9] that one can pass a formula for the derivative to the command `fsolve()` and then this derivative will be used for the iteration. This excellent feature might be very efficient, in particular for systems of equations. One should observe fewer evaluations of the function f, provided the initial value is close enough to the true solution.

Octave

```
x0 = 6.0  % choose the starting value

function [y,dy] = f2(x)
  y = besselj(0,x);
  dy = -besselj(1,x);
  [x,y]  % displayed for each evaluation of the function
endfunction

clear options          % set the options for fsolve
options.TolFun = 1e-12;
options.TolX   = 1e-12;
options.Jacobian = 'on';
options.Updating = 'off';
```

[9] The example in the current documentation of Octave 3.2.2 does not yet work as presented. The developer (Jaroslav Hajek) mentioned that this will be fixed in an upcoming version.

```
[x2, fval, info] = fsolve(@f2,x0,options)
-->
   6.00000   0.15065
   6.00000   0.15065
   5.455533  -0.022077
   5.455533  -0.022077
   5.5198e+00  -9.8715e-05
   5.5198e+00  -9.8715e-05
   5.5201e+00  -2.5912e-09
   5.5201e+00  -2.5912e-09
   5.5201e+00   2.0101e-17

x2 =  5.5201
fval =  2.0101e-17
info =  1
```

We observe that the number of correct digits is doubled for each iteration. Due to a flaw in the current version[10] the function gets called twice for each iteration, the documentation of `fsolve()` shows how to avoid the extra effort. We needed only 5 iterations to arrive at the desired accuracy.

♢

18 Example : Options of `fsolve()`
The function `fsolve()` allows to set a few options.

- `TolX` : the tolerance in x values, The default value is $1.5 \cdot 10^{-8}$.
- `FunX` : the tolerance in the function values, The default value is $1.5 \cdot 10^{-8}$.
- `MaxIter` : maximal number of iterations to be used. The default value is 400 .
- `Jacobian` : a user supplied derivative may be used.
- `Updating` : if set to "off" a Newton algorithm is used.

The default values of those options can be found in the source file for the function `fsolve()`. Type `which fsolve` on the *Octave* command promt to find the exact location of the source file and then examine the file with your favourite editor. As a example we compute the first zero of $\sin(x)$ without and with options.

Octave

```
clear options
res1 = fsolve(@(x)sin(x),3)-pi
options.TolFun = 1e-15;
options.TolX   = 1e-15
res2 = fsolve(@(x)sin(x),3,options)-pi
-->
res1 = -2.8937e-10
options = { TolFun =  1.0000e-15
            TolX   =  1.0000e-15 }
res2 =  4.4409e-16
```

♢

The command `fsolve()` is rather powerful, it can also examine overdetermined systems of equations and may be used for nonlinear regression problems, see Section 2.2.11.

[10] Soon to be fixed, thanks to open source development.

Systems of equations

The command `fsolve()` can also be used to solve systems of equations. Use some geometry (intersection of ellipses) to convince yourself that the system

$$\begin{aligned} x^2 + 4\,y^2 - 1 &= 0 \\ 4\,x^4 + y^2 - 1 &= 0 \end{aligned}$$

must have a solution close to $x \approx 1$ and $y \approx 1$. This solution can be found by the code below.

Octave

```
x0 = [1;1];  % choose the starting value

function y = f(x)  % define the system of equations
  y = [x(1)^2 + 4*x(2)^2-1;
       4*x(1)^4 + x(2)^2-1];
endfunction

[x,fval,info] = fsolve(@f,x0)  % determine one of the possible solutions
-->
x =   0.68219
      0.36559
fval =  -1.3447e-07
         1.1496e-07
info =  1
```

Implementing Newtons Algorithm

The main tool to solve a system of nonlinear equations of the form $\vec{f}(\vec{x}) = \vec{0}$ is Newtons algorithm. For a well chosen starting vector $\vec{x}_0$ apply the iteration

$$\vec{x}_{n+1} = \vec{x}_n - (DF(\vec{x}_n))^{-1}\vec{f}(\vec{x}_n)$$

where the Jacobian matrix of partial derivatives is given by

$$DF(\vec{x}) = \begin{bmatrix} \frac{\partial f_1(\vec{x})}{\partial x_1} & \frac{\partial f_1(\vec{x})}{\partial x_2} & \cdots & \frac{\partial f_1(\vec{x})}{\partial x_n} \\ \frac{\partial f_2(\vec{x})}{\partial x_1} & \frac{\partial f_2(\vec{x})}{\partial x_2} & & \frac{\partial f_2(\vec{x})}{\partial x_n} \\ \vdots & & \ddots & \vdots \\ \frac{\partial f_n(\vec{x})}{\partial x_1} & \frac{\partial f_n(\vec{x})}{\partial x_2} & \cdots & \frac{\partial f_n(\vec{x})}{\partial x_n} \end{bmatrix}$$

Consult your calculus lecture notes for information on the algorithm. Below we implement this algorithm in *Octave*. Since `MATLAB` hides the function `fsolve.m` in an expensive toolbox, we assure the code will work with basic `MATLAB`. The code will by no means replace the *Octave* function `fsolve.m`, which has more options and will examine overdetermined systems too (see Section 2.2.11).

Al the code segments below have to be in a file `fsolveNewton.m`, together with the necessary copyright statement. Then the code can be used to solve the system

$$\begin{aligned} x^2 + 4\,y^2 - 1 &= 0 \\ 4\,x^4 + y^2 - 1 &= 0 \end{aligned}$$

by calling

Octave

```
clear *
x0 = [1;1];  % choose the starting value

function y = f(x)  % define the system of equations
  y = [x(1)^2 + 4*x(2)^2-1;
       4*x(1)^4 + x(2)^2-1];
endfunction

function y = dfdx(x)  % Jacobian
  y = [2*x(1), 8*x(2);
       16*x(1)^3, 2*x(2)^2];
endfunction

[x,iter] = fsolveNewton('f',x0,1e-4*[1;1])   % use a finite difference Jacobian
[x,iter] = fsolveNewton('f',x0,1e-6)         % higher accuracy
[x,iter] = fsolveNewton('f',x0,1e-6,'dfdx')  % user provided Jacobian
```

This example was aleady solve in the previous Section 1.3.3.

- Define the function name and give the basic documentation.

```
function [x,iter] = fsolveNewton(f,x0,tolx,dfdx)

% [x,iter] = fsolveNewton(f,x0,tolx,dfdx)
%
% use Newtons method to solve a system of equations f(x)=0,
% the number of equations and unknowns have to match
% the Jacobian matrix is either given by the function dfdx or
% determined with finite difference computations
%
% input parameters:
% f    string with the function name
%      function has to return a column vector
% x0   starting value
% tolx allowed tolerances,
%      a vector with the maximal tolerance for each component
%      if tolx is a scalar, use this value for each of the components
% dfdx string with function name to compute the Jacobian
%
% output parameters:
% x    vector with the approximate solution
% iter number of required iterations
%      it iter>20 then the algorithm did not converge
```

- Verify the input arguments and set up the starting point for the loop to come.

```
  if ((nargin < 3)|(nargin>=5))
    usage('wrong number of arguments in fsolveNewton(f,x0,tolx,dfdx)');
  end
  maxit = 20;    % maximal number of iterations
  x = x0;
  iter = 0;
  if isscalar(tolx) tolx = tolx*ones(size(x0)); end
  dx = 100*abs(tolx);
  f0 = feval(f,x);
  m = length(f0);
```

```
n = length(x);
if (n ~= m) error('number of equations not equal number of unknown')
  end
if (n ~= length(dx)) error('tolerance not correctly specified')
  end
```

- Start the loop. Compute the Jacobian matrix, either by calling the provided function or by using a finite difference approximation.

```
jac = zeros(m,n); % reserve memory for the Jacobian
done = false;     % Matlab has no 'do until'
while ~done
  if nargin==4    % use the provided Jacobian
    jac = feval(dfdx,x);
  else            % use a finite difference approx for Jacobian
    dx = dx/100;
    for jj= 1:n
      xn = x; xn(jj) = xn(jj)+dx(jj);
      jac(:,jj) = ((feval(f,xn)-f0)/dx(jj));
    end
  end
```

- Apply a Newton step and close the loop.

```
  dx = jac\f0;
  x = x - dx;
  iter = iter+1;
  f0 = feval(f,x);
  if ((iter>=maxit)|(abs(dx)<tolx))
    done = true;
  end
end
```

To estimate the derivatives $\frac{\partial f(x)}{\partial x}$ we use the finite difference approximation

$$\frac{\partial f(x)}{\partial x} \approx \frac{f(x+h)-f(x)}{h} \quad \text{for } h \text{ small enough}$$

1.3.4 Optimization

In this section we will use some commands from the optimization package at SourceForge[11]. Thus have a quick look at the package, resp. its documentation. If the package is not installed on your system (hint: `pkg list all`) you will have to download, install and load the package, using the instructions in Section 1.1.1 (page 10).

19 Example : The function $f(x) = \sin(2\,x)$ has a minimum at $x_{min} = \frac{3\,\pi}{4} \approx 2.3562$. For the command `fmins()` we have to provide an initial guess and then obtain an approximate answer.

Octave

[11] in `MATLAB` with the Optimization toolbox installed you may use the function `fminsearch()` instead of `fmins()`. In *Octave* both are available.

```
xMin = fmins(@(x)sin(2*x), 2.5)
-->
xMin =  2.3560
```

If we want better accuracy of the solution we have to choose the correct options. Find the documentation with `help fmins`. In the example below we ask `fmins()` to show intermediate results and work with better accuracy, which is obtained for the final result. The intermediate results show the Nelder–Mead simplex algorithm at work.

Octave

```
options = [1, 1e-7];
xMin = fmins(@(x)sin(2*x),2.5,options)
-->
f(x0) = 9.5892e-01
Iter.  1,  how = initial    nf =   2,  f = 9.5892e-01  (0.0%)
Iter.  2,  how = shrink,    nf =   5,  f = 9.5892e-01  (0.0%)
Iter.  3,  how = shrink,    nf =   8,  f = 9.5892e-01  (0.0%)
Iter.  4,  how = shrink,    nf =  11,  f = 9.5892e-01  (0.0%)
Iter.  5,  how = contract,  nf =  13,  f = 9.9969e-01  (4.3%)
Iter.  6,  how = shrink,    nf =  16,  f = 9.9969e-01  (0.0%)
Iter.  7,  how = shrink,    nf =  19,  f = 9.9969e-01  (0.0%)
Iter.  8,  how = contract,  nf =  21,  f = 9.9990e-01  (0.0%)
Iter.  9,  how = contract,  nf =  23,  f = 9.9999e-01  (0.0%)
Iter. 10,  how = contract,  nf =  25,  f = 9.9999e-01  (0.0%)
Iter. 11,  how = contract,  nf =  27,  f = 1.0000e+00  (0.0%)
Iter. 12,  how = shrink,    nf =  30,  f = 1.0000e+00  (0.0%)
Iter. 13,  how = shrink,    nf =  33,  f = 1.0000e+00  (0.0%)
Iter. 14,  how = contract,  nf =  35,  f = 1.0000e+00  (0.0%)
Iter. 15,  how = shrink,    nf =  38,  f = 1.0000e+00  (0.0%)
Iter. 16,  how = contract,  nf =  40,  f = 1.0000e+00  (0.0%)
Iter. 17,  how = shrink,    nf =  43,  f = 1.0000e+00  (0.0%)
Iter. 18,  how = shrink,    nf =  46,  f = 1.0000e+00  (0.0%)
Iter. 19,  how = contract,  nf =  48,  f = 1.0000e+00  (0.0%)
Iter. 20,  how = shrink,    nf =  51,  f = 1.0000e+00  (0.0%)
Iter. 21,  how = shrink,    nf =  54,  f = 1.0000e+00  (0.0%)
Iter. 22,  how = contract,  nf =  56,  f = 1.0000e+00  (0.0%)
Iter. 23,  how = shrink,    nf =  59,  f = 1.0000e+00  (0.0%)
Iter. 24,  how = contract,  nf =  61,  f = 1.0000e+00  (0.0%)
Iter. 25,  how = shrink,    nf =  64,  f = 1.0000e+00  (0.0%)
Simplex size 6.3242e-08 <= 1.0000e-07...quitting
xMin =  2.3562
```

♢

If the function depends on one variable only you may also use to command `fminbnd()`. It uses a different algorithm and is usually more efficient for functions of one variable.

Octave

```
xMin = fminbnd(@(x)sin(2*x), 0,pi)
-->
xMin =  2.3562
```

20 Example : We can also optimize functions of multiple variables. Instead of a maximum of

$$f(x,y) = -2\,x^2 - 3\,x\,y - 2\,y^2 + 5\,x + 2\,y$$

we seek a minumum of $-f(x,y)$. Examine the graph of $f(x,y)$ in Figure 1.10.

Octave

```
[xx,yy] = meshgrid( [-1:0.1:4],[-2:0.1:2]);

function res = f(x,y)
  res = -2*x.^2 -3*x.*y-2*y.^2 + 5*x+2*y;
endfunction

surfc(xx,yy,f(xx,yy));    xlabel('x'); ylabel('y');
```

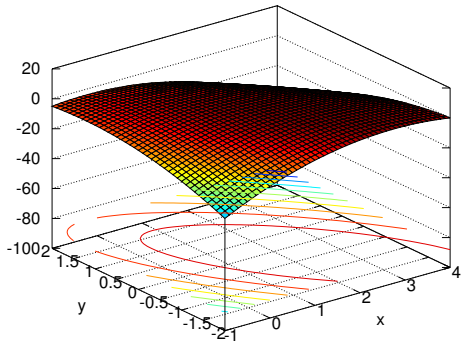


Figure 1.10: Graph of a function $h = f(x, y)$, with contour lines

Using the graph we conclude that there is a maximum not too far away from $(x, y) \approx (1.5\,,\,0)$. We use `fmins()` with the function $-f$ and the above starting values.

Octave

```
xMin = fmins(@(x)-f(x(1),x(2)),[1.5,0])
-->
xMin = 1.9996   -1.0005
```

An exact computation will find the exact position of the maximum at $(x, y) = (2\,,\,-1)$. To obtain better accuracy we can use options again, e.g.

Octave

```
xMin = fmins(@(x)-f(x(1),x(2)),[1.5,0], [0, 1e-10])
-->
xMin =  2.0000   -1.0000
```

♢

21 Example : For an efficient hardware implementation of division of floating point numbers one needs a good approximation of the function $1/x$ on the interval $[\frac{1}{2}\,,\,1]$ by a polynomial of degree 2. We want to minimize the maximal error, i.e. we seek the minimum of

$$f(a, b, c) = \max_{0.5 \le x \le 1} |\frac{1}{x} - a\,x^2 - b\,x - c|$$

As a starting guess for our parabola we use the straight line through the points $(0.5\,,\,2)$ and $(1\,,\,1)$. To improve accuracy and reliability we repeat the call of `fmins()` until the result stabilizes.

Octave

```
x = linspace(0.5,1,1001);

function res = toMin(p,x)
  res = max(abs(1./x - polyval(p,x)));
endfunction
```

```
pOptim = fmins(@(p)toMin(p,x),[0,-2,3],[0, 1e-15])
pOptim = fmins(@(p)toMin(p,x),pOptim,[0, 1e-15])
-->
pOptim =  2.7452  -6.0589   4.3284
pOptim =  2.7452  -6.0589   4.3284
```

The result can be verified visually by the code below and the resulting Figure 1.11. Obviously we have an excellent approximation of $1/x$ by a second order polynomial.

Octave

```
yOptim = polyval(pOptim,x);
figure(1)
plot(x,1./x,x,yOptim)
xlabel('x'); ylabel('1/x and polynomial approx.')
figure(2)
plot(x,yOptim-1./x)
xlabel('x'); ylabel('difference')
```

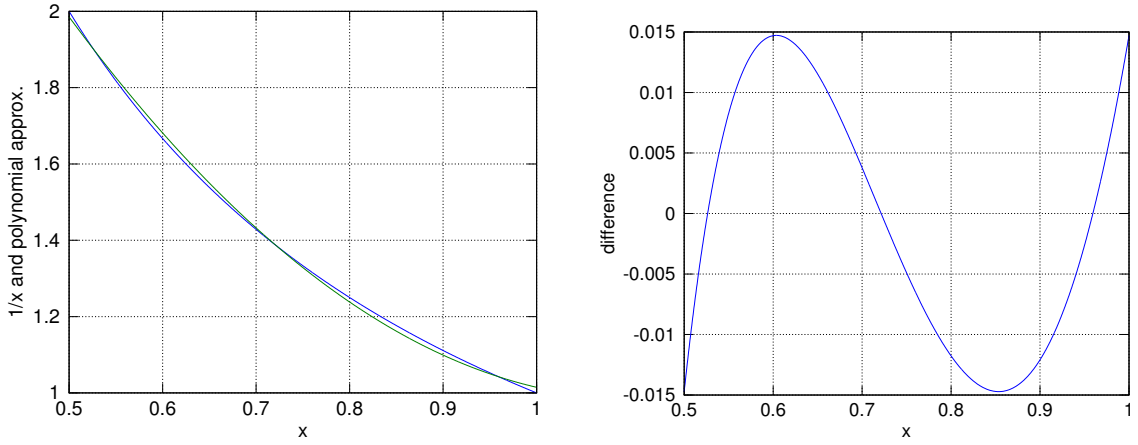


Figure 1.11: $1/x$ and its polynomial approximation

♢

Linear and nonlinear regression problems can also be considered as minimization problem. For this special type of problem there are better algorithms, see Chapter 2.2 and Sections 2.2.11.

1.4 Basic Graphics

For the graphics commands there are some noticeable differences between MATLAB and *Octave*. Thus it is necessary to consult the corresponding help files to find the documentation. In addition there are many more options and possibilities than it is possible to illustrate in the given time and space for these notes.

- *Octave* and MATLAB will by default open up a graphics window on screen to display graphics.
- After a graph is displayed you can change its appearance with many commands: choose different axis, put on labels or a title, add text, ...
- If you generate a new picture, the old one will be overwritten, You can change this behavior with `hold` or `figure()`.
- You can open up mutliple graphics windows, using the command `figure()`.
- Within a graphics window you can use the mouse to zoom, move or rotate the picture. Hitting the key `A` will through you back to the default view. Hit the key `H` to display all possible key commands.
- With the command `print()` you can write the current figure into a file, choosing from many different formats.
- When starting up *Octave* you can choose which graphics toolkit to use.
  - `gnuplot` : this is (up to now) the default. *Octave* will use *Gnuplot* as graphics engine to generate the graphics on screen or in files. This is a time tested method, but not very efficient for large 3D graphics. Use `gnuplot_binary` to find out which binary is actually used.
  - `fltk` : this is a graphics engine using OpenGL. It will use the specialized hardware on the graphics card.
  - Switching forth and back between the two toolkits within one *Octave* session is not possible.

Octave

```
graphics_toolkit        % display the current graphics toolkit
graphics_toolkit fltk   % switch to the fltk toolkit
```

In this section a few examples will be shown, but much more is possible.

1.4.1 2-D Plots

The basic `plot()` command

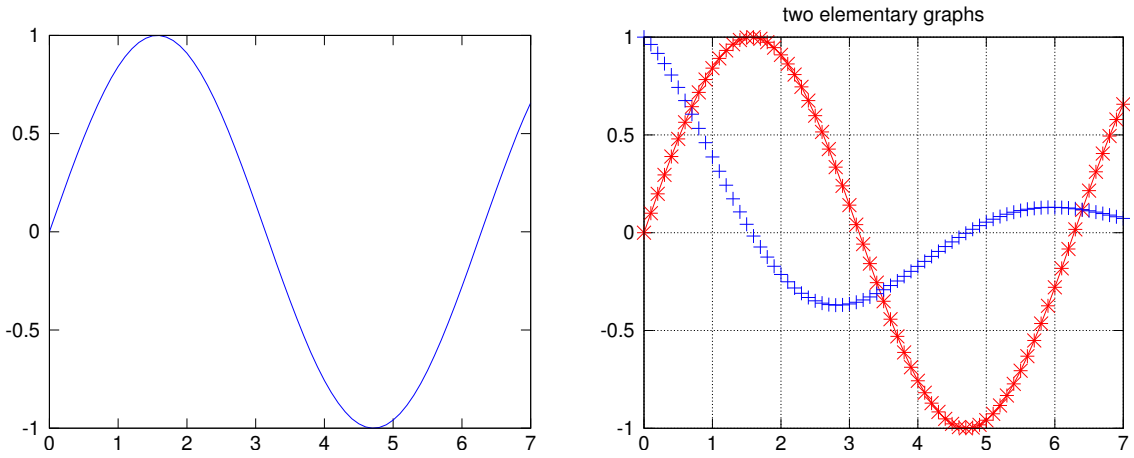
Graphs of known functions are easy to generate with MATLAB or *Octave*, as shown with the code below and the resulting figure in Figure 1.12(a).

Octave

```
x = 0:0.1:7;
y1 = sin(x);
plot(x,y1)
```

MATLAB and *Octave* will essentially plot a number of points and you can choose on how to connect the points.

- The command `plot()` can only display points and straight line connections between them. second argument.



(a) a raw graph (b) a graph with formats used

Figure 1.12: Elementary graphs of functions

- The command `plot()` with two arguments requires the values of the x coordinates as the first component and the y components as the second argument.
- A third argument of `plot()` may to be a format string, specifying how `plot()` has to display and connect the individual points. Ther are many options:
  - Choose a line style: `-` lines, `.` dots, `^` impulses, `L` steps
  - Choose the color by a letter: `k` (black), `r` (red), `g` (green), `b` (blue), `m` (megenta), `c` (cyan), `w` (white)
  - With `';title;'` choose the label for the key
  - Use `+`, `*`, `o` or `x` in combination with the lines style to choose the point style
- Multiple sets of points can be displayed with one single call to `plot()`. List the arguments sequentially.
- Use `help plot` to access further information.

The code below shows a simple example, leading to Figure 1.12(b).

Octave

```
y2 = cos(x).*exp(-x/3);
plot(x,y1,'-@*r',x,y2,'+b')
title('two elementary graphs');
grid on
```

Options and additions to `plot()` and printing

The result of the basic command `plot()` may be modified by a number of options and parameters, most of which are shown in Table 1.7. The code below is using some of the options with the result shown on the left in Figure 1.13.

- A encapsulated Postscript file `graph3.eps`, containing the graphics, will be created in the current directory. The command in the code below generates a level 2 encapsulated file, using a tight bounding box and a different font. This file is suitable to be included in LaTeX documents.

plot commands	
`plot()`	basic command to plot one or multiple functions
`semilogx()`	same as `plot()` but with logarithmic horizontal scale
`semilogy()`	same as `plot()` but with logarithmic vertical scale
`loglog()`	same as `plot()` but with double logarithmic scales
`hist()`	generate and plot a histogram
`bar()`	generate a bar chart
`plotyy()`	generate a plot with 2 independent y axis
options and settings	
`graphics_toolkit`	choose the graphics engine to be used
`figure()`	choose the display window on the screen
`title()`	set a title for the graphic
`xlabel()`	specify a label for the horizontal axis
`ylabel()`	specify a label for the vertical axis
`zlabel()`	specify a label for the third axis
`text()`	put a text at a given position in the graph
`legend()`	puts a legend on the plot or turns them on/off
`grid`	turn grid on (`grid on`) or off (`grid off`)
`axis()`	choose the viewing area, use `axis()` to reset
`hold`	toggle the hold state of the current graphic
`subplot()`	create one of the figures in a multiplot
`print()`	save the current figure in a file
`clf`	clear the current figure

Table 1.7: Generating 2D plots

- For Open-Office or Word documents the PNG format is useful. It is important to generate bitmap files with the correct size and not rescale them with the word processor! In the example below an image of size 600 by 400 is generated.
- The are many more formats available, e.g. PDF. See `help print` .

Octave

```
clf
x = -4:0.1:4;
y = (1+x.^2).*exp(3*x);
semilogy(x,y);
text(-3,2000,'Text in Graph');
title('logarithmic scale in vertical direction')
xlabel('Distance [m]'); ylabel('Temp [K]')
print('graph3.eps','-depsc2','-FTimes-Roman:20','-tight')
print('graph3.png','-S600,400')
```

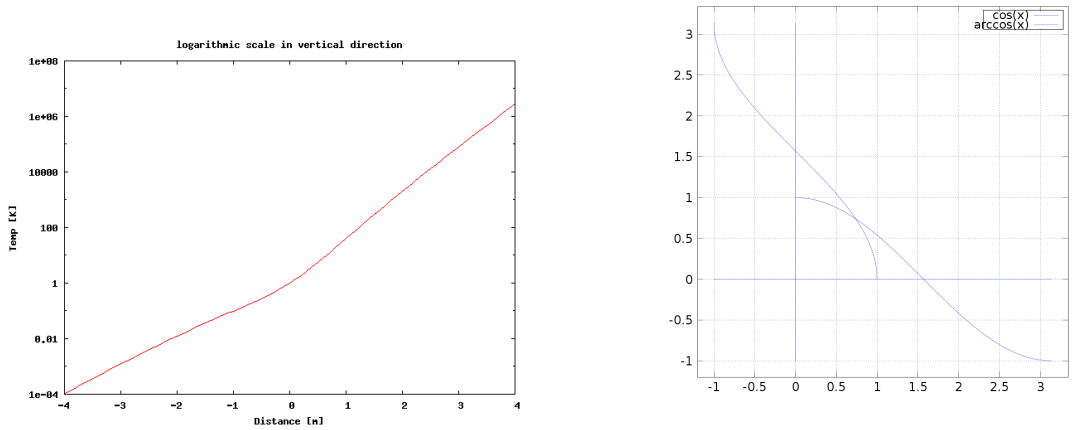


Figure 1.13: Two graphs with some decorations

Octave

```
clf
x = linspace(0,pi,50);
y = cos(x);
plot(x,y);
legend('show')
legend('cos(x)','location','northeast')
legend('boxon')
hold on
axis([-1.2 pi+0.2 -1.2 pi+0.2],'equal')
plot(y,x,';arccos(x);');
plot([-1 pi],[0 0],'b',[0 0],[-1 pi],'b');  % show coordinate axis
grid on
```

With `subplot()` one can generate multiple graphs in one figure.

Octave

```
x = linspace(-2*pi,2*pi,200);
clf
axis('normal');
axis()            % leave the scaling up to Octave
subplot(2,2,1); plot(x,sin(x));
subplot(2,2,2); plot(x,cos(x));
subplot(2,2,3); plot(x,sinh(x));
subplot(2,2,4); plot(x,cosh(x));
```

Find another example in Figure 1.23 on page 82.

A figure in a figure

Octave allows for many more tricks with pictures, e.g. you can generate a figure in a figue, as shown in Figure 1.14.

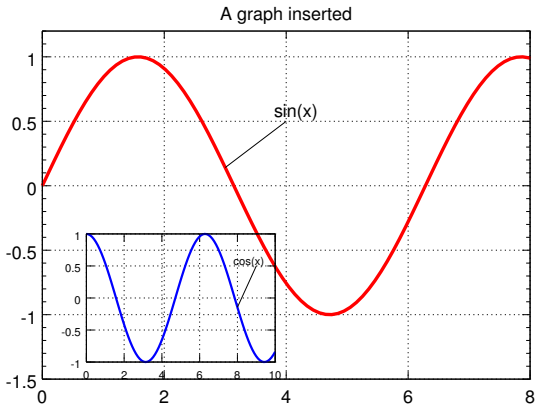


Figure 1.14: A figure in a figure

Octave

```
x = linspace(0,10);  f1 = sin(x);  f2 = cos(x);

figure(1); subplot(1,1,1)

plot(x,f1,"r","linewidth",3)
axis([0 8 -1.5 1.2])
set(gca,"fontsize",16)
grid on
line([3 4],[sin(3) 0.5])
text(3.8,0.6,"sin(x)","fontsize", 16)
title("A graph inserted")

axes("position",[0.2 0.15 0.3 0.3])
set(gca, "xlim",[3,10],"ylim",[-1.1 1.1])
axis([0 10 -1.2 1.2])
plot(x,f2,"linewidth",2)
grid on
line([8 9],[cos(8) 0.5])
text(7.8,0.6,"cos(x)")
```

1.4.2 Printing figures to files

Generating files in different formats

In the above section we already mentioned that on screen figures can be written to files, for them to be included in your favorite text procession tool or to be used with LaTeX. The basic command to be used is `print()`. It takes the name of the file to be generated and other options as parameters. The `print()` command has many options, consult the documentation by `help print` or `doc print`.

plot commands	
`print`	the basic command to write a picture in a file
options	
`-d...`	choose the device to be used
`-depsc`	colored EPS (Encapsulated PostScript)
`-dpng`	PNG (Portable Network Graphics)
`-dpdf`	PDF (Portable Document Format), full page
`-dpdfwrite`	PDF, with bounding box

Table 1.8: the `print()` command and its options

There are different types of files that might be useful. Here only 4 formats will be commented: `EPS`, `PNG`, `PDF` and `FIG`.

EPS : Encapsulated PostScript files can be used with LaTeX or other good text processing tools. Many printers, resp. their drivers, can print these files directly to paper.

- EPS files may be generated by either one of the lines below. The file `graph.eps` will contain the image.

Octave
```
print('graph.eps','-depsc','-FTimes-Roman:20','-tight')
print -depsc -FTimes-Roman:20 -tight graph.eps
```

- These figures can be rescaled without problems and the fonts for the included characters remain intact.
- For potographs the created files might be unnecassary large.
- LibreOffice/OpenOffice/Word can not handle Postscript pictures

PNG : Portable Network Graphics files are a good format for bitmaps, e.g. photos.

- The files may be generated by either of the lines below. The file `graph.png` will contain the image.

Octave
```
print('graph3.png','-S600,400')
print -S600,400 graph3.png
```

- These figures **can not be rescaled** without serious loss of image quality. Thus you have to generate it in the correct size and the above option to specify the resolution of the image is essential.
- LaTeX and LibreOffice/OpenOffice/Word can handle PNG files.

PDF : Portable Document Format can be use in LaTeXor to directly print the figure. PDF can be used instead of EPS.

- PDF files may be generated by either one of the lines below. The file `graph.pdf` will contain the image.

```
Octave
print('graph.pdf')                % for a full page
print('graph.pdf','-dpdfwrite')  % for a figure with bounding box
```

  Use the second line if you need to include the generated picture into another document, as the first line will always generate a full page.
- For potographs the created files might be unnecassary large.
- LibreOffice/OpenOffice/Word can not handle PDF pictures

fig : If you want to apply further modifications to your figure the `fig` format might be handy. You can then use the program `xfig` to modify your picture, e.g. change fonts, colors, thickness of lines, ... With `xfig` you can then safe the figure in the desired format for the final usage. To generate a colored figure use.

```
Octave
print -color graph.fig  % color might only work with fltk toolkit
```

Converting different formats

On occasion it is necessary to convert between different formats. Most Unix systems provide powerful tolls for this task.

ImageMagick is an cross platform, open source software suite for displaying, converting, and editing raster image files. It can read and write over 100 image file formats. It can not only convert, but also apply many opertaions to images: resize, rescale, rotate, ... To convert a file `graph.gif` to the PNG formart you may type `convert graph.gif graph.png` on a Unix command line. If you want to achive identical results from within *Octave* you have to use the system command.

```
Octave
system('convert graph.gif graph.png')
```

For these lecture notes I had to convert many EPS figures into the PDF format. For this I used the tool `epstopdf`, e.g. type `epstopdf graph.eps` on a Unix command line to generate the PDF file. If to be used within *Octave* use the `system()` command, as shown above.

1.4.3 Generating Histograms

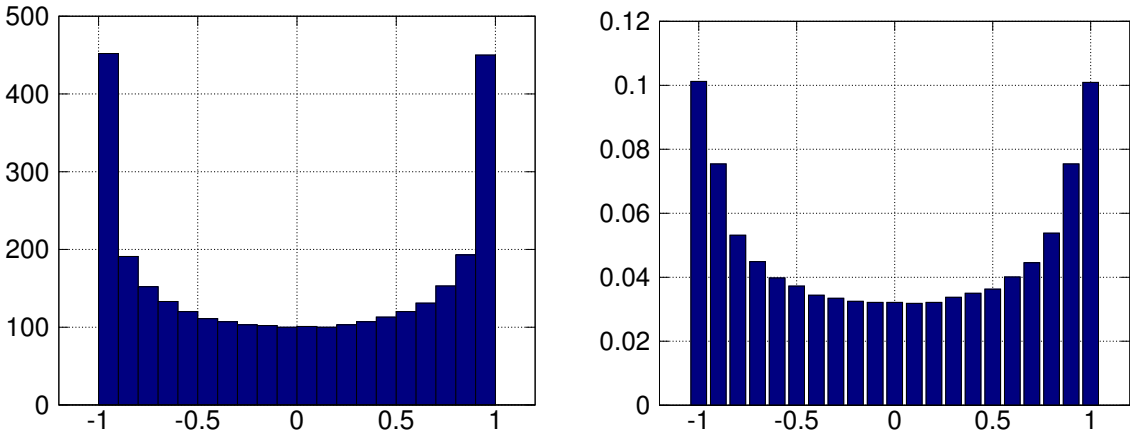
The command `hist()` will create a histogram of the values in the given vector. The following code and the resulting Figure 1.15 illustrate that the values around ± 1 are more likely to show up as results of the sin–function on $-5\,\pi \le x \le 5\,\pi$. The interval of all occurring values ($[-1\,,\,1]$) is divided up into subintervals of equal length. Then the command `hist(y,20)` counts the number of values in each subinterval and displays the result as height of the column. This leads to Figure 1.15(a). The histogram in Figure 1.15(b) is normalized, such that the sum of all heights equals 1 . Thus we can read of the probability for the values to fall into one of the bins. The values of the centers are in the vector `center` and the corresponding heights are stored in `height` and thus available for further computations. The resulting graph can also be generated by `bar(center,height)` or with `plot(center,height)`. Observe that the scaling has to be left to MATLAB/*Octave* by a call of `axis()` without arguments. The codes for *Octave* and MATLAB differ slightly and are shown below.

```
Octave
```

```
x = -5*pi:0.01:5*pi;    y = sin(x);
figure(1);
hist(y,20)
axis([-1.3  1.3]); % Matlab can not choose the x-scaling only

figure(2);
[height,center] = hist(y,-1:0.1:1,1)
height = height/sum(height);
bar(center,height);
axis([-1.2  1.2]);
```

Matlab

```
x = -5*pi:0.01:5*pi;   y = sin(x);
figure(1);
hist(y,20);
figure(2);
[height,center] = hist(y,-1:0.1:1);
height = height/sum(height);
bar(center,height)
axis([-1.1  1.1  0  0.15])
```



(a) counting histogram (b) normalized histogram

Figure 1.15: Histogram of the values of the sin–function

1.4.4 Generating 3-D Graphics

With *Octave* and MATLAB three dimensional plots can also be generated. A list of some of the commands is shown in Table 1.9.

Curves in space: `plot3()`

To examine a curve in space use the command `plot3()`. One may also plot multiple curves and choose styles, just as for the command `plot()` .

Octave

```
t = 0:0.1:5*pi;
x = cos(t);   y = 2*sin(t);   z = t/(2*pi);
plot3(x,y,z)
grid on
view(25,45);
```

plot commands	
`plot3()`	to plot a curve in space
`meshgrid()`	generate a mesh for a surface plot
`surf()`	generate a surface plot on a mesh
`surfc()`	generate a surface plot and contour lines
`mesh()`	generate a mesh plot on a mesh
`meshc()`	generate a mesh plot and contour lines
`contour()`	graph the contour lines on a surface
`quiver()`	generate a vector field
options and settings	
`view()`	set the viewing angles for 3d–plots
`caxis()`	choose the colormap and color scaling for the surfaces

Table 1.9: Generating 3D plots

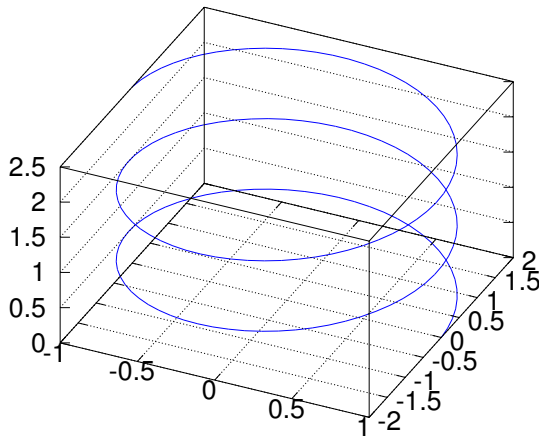


Figure 1.16: A spiral curve in space

A surface plot in space: `meshgrid()`, `surf()` **and** `mesh()`

If a surface of the type $z = f(x, y)$ in space is to be plotted then one has to apply a few steps.

- Choose the values for x and y.
- Generate matrices with values for the coordinates at each point on a mesh with the help of `meshgrid()`.
- Compute the values of the height at those points with the help of the given function $z = f(x, y)$.
- Generate the graphics with `surf()` or `mesh()` and choose a good view point and scaling.

To better understand the effect of the command `meshgrid` one may examine the result of

Octave

```
[xx,yy] = meshgrid(1:6,-1:3)
-->
xx =
   1   2   3   4   5   6
   1   2   3   4   5   6
   1   2   3   4   5   6
   1   2   3   4   5   6
   1   2   3   4   5   6

yy =
  -1  -1  -1  -1  -1  -1
   0   0   0   0   0   0
   1   1   1   1   1   1
   2   2   2   2   2   2
   3   3   3   3   3   3
```

To examine the surface generated by the function

$$z = f(x, y) = e^{-x^2-y^2} \quad \text{for} \quad -2 < x < 2 \quad \text{and} \quad -1 < y < 3$$

use the codes below to create Figure 1.17.

Octave

```
x = -2:0.1:2;  y = -1:0.1:3;
[xx,yy] = meshgrid(x,y);
zz = exp(-xx.^2-yy.^2);
mesh(xx,yy,zz)
grid on
view(120,40)
xlabel('x'); ylabel('y'); zlabel('height');
```

It is just as easy to draw contour lines of a given graph on a mesh.

Octave

```
figure(1)
clf
x = -2:0.1:2;  y = -1:0.1:2;  [xx,yy] = meshgrid(x,y);
zz = exp(-xx.^2-0.3*yy.^2);
axis('equal')
figure(2)
contour(xx,yy,zz,15)
```

Instead of a mesh, as show in Figure 1.17 we can create fully colored patches with the command `surf()`. Find the result on the left in Figure 1.19. For the graph we can also insist the the levels shown are between 0 and 1, with steps of 0.1 and we want the levels labeled, as shown on the right in Figure 1.19. We can modifiy the above code.

Octave

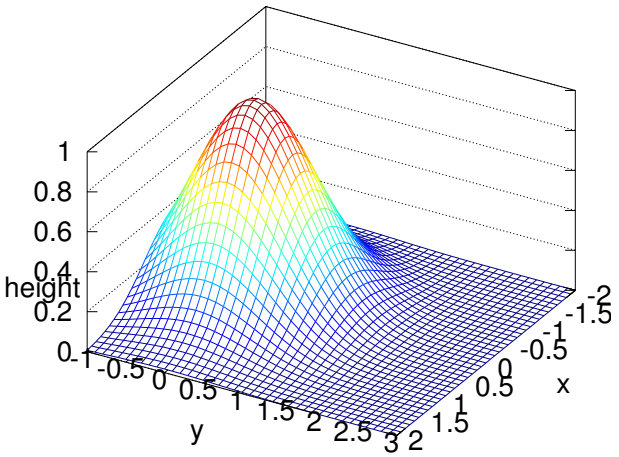


Figure 1.17: The surface $z = \exp(-x^2 - y^2)$

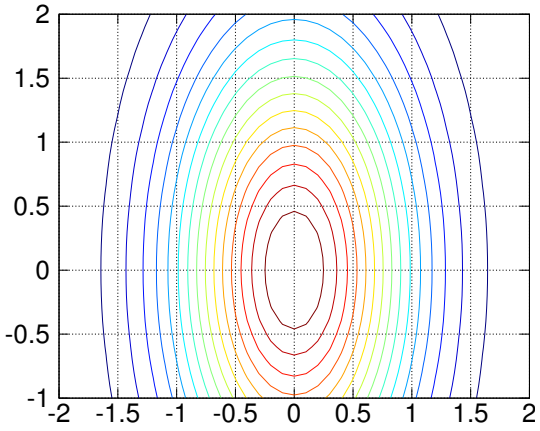


Figure 1.18: The contour lines of the function $z = \exp(-x^2 - 0.3\,y^2)$

```
x = -2:0.1:2;  y = -1:0.1:2;  [xx,yy] = meshgrid(x,y);
zz = exp(-xx.^2-0.3*yy.^2);
figure(3)
surf(xx,yy,exp(-xx.^2-yy.^2))
xlabel('x'); ylabel('y');zlabel('height')
figure(4)
cc = [0:0.1:1]                  % select the desired levels
[C,h] = contour(xx,yy,zz,cc);  % compute the level curves, no display
clabel(C,h,cc,'FontSize',10);  % display the level curves
xlabel('x'); ylabel('y');
```

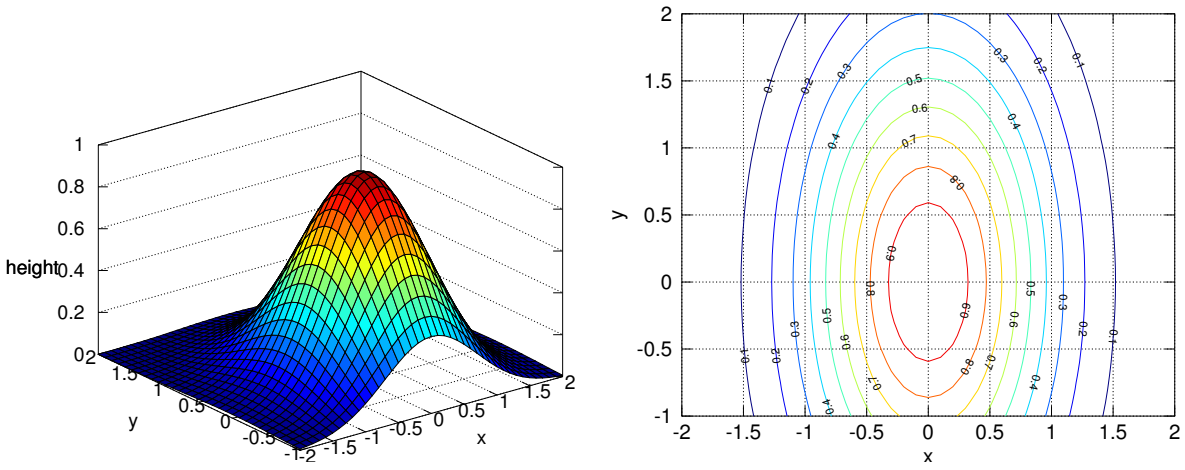


Figure 1.19: Two mofifications of the above figures

- With `mesh()` and `meshc()` only the lines connecting the points are drawn, no surface patches are used. Thus you can see through the surface.
- With `surf()` and `surfc()` the rectangles connecting the lines are filled with colored patches and thus you can not see through the surface.

The above structure of commands allows to examine rather involved surfaces. Any surface parametrized over a rectangle can be displayed. As an example we consider the torus in Figure 1.20. The torus is parametrized by the two angles u and v.

Octave

```
u1 = linspace(0,2*pi,51); v1 = linspace(pi/4,2*pi-pi/4,21);
[u,v] = meshgrid(u1,v1);
r0 = 4; r1 = 1;

x = cos(u).*(r0+r1*cos(v));
y = sin(u).*(r0+r1*cos(v));
z = r1*sin(v);
mesh(x,y,z)
```

Vector fields

Octave has commands to display vector fields. As an example we consider the planar vector field

$$\vec{F}(\vec{x}) = \begin{pmatrix} y \\ -x \end{pmatrix}$$

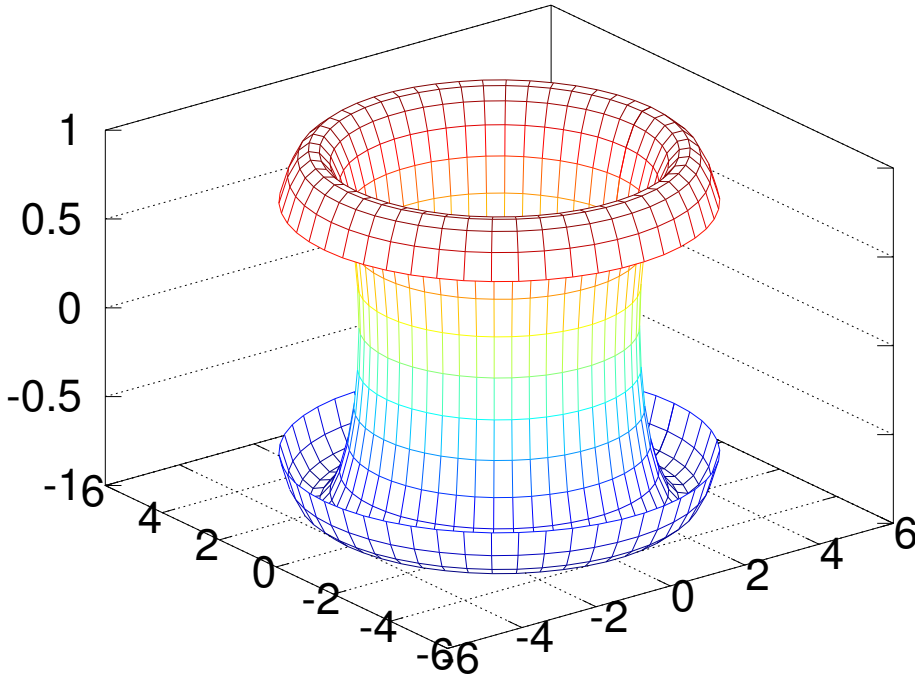


Figure 1.20: A general 3D surface

on the domain $-1 \leq x, y \leq 1.5$. Thus at a point $(x, y) \in \mathbb{R}^2$ we attach the vector $(y\,,\,-x)$. To display this vector field we have to generate a set of points $(x_i\,,\,y_i) \in \mathbb{R}^2$ at which the vectors are to be plotted. Then we construct a matrix $\mathbf{V}$ with the coordinates x_i and y_i in the first two columns. Columns 3 and 4 contain the components of the vectors at the given points. The obtain a good result the length of the vectors have to be scaled. Then the vectorfield is generated. Find the result in Figure 1.21.

Octave

```
xvec = -1:0.2:1.5; yvec = -1:0.2:1.5;
[x,y] = meshgrid(xvec,yvec);
x = x(:); y = y(:);  %%convert the matrix into a column vector.

scale = 0.1;
quiver(x,y,y,-x,scale)
```

Octave provides the command `peaks()` to generate a a nice, reasonably complicated surface. With the help of `gradient()` and `quiver()` we can also generate the gradient vector field belonging to that function.

Octave

```
[xx,yy,zz] = peaks;
figure(1);
meshc(xx,yy,zz);
figure(2);
contour(xx,yy,zz)
figure(3);
[Dx,Dy] = gradient(zz,yy(2)-yy(1));
quiver(xx,yy,Dx,Dy)
```

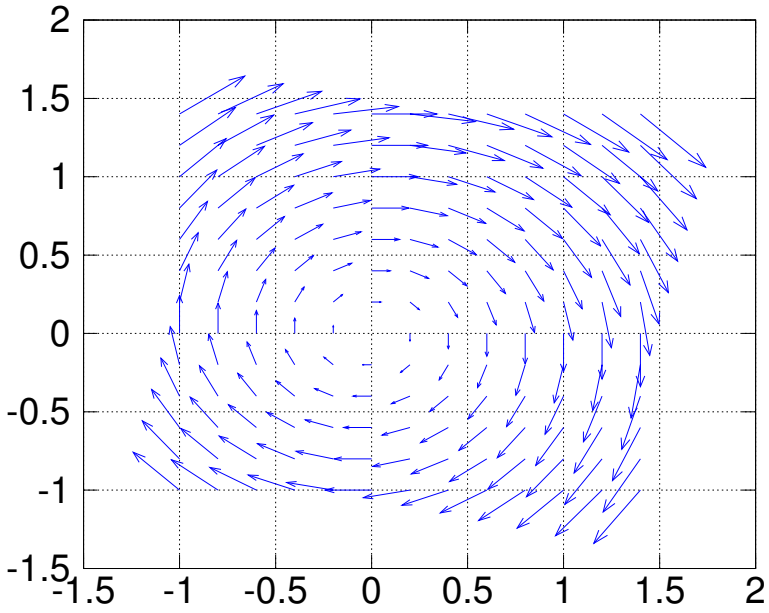


Figure 1.21: A vector field

1.5 Basic Image Processing

For the graphics commands there are some noticeable differences between MATLAB and *Octave*. Thus it is necessary to consult the corresponding help files to find the documentation. In addition there are many more options and possibilities than it is possible to illustrate in the given time and space for these notes.

1.5.1 First steps with images

Most of the information in this section is based on the image processing toolbox of *Octave* and you will need to install the toolbox and have access to its documentation.

Mathematically speaking an image is a matrix of number, or matrix of triples of numbers. If the image is represented by the $n \times m$ matrix M, then

- $M(1,1)$ contains the information about the pixel in the top left corner of the image.
- $M(1,10)$ contains the information about the tenth pixel in the top row of the image.
- $M(10,1)$ contains the information about the tenth pixel in the first column of the image.
- the vector $M(:,1)$ contains the information about all pixels in the first column of the image.

The information about each pixel can be given in different forms:

- For BW images each pixel is represented by 0 or 1, since the only two colors available are black and white.
- For grayscale images each pixel is represented by the level of gray, which can be of type `uint8`, `uint16` or `double` .
- For RGB images the intensity for each of the colors Red, Green and Blue is given by a number, which can be of type `uint8`, `uint16` or `double` .
- For **indexed** images each pixel is represented by the number of its color, i.e. an integer. Then you need the **colormap** with the translation of the number of the color to the actual color, usually given by RGB codes.

Indexed images require less memory and *Octave* uses the command `colormap()` to switch between the many colormaps (`autumn()`, `bone()`, `cool()`, `copper()`, `flag()`, `gray()`, `hot()`, `hsv()`, `jet()`, `ocean()`, `pink()`, `prism()`, `rainbow()`, `spring()`, `summer()`, `white()`, `winter()`, `contrast()`, `gpmap40()`). You can create your own colormap.

It is sometimes useful to change from one image format to another and *Octave* provides the commands:

- `rgb2gray()`: convert an RGB image to a gray scale image.
- `gray2ind()`: convert gray scale image to an index image
- `ind2gray()`: convert an indexed image to a gray scale image
- `ind2rgb()`: convert an indexed image to an RGB image
- There are more possible conversions and also the commands to detect of what type an image is. Consult the manuals.

Table 1.10 gives a very **incomplete** selection of commands related to image processing. It is essential to consult the available documentation. *Octave* and MATLAB provide basic commands and data structures to implement image processing operations efficiently. There are also many more resources on image processing with *Octave* and MATLAB on the internet, e.g.

- www.csse.uwa.edu.au/~pk/Research/MatlabFns/
- www.irit.fr/PERSONNEL/SAMOVA/joly/Teaching/M2IRR/IRR05/index.html

commands for images	
imshow()	display image
image()	display a matrix as image
imagesc()	scale image and display
imfinfo()	obtain information about an image in a file
imread()	load an image from a file
imwrite()	write an image to a file
loadimage()	load an image from a file
saveimage()	write an image to a file
colormap()	return or set the colormap
rgb2gray()	convert RGB to gray scale image
rgb2ind()	convert an RGB image to an indexed image
ind2gray()	convert indexed image to gray scale image
gray2ind()	convert a gray scale image to an indexed image
imresize()	change the size of an image
imrotate()	rotate an image matrix
fspecial()	create filters for image processing
imfilter()	apply an image filter
imsmooth()	smooth an image with different algorithms
imshear()	shear an image
edge()	use a selection of edge detection algorithms
conv(), conv2()	convolution, one and two dimensional
fft2(), ifft2()	2D Fast Fourier Transforms

Table 1.10: Image commands

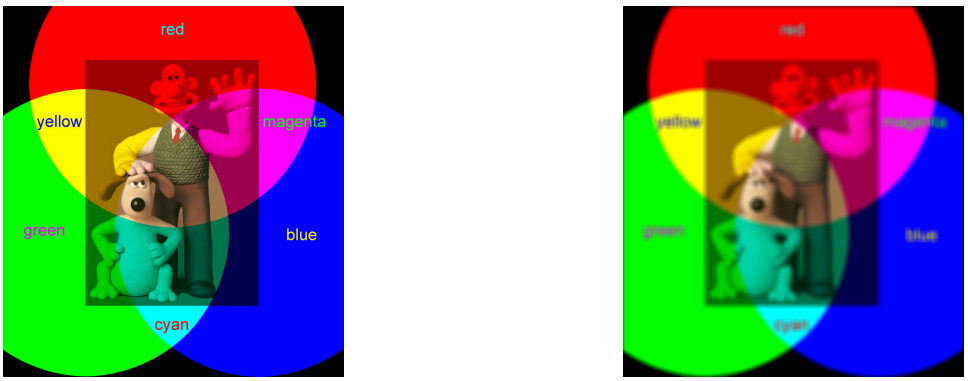
22 Example : RGB, grayscale

A picture WallaceGromit.png in the PNG (portable network graphics) is loaded into *Octave* and imfinfo() displays all available information on the image. It is an image of size 724×666 and each pixel (picture element) consists of three colors (RGB), encoded by an integer between 0 and 255. Thus the "matrix" im in the code below is of size $724 \times 622 \times 3$ and the image is shown in Figure 1.22(a).

Octave

```
imfinfo('WallaceGromit.png')        % show information on the file
im = imread('WallaceGromit.png');   % load the file
size(im)
figure(1)
imshow(im)                          % display the original picture
```

The image can be converted to a grayscale image with the help of rgb2gray() and then displayed. Each color in RGB can be displayed independently, where a white spot indicates a high intensity of this



(a) original image (b) after an averaging filter

Figure 1.22: Wallace and Gromit, original and with an averaging filter applied

color. Find the results in Figure 1.23.

Octave

```
imGray = rgb2gray(im);
imR = im(:,:,1); imG = im(:,:,2); imB = im(:,:,3);
figure(2)
subplot(2,2,1); imshow(imGray)
subplot(2,2,2); imshow(imR)
subplot(2,2,3); imshow(imG)
subplot(2,2,4); imshow(imB)
```

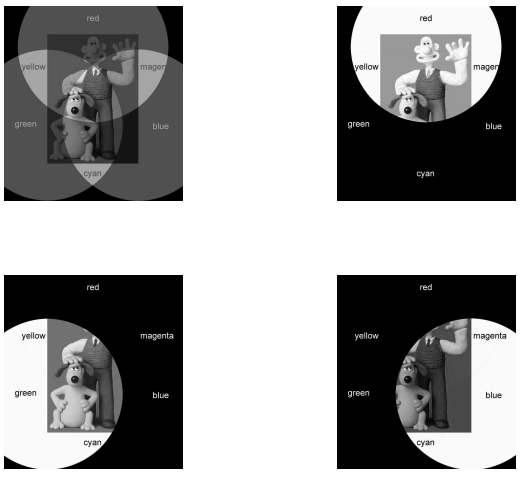


Figure 1.23: Wallace and Gromit, as grayscale and R, G and B images

With the above code all pictures are displayed as gray-scale pictures, since we provide a single intensity level as information. If you need color after all you can use a colormap. To display the red component above as a red picture use

Octave

```
redmap = zeros(256,3);              % fill the colormap with zeros
redmap(:,1) = linspace(0,1,255);    % put numbers in the first (red) column
figure(3)
imshow(imR,redmap)                  % display the image with the red colormap
```

The image processing toolbox in *Octave* contains many and powerful commands for image processing. As an elementary example we consider a filter to replace the values at each pixel with the average values of its neighbors. The result in Figure 1.22(b) is a smeared out version of the original image 1.22(a).

Octave

```
F = fspecial("average", 12);
imFilter = imfilter(im, F);
figure(3)
imshow(imFilter)
```

♢

23 Example : Edge Detection

This is a first example of edge detection, using the command provided by the SourceForge package. More information is given in a latter example. For a gray-scale image we

1. read some information about the picture, using the command `imfinfo()`.
2. load the image in *Octave* and display it on screen, using `imread()` and `imshow()`.
3. then use one of the many edge detection parameters to hopefully find all edges of the objects displayed.
4. finally we display the image with the edges only.

Find the result of the commands below in the left half of Figure 1.24.

Octave

```
imfinfo('shapessm.jpg')         % show information on the file
im = imread('shapessm.jpg');    % load the file
figure(1)
imshow(im)                      % display the original picture
edgeim = edge(im,'Canny');      % run one of the possible edge detections
figure(2)
imshow(edgeim)                  % display the picture with edges only
```

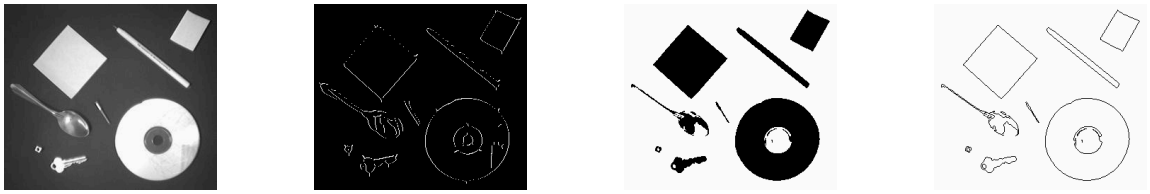


Figure 1.24: A grayscale and BW picture and edge detection

Since the sections in the original picture are either very dark, or very bright, we may convert the gray scale image into a BW (black and white) picture and try another edge detection. This might get rid of some artifacts. Find the result of the commands below in the right half of Figure 1.24. To not obtain black blobs on paper the roles of black an white are inverted by displaying `1-imbw` instead of the BW image.

Octave

```
imbw = im2bw(im,0.5);          % convert to a bw picture (0 and 1 only)
figure(3)
imshow(1-imbw)
edgeimbw = bwborder(imbw);     % run one of the possible edge detections
figure(4)
imshow(1-edgeimbw)             % display the picture with edges only
```

♢

24 Example : Filtering with FFT

Using FFT we can write an image as sum of periodic signal with different frequencies. Then we can filter high or low frequencies. As an example we examine the image in Figure 1.26. First load the image, convert it to a grayscale image and display the result.

Octave

```
imfinfo("Lenna.jpg")
im = imread("Lenna.jpg");
imG = rgb2gray(im);  % convert to a grayscale image
figure(1)
imshow(imG)          % display the result
```

Then we apply the two dimensional FFT with the help of the command `fft2()` and choose the number of frequencies to keep by `n=40` . This corresponds to a perfect low-pass filter. Due to the symmetries in the FFT of real valued signals and images we have to keep the lowest n frequencies **and** the highest $n-1$ frequencies and thus 4 blocks of the FFT of the image are copied into the FFT of the filtered image. This algorithm is visualized in Figure 1.25. Observe that the code below uses block operations instead of multiple loops. This is for speed reasons.

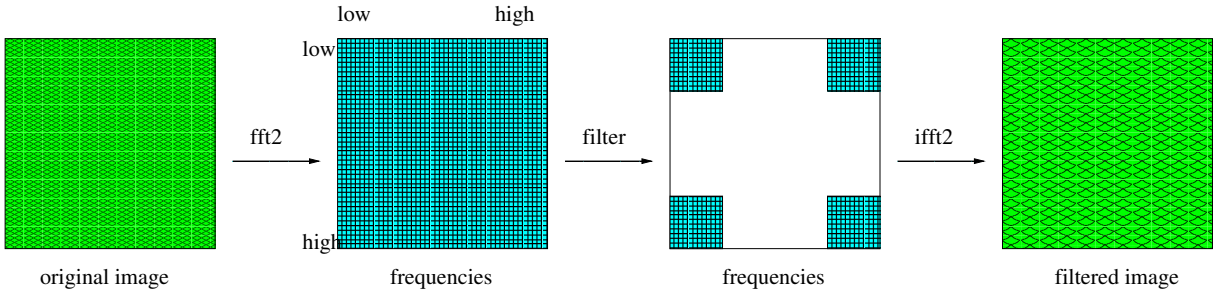


Figure 1.25: Apply a low pass filter to an image, based on FFT

Octave

```
imFFT = fft2(im2double(imG));  % convert to floating numbers and apply FFT
n = 40                         % number of frequencies to keep
[nx,ny] = size(imFFT)          % size of the image, and FFT
imFilter = zeros(nx,ny);       % zero matrix
imFilter(1:n+1,1:n+1) += imFFT(1:n+1,1:n+1);           % block top left
imFilter(1:n+1,ny-n+1:ny) += imFFT(1:n+1,ny-n+1:ny);   % block top right
imFilter(nx-n+1:nx,1:n+1) += imFFT(nx-n+1:nx,1:n+1);   % block bottom left
imFilter(nx-n+1:nx,ny-n+1:ny) += imFFT(nx-n+1:nx,ny-n+1:ny); % block bottom right
```

Finally we apply the inverse FFT by `ifft2()` and keep the real part only. Then we display the filtered image, as shown in Figure 1.26(b).

Octave

```
newIm = real(ifft2(imFilter));        % apply inverse FFT
figure(2)
imshow(newIm)                         % display the filtered image
imwrite(newIm,'LennaFiltered.png');   % save the filtered image
```

(a) original image

(b) with low pass filter

Figure 1.26: Original image of Lenna, and with a lowpass filter by FFT

♢

1.5.2 Image Processing and Vectorization, Edge Detection

25 Example : Adding Noise to a Picture

The main purpose of this example is to illustrate the power of vectorized code. We start with the Lena picture in Figure 1.26(a). Each pixel of the picture is represented by an integer value between 0 and 255 . We add some noise to this picture by adding a random number, generated by a normal distribution with average 0 and a standard deviation given by `NoiseAmp=20` . The code below applies this idea with a double loop.

Octave

```
im  = imread("Lenna.jpg");
imG = rgb2gray(im);  % convert to a grayscale image
figure(1)
imshow(imG)          % display the result

[Nlines,Ncols] = size(imG);  % compute the size of the picture
NoiseAmp = 20;               % amplitude of noise
newIm = imG;                 % copy the image

t0 = cputime();
for lin = 1:Nlines           % loop over al rows
  for col = 1:Ncols          % loop over al columns
    newIm(col,lin) += NoiseAmp*randn(1);  % add noise to the pixel
  endfor
endfor
timingLoop = cputime()-t0
figure(2); imshow(newIm)
```

A sample run took 32 seconds and produced the expected, noisy result. The same algorithm can be applied using vectorized code, getting rid of the loops. Generate a matrix of random numbers with one command (`NoiseAmp*randn(Ncols,Nlines)`) and add it to the original matrix.

Octave

```
t0 = cputime();
newIm2 = imG + NoiseAmp*randn(Ncols,Nlines);
timingVectorized = cputime()-t0
figure(3); imshow(newIm2)
```

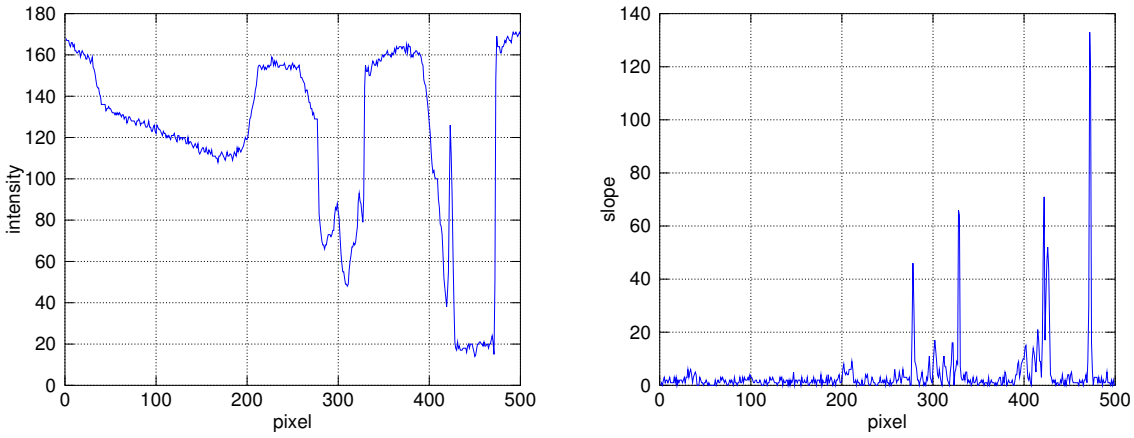
This code only used 0.048 sec of CPU time, i.e. the code is 670 times faster. ♢

26 Example : Edge detection

In many application the first step of image processing is edge detection, e.g. to identify objects. As example consider Figure 1.27 and the goal is to mark the edges of the different objects.

Figure 1.27: A few objects, for edge detection

- **The basic idea**
  We illustrate the basic idea by analyzing one line in the picture. The size of the picture is 350×500 and we pick a horizontal line, cutting through the Pritt stick and the pocket knife. The darker sections correspond to lower values on in Figure 1.28(a).



(a) intensity (b) absolute value of the derivative

Figure 1.28: Intensity along a horizontal line through the objects

The basic idea of an edge detection is to look for steep slopes in the above graph. Based on the definition of the derivative we examine

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2\,h}$$

For the discrete values $u(k)$ of the intensity we define

$$\text{edge}(k) = -u(k-1) + u(k+1) \quad \text{for} \quad 2 \le k \le n-1$$

or with *Octave*

Octave

```
imRaw = imread('Edgetest.png');
figure(1); imshow(imRaw);
hold("on")
plot([1,500],[200,200],"r");

test_line = double(imRaw(200,:)); % pick one line to be examined
                                  % convert to data type double
figure(2)
plot(test_line)
xlabel('pixel'); ylabel('intensity')

n = length(test_line);
edge = zeros(1,n);
for k = 2:n-1
  edge(k) = -test_line(k-1)+test_line(k+1);
endfor
figure(3)
plot(abs(edge))
xlabel('pixel'); ylabel('slope')
```

This leads to Figure 1.28(b). Now we can choose a cutoff level, e.g. 40, to decide where we see an edge. This will point towards four points sitting on an edge in Figure 1.27, which is visually confirmed by scanning along the thin horizontal line in that figure.

The above implementation uses a `for...endfor` loop, which can be replaced by a vector operation, mainly for speed reasons.

Octave

```
edge = [0 , -test_line(1:n-2) + test_line(3:n) , 0];
```

The above can also be considered as a convolution of the vector of the intensity values along the line to be examined with the vector[12]

-1	0	1

- **Detecting horizontal edges**
  The above idea has to be carried over to the full image. We replace the vector by the 3 matrix

-1	0	1
-2	0	2
-1	0	1

[12] Check you math lecture notes for the definition of convolution, either in the chapter on Laplace or Fourier transforms.

This corresponds to a weighted average of the slopes in three lines. To apply the procedure to the matrix

$$\mathbf{A} = \begin{bmatrix} 1 & 11 & 11 & 1 & 1 & 1 \\ 2 & 12 & 12 & 2 & 2 & 2 \\ 3 & 13 & 13 & 3 & 3 & 3 \\ 4 & 14 & 14 & 3 & 3 & 3 \\ 5 & 15 & 15 & 3 & 3 & 3 \\ 6 & 16 & 16 & 3 & 3 & 3 \end{bmatrix}$$

we proceed as follows:

1. Put the central element of the 3×3 filter matrix over one entry in the matrix $\mathbf{A}$.
2. Multiply and add the overlapping numbers.
3. Put the result in the new, filtered matrix.

Let us examine a few examples:

- In the second row and second column we obtain

$$b_{2,2} = \left\{ \begin{array}{ccccc} +(-1)\cdot 1 & + & (0)\cdot 11 & + & (1)\cdot 11 \\ +(-2)\cdot 2 & + & (0)\cdot 12 & + & (2)\cdot 12 \\ +(-1)\cdot 3 & + & (0)\cdot 13 & + & (1)\cdot 13 \end{array} \right\} = 30$$

  This indicatetes an edge with positive slope.

- In the second row and fourth column we obtain

$$b_{2,4} = \left\{ \begin{array}{ccccc} +(-1)\cdot 11 & + & (0)\cdot 1 & + & (1)\cdot 1 \\ +(-2)\cdot 12 & + & (0)\cdot 1 & + & (2)\cdot 2 \\ +(-1)\cdot 13 & + & (0)\cdot 1 & + & (1)\cdot 3 \end{array} \right\} = -30$$

  This indicatetes an edge with negative slope.

- In the second row and fifth column we obtain

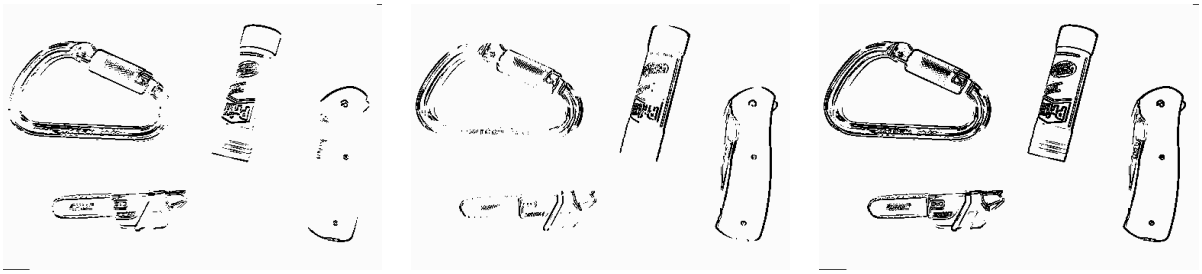
$$b_{2,3} = \left\{ \begin{array}{ccccc} +(-1)\cdot 1 & + & (0)\cdot 1 & + & (1)\cdot 1 \\ +(-2)\cdot 2 & + & (0)\cdot 2 & + & (2)\cdot 2 \\ +(-1)\cdot 3 & + & (0)\cdot 3 & + & (1)\cdot 3 \end{array} \right\} = 0$$

  This indicates no edge.

We implement this directly by matrix operations and apply it to the given image. Observe the code without loops, leading to fast computations. Since the x coordinate corresponds to vertical lines, we detect horizontal edges.

Octave

```
[nx,ny] = size(imRaw);      % size of picture
ix = 2:nx-1; iy =  2:ny-1; % indices, unshifted
imRaw = double(imRaw);
Gx = -1*imRaw(ix-1,iy-1) + 1*imRaw(ix+1,iy-1)...
     -2*imRaw(ix-1,iy  ) + 2*imRaw(ix+1,iy  )...
     -1*imRaw(ix-1,iy+1) + 1*imRaw(ix+1,iy+1);

edgeLevel = 100;  % choose the detection level
imshow(1-(abs(Gx)>edgeLevel))
```



(a) horizontal (b) vertical (c) combined

Figure 1.29: Sobel edge detection

Find the result on in Figure 1.29(a). Observe that we only marked horizontal edges. The obvious vertical edges in the original image are not detected.

- **Detecting vertical edges**
  For vertical edges we apply a similar procedure, but use the matrix

$+1$	$+2$	$+1$
0	0	0
-1	-2	-1

  and use the code

Octave
```
Gy = +1*imRaw(ix-1,iy-1) + 2*imRaw(ix,iy-1) + 1*imRaw(ix+1,iy-1)...
     -1*imRaw(ix-1,iy+1) - 2*imRaw(ix,iy+1) - 1*imRaw(ix+1,iy+1);
```

  leading to the result in Figure 1.29(b).

- **Combining horizontal and vertical edges**
  Now we combine the two basic detection algorithms, leading to Figure 1.29(c). We finally see all edges.

Octave
```
imshow(1-((sqrt(Gx.^2+Gy.^2))>edgeLevel))
```

- **The function** `edge()`
  The image package has a built in function `edge()`,which can be used to apply the Sobel edge detection algorithm, leading to Figure 1.30. The function `edge()` allow to use a few other filters for edge detection, e.g. Sobel, Prewitt, Roberts, Canny, ... All those algorithms are using the above idea, with different filter matrices. Examine the result of `help edge` or the source code of `edge.m` to find out more.

Octave
```
imSobel = edge(uint8(imRaw),'Sobel');
imshow(1-imSobel)
```

♢

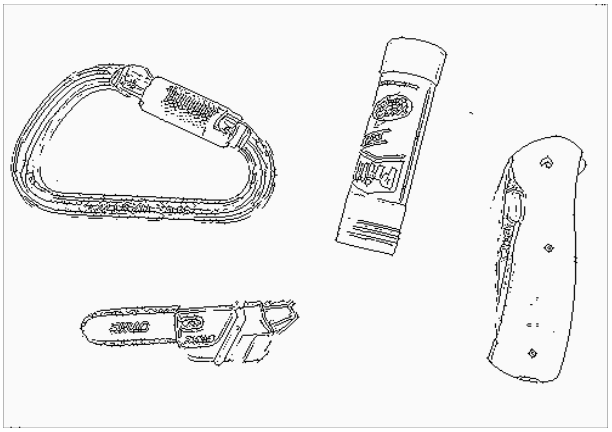


Figure 1.30: Result of a Sobel edge detection

27 Example : Observations on edge detection
The above idea can be modified in many different ways.

- We may use other filters, e.g. the matrices

+3	0	−3
+10	0	−10
+3	0	−3

and

+3	+10	+3
0	0	0
−3	−10	−3

  Since the above filter operations can be written as convolution, we can use the command `conv2()` in *Octave* to apply the edge detection filters. Particular attention has to be paid to the behavior of the convolution at the boundary of the images, consult the documentation on `conv()` and `conv2()`. This leads to very efficient code and Figure 1.31(a) as result.

Octave
```
imRaw = imread('Edgetest.png');

Sx = single([ 3 0 -3 ; 10 0 -10 ; 3 0 -3 ]);
Sy = single([ 3 10 3 ; 0 0 0 ; -3 -10 -3 ]);

imRawEdge = sqrt(conv2(imRaw,Sx).^2 + conv2(imRaw,Sy).^2);
figure(2)
imshow(1-(imRawEdge>250))
```

- The above fails miserably if noise is added, as can be seen in Figure 1.31(b). Our eye and brain can still see the real edges, but the code does not.

Octave
```
[n,m] = size(imRaw);
imNoise = imRaw + 10*randn(n,m);
figure(3); imshow(imNoiseEdge)

imNoiseEdge = sqrt(conv2(imNoise,Sx).^2 + conv2(imNoise,Sy).^2);
figure(4); imshow(1-(imNoiseEdge>250))
```

- The effect of noise can sometimes be controlled by an averaging filter. The value at one pixel is replaced by a weighted average of points close to this pixel. To average over a 5×5 section we can

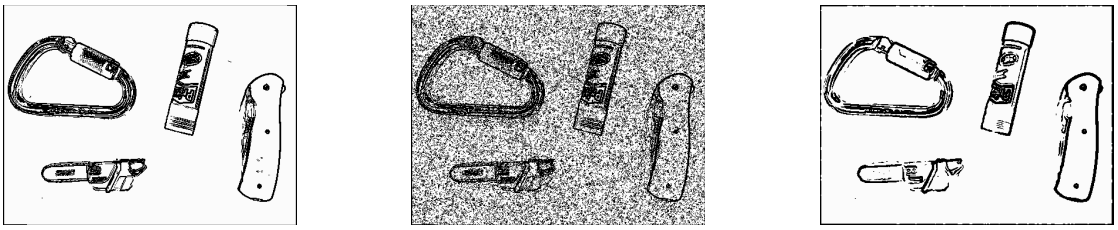
(many other options are possible) use the matrix

$$\mathbf{A} = \frac{1}{m}\begin{bmatrix} 1 & 3 & 6 & 3 & 1 \\ 3 & 8 & 10 & 8 & 3 \\ 6 & 10 & 12 & 10 & 6 \\ 3 & 8 & 10 & 8 & 3 \\ 1 & 3 & 6 & 3 & 1 \end{bmatrix}$$

where m is chosen such that the sum of all values in $\mathbf{A}$ equals 1 . This assures that an image with constant intensity in not modified. Use a convolution of the noisy image matrix with this averaging matrix to generate a new picture. Now we can detect the edges in a noisy image, as seen in Figure 1.31(c).

Octave

```
AvgMat = [1 3 6 3 1; 3 8 10 8 3;6 10 12 10 6; 3 8 10 8 3; 1 3 6 3 1];
AvgMat = AvgMat/sum(AvgMat(:));
imNoiseAvg = conv2(imNoiseEdge,AvgMat,'same');

imNoiseAvgEdge = sqrt(conv2(imNoiseAvg,Sx).^2 + conv2(imNoiseAvg,Sy).^2);
figure(5); imshow(1-(imNoiseAvgEdge>250))
```



(a) without noise (b) with noise (c) with noise and averaging filter

Figure 1.31: Edge detection, using a different filter

♢

28 Example : Filters can also be applied directly with the help of the commands `fspecial()` and `imfilter()`. As an example we try to detect edges in the Wallace and Gromit picture.

GromitEdge.m

```
im = imread ('WallaceGromit.png');
imH = imfilter(im,fspecial('Sobel') ,'replicate');
imV = imfilter(im,fspecial('Sobel')','replicate');

figure(11)
subplot(1,3,1); imshow(im);
subplot(1,3,2); imshow(imH);
subplot(1,3,3); imshow(imV);
```

♢

1.6 Ordinary Differential Equations

From your class on Engineering Mathematics or Ordinary Differential Equations you should have some basics knowledge and suitable examples for fixed step size algorithms, e.g. Euler, Heun and Runge-Kutta. Thus we concentrate on the usage of the *Octave* commands to solve differential equations. It is assumed that you are familiar with the theoretical aspects of ODEs (Ordinary Differential Equations).

For a given, smooth function $f(x,t)$ and given initial time t_o and initial values x_0 the initial value problem

$$\frac{d}{d\,t}\,x(t) = f(x(t),t) \quad \text{with} \quad x(t_0 = x_0)$$

has exactly one solution, a function $x(t)$. One can attempt to find a solution, by analytical or numerical methods. *Octave* and `MATLAB` use numerical methods to determine solutions of differential equations. In this section we present a few basic ideas:

1. With *Octave* use `lsode()` to solve a single ODE or a system. We use the Volterra-Lotka model as an example.
2. Show how to use the option provided by `lsode.m`.
3. Examine how to use `C++` code within *Octave* to improve the speed.
4. Examine how to perform further calculations with solutions of ODEs. We examine the period of a Volterra-Lotka solution.
5. Examine the functions provided by the ODE package on Octave-Forge.
6. To close the section a code from your authors lecture notes is examined.

Unfortunately `MATLAB` and *Octave* (resp. `lsode()`) show a minor, but annoying difference, as pointed out in subsection 1.6.5 on page 99. `MATLAB` does not provide the command `lsode()`, you are restricted to `ode45()` and its friends.

1.6.1 Using `lsode()` to solve systems of ordinary differential equations

Octave provides the standard command `lsode()` to solve ordinary differential equations. Find two carefully worked out examples, the first for a single differential equation, the second for a system.

29 Example : Logistic equation
As a first example we consider the equation

$$\frac{d}{dt}\,x(t) = x(t) - x(t)^2 \quad \text{with} \quad x(0) = 0.2$$

To find a numerical solution we have to provide *Octave* with a function describing the function $f(x,t) = x - x^2$, the initial time and value and the times at which we want to know the solution.

Octave

```
%% script file to solve a logistic differential equation
x0 = 0.2;  % initial value
t0 = 0;    % initial time
Tend = 10; % time interval for which solution has to be computed
n = 50;    % number of intermediate times

%% define the function describing the right hand side
function y = logF(x,t)
  y = x-x.*x ;
```

```
endfunction

% generate vector with the times at which solution is desired
T = t0+linspace(0,Tend,n);
```

Then a simple call of the function `lsode()` yields the desired solution and we may plot a single or multiple solutions, as shown in Figure 1.32.

Octave

```
X = lsode('logF', x0, T);

plot(T,X)
axis([0,Tend,0,1]); grid on

X2 = lsode('logF', 2*x0, T);
X3 = lsode('logF', 0.2*x0, T);

plot(T,[X X2 X3])
xlabel('time t'); ylabel('population'); grid on
```

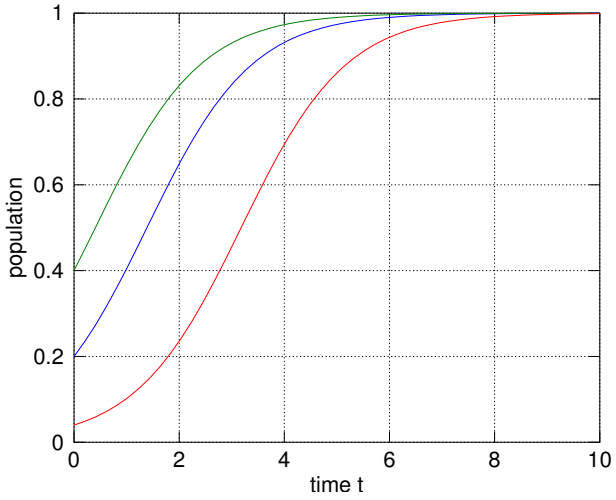


Figure 1.32: Some solutions of the logistic differential equation

♢

The above code may easily be adapted to solve systems of ODEs, as illustrated by the Volterra-Lotka simulation.

30 Example : Volterra-Lotka model

Consider two different species with the size of their population given by $x(t)$ and $y(t)$. The predators y (e.g. sharks) are feeding of the pray x (e.g. small fish). The food supply for the pray is limited by the environment.

$x(t)$ population size of pray at time t

$y(t)$ population size of predator at time t

The behavior of these two populations can be described by a system of first order differential equations.

$$\begin{aligned} \dot{x}(t) &= (c_1 - c_2\, y(t))\, x(t) \\ \dot{y}(t) &= (c_3\, x(t) - c_4)\, y(t) \end{aligned}$$

where c_i are positive constants. This function can be implementd in a function file `VolterraLotka.m` in *Octave*.

VolterraLotka.m

```
function res = VolterraLotka(x,t)
  c1 = 1; c2 = 2; c3 = 1; c4 = 1;
  res = [(c1-c2*x(2))*x(1);
         (c3*x(1)-c4)*x(2)];
endfunction
```

With the help of the above function we can creat a vector field plot for this system of two differential equations. Find the result as vector field in Figure 1.33.

Octave

```
x = 0:0.2:2.6;  % define the x values to be examined
y = 0:0.2:2.0;  % define the y values to be examined

n  = length(x);  m  = length(y);
Vx = zeros(n,m); Vy = Vx; % create zero vectors for the vector field

for i = 1:n
  for j = 1:m
    v = VolterraLotka([x(i),y(j)],0); % compute the vector
    Vx(i,j) = v(1); Vy(i,j) = v(2);
  endfor
endfor

figure(1);
quiver(x,y,Vx',Vy',3);
axis([min(x),max(x),min(y),max(y)]);
grid on; xlabel('prey'); ylabel('predator');
```

Again using the above defined function `VolterraLotka` we can solve the differential equation for times $0 \leq t \leq 15$ with the initial conditions $x(0) = 2$ and $y(0) = 1$. In the code below we choose to use 100 different values for the time t to display the solution. Observe that the algorithm `lsode()` internally uses considerably more points.

Octave

```
t  = linspace(0,15,100);
XY = lsode('VolterraLotka',[2,1],t);
```

The resulting solution can now be used to visualize the solution.

- Find the size of the two populations as function of time on the left in Figure 1.33. One observes that the solution might be periodic, with a period of $T \approx 7$.
- Find the size of the two populations directly on the right in Figure 1.33, together with the corresponding vector field. The periodicity of the solution is confirmed.

Octave

```
figure(2);
plot(t,XY)
xlabel('time'); legend('prey','predator'); axis([0,15,0,3]); grid on

figure(3);
plot(XY(:,1),XY(:,2));
axis([min(x),max(x),min(y),max(y)]); hold on
quiver(x,y,Vx',Vy',2);
grid on; xlabel('prey'); ylabel('predator'); hold off
```

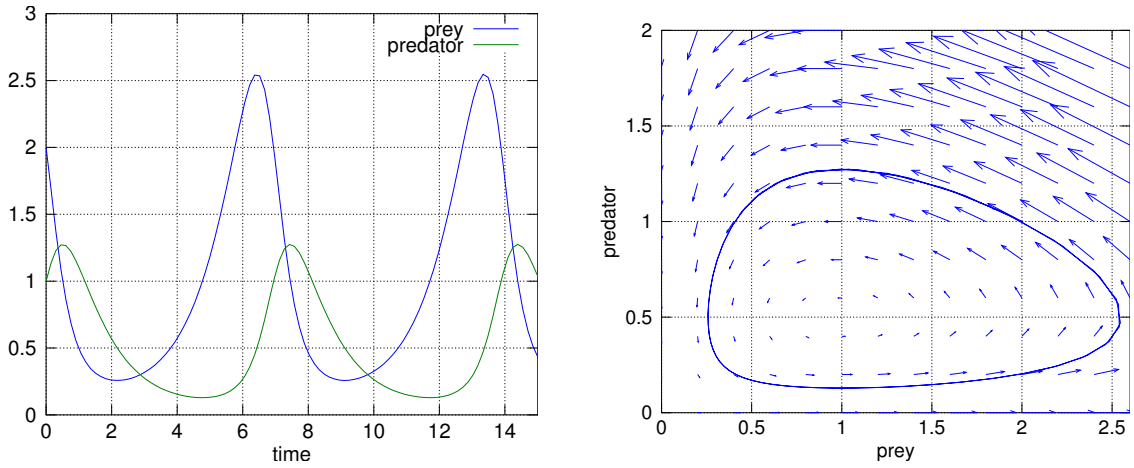


Figure 1.33: One solution and the vector field for the Volterra-Lotka problem

♢

31 Example : Converting a second order problem to a system of first order differential equations
A second order differential equation for one dependent variable $x(t)$ can always be transformed into a system of two differential equations of order one. We illustrate this with an example. The equation

$$\ddot{x}(t) + \alpha\,\dot{x}(t) + k\,x(t) = f(t)$$

might be generated by a mass attached to a spring with an additional damping term $\alpha\,\dot{x}$. We introduce the new variables

$$y_1(t) = x(t) \quad \text{and} \quad y_2(t) = \dot{x}(t)$$

This leads to

$$\frac{d}{dt}\,y_1(t) = \dot{x}(t) = y_2(t)$$

and

$$\frac{d}{dt}\,y_2(t) = \frac{d}{dt}\,\dot{x}(t) = \ddot{x}(t) = f(t) - \alpha\,\dot{x}(t) - k\,x(t) = f(t) - \alpha\,y_2(t)(t) - k\,y_1(t)$$

This can be written as a system of first order equations

$$\frac{d}{dt}\begin{pmatrix} y_1(t) \\ y_2(t) \end{pmatrix} = \begin{pmatrix} \dot{y}_1(t) \\ \dot{y}_2(t) \end{pmatrix} = \begin{pmatrix} y_2(t) \\ f(t) - k\,y_1(t) - \alpha\,y_2(t)(t) \end{pmatrix}$$

or

$$\frac{d}{dt}\,\vec{y}(t) = \vec{F}(\vec{y}(t))$$

and with the help of a function file the problem can be solved with computations very similar to the above Volterra-Lotka example. The code below will compute a solution with the initial conditions $x(0) = 0$ and $\dot{x}(0) = 1$. Then the Figure 1.34 will be generated.

Octave

```
y = -1:0.2:1;
v = -1:0.2:1;

n = length(y); m = length(v);
Vx = zeros(n,m); Vy = Vx; % create zero vectors for the vector field

function ydot = Spring(y,t)
  ydot = zeros(size(y));
  k = 1; al = 0.1;
  ydot(1) = y(2);
  ydot(2) = -k*y(1)-al*y(2);
endfunction

for i = 1:n
  for j =1 :m
    z = Spring([y(i),v(j)],0);       % compute the vector
    Vx(i,j) = z(1); Vy(i,j) = z(2); % store the components
  endfor
endfor

t = linspace(0,25,100);
XY = lsode('Spring',[0,1],t);

figure(1);
plot(t,XY)
xlabel('time'); legend('position','velocity')
axis(); grid on
```

To generate the vector field on the left in Figure 1.34 use the command `quiver()`.

Octave

```
figure(2);
plot(XY(:,1),XY(:,2));              % plot solution in phase portrait
axis([min(y),max(y),min(v),max(v)]);
hold on
quiver(y,v,Vx',Vy');
xlabel('position'); ylabel('velocity');
grid on; hold off
```

In the left part of Figure 1.34 find the vector field and the computed solution. The horizontal axis represents the displacement x and the vertical axis indicates the velocity $v = \dot{x}$. In the right part find the graphs of $x(t)$ and $v(t)$ as function of the time t. The effect of the damping term $-\alpha\, v(t) = -0.1\, v(t)$ is clearly visible. ♢

1.6.2 Options of `lsode`

The algorithms used by the command `lsode()` (Livermore Solver for Ordinary Differential Equations) were developed by Alan Hindmarsh [Hind93]. The code in *Octave* allows to set many options:

- integration method (Adams, stiff, bdf)
- absolute tolerance
- relative tolerance
- initial step size
- minimal and maximal step size

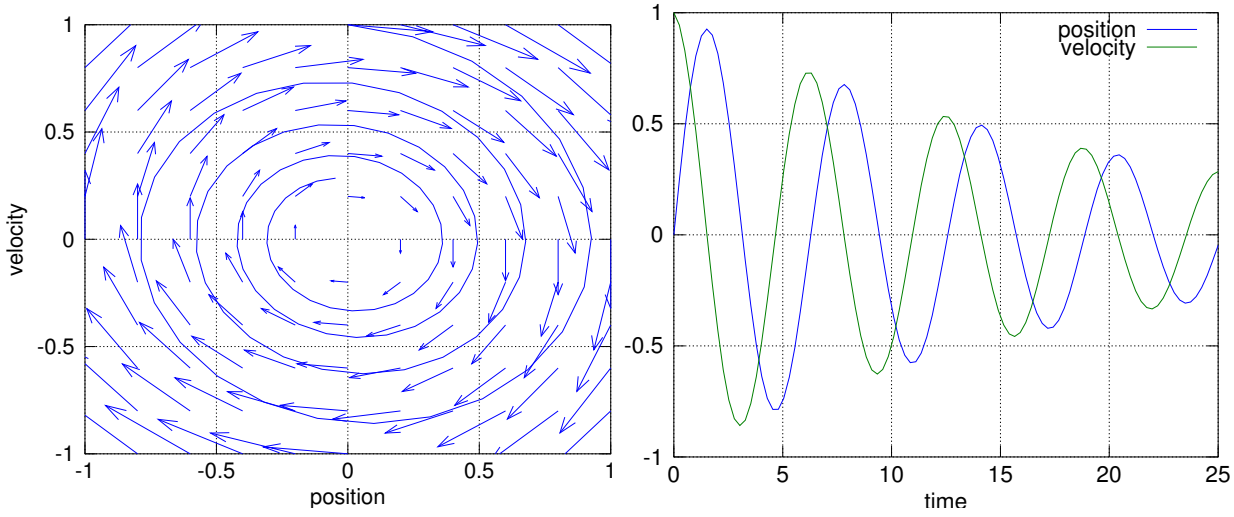


Figure 1.34: Vector field and a solution and for a spring-mass problem

This is done by the command `lsode_options()`. If called without arguments the current values will be returned, e.g.

Octave

```
lsode_options()
—>
Options for LSODE include:

  keyword                                value
  ———————                                ———————
  absolute tolerance                     1.49012e−08
  relative tolerance                     1.49012e−08
  integration method                     stiff
  initial step size                      −1
  maximum order                          −1
  maximum step size                      −1
  minimum step size                      0
  step limit                             100000
```

Find more documentation in the on-line manual. As an example we might ask for more an abolute and relative tolerance of 10^{-10} by

Octave

```
lsode_options("relative tolerance",1e−10)
lsode_options("absolute tolerance",1e−10)
```

Solving the above differential equations will now require more computation time.

1.6.3 Using C++ code to speed up computations

When solving a differential equation $\dot{x}(t) = \vec{F}(\vec{x}(t))$ numerically the function $\vec{F}$ will have to be called many times. Thus we have to look out for fast computations. *Octave* has a good interface for C++ code to be integrated into the *Octave* environment. As an example we rewrite the *Octave* function file `VolterraLotka.m` as `C++` code. Observe that within *Octave* the indexing of arrays starts with 1, but in `C` and `C++` the first index is 0. Thus the components $x(1)$ and $x(2)$ in *Octave* now become $x(0)$ and $x(1)$ in `C++`.

VolterraLotkaC.cc

```
#include <octave/oct.h>
DEFUN_DLD (VolterraLotkaC, args, ,"Function for a Volterra Lotka model")
{
  ColumnVector dx (2);
  ColumnVector x (args(0).vector_value ());

  double c1=1.0, c2=2.0, c3=1.0, c4=1.0;
  dx(0) = (c1-c2*x(1))*x(0);
  dx(1) = (c3*x(0)-c4)*x(1);

  return octave_value (dx);
}
```

Then we have to launch the *Octave* compiler in a shell (or within the *Octave* environment) in the current directory by the command

```
mkoctfile VolterraLotkaC.cc
```

A compiled version `VolterraLotkaC.oct` will be created. If the command `VolterraLotkaC()` is launched in *Octave* and this file is in the current directory we can now use compiled code. To test the code we may compare the function file and the compiled code.

Octave

```
[VolterraLotka([2.22,1.12]), VolterraLotkaC([2.22,1.12])]
-->
  -2.7528  -2.7528
   1.3664   1.3664
```

The main advantage of `C++` code is speed. With the code below one can compare the performence of the script file with the `C++` code.

Octave

```
t = linspace(0,500,100);
lsode_options("relative tolerance",1e-10);
lsode_options("absolute tolerance",1e-10);

t0 = cputime();
XY = lsode('VolterraLotka',[2,1],t);
TimeScript = cputime()-t0

t0 = cputime();
XY = lsode('VolterraLotkaC',[2,1],t);
TimeCPP = cputime()-t0

ratio = TimeScript/TimeCPP
```

On one test system the `C++` ran 8 times faster than the function file. The difference for more complicated examples can be more drastic.

Other examples are provided with the *Octave* distribution, e.g. `oregonator`.

1.6.4 Determine the period of a Volterra-Lotka solution

Using Figure 1.33 we may guess that the solution of the Volterra-Lotka equation is periodic with a period $6.5 \leq T \leq 7$. We use *Octave* to confirm this proposition.

- We first choose the initial values and solve the system of differential equations using `lsode()`. We use the inital time 0 and generate values of the solution at 1000 times between 6.5 and 7.0 . We require

an absolute an relative tolerance of 10^{-10}.

Octave

```
x0 = 2; y0 = 1; % initial values
t = [0,linspace(6,7,1000)]; % examine times between 6 and 7
lsode_options("relative tolerance",1e-10)
lsode_options("absolute tolerance",1e-10)
XY = lsode('VolterraLotkaC',[x0,y0],t); % solve the ODE
```

- We examine the first component (prey) of the solution only and want to determine at what time its value crosses the initial value. For this we detect a sign change of $x(t) - x(0)$ by multiplying two subsequent values and examine the sign. At the crossing we will find a negative sign. As a result we know in which time interval the period will be.

Octave

```
y = XY(2:end,1)-x0; t = t(2:end);      % examine the first component only
plot(t,y); % visual test for zero
grid on
s = sign((XY(2:end,1)-x0).*(XY(1:end-1,1)-x0)); % detect sign changes
pos = find(s<0);                                % position of sign change
```

- To increase **accuracy** we use linear interpolation. If a function $f(t)$ crosses zero between a and b we replace the actual function by a straight line and search the zero of this linear interpolation. By solving

$$f(a + \Delta t) \approx g(\Delta t) = f(a) + \frac{f(b) - f(a)}{b - a} \Delta t = 0$$

we find

$$\Delta t = \frac{-f(a)}{f(b) - f(a)} (b - a)$$

Using this idea we can solve the Volterra-Lotka equation again with initial time give by the time just before the first component of the solution crosses its initial value again. Thus we only have to solve for a very short time interval.

Octave

```
% use linear interpolation to determine the partial time step
dt = (t(pos)-t(pos-1))*y(pos-1)/(y(pos-1)-y(pos))
T = t(pos-1)+dt                                  % estimate the period
XYt = lsode('VolterraLotkaC',XY(pos,:),[T-dt,T]); % compute the value at T
XYt(2,:)-[x0,y0] % difference with initial values
-->
dt =  1.6494e-04
T =  6.9411
      1.3717e-07  -7.5397e-08
```

The numerical result confirms that **both** components are periodic with a period of $T \approx 6.9411$.

1.6.5 The ODE Package on Octave-Forge

The standard command in *Octave* to solve ordinary differential equations is `lsode()`, as used in the previous section. On OctaveForge at `http://octave.sourceforge.net/` you can find an package with additional commands to solve ODEs.

- Dowload the package `odepkg` in a local directory

- Launch *Octave* and install the package with the command
  `pkg install odepkg-0.8.0.tar.gz`
- Depending on your local configuration you might have to load the package with
  `pkg load odepkg`
- With this package many commands from `MATLAB` are now available in *Octave*, and some additional commands. Table 1.11 shows some of the commands.
- Observe a minor, but annoying difference to the command `lsode()`: the arguments in the function describing the differential equation have to be swapped.

```
lsode()   <-->   dx = f(x,t)
ode??()   <-->   dx = f(t,x)
```

Solver	Description
`lsode()`	efficient, addaptive solver based on Hindmarsh's work ([Hind93])
`ode23()`	addaptive, explicit,solver, based on Heun's method
`ode45()`	addaptive, explicit solver, based on Runge-Kutta method of order 4, resp. 5
`ode54()`	Runge Kutta solver
`ode78()`	addaptive, explicit solver, based on Runge-Kutta method of order 7, resp. 8
`ode2r()`	solver for stiff problems, based on Hairer and Wanner's code
`ode5r()`	solver for stiff problems, based on Hairer and Wanner's code

Table 1.11: *Octave* commands to solve ordinary differential equations

The package provides many additional commands, some of them shown in Table 1.12. Find a description of the algorithms, their advantages and disadvantages in the file `odepkg.pdf`, to be found in the subdirectory with the package.

Command	Description
`odeexamples()`	launch demos for ordinary differential equations
`ode23d()`	solver for delay differential equations
`ode45d()`	solver for delay differential equations
`ode78d()`	solver for delay differential equations

Table 1.12: Additional commands in the ODE package

Examples for `ode23()`, `ode45()` and `ode78()`

As an example we consider again the pendulum equation

$$\frac{d}{dt}\begin{pmatrix} y(y) \\ v(t) \end{pmatrix} = \begin{pmatrix} v(t) \\ -y(t) - 0.1\,v(t) \end{pmatrix} \quad \text{with} \quad \begin{pmatrix} y(0) \\ v(0) \end{pmatrix} = \begin{pmatrix} 0 \\ 0.9 \end{pmatrix}$$

Thus a function file with this function may be generated and then used by all examples below.

ODEPend.m

```
function dy = ODEPend(t,y)
  k  = 1; alpha = 0.1;
  dy = [y(2);-k*y(1)-alpha*y(2)];
endfunction
```

As a general rule we first choose the parameters for the solver. As a first example we choose a relative tolerance of 10^{-3} and an absolute tolerance of 10^{-3}. We want a graph to be generated while the differential equation is solved.

Octave

```
vopt = odeset("RelTol", 1e-3, "AbsTol", 1e-3,"NormControl", "on",\
    "OutputFcn", @odeplot);
```

Then we use `ode78()` to solve the system of equations.

Octave

```
ode78(@ODEPend, [0 25], [0 0.9], vopt);
```

The resulting animation and final solution will look rather ragged. Since the Runge–Kutta algorithm of order 7 is very efficient, only very few points have to be computed. Thus the graphic does not look nice, but the numerical results are reliable. The command

Octave

```
ode23(@ODEPend, [0 25], [0 0.9], vopt);
```

will generate a nice looking graph, but require more computation time.

With all of the above codes the numerical values will not be returned and are thus not available for further computation. Use the code below if further computations have to be performed. You will find a plot of position and velocity as function of time and a phase plot.

Octave

```
vopt = odeset('RelTol', 1e-10, 'AbsTol', 1e-10,'NormControl', 'on');
[t,y] = ode78(@ODEPend, [0 25], [0 0.9], vopt);
figure(1); plot(t,y);
xlabel('time');ylabel('position and velocity');grid on
figure(2); plot(y(:,1),y(:,2));
xlabel('position');ylabel('velocity');  grid on
```

1.6.6 Codes from lecture notes by this author

To illustrate the codes presented classe by this author we use the example of a diode circuit examined in the corresponding lecture notes. The behavior of the diode is given by a function

$$i = D(u) = \begin{cases} 0 & \text{for} \quad u \geq -u_s \\ R_D(u + u_s) & \text{for} \quad u < -u_s \end{cases}$$

Based on Kirchhoff's law we find the differential equations

$$\begin{aligned} \dot{u}_h(t) &= \frac{1}{C_1}\left(-D(u_h(t) - u_{in}(t)) + D(u_{out}(t) - u_h(t))\right) \\ \dot{u}_{out}(t) &= \dot{u}_{in}(t) - \frac{1}{C_2} D(u_{out}(t) - u_h(t)) \end{aligned}$$

We define the initial conditions and the two function in a script file. We examine an input voltage of $u_{in}(t) = 10\cos(t)$.

Octave

```
Tend = 30; u0 = [0;0];

function curr = Diode(u)
  Rd = 10; us = 0.7;
  if (u>=-us)  curr = 0;
  else curr = Rd*(u+us);
  endif
endfunction

function y = circuit(t,u)
  C1 = 1; C2 = 1;
  y  = [-1/C1*(Diode(u(1)-10*sin(t))-Diode(u(2)-u(1)));
        10*cos(t)-1/C2*Diode(u(2)-u(1))];
endfunction
```

Using `RK45()`, Runge-Kutta adaptiv

We can use the adaptive Runge-Kutta algorithm with relative and absolute tolerance of 10^{-5} and generate the plot by

Octave

```
t0 = cputime();
[t,u] = rk45('circuit',0,Tend,u0,1e-5,1e-5); % Runge Kutta adaptiv
timer = cputime()-t0
figure(1);
plot(t,u(:,2)'.')
grid on; xlabel('time'); ylabel('tension');
```

The result in Figure 1.35 seems reasonable, but it took 8 seconds of CPU time to compute.

Using `ode_Runge()`, Runge-Kutta with fixed step

We can compare the result with a Runge-Kutta calculation with 100 steps, resulting in Figure 1.35.

Octave

```
tFix = linspace(0,Tend,100);
t0 = cputime();
[tFix,uFix] = ode_Runge('circuit',tFix,u0,1); % Runge Kutta
timer = cputime()-t0
plot(tFix,uFix(:,2),t,u(:,2))
grid on; xlabel('time'); ylabel('tension');
legend('u fix','u adapt')
```

It took only 0.15 seconds, but the solution is ragged at the turning points. This can be improved by using 10 intermediate steps between the output times. Use

Octave

```
[tFix,uFix] = ode_Runge('circuit',tFix,u0,10); % Runge Kutta
```

to find a competitive solution in 1.3 seconds. This is one of the rare occasion where a fixed size algorithm outperforms an adaptive algorithm.

Using `lsode()`

We can compare the above result with the performance of `lsode()`. Unfortunately the arguments t and u have to be given in reverse order for `lsode()` and the above codes and thus the header of the function `circuit` has to be modified slightly. We have to specify the tolerances. With a computation time of 0.48

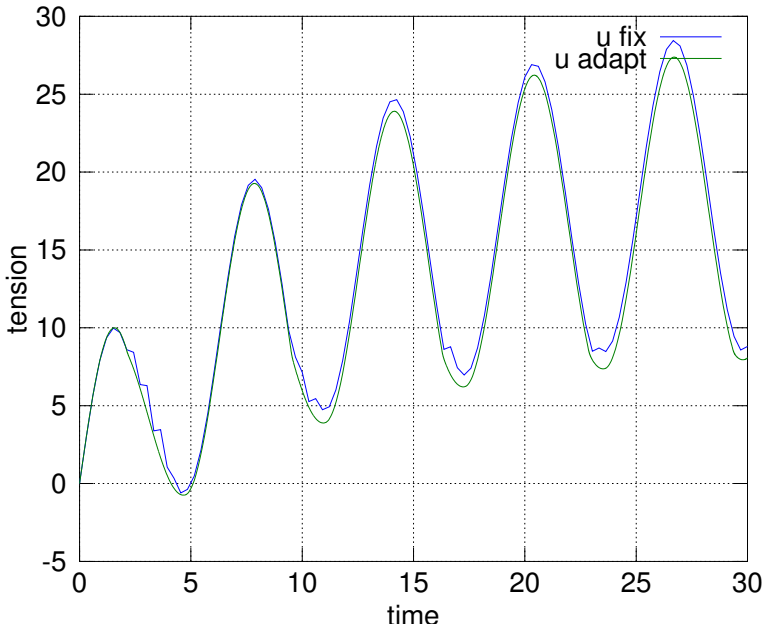


Figure 1.35: Solution for the diode circuit with Runge-Kutta, fixed step and adaptive

seconds we find a good solution. This illustrates the quality of the algorithm in `lsode.m`.

DoubleTensionLSODE.m

```
1;
function y = circuit(u,t)
  C1 = 1; C2 = 1;
  y  = [-1/C1*(Diode(u(1)-10*sin(t))-Diode(u(2)-u(1)));
        10*cos(t)-1/C2*Diode(u(2)-u(1))];
endfunction

t = linspace(0,Tend,100);
lsode_options("absolute tolerance",1e-5);
lsode_options("relative tolerance",1e-5);

t0 = cputime();
u  = lsode('circuit',u0,t);
timer = cputime()-t0
plot(t,u(:,2))
grid on; xlabel('time'); ylabel('tension');
```

Exercise 1.6–1 As an exercise you may solve the differential equations for the above diode circuit, using the codes form the *Octave*-package: `ode23()`, `ode45()`, `ode78()`, `ode3r()` and `ode5r()`. Aim for relative and absolute errors of 10^{-5}, measure and compare the computation times.

1.6.7 List of files

In the previous section the codes and data files in Table 1.13 were used.

filename	function
`logistic.m`	script file to solve the logistic equation
`VolterraLotka.m`	function file for the Volterra-Lotka model
`VolterraLotkaField.m`	script file to solve the Volterra-Lotka model
`VolterraLotkaC.cc`	`C++` code file for the Volterra-Lotka model
`VolterraLotkaPeriod.m`	script file to determine the period of solutions
`SpringODE.m`	script file to solved the damped spring model
`ode_Euler.m`	algorithm of Euler, fixed step size
`ode_Heun.m`	algorithm of Heun, fixed step size
`ode_Runge.m`	algorithm of Runge-Kutta, fixed step size
`rk45.m`	adaptive Runke Kutta algorithm
`DoubleTension.m`	sample code for the diode circuit
`DoubleTensionLSODE.m`	using `lsode()`

Table 1.13: Codes and data files for section 1.6

1.6.8 Exercises

The exercises

Exercise 1.6–2 The physical pendulum, large angles
The differential equation

$$\ddot{\alpha}(t) = -k^2 \sin(\alpha(t))$$

corresponds to a pendulum with possible large angles α. With $k = 1$ the period for small angles α is given by $T = 2\,\pi$.

(a) Rewrite the single differential equation as a system of equations of order 1.

(b) Generate a vector field plot for the domain $-0.2 \leq \alpha \leq 0.2$ and $-0.2 \leq \dot{\alpha} \leq 0.2$.

(c) Use `lsode()` to compute a solution with a small starting angle $\alpha(0) = 0.1 \approx 5.7^\circ$ and initial velocity $v(0) = 0$. Plot the solution for times $0 \leq t \leq 6\,\pi$, i.e. 3 periods for small angles.

(d) Generate a vector field plot for the domain $5 \leq \alpha \leq 5$ and $-2 \leq \dot{\alpha} \leq 2$.

(e) Use `lsode()` to compute a solution with a starting angle $\alpha(0) = 3 \approx 172^\circ$ initial velocity $v(0) = 0$.

Exercise 1.6–3 The physical pendulum with damping
Repeat the above exercise with an additional small damping term, i.e. examine the differential equation

$$\ddot{\alpha}(t) = -k^2 \sin(\alpha(t)) - \mu\,\dot{\alpha}(t)$$

Use the values $k = 1$ and $\mu = 0.1$.

Exercise 1.6–4 A series expansion of the solution of the differential equation

$$u''(x) = -x\,u(x) \quad \text{with} \quad u(0) = 1 \quad \text{and} \quad u'(0) = 0$$

is given by

$$u(x) = 1 - \frac{x^3}{6} + \frac{x^6}{180} - \frac{x^9}{12960} + \dots$$

Thus we can use the first terms to determine the first positive zero x_1 of the solution. We will find $x_1 = \sqrt[3]{6} \approx 1.81$ (2 terms) or better $x_1 \approx 2.024$ (3 terms). Solve the differential equation numerically and determine the zero.

The solution of this differential equation and its first zero are used to determine the theoretical maximal length of a stable upright column (Euler buckling).

Chapter 2

Applications of *Octave*

In this chapter we examine a number of applications of *Octave*. In each the question or problem is formulated and then solved with the help of *Octave*. For some of the necessary mathematical tools brief explanations are provided. But the notes are assuming that the reader is familiar with the Math and Physics of a typical engineering curriculum.

This small set of applications with solutions shall help you to use *Octave* to solve **your** engineering problems. The selection is strongly influenced by my personal preference and some of the topics students we working on.

- Numerical integration to examine magnetic fields, Section 2.1.
- A careful examination of linear and nonlinear regression and its applications, Section 2.2.
- Develop and test an integer arithmetic algorithm, to be implemented on a micro controller, Section 2.4.
- A probabilistic analysis of stock performance, leading to the Black–Scholes–Merton approach to put a price tag on a stock option, Section 2.5.
- Decompose the motion of a falling watch caliber into displacement and deformation, visualize with a movie, Section 2.6.
- Analyze the motion of a damped vibrating cord, used in a balance. Use an external program (Gnuplot) to generate graphs, Section 2.7.

2.1 Numerical Integration and Magnetic Fields

2.1.1 Basic integration methods

Trapezoidal integration using `trapz()`

The simples integration in *Octave* is based on the trapezoidal rule and implemented in the command `trapz()`. Examine the on-line help. The code below computes

$$\int_0^\pi \sin(x)\, dx$$

with 100 subintervalls of equal length.

Octave

```
x = 0:pi/100:pi;
y = sin(x);
trapz(x,y)
```

The returned value of 1.9998 is rather close to the exact value of 2 .

Numerical analysis indicates that the approximation error of the trapezoidal rule is proportional to h^2, where h the the length of the subintervals. This is confirmed by the graphic created by the code below.

- for $n = 10,\ 20,\ 40, \ldots, 10 \cdot 2^9$ the integral is computed with n subintervals.
- The error is then plotted with double logarithmic scales. Since

$$\begin{aligned} \text{error} &\approx c \cdot h^2 \\ \ln(\text{error}) &\approx \ln(c) + 2\ \ln h = \ln(c) + 2\ \ln\frac{\pi}{n} = \ln(c) + 2\ln\pi - 2\ \ln n \end{aligned}$$

the result should be a straight line with slope -2. This is confirmed in Figure 2.2.

Octave

```
Nrun = 10;  n = zeros(1,Nrun);  err = zeros(1,Nrun);
for k = 1:Nrun
  n(k) = 10*2^(k-1);
  x = linspace(0,pi,n(k)+1);
  err(k) = abs(2-trapz(x,sin(x)));
endfor

loglog(n,err);
```

Using the linear regression commands

Octave

```
F = [ones(size(n))', log(n')];
LinearRegression(F,log(err'))
```

we find

$$\begin{aligned} \ln(\text{err}(n)) &\approx 0.5 - 2\ \ln(n) \\ \text{err}(n)) &\approx \frac{1.6}{n^2} \end{aligned}$$

and this confirms the error estimate for the trapezoidal integration method.

With the command `cumtrapz()` we can not only compute the integral over the complete interval, but also the values of the integral at the intermediate points, i.e. the code

Octave

```
x  = 0:pi/100:pi;
y  = sin(x);
ys = cumtrapz(x,y);
plot(x,ys)
xlabel('position x'); ylabel('integral of sin(x)'); grid on
```

will compute

$$\int_0^x \sin(s)\, ds$$

for 101 values of x evenly distributed form 0 to π . The result is shown in Figure 2.1.

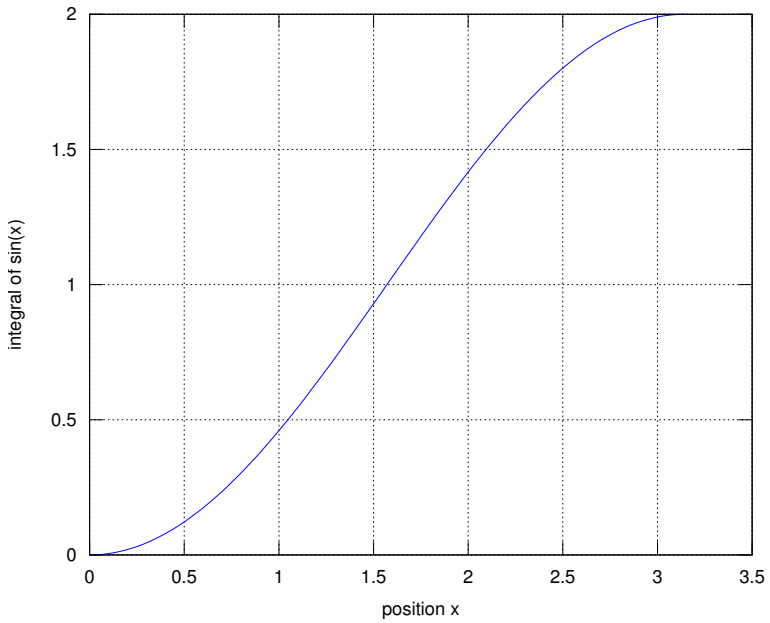


Figure 2.1: Cumulative trapezoidal integration of $\sin(x)$

Simpson integration

In your (numerical) analysis course you should have learned about the Simpson method for numerical integrals. Below find an implementation in *Octave*. We have the following requirements for the code:

- Simpsons integration formula for an even number of subintervals has to be applied. The code can only handle subintervals of equal length.
- The function can be given either as a function name or by a list of values.

simpson.m

```
function res = simpson(f,a,b,n)

%% simpson(integrand,a,b,n) compute the integral of the function f
%% on the interval [a,b] with using Simpsons rule
%% use n subintervals of equal length , n has to be even, otherwise n+1 is used
%% f is either a function name, e.g  'sin' or a vector of values

if is_vector(f)
  n = length(f);
  if (floor(n/2)-n/2==0)
    error("simpson: odd number of data points required");
```

```
    else
      n   = n-1;
      h   = (b-a)/n;
      f_x = f(:)';
    endif
  else  %% compute the function values using the function name
    n = round(n/2+0.1)*2; %% assure even number of subintervals
    h = (b-a)/n;
    x = linspace(a,b,n+1);
    f_x = x;
    for k = 0:n
      f_x(k+1) = feval(f,x(k+1));
    end
  endif

  w = 2*[ones(1,n/2); 2*ones(1,n/2)](:); % construct the simpson weights
  w = [w;1]; w(1) = 1;
  res = (b-a)/(3*n)*f_x*w;
```

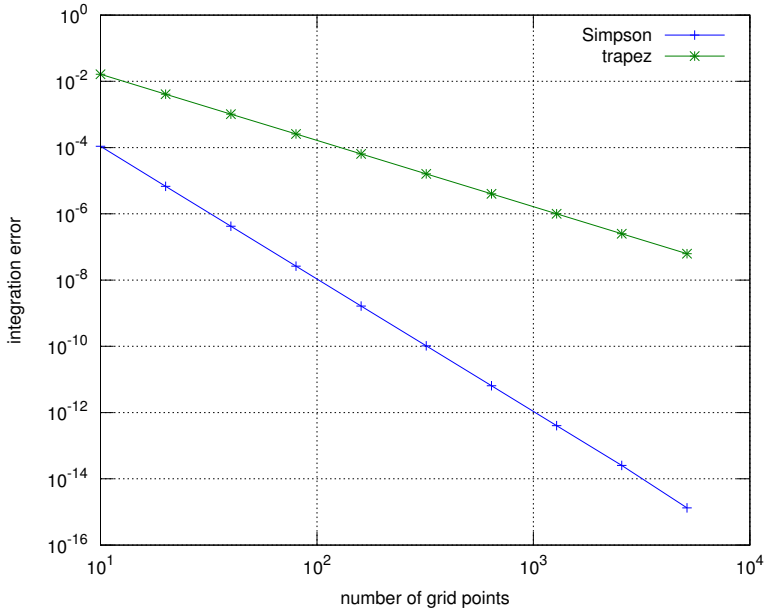


Figure 2.2: Error of trapezoidal and Simpsons method

This integration can now be tested similarly to the above tests. The graphical result for the trapezoidal and Simpson integration is shown in Figure 2.2.

Octave

```
Nrun = 10;  n = zeros(1,Nrun); err = zeros(1,Nrun);
for k = 1:Nrun
  n(k)   = 10*2^(k-1);
  err(k) = abs(2-simpson('sin',0,pi,n(k)));
endfor
loglog(n,err,'-@+;Simson;',n,errTrap,'-@*;trapez;');
xlabel('number of grid points'); ylabel('integration error'); grid on

F = [ones(size(n))' log(n')];
LinearRegression(F,log(err'))
```

The result of the regression confirms that the error is proportional to h^4 . This is confirmed in Figure 2.2.

Observe that the accuracy of the integration methods can not be better than machine accuracy. This effect is starting to show in the lower right corner of Figure 2.2.

Adaptive integration using `quad()`, anonymous functions

The built-in *Octave* command `quad()` (short for quadrature) is based on the **Quadpack** software to compute integrals numerically. This is a well tested, reliable package. Its usage in *Octave* is rather simple, as shown by the example below.

Octave

```
1; % assure it is a script file
function y = f(x)
  y = 4/(1+x^2);
endfunction

nInt = quad('f',0,1,1e-5)
```

Read the on-line help of `help quad` to learn how to set absolute and relative error requirements. The return results of `quad()` can also include information on the number of function evaluations and estimates on the error. Internally `quad()` is using an adaptive method of integration.

With `quad()` a function can be integrated with respect to one variable. Very often the function to be integrated depends on parameters. As an example consider

$$I(p) = \int_0^1 \sin(p\,x\,2\,\pi)\;dx$$

The result will depend on the parameter p. the function $f(x,p) = \sin(p\,x\,2\,\pi)$ can be integrated with respect to x using an anonymous function, as illustrated below.

Octave

```
%% integration using an anonymous function
p = 2;  % value of parameter

function y = f(x,p)  % function to be integrated with respect to x
  y = sin(p*x*2*pi);
endfunction

quad(@(x)f(x,p),0,1)  % in p is an integer number, then the exact value is 0
```

2.1.2 Comparison of integration commands in *Octave*

Above three different commands for numerical integration are shown. For any given integration one has to choose the best method. In Table 2.1 find a brief description.

For each situation the best algorithm has to be chosen. A comparison is given in Table 2.2.

> The command `quad()` should be used whenever possible.

2.1.3 From Biot–Savart to magnetic fields

The *Octave* command for numerical integration will be used to determine the magnetic field of a circular conductor. The situation is shown in Figure 2.3. If a short segment $\vec{ds}$ of a conductor carries a current I then the contribution $d\vec{H}$ to the magnetic field is given by the law of Biot–Savart

$$d\vec{H} = \frac{I}{4\,\pi\,r^3}\;\vec{ds} \times \vec{r}$$

`trapz()`, `cumtrapz()`	uses trapezoidal rule to be used for discretized values only uneven spacing is possible
`simpson()`	uses Simpson's method for discretized values of function name even number of subintervals of equal length
`quad()`	uses **Quadpack**, adaptive algorithm function name has to be given

Table 2.1: Integration commands in *Octave*

	`trapz()`	`simpson()`	`quad()`
accuracy	poor	intermediate	excellent
built–in error control	no	no	yes
applicable if values only given	yes	yes	no
applicable if function name is given	no	yes	yes
applicable if subintervals have unequal length	yes	no	

Table 2.2: Comparison of the integration commands in *Octave*

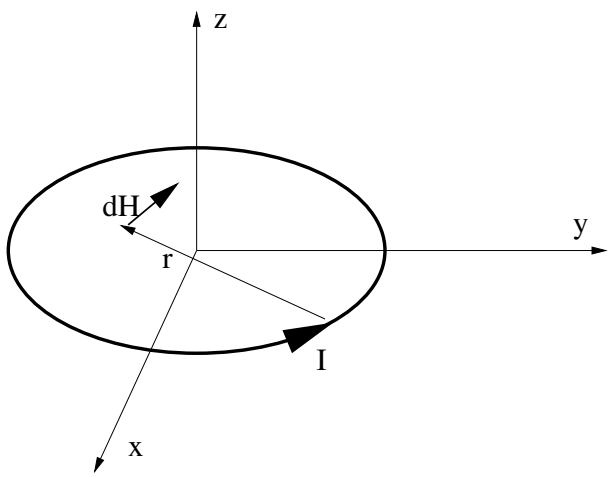


Figure 2.3: Circular conductor for which the magnetic field has to be computed

where $\vec{r}$ is the vector connecting the point on the conductor to the points at which the field is to be computed.

A parametrization of the circle is given by

$$\begin{pmatrix} R\cos\phi \\ R\sin\phi \\ 0 \end{pmatrix} \quad \text{where} \quad 0 \le \phi \le 2\pi$$

leading to a line segment $\vec{ds}$ of

$$\vec{ds} = \begin{pmatrix} -R\sin\phi \\ R\cos\phi \\ 0 \end{pmatrix} d\phi$$

The field $\vec{H}$ generated will have a radial symmetry and we may examine the field in the xz–plane only, i.e. at points $(x, 0, z)$. We find

$$\vec{r} = \begin{pmatrix} x \\ 0 \\ z \end{pmatrix} - \begin{pmatrix} R\cos\phi \\ R\sin\phi \\ 0 \end{pmatrix}$$

and

$$\begin{aligned} r^2 &= (R\cos\phi - x)^2 + R^2\sin^2\phi + z^2 \\ &= R^2 - 2\,x\,R\cos\phi + x^2 + z^2 \end{aligned}$$

To apply Biot–Savart we need the expression

$$\vec{ds}\times\vec{r} = \begin{pmatrix} -R\sin\phi \\ R\cos\phi \\ 0 \end{pmatrix} \times \begin{pmatrix} x - R\cos\phi \\ -R\sin\phi \\ z \end{pmatrix} d\phi = \begin{pmatrix} z\,R\cos\phi \\ z\,R\sin\phi \\ R^2 - x\,R\cos\phi \end{pmatrix} d\phi$$

and thus obtain an integral for the 3 components of the field $\vec{H}$ at the point $(x, 0, z)$

$$\vec{H}(x,y,z) = \frac{I}{4\,\pi}\int_0^{2\pi} \frac{1}{(R^2 - 2\,x\,R\cos\phi + x^2 + z^2)^{3/2}} \begin{pmatrix} z\,R\cos\phi \\ z\,R\sin\phi \\ R^2 - x\,R\cos\phi \end{pmatrix} d\phi \qquad (2.1)$$

For each of the three components of the field we find one integral to be computed.

In the following sections we examine the special situation $R = 1$ and $I = 1$.

2.1.4 Field along the central axis and the Helmholtz configuration

Along the z–axis we use $x = 0$ and the above integral simplifies to

$$\vec{H} = \frac{I}{4\,\pi}\int_0^{2\pi} \frac{1}{(R^2 + z^2)^{3/2}} \begin{pmatrix} z\,R\cos\phi \\ z\,R\sin\phi \\ R^2 \end{pmatrix} d\phi$$

Verify that the x- and y component of $\vec{H}$ vanish, as they should because of the radial symmetry. For the z component $H_z(z)$ we obtain

$$H_z(z) = \frac{I}{4\,\pi}\int_0^{2\pi} \frac{R^2}{(R^2 + z^2)^{3/2}}\,d\phi = \frac{I}{2}\,\frac{R^2}{(R^2 + z^2)^{3/2}}$$

For very small and large values of z the above may be simplified to

$$H_{z \ll R} \approx \frac{I}{2}\,\frac{1}{R} \quad \text{and} \quad H_{z \gg R} \approx \frac{I}{2}\,\frac{R^2}{z^3}$$

The above approximations allow to compute the field at the center of the coil and show that the field along the center axis converges to 0 like $1/z^3$.

For many applications is is important that the magnetic field should be constant over the domain to be examined. The above computations show that the field generated by a single coil is far from constant. For a Helmholtz configuration we place two of the above coils, at the heights $z = \pm h$. The value of h has to be such that the field around the center is as homogeneous as possible. To examine this situation we shift one coil up by h and another coil down by $-h$ and then examine the resulting field. On the left in Figure 2.4 we find the results if the two coils are close together, on the right if they are far apart. Neither situation is optimal for a homogeneous magnetic field.

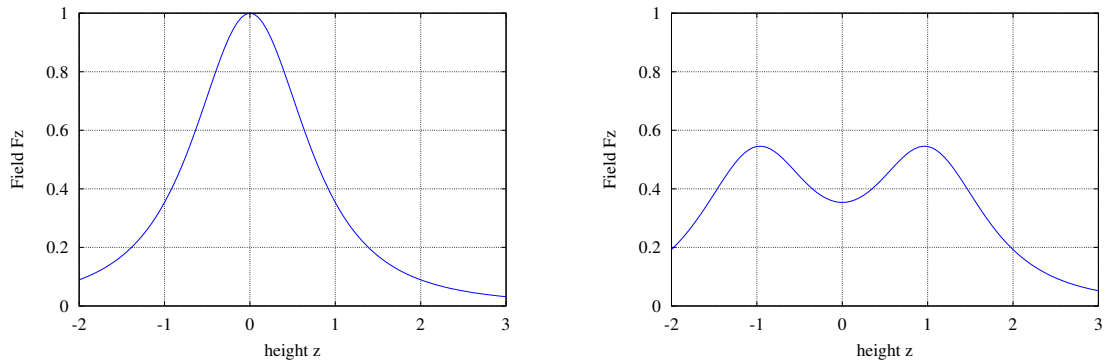


Figure 2.4: Magnetic field along the central axis

We have to examine the field G generated by both coils and thus G is given as the sum of the two fields by the individual coils at height $z = \pm h$.

$$G(z) = H_z(z+h) + H_z(z-h) = \frac{I}{2}\,\left(\frac{R^2}{(R^2+(z-h)^2)^{3/2}} + \frac{R^2}{(R^2+(z+h)^2)^{3/2}}\right)$$

The field at $z = 0$ is as homogeneous as possible if as many terms as possible in the Taylor expansion vanish.

$$G(z) \approx G(0) + \frac{d\,G(0)}{dz}\,z + \frac{1}{2}\,\frac{d^2\,G(0)}{dz^2}\,z^2 + \frac{1}{6}\,\frac{d^3\,G(0)}{dz^3}\,z^3 + \ldots$$

Since H_z is an even function know that the first derivative is an odd function and the second derivative is an even function. Thus we find

$$\frac{d\,G(0)}{dz} = \frac{d}{dz}\,H(h) + \frac{d}{dz}\,H(-h) = 0$$

and

$$\frac{d^2\,G(0)}{dz^2} = \frac{d^2}{dz^2}\,H_z(h) + \frac{d^2}{dz^2}\,H_z(-h) = 2\,\frac{d^2}{dz^2}\,H_z(h)$$

Thus the optimal solution is characterized as zero of the second derivative of $H_z(z)$.

$$\frac{d^2}{dz^2}\,H_x(z) = \frac{I\,R^2}{2}\,\frac{d^2}{dz^2}\,\left(\frac{1}{(R^2+z^2)^{3/2}}\right) = 0$$

We find

$$\frac{d}{dz}\,\frac{1}{(R^2+z^2)^{3/2}} \quad = \quad \frac{-3\cdot 2\,z}{2\,(R^2+z^2)^{5/2}} = \frac{-3\,z}{(R^2+z^2)^{5/2}}$$

$$\frac{d^2}{dz^2}\,\frac{1}{(R^2+z^2)^{3/2}} = \frac{-3\,(R^2+z^2)^{5/2} + 3\,z\,\frac{5}{2}(R^2+z^2)^{3/2}\,2\,z}{(R^2+z^2)^5}$$
$$= \frac{-3\,(R^2+z^2) + 3\,z\,5\,z}{(R^2+z^2)^{7/2}} = 3\,\frac{4\,z^2 - R^2}{(R^2+z^2)^{7/2}}$$

Thus the second derivative of $G(0)$ vanishes if $h = \pm\frac{R}{2}$. This implies the the distance between the centers of the coil should be equal to the Radius R. This is confirmed by the results in Figure 2.5.

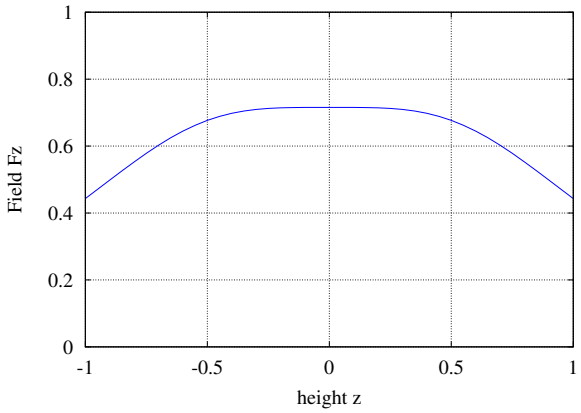


Figure 2.5: Magnetic field along the central axis, Helmholtz configuration

The above figures were generated by *Octave* with the help of a function file `HzAxis.m` to compute the field along the axis

HzAxis.m

```
function H = HzAxis(z)
  R = 1;
  H = R^2/2*(R^2+z.^2).^(-3/2);
endfunction
```

and the commands

Octave

```
z = linspace(-2,3,101);
figure(1);
dz = 0.0;
plot(z,HzAxis(z-dz)+HzAxis(z+dz))
axis([-2,3,0,1])
grid on; xlabel('height z'); ylabel('Field Fz');

figure(2);
dz = 1;
plot(z,HzAxis(z-dz)+HzAxis(z+dz))
axis([-2,3,0,1])
grid on; xlabel('height z'); ylabel('Field Fz');

figure(3);
dz = 1/2;
plot(z,HzAxis(z-dz)+HzAxis(z+dz))
axis([-1,1,0,1])
grid on; xlabel('height z'); ylabel('Field Fz');
```

2.1.5 Field in the plane of the conductor

In the plane $z = 0$ of the conductor the field will show a radial symmetry again, the field at the point $(x, y, 0)$ is given by a rotation of the field at the point $(\sqrt{x^2 + y^2}, 0, 0)$. Thus we compute the field along the x–axis only. Based on equation (2.1) we have to compute three integrals.

$$\vec{H}(x, y, z) = \frac{I}{4\,\pi} \int_0^{2\pi} \frac{1}{(R^2 - 2\,x\,R\,\cos\,\phi + x^2 + z^2)^{3/2}} \begin{pmatrix} z\,R\,\cos\,\phi \\ z\,R\,\sin\,\phi \\ R^2 - x\,R\,\cos\,\phi \end{pmatrix} d\phi$$

For the z component H_z we need to integrate a scalar valued function, depending on the variable angle ϕ and the parameters R, x, y and z. We define an *Octave* function `dHz()`.

dHz.m

```
function res = dHz(phi,R,x,z)
  res = R*(R-x.*cos(phi))./sqrt(R^2-2*x.*R.*cos(phi)+x.^2 +z.^2).^3;
endfunction
```

Currently we are only interested in $_z$ along the x–axis, i.e. $y = z = 0$ and we want to compute

$$H_z(x, 0, 0) = \frac{I}{4\,\pi} \int_0^{2\pi} \frac{R^2 - x\,R\,\cos\,\phi}{(R^2 - 2\,x\,R\,\cos\,\phi + x^2)^{3/2}}\, d\phi$$

An analytical formula for this integral can be given, but the expression is very complicated. Thus we prefer a numerical approach. The integral to be computed will depend on the parameters x, y and R representing the position at which the magnetic field will be computed. We use function handles and anonymous functions to deal with these parameters for the integration. We examine a coil with diameter $R = 1$ and first compute the field for values $-0.5 \le x \le 0.8$ and then for $1.2 \le x \le 3$. The results are shown in Figure 2.6. Observe that the field is large if we are close to the wire at $x \approx R = 1$ and the z component changes sign outside of the circular coil. As x increases H_z converges to 0 . This is confirmed by physical facts.

Octave

```
x  = -0.5:0.05:0.8;
Fz = zeros(size(x));
for k = 1:length(x)
  fz = @(al)dHz(al,1,x(k),0);      % define the anonymous function
  Fz(k) = quad(fz,0,2*pi)/(4*pi); % integrate
endfor

figure(1)
plot(x,Fz)
grid on
axis([-0.5 0.8 0 1.2]);
xlabel('position x'); ylabel('Field Fz');

x2 = 1.2:0.05:3;
Fz2 = zeros(size(x2));
for k = 1:length(x2)
  fz = @(al)dHz(al,1,x2(k),0);      % define the anonymous function
  Fz2(k) = quad(fz,0,2*pi)/(4*pi); % integrate
endfor

figure(2)
plot(x,Fz,x2,Fz2)
grid on
axis([-0.5 3 -0.6 1.2]);
xlabel('position x'); ylabel('Field Fz');
```

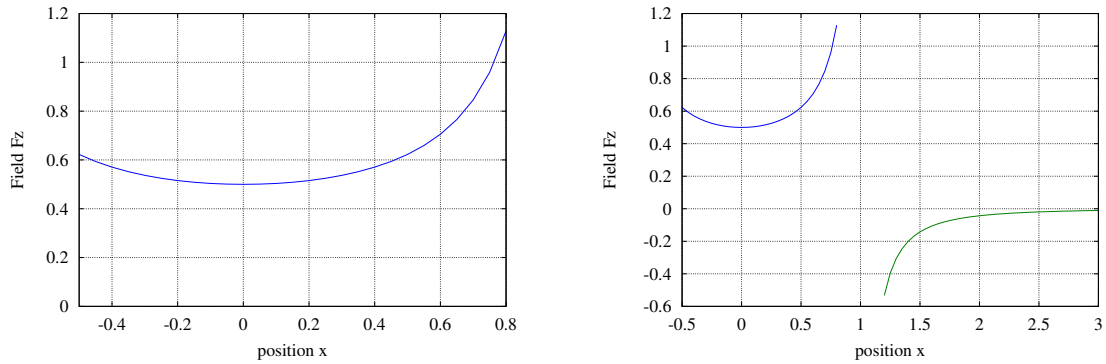


Figure 2.6: Magnetic field along the x axis

2.1.6 Field in the xz–plane

In the xz plane we have to examine both components of the field and thus we need to compute $H_x(x, 0, y)$ too. Using equation (2.1) we find

$$H_x(x, 0, z) = \frac{I}{4\,\pi} \int_0^{2\pi} \frac{z\,R\,\cos\,\phi}{(R^2 - 2\,x\,R\,\cos\,\phi + x^2 + z^2)^{3/2}}\,d\phi$$

We write a *Octave* function for the expression to be integrated.

dHx.m

```
function res = dHx(phi,R,x,z)
  res = R*z.*cos(phi)/sqrt(R^2-2*x.*R.*cos(phi)+x.^2 +z.^2).^3;
endfunction
```

We proceed as follows:

1. Choose the domain of $-0.4 \leq x \leq 0.7$ and $-1 \leq z \leq 2$. Generate vectors with the values of x and z for which the field $\vec{H}$ will be computed.
2. Generate a mesh of points with the command `meshgrid()` .
3. Create the empty matrices `Hx` and `Hz` for the components of the field.
4. Use a for loop to fill in the values of both components of $\vec{H}$, using the integrals based on (2.1).

Octave

```
z = -1:0.2:2; x = -0.4:0.1:0.7;
[xx,zz] = meshgrid(x,z);
x = xx(:); z = zz(:);
Hx = zeros(size(x)); Hz = Hx;

for k = 1:length(x)
  fx    = @(al)dHx(al,1,x(k),z(k));   % define the anonymous function
  Hx(k) = quad(fx,0,2*pi)/(4*pi);     % integrate
  fz    = @(al)dHz(al,1,x(k),z(k));   % define the anonymous function
  Hz(k) = quad(fz,0,2*pi)/(4*pi);     % integrate
endfor
```

The next step is to visualize the vector field $\vec{H}$ in the xz plane in the center of the circular coil. To arrive at Figure 2.7 we use the command `quiver()` to display the vector field.

In the left part of Figure 2.7 we find magnetic fields of drastically different sizes, in particular close to the conductor. For a good visualization it is often useful to normalize all vectors to have equal length. Find the result of the code below in the right part of Figure 2.7.

Octave

```
subplot(1,2,1)
quiver(x,z,Hx,Hz,0.2)
grid on
axis('equal')

scal = 1./sqrt(Hx(:).^2+Hz(:).^2);  % length of each vector
Hx = scal.*Hx; Hz = scal.*Hz;       % normalize length

subplot(1,2,2)
quiver(x,z,Hx,Hz,0.1)
grid on
axis('equal')
```

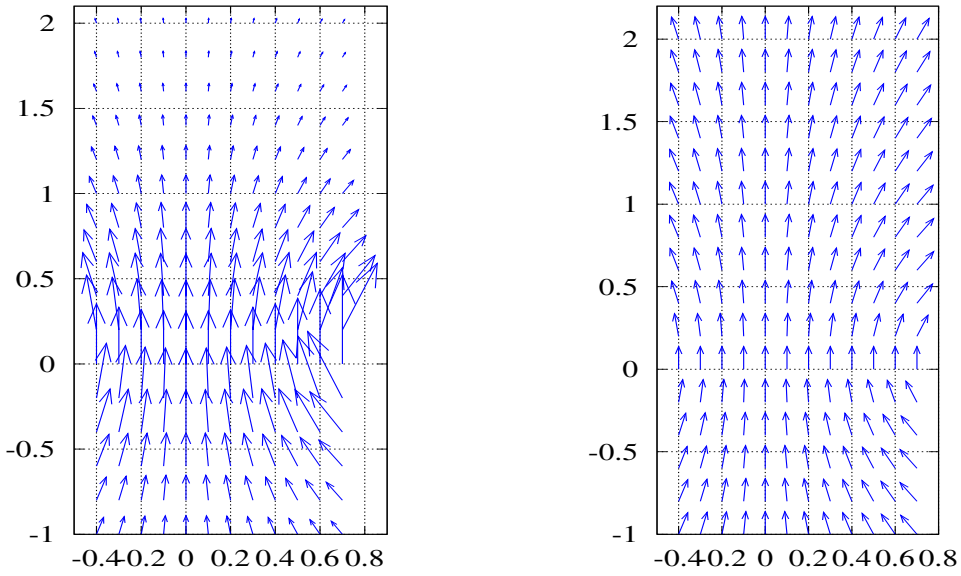


Figure 2.7: Magnetic vector field in a plane, actual length and normalized

2.1.7 The Helmholtz configuration

To obtain a homogeneous field in the center of two coils we have to place them at a distance equal to the radii of the circular coils. We can compute and visualize the field of this configuration using the same ideas and codes as in the section above. Find the result in Figure 2.8.

Octave

```
clf
x = -0.3:0.05:0.3; z = x;
h = 0.5; % optimal distance for Helmholtz configuration is 2*h=R

[xx,zz] = meshgrid(x,z);
x = xx(:); z = zz(:);
Hx = zeros(size(x)); Hz = Hx;
```

```
for k = 1:length(x)
  fx     = @(al)(dHx(al,1,x(k),z(k)-h)+dHx(al,1,x(k),z(k)+h));
  Hx(k) = quad(fx,0,2*pi)/(4*pi);
  fz     = @(al)(dHz(al,1,x(k),z(k)-h)+dHz(al,1,x(k),z(k)+h));
  Hz(k) = quad(fz,0,2*pi)/(4*pi);
endfor

quiver(x,z,Hx,Hz,0.001)
grid on
```

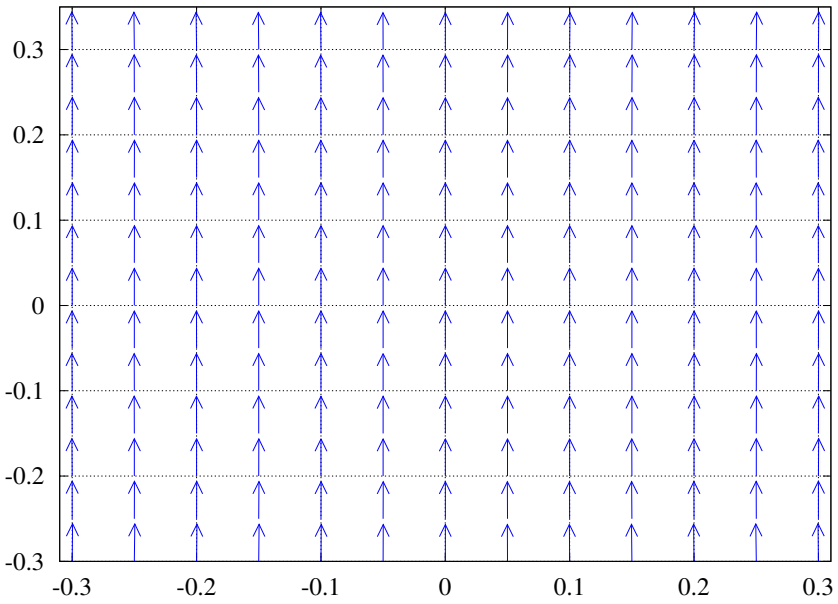


Figure 2.8: Magnetic field for two Helmholtz coils

Analysis of homogeneity of the magnetic field

The main purpose of the Helmholtz configuration is to provide a homogeneous field at the center of the coils. Thus we want the all components of the field to be constant. It is not obvious how to quantify the deviation from a constant magnetic field. We suggest three options:

1. Variation in z component only
   The z component H_z is clearly the largest component. Thus we might examine the variations of H_z only. One possible method is to generate level curves for the relative deviation

$$\text{relative deviation in } H_z \quad = \left| \frac{H_z(x,y,z) - H_z(0,0,0)}{H_z(0,0,0)} \right|$$

2. Variation in all components
   We might also take the other components into account and examine the deviation vector

$$\vec{H}(x,y,z) - \vec{H}(0,0,0) = \begin{pmatrix} H_x(x,y,z) \\ H_y(x,y,z) \\ H_z(x,y,z) \end{pmatrix} - \begin{pmatrix} 0 \\ 0 \\ H_z(0,0,0) \end{pmatrix}$$

and then generate level curves for the relative deviation

$$\text{relative deviation in } \vec{H} \quad = \frac{\|\vec{H}(x,y,z) - \vec{H}_z(0,0,0)\|}{H_z(0,0,0)}$$

3. Variation in the strength of the magnetic field
   If only the strength $\|\vec{H}\|$ matters and the direction of the magnetic field is irrelevant we might examine level curves for

$$\text{relative deviation in strength } \|\vec{H}\| \quad = \left| \frac{\|\vec{H}(x,y,z)\| - H_z(0,0,0)}{H_z(0,0,0)} \right|$$

The above ideas can be implemented in *Octave*, leading to the result in Figure 2.9 for the relative deviation in H_z. The deviation is examined in the xz–plane, i.e. for $y = 0$. The result in Figure 2.9 for the relative deviation shows that the relative deviation is rather small at the center $(x, z) \approx (0, 0)$ but increases shaply at the corners of the examined domain of $-0.3 \le x \le 0.3$ and $-0.3 \le z \le 0.3$.

Octave

```
n    = sqrt(length(Hz))
HzM = reshape(Hz,n,n);
Hz0 = HzM(floor(n/2)+1,floor(n/2)+1)
reldev = abs(HzM-Hz0)/Hz0;
mesh(xx,zz,reldev)
```

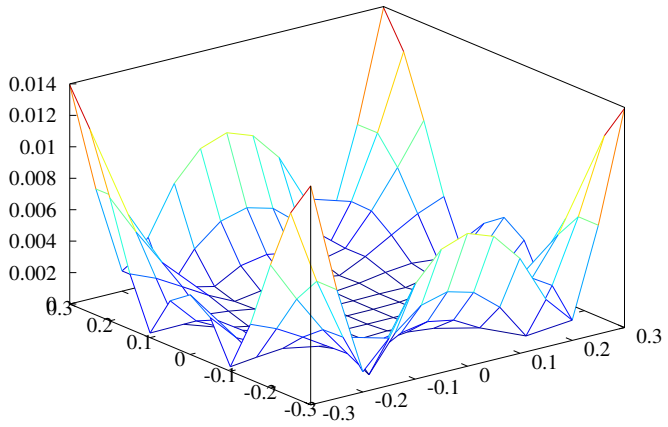


Figure 2.9: Relative changes of H_z in the plane $y = 0$

Level curves for relative deviations

To estimate the domain for which the relative deviation is small we can use level curves. We use a fine mesh[1] to obtain smoother curves. In Figure 2.10 we find the level curves for relative deviation in H_z at levels 0.001, 0.002, 0.005 and 0.01 . We see that the deviation remains small along a few lines, even if we move away from the center. This is confirmed by Figure 2.9. On might have to pay attention to the computation time. If a grid on $n \times n$ points is examined, then $2\,n^2$ integrals have to be computed. For the sample code below this translates to 5202 integrals.

Octave

[1]The price to pay is some CPU time. For a quick check one may work at a lower resolution.

```
n = 51; x = linspace(-0.3,0.3,n); z = x;
h = 0.5; % optimal distance for Helmholtz configuration

[xx,zz] = meshgrid(x,z);
x = xx(:); z = zz(:);
Hx = zeros(size(x)); Hz = Hx;

for k = 1:length(x)
  fx    = @(al)(dHx(al,1,x(k),z(k)-h)+dHx(al,1,x(k),z(k)+h));
  Hx(k) = quad(fx,0,2*pi)/(4*pi);
  fz    = @(al)(dHz(al,1,x(k),z(k)-h)+dHz(al,1,x(k),z(k)+h));
  Hz(k) = quad(fz,0,2*pi)/(4*pi);
endfor
HzM = reshape(Hz,n,n);
Hz0 = HzM(floor(n/2)+1,floor(n/2)+1)
reldev = abs(HzM-Hz0)/Hz0;
contour(xx,zz,reldev,[0.001,0.002,0.005,0.01])
axis('equal'); grid on
xlabel('x'); ylabel('z');
```

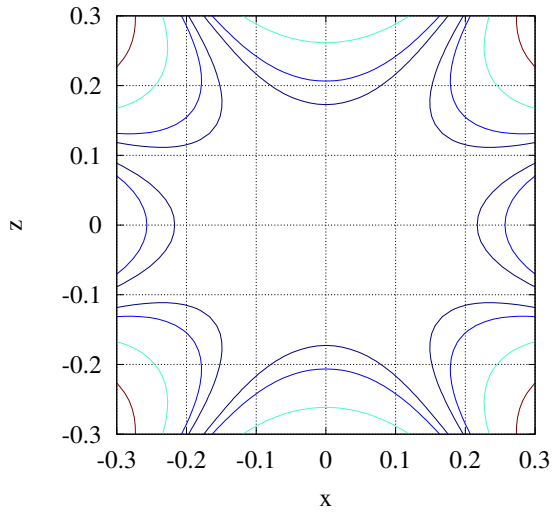


Figure 2.10: Level curves for the relative changes of H_z at levels 0.001, 0.002, 0.005 and 0.01

It might be a better approach to examine the relative deviation in $\vec{H}$ and not the z component only. Find the code below and the result in Figure 2.11 we see that the relative deviation of $\vec{H}$ increases uniformly as we move away from the center. For Helmholtz coils with radius $R = 1$ we find that in an approximate cylinder with radius 0.2 and height 0.4 the relative deviation in the magnetic field is smaller than 0.001, thus the field is rather homogeneous.

Octave

```
HxM = reshape(Hx,n,n);
HDev = sqrt(HxM.^2 + (HzM-Hz0).^2)/Hz0;
contour(xx,zz,HDev,[0.001,0.002,0.005,0.01])
axis('equal');grid on
xlabel('x'); ylabel('z');
```

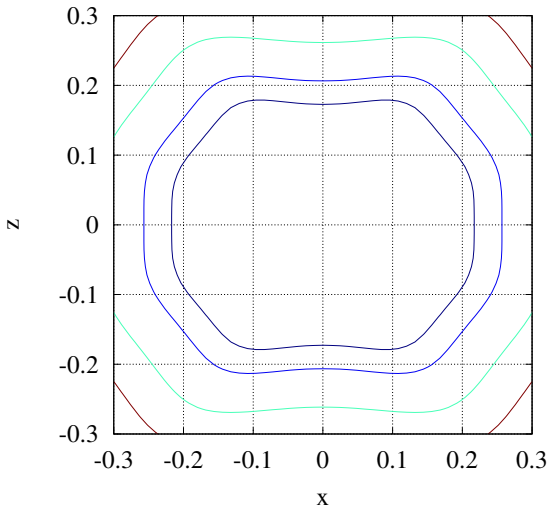


Figure 2.11: Level curves for the relative deviation of $\vec{H}$ at levels 0.001, 0.002, 0.005 and 0.01

2.1.8 Flowlines

Use the vector fields above, `interp2` and an ODE solver to generate flow lines

2.1.9 List of codes and data files

In the previous section the codes and data files in Table 2.3 were used.

filename	function
`testtrapez.m`	script file for test of `trapz()`
`simpson.m`	function file, implementing Simpson's algorithm
`testsimpson.m`	script file for test of `simpson()`
`dHx.m` `dHz.m`	function files for integrands of the x and y components of the magnetic field
`Hz_along_x_axis.m`	script file to compute z–component of field along z–axis
`VectorFields.m`	script file to compute vector field in xz–plane
`VectorFieldsHelmholtz.m`	script file to compute vector field for Helmholtz configuration
`HelmholtzContours.m`	script file to compute level curves for Helmholtz configuration

Table 2.3: Codes and data files for section 2.1

2.1.10 Exercises

The exercises

Exercise 2.1–1 Rewrite the function files `Hx.m` and `Hy.m` such that they use a Simpson integration with 100 subintervals.

The answers

Exercise 2.1–1

Octave

```
function res = Hx(x,z);
  global xt
  global zt
  xt = x;  zt = z;
  res = simpson('dHx',0,2*pi,100)/(4*pi);
endfunction
```

2.2 Linear and Nonlinear Regression

One of the most common engineering problems is to find optimal parameters for your model to be as close as possible to some measured data. This very often leads to a regression problem and there is a fast literature and many pieces of code are available. Obviously *Octave* also provides a set of tools for this task. This section shall serve as an introduction on when and how to use those codes. The structure of the section is as follows:

- Show a first example of a straight line regression, the most common case. Only basic *Octave* commands are used.
- Present the matrix notation for general linear regression problems.
- Examine the variance (accuracy) of the parameters to be determined.
- Present an example where the basic ideas will lead to serious problems, as is the case for many real world problems. Point out how to avoid or eliminate those problems. Give some of the mathematical background (QR factorization).
- Give some information on weighted regression problems.
- All of the above will lead to the code in `LinearRegression.m`, which will then be used to solve three real world engineering problems.
- Finally the commands `leasqr()` and `fsolve()` are used to solve nonlinear regression problems, illustrated by examples.

2.2.1 Linear regression for a straight line

For n given points $(x_i\,,\,y_i)$ in a plane we try to determine a straight line $y(x) = p_1 \cdot 1 + p_2 \cdot x$ to match those points as good as possible. One good option is to examine the residuals $r_i = p_1 \cdot 1 + p_2 \cdot x_i - y_i$. Using matrix notations we find

$$\vec{r} = \mathbf{F} \cdot \vec{p} - \vec{y} = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ 1 & x_3 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix} \cdot \begin{pmatrix} p_1 \\ p_2 \end{pmatrix} - \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_n \end{pmatrix}$$

Linear regression corresponds to minimization of the norm of $\vec{r}$, i.e. minimize

$$\|\vec{r}\|^2 = \|\mathbf{F} \cdot \vec{p} - \vec{y}\|^2 = \langle \mathbf{F} \cdot \vec{p} - \vec{y}\,,\, \mathbf{F} \cdot \vec{p} - \vec{y} \rangle$$

Consider $\|\vec{r}\|^2$ as a function of p_1 and p_2. At the minimal point the two partial derivatives have to vanish. This leads to a system of linear equations for the vector $\vec{p}$.

$$\mathbf{X} \cdot \vec{p} = \left(\mathbf{F}^T \cdot \mathbf{F}\right) \cdot \vec{p} = \mathbf{F}^T \cdot \vec{y}$$

This can easily be implemented in *Octave*, leading to the result in Figure 2.12 and a residual of $\|\vec{r}\|^2 \approx 1.23$.

Octave

```
x = [0; 1; 2; 3.5; 4]
y = [-0.5; 1; 2.4; 2.0; 3.1]

F = [ones(size(x)) x]
p = (F'*F)\(F'*y)
residual = norm(F*p-y)

xn = [-1 5]; yn = p(1)+p(2)*xn;
plot(x,y,'+r',xn,yn)
```

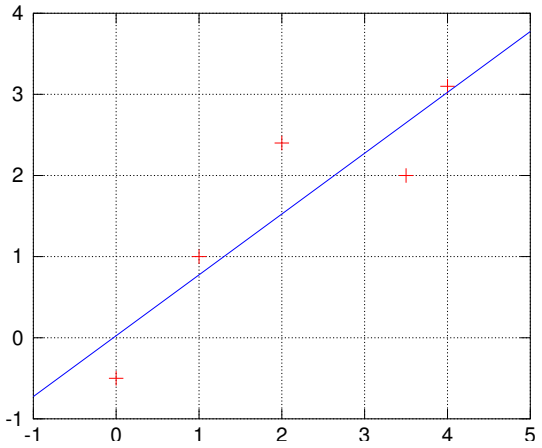


Figure 2.12: Regression of a straight line

2.2.2 General linear regression, matrix notation

The above idea carries over to a linear combination of functions $f_j(x)$ for $1 \leq j \leq m$. For a vector $\vec{x} = (x_1, x_2, \ldots, x_k)^T$ we examine a function of the form

$$f(\vec{x}) = \sum_{j=1}^{m} p_j \cdot f_j(\vec{x})$$

The optimal values of the parameter vector $\vec{p} = (p_1, p_2, \ldots, p_m)^T$ have to be determined. Thus we try to minimize the expression

$$\chi^2 = \|\vec{r}\|^2 = \sum_{i=1}^{n} (f(x_i) - y_i)^2 = \sum_{i=1}^{n} \left(\left(\sum_{j=1}^{m} p_j \cdot f_j(x_i) \right) - y_i \right)^2$$

Using the vector and matrix notations

$$\vec{p} = \begin{pmatrix} p_1 \\ p_2 \\ \vdots \\ p_m \end{pmatrix} \quad , \quad \vec{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} \quad , \quad \mathbf{F} = \begin{bmatrix} f_1(x_1) & f_2(x_1) & \ldots & f_m(x_1) \\ f_1(x_2) & f_2(x_2) & \ldots & f_m(x_2) \\ \vdots & \vdots & \ddots & \vdots \\ f_1(x_n) & f_2(x_n) & \ldots & f_m(x_n) \end{bmatrix}$$

we have to minimize the expression

$$\|\vec{r}\|^2 = \|\mathbf{F} \cdot \vec{p} - \vec{y}\|^2 = \langle \mathbf{F} \cdot \vec{p} - \vec{y},\, \mathbf{F} \cdot \vec{p} - \vec{y} \rangle$$

leading again to the necessary condition

$$\mathbf{X} \cdot \vec{p} = \left(\mathbf{F}^T \cdot \mathbf{F}\right) \cdot \vec{p} = \mathbf{F}^T \cdot \vec{y}$$

This is a system of n linear equations for the unknown n–vector $\vec{p}$. Once we have the optimal parameter vector $\vec{p}$ we can compute the values of the regression curve with a matrix multiplication.

$$(\mathbf{F} \cdot \vec{p})_i = \sum_{j=1}^{m} f_j(x_i) \cdot y_j$$

As an example we try to fit a parabola

$$y = p_1 \cdot 1 + p_2 \cdot x + p_3 \cdot x^2$$

through the points given in the above example. The matrix $\mathbf{F}$ is given by

$$\mathbf{F} = \begin{bmatrix} 1 & x_1 & x_1^2 \\ 1 & x_2 & x_2^2 \\ 1 & x_3 & x_3^2 \\ 1 & x_4 & x_4^2 \\ 1 & x_5 & x_5^2 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 1 & 1 \\ 1 & 2 & 2^2 \\ 1 & 3.5 & 3.5^2 \\ 1 & 4 & 4^2 \end{bmatrix}$$

This can be coded leading to the result in Figure 2.13 and a residual of $\|\vec{r}\|^2 \approx 0.89$. This residual is, as expected, smaller than the residual for a straight line fit.

Octave

```
x = [0; 1; 2; 3.5; 4];
y = [-0.5; 1; 2.4; 2.0; 3.1];

F = [ones(length(x),1) x x.^2]
p = (F'*F)\(F'*y)
residual = norm(F*p-y)

xn = [-1:0.1:5]';
yn = p(1) + p(2)*xn + p(3)*xn.^2;
plot(x,y,'+r',xn,yn)
```

2.2.3 Estimation of the Variance of parameters

Using the above results (for the parabola fit) we can determine the residual vector

$$\vec{r} = \mathbf{F} \cdot \vec{p} - \vec{y}$$

and then the mean and variance $V = \sigma^2$ of the y–errors can be estimated. The estimation is valid if all y–errors are assumed to be of equal size, i.e. we assume a-priori that the errors are given by a normal distribution.

Octave

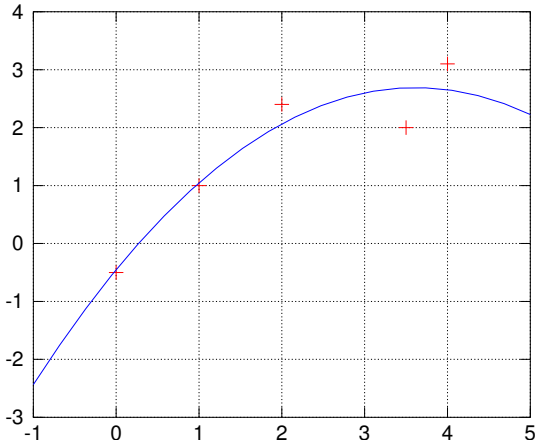


Figure 2.13: Regression of a parabola

```
residual = F*p-y;
mean(residual)
sum(residual.^2)/(length(residual)-3)  % 3 parameters in parabola
```

The mean should equal zero and the standard deviation $\sigma \approx \sqrt{0.39} \approx 0.63$ is an estimate for the errors in the y–values. Smaller values of σ indicate that the values of y are closer of the regression curve.

In most applications the values of the parameters p_j contain the essential information. It is often important to know how reliable the obtained results are, i.e. we want to know the variance of the determined parameter values. To this end consider

$$\left(\mathbf{F}^T \cdot \mathbf{F}\right) \cdot \vec{p} = \mathbf{F}^T \cdot \vec{y}$$

and thus

$$\vec{p} = \left(\mathbf{F}^T \cdot \mathbf{F}\right)^{-1} \cdot \mathbf{F}^T \cdot \vec{y} = \mathbf{M} \cdot \vec{y}$$

or

$$p_j = \sum_{i=1}^{n} m_{j,i}\, y_i \quad \text{for} \quad 1 \le j \le m$$

where

$$\mathbf{M} = [m_{j,i}]_{1\le j\le m\,,1\le i\le n} = \left(\mathbf{F}^T \cdot \mathbf{F}\right)^{-1} \cdot \mathbf{F}^T$$

is a $m \times n$–matrix, where $m < n$ (more columns than rows).

This explicit representation of p_j allows[2] to compute the variance $V(p_j)$ of the parameters p_j, using the estimated variance σ^2 of the y–values. The result is

$$V(p_j) = \sum_{i=1}^{n} m_{j,i}^2\, \sigma^2 \quad \text{where} \quad \sigma^2 = \frac{1}{n-m} \sum_{i=1}^{n} r_1^2$$

[2] If z_k are **independent** random variables given by a normal distribution with variances $V(z_k)$, then a linear combination of the z_i also leads to a normal distribution. The variances are given by the following rules:

$$\begin{aligned} V\left(z_1 + y_2\right) &= V\left(z_1\right) + V\left(z_2\right) \\ V\left(\alpha_1\, z_1\right) &= \alpha_1^2\, V\left(z_1\right) \\ V\left(\sum \alpha_i\, z_i\right) &= \sum \alpha_i^2\, V\left(z_i\right) \end{aligned}$$

All the above computations can be packed in a function file `LinearRegression.m`[3] to compute the optimal values of the parameters and the estimated variances.

Octave

```
function [p,y_var,r,p_var] = LinearRegression1(F,y)

p = (F'*F)\(F'*y);          % estimate the values of the parameters

residual = F*p-y;           % compute the residual vector
r = norm(residual);         % and its norm
y_var = var(residual);      % variance of the y-errors

M = inv(F'*F)*F';
M = M.*M;                   % square each entry in the matrix M
p_var = sum(M,2)*y_var;     % variance of the parameters
```

The function `LinearRegression()` now allows to solve the straight line problem leading to Figure 2.12 with only a few lines of code.

Octave

```
x = [0; 1; 2; 3.5; 4];  y = [-0.5; 1; 2.4; 2.0; 3.1];
F = [ones(length(x),1) x];
[p,y_v,r,p_v] = LinearRegression(F,y)
sqrt(p_v)
```

The result shows that the equation for the optimal straight line is

$$y = 0.025 + 0.75 \cdot x$$

where the constant contribution (0.025) has a standard deviation of 0.475 and the standard deviation of the slope (0.75) is given by 0.184 . This information should prevent you from showing too many digits when analyzing measured data.

To fit a parabola through the same points replace one line only by

Octave

```
F = [ones(length(x),1) x x.^2];
```

2.2.4 Example 1: Intensity of light of an LED depending on the angle of observation

The intensity of the light emitted by an LED will depend on the angle α of observation. The data sheets of the supplier should show this information. A sample of real data is stored in the file `LEDdata.txt`.The script `LEDdata.m` also contains the data. In section 2.9.2 you find the information on how to import the data from the data sheet into *Octave*. Then Figure 2.14(b) may be then generated by the code below.

Octave

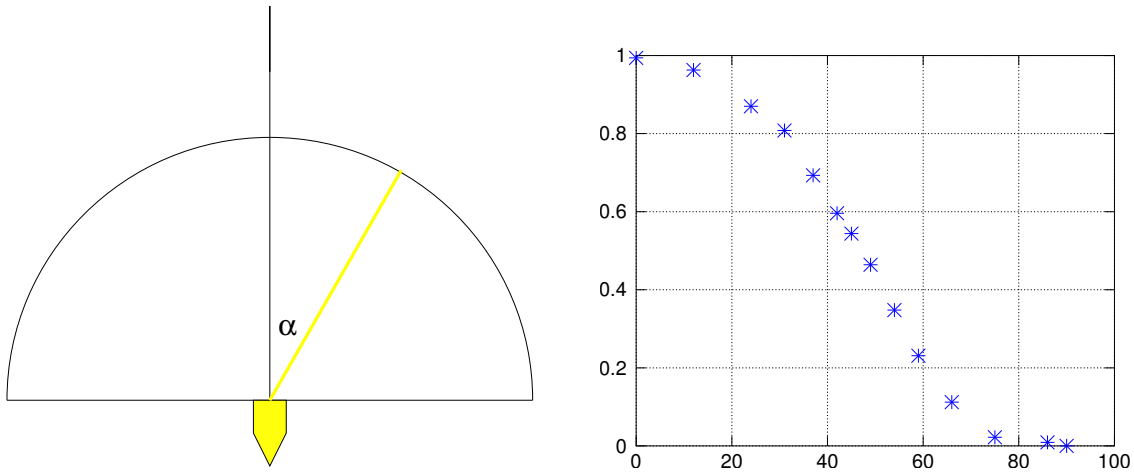
```
LEDdata; % load the data
figure(1);
plot(angle,intensity,'*');
```

To do further analysis it can be useful to have a formula for the intensity as function of the angle and linear regression is one of the options on how to obtain such a formula. The following code will fit a polynomial of degree 4 through those points and then display the result in Figure 2.15. The resulting parameters point towards an intensity function

$$T(\alpha) = 124.28 + 0.1111\,\alpha - 4.0576 \cdot 10^{-3}\,\alpha^2 + 5.0299 \cdot 10^{-5}\,\alpha^3 - 2.1087 \cdot 10^{-7}\,\alpha^4$$

Octave

[3] A better implementation is given in Figure 2.17 on page 136 and thus the function name is temporarily set to `LinearRegression1()`



(a) setup of LED (b) relative intensity

Figure 2.14: Intensity of light as function of the angle

```
LEDdata; % load the data
n = 5;
F = ones(length(angle),n);
for k = 1:n
  F(:,k) = angle.^(k-1);
end

[p,int_var,r,p_var] = LinearRegression1(F,intensity);
[p,sqrt(p_var)]              % display the estimated values for the parameters

al = (0:1:90)'; % consider angles from 0 to 90 degree
Fnew = ones(length(al),n);
for k = 1:n
  Fnew(:,k) = al.^(k-1);
end

Inew = Fnew*p;
plot(angle,intensity,'*',al,Inew)
grid on
xlabel('angle');ylabel('intensity')
```

The result in Figure 2.15 is useless since the estimated variances of the parameters are of the same order of magnitude as the values[4]. We need to find the reason for the failure and how to eliminate the problems.

The previous implementation of the linear regression algorithm has to solve a system of equations with the matrix $\mathbf{F}' \cdot \mathbf{F}$. With the help of

Octave

```
F'*F
-->
   1.4000e+01   6.7000e+02   4.1114e+04   2.8161e+06   2.0767e+08
   6.7000e+02   4.1114e+04   2.8161e+06   2.0767e+08   1.6113e+10
   4.1114e+04   2.8161e+06   2.0767e+08   1.6113e+10   1.2949e+12
   2.8161e+06   2.0767e+08   1.6113e+10   1.2949e+12   1.0666e+14
   2.0767e+08   1.6113e+10   1.2949e+12   1.0666e+14   8.9414e+15
```

[4]Previous releases of MATLAB and *Octave* generated numbers which were obviously wrong. This was very useful for didactical purposes, but less so for real world problems.

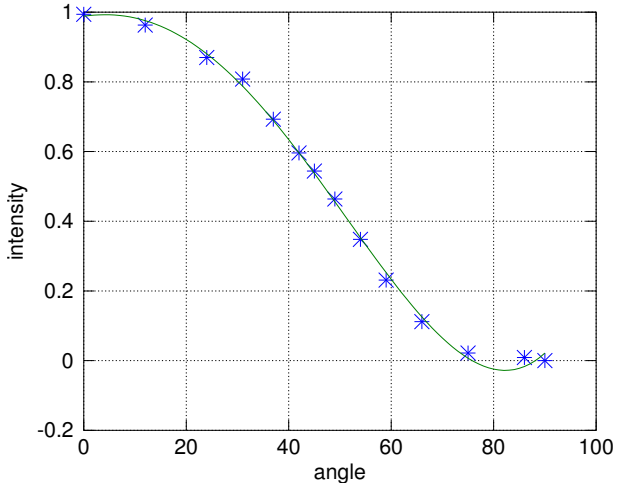


Figure 2.15: Intensity of light as function of the angle and a first regression curve

we see that the matrix contains numbers of the order 1 and of the order 10^{16} and one should not be surprised by trouble when solving such a system of equations. Mathematically speaking we have a **condition number** that is very large (10^{16}) and thus we will loose many digits of precision. Entries of vastly different sizes are an indication for large condition numbers, but other effects also matter and you will have to consult specialized literature or a mathematician to obtain more information.

There are different measures to be taken to avoid the problem. For a good solution they should all be taken into account.

1. **Rescaling**
   For a polynomial for degree 4 and angles of $90°$ the matrix $\mathbf{F}$ will contain numbers of the size 1 and 90^4. Thus $\mathbf{F}' \cdot \mathbf{F}$ will contain number of the size $90^8 \approx 100^8 = 10^{16}$. If we switch to radians instead of degrees this will be reduced to $(\frac{\pi}{2})^8 \approx 40$ and thus should avoid the problem. The code below will generate a good solution.

Octave

```
LEDdata;
scalefactor = 180/pi;
angle = angle/scalefactor;

n = 5;
F = ones(length(angle),n);
for k = 1:n
  F(:,k) = angle.^(k-1);
end

[p,int_var,r,p_var] = LinearRegression1(F,intensity);
result = [p sqrt(p_var)]      % display the estimated values for the parameters

al = ((0:1:90)')/scalefactor; % consider angles from 0 to 90 degree

Fnew = ones(length(al),n);
for k = 1:n
  Fnew(:,k) = al.^(k-1);
end

Inew = Fnew*p;
```

```
plot(angle*scalefactor,intensity,'*',al*scalefactor,Inew)
grid on
xlabel('angle');ylabel('intensity')
```

This is confirmed by the smaller condition number.

Octave

```
cond(F'*F)
-->
2.1427e+05
```

2. **Better choice of basis functions**
Since the intensity function $I(\alpha)$ has to be symmetric with respect to α, i.e. $I(-\alpha) = I(\alpha)$, there can be no contributions of the form α, α^3 or α^5. Thus we seek a good fit for a function of the type

$$I(\alpha) = p_1 + p_2\,\alpha^2 + p_3\,\alpha^4$$

The code below leads to the result in Figure 2.16. The condition number of $\mathbf{F}'\cdot\mathbf{F}$ is approximately 200 and thus poses no problem. The result in Figure 2.16 is now useful for further investigations and the computations indicate that the intensity is approximated by

$$I(\alpha) = 1.02951 - 0.95635\,\alpha^2 + 0.21890\,\alpha^4$$

The code is a slight modification of the previous code.

Octave

```
LEDdata;
scalefactor = 180/pi;
angle = angle/scalefactor;
n = 3;
F = ones(length(angle),n);
for k = 1:n
  F(:,k) = angle.^(2*(k-1));
end

[p,int_var,r,p_var] = LinearRegression1(F,intensity);
result = [p,sqrt(p_var)]        % display the estimated values for the parameters

al = ((0:1:90)')/scalefactor; % consider angles from 0 to 90 degree

Fnew = ones(length(al),n);
for k = 1:n
  Fnew(:,k) = al.^(2*(k-1));
end

Inew = Fnew*p;
plot(angle*scalefactor,intensity,'*',al*scalefactor,Inew)
grid on
xlabel('angle');ylabel('intensity')
```

This point is by far the most important aspect to consider when using the linear regression method.

> Choose your basis function for linear regression very carefully,
> based on information about the system to be examined.

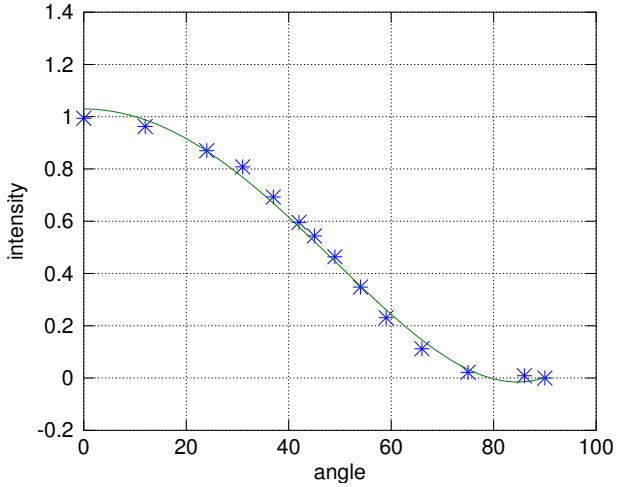


Figure 2.16: Intensity of light as function of the angle and regression with an even function

There are many software packages (*Mathematica*, `MATLAB`, *Octave*, Excel, ...) that allow to perform linear regression with polynomials of high degrees. This author is not aware of **one single problem** where a polynomial of high degree leads to useful information. All software behave according to the **GIGO**[5] principle.

3. **QR decomposition instead of $\mathbf{F}' \cdot \mathbf{F}$ matrix**
   Idea and consequences of this change in algorithm are based on QR factorization and are given in the nextb section. Any serious implementation of a linear regression method should use this modification. In all the above code the function `LinearRegression1()` has to be replaced by `LinearRegression()` to take advantage of the improved algorithm.

2.2.5 QR factorization and linear regression

For a $n \times m$ matrix $\mathbf{F}$ with more rows than columns ($n > m$) a **QR** decomposition of the matrix can be computed.

$$\mathbf{F} = \mathbf{Q} \cdot \mathbf{R}$$

where the $n \times n$ matrix $\mathbf{Q}$ is orthogonal ($\mathbf{Q}^{-1} = \mathbf{Q}^T$) and the $n \times m$ matrix $\mathbf{R}$ has an upper triangular structure.

$$\mathbf{R} = \begin{bmatrix} \mathbf{R}_u \\ \mathbf{0} \end{bmatrix} \quad \text{and} \quad \mathbf{Q} = \begin{bmatrix} \mathbf{Q}_l & \mathbf{Q}_r \end{bmatrix}$$

The two $m \times m$ matrices $\mathbf{R}_u$ and $\mathbf{Q}_l$ both square. Multiplying a vector $\vec{r} \in \mathbb{R}^n$ with the orthogonal matrix $\mathbf{Q}$ or its inverse $\mathbf{Q}^T$ corresponds to a rotation of the vector and thus will not change its length. This observation can be used to rewrite the linear regression problem from Section 2.2.2.

$$\begin{aligned}
\mathbf{F} \cdot \vec{p} - \vec{y} &= \vec{r} \quad \text{length to be minimized} \\
\mathbf{Q} \cdot \mathbf{R} \cdot \vec{p} - \vec{y} &= \vec{r} \quad \text{length to be minimized} \\
\mathbf{R} \cdot \vec{p} - \mathbf{Q}^T \cdot \vec{y} &= \mathbf{Q}^T \cdot \vec{r} \\
\begin{bmatrix} \mathbf{R}_u \cdot \vec{p} \\ \mathbf{0} \end{bmatrix} - \begin{bmatrix} \mathbf{Q}_l^T \cdot \vec{y} \\ \mathbf{Q}_r^T \cdot \vec{y} \end{bmatrix} &= \begin{bmatrix} \mathbf{Q}_l^T \cdot \vec{r} \\ \mathbf{Q}_r^T \cdot \vec{r} \end{bmatrix}
\end{aligned}$$

[5] Garbage In, Garbage Out

Since the vector $\vec{p}$ does not change the lower part of the above system, the problem can be replaced by the smaller system of equations shown below.

$$\mathbf{R}_u \cdot \vec{p} - \mathbf{Q}_l^T \cdot \vec{y} = \mathbf{Q}_l^T \cdot \vec{r} \quad \text{length to be minimized}$$

Obviously this length is minimized if $\mathbf{Q}_l^T \cdot \vec{r} = \vec{0}$ and thus we find the reduced equations for the vector $\vec{p}$.

$$\begin{aligned} \mathbf{R}_o \cdot \vec{p} &= \mathbf{Q}_l^T \cdot \vec{y} \\ \vec{p} &= \mathbf{R}_o^{-1} \cdot \mathbf{Q}_l^T \cdot \vec{y} \end{aligned}$$

In *Octave* the above algorithm can be implemented with two commands only.

Octave

```
[Q,R] = qr(F,0);
p = R\(Q'*y);
```

It can be shown that the condition number for the $\mathbf{QR}$ algorithm is much smaller that the condition number for the algorithm based on $\mathbf{F}^T \cdot \mathbf{F} \cdot \vec{p} = \mathbf{F}^T \cdot \vec{y}$. Thus there are fewer accuracy problems to be expected and we obtain results with higher reliability.

2.2.6 Weighted linear regression

The general method

So far we minimized the length of the residual vector

$$\vec{r} = \mathbf{F} \cdot \vec{p} - \vec{y}$$

using the standard length $\|\vec{r}\|^2 = \sum_{i=1}^{n} r_1^2$. There are situations where not all errors have equal weight and thus we try to minimize a weighted length

$$\|\vec{r}\|_W^2 = \sum_{i=1}^{n} w_i^2 \, r_1^2 = \langle \mathbf{W} \cdot \vec{r}, \, \mathbf{W} \cdot \vec{r} \rangle$$

where the weight matrix $\mathbf{W}$ is given by

$$\mathbf{W} = \operatorname{diag}(\vec{w}) = \begin{bmatrix} w_1 & & & \\ & w_2 & & \\ & & \ddots & \\ & & & w_n \end{bmatrix}$$

A large value of the weight w_i implies that an error r_i in that component has large weight. Thus the algorithm will try to keep r_i small.

Now an algorithm similar to the previous section can be applied to estimate the optimal values for the parameters $\vec{p}$.

$$\begin{aligned} \mathbf{F} \cdot \vec{p} - \vec{y} &= \vec{r} \quad \text{weighted length to be minimized} \\ \mathbf{W} \cdot \mathbf{F} \cdot \vec{p} - \mathbf{W} \cdot \vec{y} &= \mathbf{W} \cdot \vec{r} \quad \text{standard length to be minimized} \\ \mathbf{Q} \cdot \mathbf{R} \cdot \vec{p} - \mathbf{W} \cdot \vec{y} &= \mathbf{W} \cdot \vec{r} \quad \text{standard length to be minimized} \\ \mathbf{R} \cdot \vec{p} - \mathbf{Q}^T \cdot \mathbf{W} \cdot \vec{y} &= \mathbf{Q}^T \cdot \mathbf{W} \cdot \vec{r} \\ \begin{bmatrix} \mathbf{R}_u \cdot \vec{p} \\ \mathbf{0} \end{bmatrix} - \begin{bmatrix} \mathbf{Q}_l^T \cdot \mathbf{W} \cdot \vec{y} \\ \mathbf{Q}_r^T \cdot \mathbf{W} \cdot \vec{y} \end{bmatrix} &= \begin{bmatrix} \mathbf{Q}_l^T \cdot \mathbf{W} \cdot \vec{r} \\ \mathbf{Q}_r^T \cdot \mathbf{W} \cdot \vec{r} \end{bmatrix} \\ \mathbf{R}_u \cdot \vec{p} &= \mathbf{Q}_l^T \cdot \mathbf{W} \cdot \vec{y} \\ \vec{p} &= \mathbf{R}_u^{-1} \cdot \mathbf{Q}_l^T \cdot \mathbf{W} \cdot \vec{y} \end{aligned}$$

This algorithm is implemented in Figure 2.17 (see page 136).

To estimate the variances of the parameters $\vec{p}$ we have to use assumptions on the variances σ_i of the y_i values. A heuristic argument in the next section motivates the estimate

$$\sigma_j^2 \approx \frac{1}{w_j^4} \frac{1}{n-m} \sum_{i=1}^{n} r_i^2 \, w_i^4$$

and then use

$$\vec{p} = \mathbf{R}_u^{-1} \cdot \mathbf{Q}_l^T \cdot \mathbf{W} \cdot \vec{y} = \mathbf{M} \cdot \vec{y}$$

to conclude

$$\begin{aligned} p_j &= \sum_{i=1}^{n} m_{j,i} \, y_i \quad \text{for} \quad 1 \le j \le m \\ V(p_j) &= \sum_{i=1}^{n} m_{j,i}^2 \, \sigma_i^2 \quad \text{for} \quad 1 \le j \le m \end{aligned}$$

If we set all weights to $w_i = 1$ this leads back to the results in section 2.2.3 .

Geometric interpretation of the weights

Let $\vec{y}$ be a vector and weights w_i. Then find a such that

$$\chi^2 = \sum_{i=1}^{n} (a - y_i)^2 \, w_i^2$$

is minimized. This leads to the necessary condition

$$\begin{aligned} 0 &= \frac{\partial}{\partial a} \sum_{i=1}^{n} (a - y_i)^2 \, w_i^2 = 2 \sum_{i=1}^{n} (a - y_i) \, w_i^2 \\ a &= \frac{\sum_{i=1}^{n} w_i^2 \, y_i}{\sum_{i=1}^{n} w_i^2} \end{aligned}$$

To obtain an interpretation of the effect of the weights ω_i we seek a condition on the values y_i such that the weighted error

$$\chi^2 = \sum_{i=1}^{n} (y_i - a)^2 \, w_i^2$$

is minimized. Using the Lagrange multiplier rule we find the necessary condition

$$\begin{aligned} \frac{\partial}{\partial y_j} \sum_{i=1}^{n} |y_i - a| &= \lambda \, \frac{\partial}{\partial y_j} \sum_{i=1}^{n} (y_i - a)^2 \, w_i^2 \\ \pm 1 &= \lambda \, 2 \, (y_j - a) \, w_j^2 \\ (y_j - a)^2 \, w_j^4 &= \text{independent on } j \end{aligned}$$

1. For the uniform weights $w_i = 1$ we rediscover the arithmetic average

$$a = \frac{1}{n} \sum_{i=1}^{n} y_i$$

and the total quadratic error is minimized if $|y_i - a|$ is independent on i. Thus this weight is appropriate if the absolute errors are uniformly distributed.

2. Choose $w_i = 1/\sqrt{y_i}$ to find

$$a = \frac{n}{\sum_{i=1}^{n}(1/y_i)}$$

and the total quadratic error is minimized if

$$(y_i - a)^2 \, w_i^4 = \left(\frac{y_i - a}{y_i}\right)^2$$

is independent on i. Thus this weight is appropriate if the relative errors are uniformly distributed.

In the previous section we assumed that the relative errors are given by a normal distribution and then we estimated σ_i^2 (the variance of y_i). For this purpose we first estimate the variance of the relative errors. Use the fact that the average relative error equals 0 to conclude that

$$\frac{\sigma_j^2}{y_j^2} \approx \frac{1}{n} \sum_{i=1}^{n} \frac{r_i^2}{y_i^2}$$

3. For the general weighted average we conclude in a similar fashion that the weights w_j are appropriate if the weighted errors $|y_i - a| \, w_i^2$ are evenly spread. This can only be justified with knowledge about the problem at hand. Then we use the estimated variance of this expression to conclude

$$\sigma_j^2 \, w_j^4 \approx \frac{1}{n} \sum_{i=1}^{n} w_i^4 \, r_i^2$$

This leads to the estimate for σ_j in the previous section. The method is implemented in the code of `LinearRegression()` in Figure 2.17.

Minimize relative errors

If $y_i > 0$ we can consider the special weights $w_i = 1/\sqrt{y_i}$ and we will minimize the expression

$$\chi^2 = \sum_{i=1}^{n} \frac{r_i^2}{y_i}$$

As an example consider the results of

Octave

```
x = [0;4;4];   y = [1;0.5;1.5];
F = [ones(length(x),1) x];

p1 = LinearRegression(F,y)
y1 = F*p1;
p2 = LinearRegression(F,y,1./sqrt(abs(y)))
y2 = F*p2;

axis([-0.5 4.5 0 2]);
plot(x,y,'*r',x,y1,'b',x,y2,'g')
```

Both regression lines will pass through the point $(0\,,\,1)$. The uniform weights lead to a horizontal line through the point $(4\,,\,1)$ and the two errors $|0.5 - 1| = |1.5 - 1|$ coincide. The weights $1/\sqrt{y}$ lead to a large weight for the point $(4\,,\,0.5)$ and a smaller weight for $(4\,,\,1.5)$. Thus the second line will move closer to the bottom point. The line passes through the point $(4\,,\,0.75)$. The relative errors $\frac{|0.5-0.75|}{0.5} = \frac{|1.5-0.75|}{1.5}$ coincide.

2.2.7 Code for the function `LinearRegression()`

The structure of the function file has the typical structure of a well written *Octave* function file.

- The first line has to list the function name, the parameters and the return values.
- The subsequent lines (starting with %) give some documentation and instructions on the command `LinearRegression()`. This text will be displayed by the command `help LinearRegression`. A description of the parameters and the return values is given.
- The function verifies that the correct number of arguments (2 or 3) is given, otherwise returns with a message.
- The correct size of the arguments (`F` and `y`) is verified. An error message is displayed if the size of matrix and vector do not match.
- Finally the necessary computations are carried out.
- The estimated variances of the parameters are only computed if the output is also used. This is implemented by counting the return arguments of the call of the function (`nargout`).

The resulting function can be called with 1, 2, 3 or 4 return arguments. The function will return only the necessary values.

- `p = LinearRegression(F,y)` will return the estimated value of the parameters $\vec{p}$ only .
- `[p,y_var] = LinearRegression(F,y)` will also return the variance of the y–error.
- `[p,y_var,r,p_var] = LinearRegression(F,y)` will return all 4 results.

Find the complete code in Figure 2.17.

LinearRegression.m

```
function [p,y_var,r,p_var] = LinearRegression(F,y,weight)

% general linear regression
%
% [p,y_var,r,p_var] = LinearRegression(F,y)
% [p,y_var,r,p_var] = LinearRegression(F,y,weight)
%
% determine the parameters p_j  (j=1,2,...,m) such that the function
% f(x) = sum_(i=1,...,m) p_j*f_j(x) fits as good as possible to the
% given values y_i = f(x_i)
%
% parameters
% F  n*m matrix with the values of the basis functions at the support points
%    in column j give the values of f_j at the points x_i  (i=1,2,...,n)
% y  n column vector of given values
% weight  n column vector of given weights
%
% return values
% p     m vector with the estimated values of the parameters
% y_var estimated variance of the error
% r     weighted norm of residual
% p_var estimated variance of the parameters p_j

if ((nargin < 2)|(nargin>=4))
 usage('wrong number of arguments in [p,y_var,r,p_var]=LinearRegression(F,y)');
end

[rF, cF] = size(F);  [ry, cy] = size(y);
if ( (rF ~= ry)|(cy>1))
  error ('LinearRegression: incorrect matrix dimensions');
end

if (nargin==2) % set uniform weights if not provided
  weight = ones(size(y));
end

wF = spdiags(weight,0,ry,ry)*F;

[Q,R] = qr(wF,0);                 % estimate the values of the parameters
p = R\(Q'*(weight.*y));

residual = F*p-y;                 % compute the residual vector
r = norm(weight.*residual);       % and its weighted norm
% variance of the weighted y-errors
y_var = sum((residual.^2).*(weight.^4))/(rF-cF);

if nargout>3    % compute variance of parameters only if needed
  M = inv(R)*Q'*spdiags(weight,0,ry,ry);
  M = M.*M;                         % square each entry in the matrix M
   p_var = M*(y_var./(weight.^4));  % variance of the parameters
end
```

Figure 2.17: Code for the command `LinearRegression()`

2.2.8 Example 2: Performance of a linear motor

In his diploma thesis in 2005 Aloïs Pfenniger examined the forces of a linear magnetic motor as function of length and diameter of the coils used to construct the motor. A typical configuration is displayed in Figure 2.18. With a lengthy computation (approximately 4 hours per configuration) he computed the forces for 25 different configurations. The result is shown in Figure 2.19.

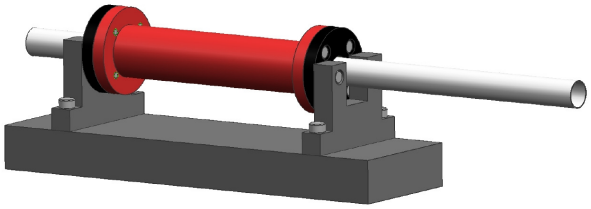


Figure 2.18: A magnetic linear motor

Octave

```
PfennigerData;
plot(long(:,1),force(:,1),long(:,2),force(:,2),long(:,3),force(:,3),...
     long(:,4),force(:,4),long(:,5),force(:,5));
xlabel('length of coil'); ylabel('force');

mesh(diam,long,force)
xlabel('diameter of coil'); ylabel('length of coil'); zlabel('force');
view(-10,30);
```

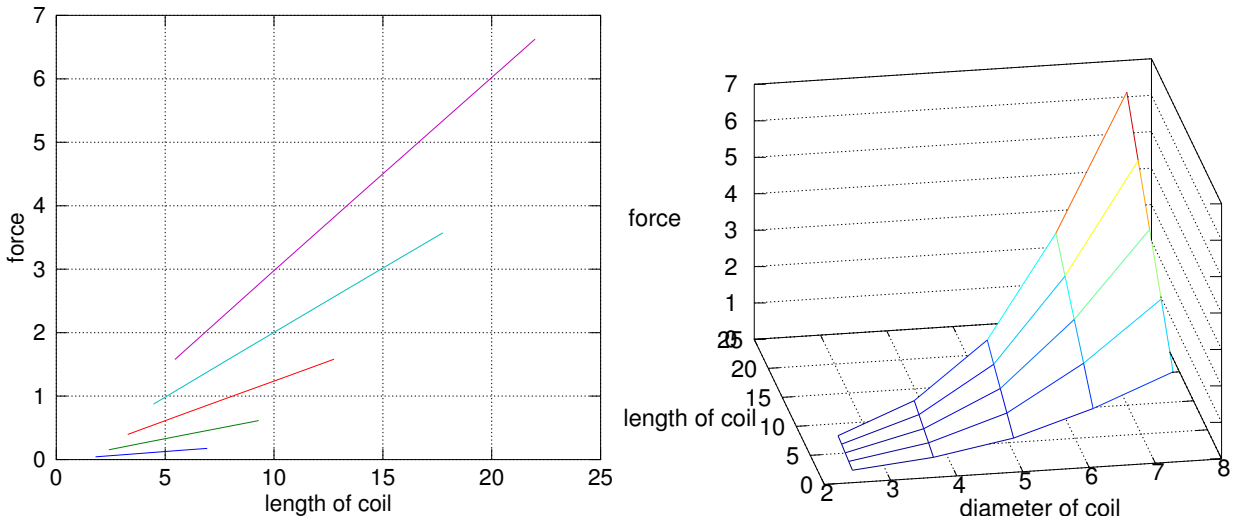


Figure 2.19: Force as function of length of coils, for 5 different diameters

General function

These graphs indicate that the force f might depend linearly on the length l and quadratically on the diameter d.

$$f(l,d) = p_1 + p_2\, l + p_3\, l\, d + p_4\, l\, d^2$$

A call of `LinearRegression()` and `Mesh()`

Octave

```
diam1 = diam(:); long1=long(:); force1=force(:);

F = [ones(size(long1)) long1 long1.*diam1 long1.*(diam1.^2)];
coef = LinearRegression(F,force1)

[L,DIA] = meshgrid(2:30,2:0.5:8);
forceA = coef(1)+L.*(coef(2)+coef(3)*DIA+coef(4)*DIA.^2);
figure(2);
mesh(DIA,L,forceA)
xlabel('diameter of coil'); ylabel('length of coil'); zlabel('force');
view(-10,30);
```

leads to the approximate function

$$f(l,d) = -0.0252 + 0.0193\,l - 0.0114\,l\,d + 0.0065\,l\,d^2$$

and the residual of $r \approx 0.065$ gives an indication on the size of the error. The results generated by the code

Octave

```
forceA2  = coef(1)+long.*(coef(4)*diam.^2+coef(3)*diam+coef(2));
maxerror = max(max(abs(forceA2-force)))
maxrelerror = max(max(abs(forceA2-force)./force))
```

show the maximal error of 0.04 and a relative error of 10% .

If we seek to minimize the relative error we have to replace the call of `LinearRegression()` by

Octave

```
[coef,f_var,r,coef_var] = LinearRegression(F,force1,1./sqrt(force1))
```

and will find a larger maximal error of 0.05 but a smaller relative error of only 3% . The approximate function is

$$f(l,d) = -0.00639 + 0.00662\,l - 0.00730\,l\,d + 0.00617\,l\,d^2$$

The contour plot in Figure 2.20 is generated by the code below. The levelcurves are 0.5 apart, with values from 0.5 to 8 .

Octave

```
contour(DIA,L,forceA,[0.5:0.5:8])
xlabel('diameter of coil'); ylabel('length of coil');
```

Adapted function

Physical reasoning might make believe that the form of the function should be simpler than in the previous section. We search a solution of the form

$$f(l,d) = p_1\,l + p_2\,l\,d^2$$

and apply a weighted linear regression to keep the relative errors small.

Octave

```
F = [long1 long1.*(diam1.^2)];
[coef,f_var,r,coef_var] = LinearRegression(F,force1,1./sqrt(force1))

forceB = L.*(coef(1)+coef(2)*DIA.^2);

figure(1);
```

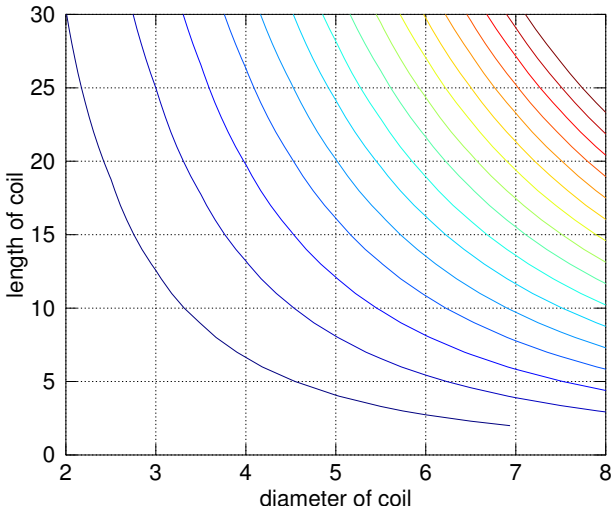


Figure 2.20: Level curves for force as function of length and diameter of coil

```
mesh(DIA,L,forceB)
xlabel('diameter of coil'); ylabel('length of coil'); zlabel('force');
view(-10,30);
figure(2);
contour(DIA,L,forceA,[0.5:0.5:8])
xlabel('diameter of coil'); ylabel('length of coil');

forceB2 = long.*(coef(1)+coef(2)*diam.^2);
maxrelerror = max(max(abs(forceB2-force)./force))
maxerror = max(max(abs(forceB2-force)))
```

The graphical result can be seen in Figure 2.21 and the numerical results indicates a solution

$$f(l,d) = -0.00990\, l + 0.00543975\, l\, d^2$$

The maximal error is 0.1 and the maximal relative error is 5% . With the above function further computations can be carried out quite easily.

2.2.9 Example 3: Calibration of an orientation sensor

Description of the problem

With the help of two accelerations sensors one can determine the vertical (x) and horizontal (y) components of the gravitational field. Under perfect conditions we would find

$$x = g\,\cos(\alpha) \quad \text{and} \quad y = g\,\sin(\alpha)$$

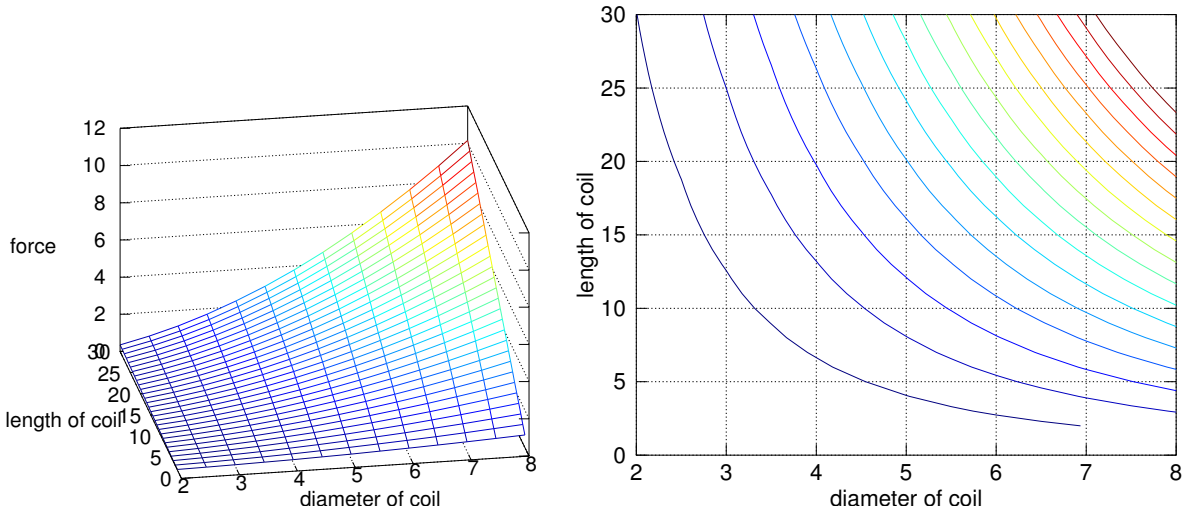
where α is the angle by which the device was rotated, clockwise. Typical sensor yield a signal proportional to the applied field, but there might be an offset. The sensor might not be perfectly orthogonal and not be mounted perfectly. Thus we actually receive signals of the type

$$x = x_0 + r_x\,\cos(\alpha - \phi_x) \quad \text{and} \quad y = y_0 + r_y\,\sin(\alpha - \phi_y)$$

If the orientation of the device is to be determined we have to compute α, given the values of x and y. Use

$$\frac{x - x_0}{r_x} = \cos(\alpha - \phi_x) \quad \text{and} \quad \frac{y - y_0}{r_y} = \sin(\alpha - \phi_y)$$

where the parameters x_0, y_0, r_x, r_y, ϕ_x and ϕ_y might be different for each sensor.



(a) the surface (b) the level curves

Figure 2.21: Computations with simplified function

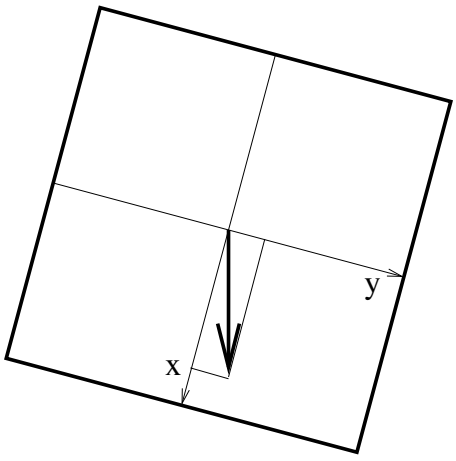


Figure 2.22: A slightly rotated direction sensor

Solution with the help of linear regression

Assume that the x direction sensor is mounted in the direction given by a vector $\vec{m}_x$. Its sensitivity is given by $\|\vec{m}_x\|$. Then the signal on the x–sensor is given by

$$s_x = \langle \vec{g}\,,\, \vec{m}_x \rangle + c_x$$

The constant c_x corresponds to the offset of the sensor, i.e. the sensors output signal for a zero input. For a number of given vectors $\vec{g}_i$ $(1 \leq i \leq n)$ and the resulting signals s_i we have to minimize the residual vector $\vec{r}$ determined by

$$\begin{bmatrix} g_{x,1} & g_{y,1} & 1 \\ g_{x,2} & g_{y,2} & 1 \\ g_{x,3} & g_{y,3} & 1 \\ & \vdots & \\ g_{x,n} & g_{y,n} & 1 \end{bmatrix} \cdot \begin{pmatrix} m_{x,1} \\ m_{x,2} \\ c_x \end{pmatrix} - \begin{pmatrix} s_1 \\ s_2 \\ s_3 \\ \vdots \\ s_n \end{pmatrix} = \begin{pmatrix} r_1 \\ r_2 \\ r_3 \\ \vdots \\ r_n \end{pmatrix}$$

A linear regression will give the optimal values vor $\vec{m}_x$ and c_x. Similar calculations can be applied for the y–sensor, leading to the best values for $\vec{m}_y$ and c_y.

Once the parameter values are determined we can compute the signal at the sensors for a given orientation of the $\vec{g}$ vector by

$$\vec{s} = \begin{pmatrix} s_x \\ s_y \end{pmatrix} = \begin{bmatrix} m_{x,1} & m_{x,2} \\ m_{y,1} & m_{y,2} \end{bmatrix} \cdot \begin{pmatrix} g_1 \\ g_2 \end{pmatrix} + \begin{pmatrix} c_x \\ c_y \end{pmatrix} = \mathbf{M} \cdot \vec{g} + \vec{c}$$

This can be solved for the vector g by

$$\vec{g} = \mathbf{M}^{-1}\,(\vec{s} - \vec{c})$$

This is the expression to determine the direction of the $\vec{g}$ vector as function of the signals $\vec{s}$ at the sensors. The angle β between the x axis and the $\vec{g}$ field the given by

$$\tan\beta = \frac{g_y}{g_x}$$

The above algorithm is implemented in the code below, using some simulated data.

Octave

```
OrientationData; %% read the values of alpha, x and y

axis('equal')
plot(x,y);
gx = cos(al); gy = sin(al);

F = [gx gy ones(size(al))];
[px,xvar,r,pvar] = LinearRegression(F,x);
[py,xvar,r,pvar] = LinearRegression(F,y);

mx = px(1:2); cx = px(3); my = py(1:2); cy = py(3);

m = [mx my]
c = [cx;cy]

minv = inv(m);

xn = F*px;  yn = F*py;
hold on
plot(xn,yn,'b')
```

This computation leads to Figure 2.23 and the numerical results below.

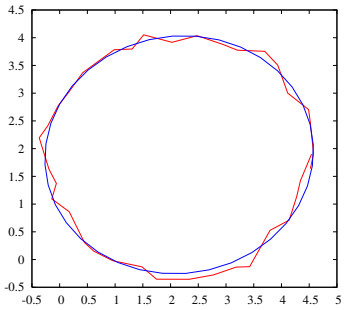


Figure 2.23: Measured data and the fitted circle

$$\vec{s} = \begin{pmatrix} s_x \\ s_y \end{pmatrix} = \begin{bmatrix} 2.40299 & -0.19664 \\ 0.30382 & 2.13793 \end{bmatrix} \cdot \begin{pmatrix} g_1 \\ g_2 \end{pmatrix} + \begin{pmatrix} 2.1549 \\ 1.8899 \end{pmatrix} = \mathbf{M} \cdot \vec{g} + \vec{c}$$

The diagonal dominance of this matrix indicates the two sensor have (almost) the same orientation as the coordinate axis. The numbers show that the x sensor has an offset of $x_0 \approx 2.155$ and an amplification of $r_x = \sqrt{m_{1,x}^2 + m_{x,2}^2} \approx 2.4221$. Similarly we determine the offset of the y–sensor as $y_0 \approx 1.89$ and an amplification of $r_y \approx 2.15$.

The results also allow to determine the angles of the sensors with respect to their axis. If $\vec{g}$ points in x–direction then we should obtain a maximal signal on the x sensor and if $\vec{g}$ points in y–direction we expect no signal on the x sensor. Thus the angle at which the sensor is mounted can be estimated by

$$\phi_x \approx \arctan\left(\frac{m_{x,1}}{m_{x,2}}\right)$$

and similary for the y–sensor. The code

Octave

```
atan2(mx(2),mx(1))*180/pi
atan2(my(2),my(1))*180/pi-90
```

leads to deviations of $\phi_x \approx 7.21°$ and $\phi_y \approx 5.26°$. The difference of these two angles corresponds to the angle between the two sensors.

To determine the direction of $\vec{g}$ using the measurements s_x and s_y we will use

$$\vec{g} = \mathbf{M}^{-1} \cdot (\vec{s} - \vec{c}) = \begin{bmatrix} 0.411365 & 0.037835 \\ -0.058458 & 0.462365 \end{bmatrix} \cdot \begin{pmatrix} s_x - 2.1549 \\ s_y - 1.8899 \end{pmatrix}$$

This formula contains all calibration data for this (simulated) sensor.

Estimation of errors

In this subsection we want to estimate the variances of the parameters. The variances of $\mathbf{M}$, x_0 and y_0 are directly given by the return parameters of the command `p_var` of `LinearRegression()`. This might be sufficient to estimate the measurement errors for the vector $\vec{g}$.

As a next step we estimate the variances or r_x, r_y and the two angles ϕ_x and ϕ_y. Use the notation $p_2 = m_{x,1}$ and $p_3 = m_{x,2}$ and

$$r_x = \sqrt{m_{x,1}^2 + m_{x,2}^2} = \sqrt{p_2^2 + p_3^2} \quad , \quad \frac{\partial\, r_x}{\partial p_2} = \frac{p_2}{r_x} \quad \text{and} \quad \frac{\partial\, r_y}{\partial p_3} = \frac{p_3}{r_x}$$

to determine the variance of r_x as

$$V(r_x) = \frac{p_2^2}{r_x^2}\, V(p_2) + \frac{p_3^2}{r_x^2}\, V(p_3)$$

If $V(p_2) \approx V(p_3)$ this simplifies to $V(r_x) \approx V(p_2)$. The similar result is valid for $V(r_y)$.

Since $\frac{\partial}{\partial x} \arctan x = \frac{1}{1+x^2}$ we conclude

$$\begin{aligned}
\phi_x &= \arctan \frac{p_3}{p_2} \\
\frac{\partial}{\partial p_2}\, \phi_x &= \frac{1}{1 + (p_3/p_2)^2}\, \frac{-p_3}{p_2^2} = \frac{-p_3}{p_2^2 + p_3^2} = \frac{-p_3}{r_x^2} \\
\frac{\partial}{\partial p_3}\, \phi_x &= \frac{1}{1 + (p_3/p_2)^2}\, \frac{1}{p_2} = \frac{p_2}{p_2^2 + p_3^2} = \frac{p_2}{r_x^2} \\
V(\phi_x) &\approx \frac{1}{r_x^4}\, \left(p_3^2\, V(p_2) + p_2^2\, V(p_3)\right) \\
\sigma(\phi_x) &= \sqrt{V(\phi_x)} \approx \frac{1}{r_x^2}\, \sqrt{p_3^2\, V(p_2) + p_2^2\, V(p_3)}
\end{aligned}$$

and similarly[6] for ϕ_y. If $V(p_2) = V(p_3)$ this simplifies drastically to

$$\sigma(\phi_x) \approx \frac{\sqrt{V(p_2)}}{r_x} = \frac{\sigma(p_2)}{r_x}$$

If we redo the simulation with the data

$$x_0 = 0.5 \quad , \quad y_0 = 0 \quad , \quad r_x = 1 \quad , \quad r_y = 1.1 \quad , \quad \phi_x = 0^\circ \quad , \quad \phi_y = 5^\circ$$

and add a random perturbation to x and y of the size 0.001 (variance of the simulated values) then we find with identical computations the approximated values

$$x_0 \approx 0.5 \quad , \quad y_0 \approx 0 \quad , \quad r_x \approx 1 \quad , \quad r_y \approx 1.1 \quad , \quad \phi_x \approx 0.01^\circ \quad , \quad \phi_y \approx 4.99^\circ$$

and all variances $V(p_i)$ are of the order 10^{-8} and thus the standard deviations of the order 10^{-4}. This is small compared to the standard deviations of x and y, i.e. $\sigma(x) = \sigma(y) = 0.001$. One can verify that the standard deviation of ϕ_x for the above simulation is approximately 0.013° and thus explains the deviation of ϕ_x from zero.

2.2.10 Example 4: Analysis of a sphere using an AFM

In his diploma thesis in 2006 Ralph Schmidhalter used an atomic force microscope (AFM) to examine the surface of ball bearing balls, produced by the local company Micro Precision Systems (MPS). The AFM yields a measured height $h(x, y)$ as function of the horizontal coordinates x and y. One can then try to determine the radius R of the ball with the given data.

6

$$\tan \phi_y = \frac{-p_2}{p_3} \quad \Longrightarrow \quad \begin{array}{rcl} \frac{\partial}{\partial p_2}\, \phi_y &=& \frac{1}{1+(p_2/p_3)^2}\, \frac{-1}{p_3} = \frac{-p_3}{r_x^2} \\ \frac{\partial}{\partial p_3}\, \phi_y &=& \frac{1}{1+(p_2/p_3)^2}\, \frac{+p_2}{p_3^2} = \frac{p_2}{r_x^2} \end{array} \quad \Longrightarrow \quad V(\phi_x) \approx \frac{1}{r_x^4}\, \left(p_3^2\, V(p_2) + p_2^2\, V(p_3)\right)$$

Approximation of the sphere

Examine the height of a sphere with radius R and the highest point at $(x_0\,,\,y_0)$. Use the Taylor approximation $\sqrt{1+z} \approx 1 + \frac{1}{2}\,z$ to express the height h as a linear combination of the four functions 1, x, y and (x^2+y^2).

$$\begin{aligned} h(x,y) &= h_0 + \sqrt{R^2 - (x-x_0)^2 - (y-y_0)^2} \\ &= h_0 + R\,\sqrt{1 - \frac{1}{R^2}\,((x-x_0)^2 + (y-y_0)^2)} \\ &\approx h_0 + R - \frac{(x-x_0)^2}{2\,R} - \frac{(y-y_0)^2}{2\,R} \\ &= h_0 + R - \frac{x_0^2+y_0^2}{2\,R} + \frac{x_0}{R}\,x + \frac{y_0}{R}\,y - \frac{1}{2\,R}\,(x^2+y^2) \\ &= p_1 + p_2\,x + p_3\,y + p_4\,(x^2+y^2) \end{aligned}$$

where

$$\begin{aligned} p_1 &= h_0 + R - \frac{x_0^2+y_0^2}{2\,R} \\ p_2 &= \frac{x_0}{R} \\ p_3 &= \frac{y_0}{R} \\ p_4 &= -\frac{1}{2\,R} \end{aligned}$$

If all values of p_i are known we can solve for the parameters of the sphere.

$$\begin{aligned} R &= -\frac{1}{2\,p_4} \\ x_0 &= R\,p_2 \\ y_0 &= R\,p_3 \\ h_0 &= p_1 - R + \frac{x_0^2+y_0^2}{2\,R} \end{aligned}$$

In particular we can read of the estimated radius R of the sphere.

Reading the data, visualize and apply linear regression

The data is measured and then stored in a file `SphereData.csv`. The first few lines of the file are shown below. For each of 5 different values of y, ranging from 0 to 14 μm, 256 values of x were examined, also ranging from 0 to 14 μm.

SphereData.csv

```
0,0,5.044e-006
5.491e-008,0,5.044e-006
1.098e-007,0,5.042e-006
1.647e-007,0,5.044e-006
2.196e-007,0,5.048e-006
2.745e-007,0,5.05e-006
3.294e-007,0,5.052e-006
3.844e-007,0,5.054e-006
4.393e-007,0,5.055e-006
4.942e-007,0,5.058e-006
5.491e-007,0,5.06e-006
6.04e-007,0,5.06e-006
6.589e-007,0,5.06e-006
...
```

Each row contains the values of x, y and the height z. These values have to be read into variables in *Octave*. We may use the command `dlmread()` introduced in Section 1.2.8 .

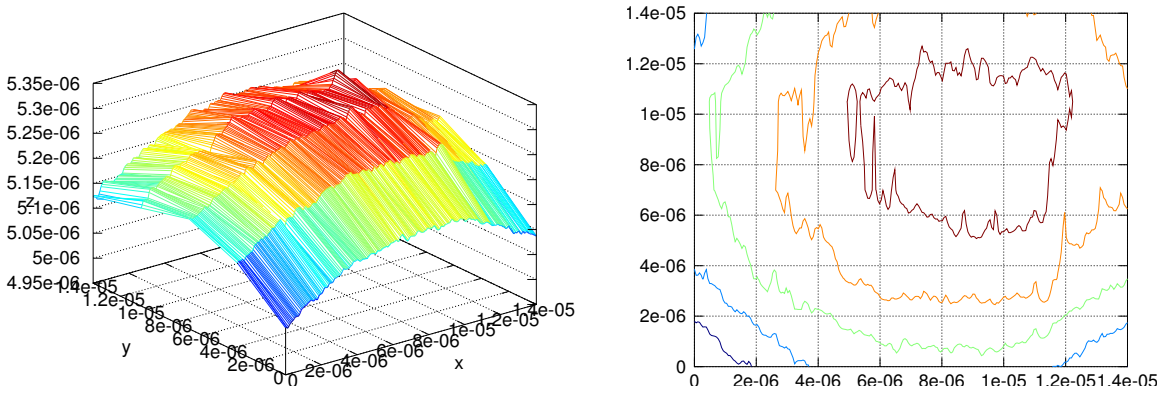
Octave

```
ttt = dlmread ('SphereData.csv');
x = tt(:,1); y = tt(:,2); z = tt(:,3);
```

As a next step we generate the plots with the surface and another plot with the level curves. Find the results in Figure 2.24.

Octave

```
steps = 5;
xx = reshape(x,N/steps,steps);
yy = reshape(y,N/steps,steps);
zz = reshape(z,N/steps,steps);

figure(1);    %% create a contour plot
contour(xx,yy,zz,5);
axis('equal')

figure(2);    %% create a surface plot
mesh(xx,yy,zz);
axis('normal');
```



(a) the surface

(b) the level curves

Figure 2.24: The surface of a ball and the level curves

A quick look at Figure 2.24 confirms that the top of the ball is within the scanned area. This allows for a quick check of the validity of the Taylor approximation at the start of this section.

The radius of the ball is approximately 300 μm and since the top is part of the scanned area we may estimate $|x - x_0| \leq 14\ \mu m$ and $|y - y_0| \leq 14\ \mu m$. This leads to

$$z = \frac{1}{R^2}\left((x - x_0)^2 + (y - y_0)^2\right) \leq 0.0044$$

and since the error of the approximation $\sqrt{1+z} \approx 1 + \frac{1}{2}z$ is typically given by $\frac{1}{8}z^2 \leq 2.5 \cdot 10^{-6}$. This this approximation error is considerably smaller than the variation in the measured values. This justifies the simplifying approximation.

Linear regression and an error analysis

The height is written as a linear combination of the functions 1, x, y and $x^2 + y^2$ and thus we have to construct the matrix

$$\mathbf{F} = \begin{bmatrix} 1 & x_1 & y_1 & x_1^2 + y_1^2 \\ 1 & x_2 & y_2 & x_2^2 + y_2^2 \\ 1 & x_3 & y_1 & x_3^2 + y_3^2 \\ & & \vdots & \\ 1 & x_n & y_n & x_n^2 + y_n^2 \end{bmatrix}$$

The we can determine the estimates for the parameters p_i and their standard deviations Δp_i and thus for the radius R and the center (x_0, y_0) .

Octave

```
F = [ones(size(x)) x y x.^2+y.^2];
[p,y_var,r,p_var] = LinearRegression(F,z);
Radius = -1/(2*p(4))
x0 = Radius*p(2)
y0 = Radius*p(3)
```

To estimate the standard deviations for R, x_0 and y_0 we need to apply the rules of error propagation and we find:

$$\begin{aligned} R &= \frac{-1}{2\,p_4} \\ \Delta R &\approx \left|\frac{\partial\, R}{\partial p_4}\right| \Delta p_4 = \frac{1}{2\,p_4^2}\,\Delta p_4 = 2\,R^2\,\Delta p_4 \\ x_0 &= R\,p_2 \\ \Delta x_0^2 &\approx \left(\frac{\partial\, x_0}{\partial p_2}\,\Delta p_2\right)^2 + \left(\frac{\partial\, x_0}{\partial R}\,\Delta R\right)^2 = (R\,\Delta p_2)^2 + (p_2\,\Delta R)^2 \\ \Delta x_0 &\approx \sqrt{(R\,\Delta p_2)^2 + (p_2\,\Delta R)^2} \\ \Delta y_0 &\approx \sqrt{(R\,\Delta p_3)^2 + (p_3\,\Delta R)^2} \end{aligned}$$

These results are readily translated into *Octave* code

Octave

```
deltaRadius = 2*Radius^2*sqrt(p_var(4))
deltaX0 = sqrt(Radius^2*p_var(2) + p(2)^2*deltaRadius^2)
deltaY0 = sqrt(Radius^2*p_var(3) + p(3)^2*deltaRadius^2)
```

leading to the results

$$\begin{aligned} R \pm \Delta R &\approx 296.4 \pm 1.7\ \mu m \\ x_0 \pm \Delta x_0 &\approx 8.46 \pm 0.07\ \mu m \\ y_0 \pm \Delta y_0 &\approx 8.77 \pm 0.07\ \mu m \end{aligned}$$

Thus we seem to have a valid measurement of the radius R and the center (x_0, y_0) of the circle.

Unfortunately different measurements of R lead to vastly different results, thus the problems requires some further analysis.

Regression with general second order surface

If we replace the approximation of a sphere by general surface of second order

$$h(x,y) = p_1 + p_2\,x + p_3\,y + p_4\,x^2 + p_5\,y^2 + p_6\,x\,y$$

The radii of curvature are determined by the function

$$f(x,y) = p_4\,x^2 + p_5\,y^2 + p_6\,x\,y = \langle \begin{pmatrix} x \\ y \end{pmatrix}, \begin{bmatrix} p_4 & p_6/2 \\ p_6/2 & p_5 \end{bmatrix} \cdot \begin{pmatrix} x \\ y \end{pmatrix} \rangle$$

If λ_i and $\vec{e}_i$ are the two eigenvalues and eigenvectors of the symmetric matrix

$$\mathbf{A} = \begin{bmatrix} p_4 & p_6/2 \\ p_6/2 & p_5 \end{bmatrix}$$

Then any vector $(x,y)^T$ can be written in the form $t\,\vec{e}_i + s\,\vec{e}_2$ and

$$f(x,y) = \lambda_1\,t^2 + \lambda_2\,s^2$$

and consequently the two principal radii are given by

$$R_1 = \frac{-1}{2\,\lambda_1} \quad \text{and} \quad R_2 = \frac{-1}{2\,\lambda_2}$$

This leads to *Octave* code

Octave

```
F2  = [ones(size(x)) x y x.^2 y.^2 x.*y];
[p,y_var,r,p_var] = LinearRegression(F2,z);
RadiusNew = -0.5./eig([p(4), p(6)/2;p(6)/2,p(5)])
```

and the results

$$R_1 \approx 267\,\mu m \quad \text{and} \quad R_2 \approx 316\,\mu m$$

We seem to have an enormous difference between the two radii, which does certainly not correspond to reality. This was confirmed by different measurements. Thus there must be a systematic error in the measurements. A possible candidate is an inadequate calibration of the AFM.

2.2.11 Nonlinear Regression

The commands in the above section are well suited for linear regression problems, but there are many important **nonlinear** regression problems, as shown in Table 2.4. Unfortunately nonlinear regression problems are considerably more delicate to work with and special algorithm are to be used. It is in many problems critical to find good initial guesses for the parameter to be determined. Linear and nonlinear regression problems may also be treated as minimization problems. It is not a good ideas, as they have special properties that one can take advantage of.

Nonlinear Least Square Fit with `leasqr()`

The optimization package of *Octave* provides the command `leasqr()`. It is an excellent implementation of the Levenberg–Marquardt algorithm. The package also provides one example as `leasqrdemo()` and you can examine its source.

As a further example we try to fit a function of the type

$$f(t) = A\,e^{-\alpha t}\,\cos(\omega\,t + \phi)$$

function	parameter	
$y = a + m\,x$	a, m	linear
$y = a\,x^2 + b\,x + c$	a, b, c	linear
$y = a\,e^{c\,x}$	a, c	nonlinear
$y = d + a\,e^{c\,x}$	a, c, d	nonlinear
$y = a\,e^{c\,x}$	a	linear
$y = a\,\sin(\omega t + \delta)$	a, ω, δ	nonlinear
$y = a\,\cos(\omega t) + b\,\sin(\omega t)$	a, b	linear

Table 2.4: Examples for linear and nonlinear regression

through a number of measured points (t_i, y_i). Choose the values for the parameters A, α, ω and ϕ to minimize

$$\sum_i |f(t_i) - y_i|^2$$

Since the function is nonlinear with respect to the parameters A, α, ω and ϕ we can **not** use linear regression. In *Octave*the command `leasqr()` will solve nonlinear regression problems. As an example we will:

1. Choose ”exact” values for the parameters.
2. Generate normaly distributed random numbers as perturbation of the ”exact” result.
3. Define the appropriate function and generate the data.

Find the code below and the generated data points are shown in Figure 2.25.

Octave

```
Ae = 1.5; ale = 0.1; omegae = 0.9 ; phie = 1.5;
noise = 0.1;
t = linspace(0,10,50)'; n = noise*randn(size(t));
function y = f(t,p)
  y = p(1)*exp(-p(2)*t).*cos(p(3)*t + p(4));
endfunction
y =  f(t,[Ae,ale,omegae,phie])+n;
plot(t,y,'+;data;')
```

You have to provide the function `leasqr()` with good initial estimates for the parameters. Examining the selection of points in Figure 2.25 we estimate

- $A \approx 1.5$: this might be the amplitude at $t = 0$.
- $\alpha \approx 0$: there seems to be very little damping.
- $\omega \approx 0.9$: the period seems to be slightly larger than $2\,\pi$, thus ω slightly smaller than 1.
- $\psi \approx \pi/2$: the graph seems to start out like $-\sin(\omega\,t) = \cos(\omega\,t + \frac{\pi}{2})$

The results of your simulation might vary slightly, caused by the random numbers involved.

Octave

```
A0 = 2; al0 = 0; omega0 = 1; phi0 = pi/2;
[fr,p]= leasqr(t,y,[A0,al0,omega0,phi0],'f',1e-10);
p'

yFit = f(t,p);
plot(t,y,'+;data;', t,yFit,';fit;')
-->
p =   1.523957   0.098949   0.891675   1.545294
```

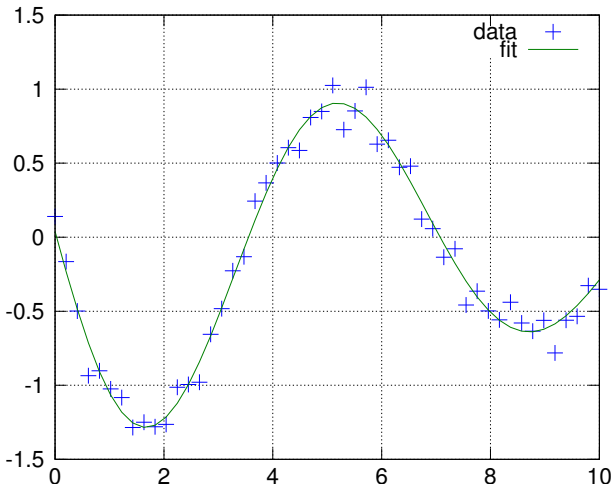


Figure 2.25: Least square approximation of a damped oscillation

The above result contains the estimates for the parameters. For many problems the deviations from the true curve are randomly distributed, with a normal distribution, with small variance. In this case the parameters are also randomly distributed with a normal distribution. The diagonal of the covariance matrix contains the variances of the parameters and thus we can estimate the standard deviations by taking the square root.

Octave

```
[fr,p,kvg,iter,corp,covp,covr,stdresid,Z,r2] =...
      leasqr(t,y,[A0,al0,omega0,phi0],'f',1e-10);
pDev = sqrt(diag(covp))'
-->
pDev =   0.0545981   0.0077622   0.0073468   0.0307322
```

With the above results we obtain Table 2.5. observe that the results are consistent, i.e. the estimated parameters are rather close to the ”exact” values. To obtain even better estimates, rerun the simulation with less noise or more points.

parameter	estimated value	standard dev.	”exact” value
A	1.52	0.055	1.5
α	0.099	0.0078	0.1
ω	0.892	0.0073	0.9
ϕ	1.54	0.031	1.5

Table 2.5: Estimated and ”exact” parameters

The above algorithm is applicable if we have only very few periods of the signal to examine. For a

longer signal it typically fails miserably. Consider Fourier methods or ideas examined in Section 2.7 on a vibrating cord.

Nonlinear Regession with `fsolve()`

The command `fsolve()` is used to solve systems of nonlinear equations, see Section 1.3.3. Assume that a function depends on parameters $\vec{p} \in \mathbb{R}^m$ and the actual variable x, i.e.

$$y = f(\vec{p}, x)$$

If many points $\vec{x} \in \mathbb{R}^n$ are given and the same number of values of $\vec{y}_d \in \mathbb{R}^n$ are measured and for precise measurements we expect $\vec{d}_d \approx \vec{y} = f(\vec{p}, \vec{x})$. Then we can search for the optimal parameters $\vec{p} \in \mathbb{R}^m$ such that

$$f(\vec{p}, \vec{x}) - \vec{y}_d = \vec{0}$$

If $m < n$ this is an **overdetermind** system of n equation for the m unknowns $\vec{p} \in \mathbb{R}^m$. In this case the command `fsolve()` will convert the system of equations to a minimization problem

$$\|f(\vec{p}, \vec{x}) - \vec{y}_d\| \quad \text{is minimized with respect to } \vec{p} \in \mathbb{R}^m$$

It is also possible[7] to estimate the variances of the optimal parameters, using the techniques from Section 2.2.3.

In the example below some data $y = \exp(-0.2\,x)+3$ is generated and then some noise added. As initial paramter we use the naive guess $y(x) = \exp(0 \cdot x) + 0$. The best possible fit is determined and displayed in Figure 2.26.

Octave

```
b0 = 3; a0 = 0.2;  % chose the data
x = 0:.5:5;
noise = 0.1 * sin (100*x);
y = exp (-a0*x) + b0 + noise;

[c, fval, info, output] =  fsolve (@(p) (exp(-p(1)*x) + p(2) - y), [0, 0]);
plot(x,y,'+', x,exp(-p(1)*x)+p(2))
```

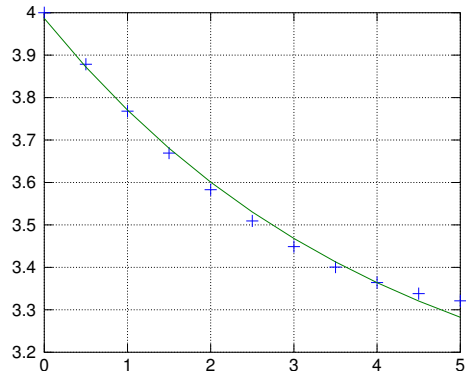


Figure 2.26: Nonlinear least square approximation with `fsolve()`

[7] Ask this author for a sample code.

2.2.12 A real world nonlinear regression problem

For her Bachelor project Linda Welter had to solve a nontrivial nonlinear regression problem. The dependent variable was the sum of a linear function and an trigonometric function with exponentially decaying amplitude. For a given set of points a function of the form

$$y = f(t) = p_1 \cdot \exp(-p_2 \cdot t) \cdot \cos(p_3 \cdot t + p_4) + p_5 + p_6 \cdot t$$

and one has to find the optimal values for the six parameters p_i. At first sight this is a straight application for the function `leasqr()`, presented in the previous section. Thus we run the code below.

Octave

```
nReadData  % read the data

function y = f_exp_trig_lin(t,p)
  y = p(1)*exp(-p(2)*t).*cos(p(3)*t + p(4)) + p(5) + p(6)*t;
endfunction

p_in = zeros(6,1);  % guess for initial values for parameters
[fr,p] = leasqr(t,y,p_in,'f_exp_trig_lin',1e-8);

y_fit1 = f_exp_trig_lin(t,p);
figure(1)
plot(t,y,t,y_fit1)
xlabel('t'); legend('y','y_fit1'); grid on
```

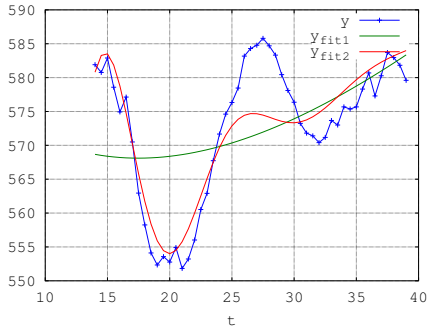


Figure 2.27: Raw data and a first fit

This first result is clearly of low quality and we try to improve by using better initial estimates for the parameters. Examine the graph carefully and estimate the values, leading to the code and second regression result in Figure 2.27.

Octave

```
p_in = [1,0,0.5,0,570,0]; % guess for initial values for parameters
[fr,p] = leasqr(t,y,p_in,'f_exp_trig_lin',1e-8);
y_fit2 = f_exp_trig_lin(t,p);
figure(1)
plot(t,y,t,y_fit1,t,y_fit2)
xlabel('t'); legend('y','y_fit1','y_fit2'); grid on
```

To improve upon the above result we need a plan on how to proceed, and then implement the plan.

1. First get a good estimate on the linear function by fitting a straight line through those points.

2. The difference of the straight line and the given data should be an trigonometric function with exponentially decaying amplitude. Use a nonlinear regression to determine those parameters.

3. Use the above parameter results to run a full nonlinear regression, but now with good initial guesses.

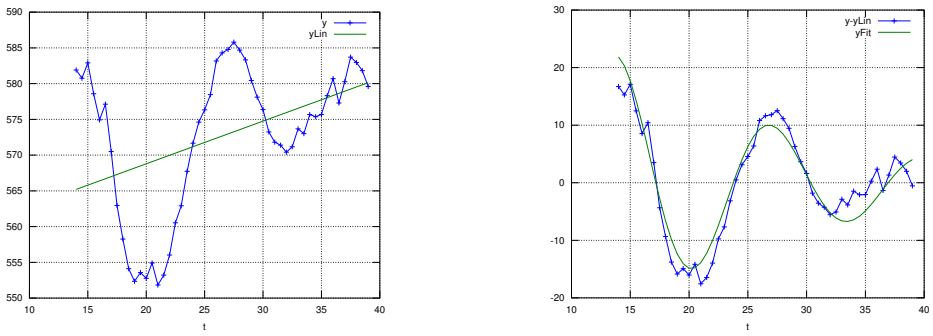
Now we implement and test the above, step by step.

1. Using `LinearRegression()` we fit a straight line through the given data points.

Octave

```
%%% fitting a straight line
F = ones(length(t),2); F(:,2) = t;
pLin = LinearRegression(F,y)
yLin = F*pLin;

figure(2)
plot(t,y,'+-',t,yLin)
xlabel('t'); legend('y','yLin'); grid on
-->
pLin =   556.84180
           0.59710
```

Thus the best possible line has a slope of approximately 0.6 and a y–intercept at $y \approx 557$. This is confirmed by Figure 2.28(a) .



(a) the straigh line fit (b) exponetial regression to difference

Figure 2.28: Regression by straight line and pure exonential

2. Now we examine the difference of the optimal straight line and the actual data. Using a new function and `leasqr()` we find the best optimal fit. The initial parameters are estimated by using Figure 2.28(b) . We find the estimated standard deviations in the square roots of the diagonal elements of the covariance matrix.

Octave

```
% nonlinear regression with leasqr
AEst = 50; alphaEst = log(16/12)/14; omegaEst = 0.5 ; phiEst = -15;

function y = f_exp_trig(t,p)
  y = p(1)*exp(-p(2)*t).*cos(p(3)*t + p(4));
endfunction

[fr,p,kvg,iter,corp,covp] = ...
   leasqr(t,y-yLin,[AEst,alphaEst,omegaEst,phiEst],'f_exp_trig',1e-4);
pVal = p'
pDev = sqrt(diag(covp))'
```

```
-->
pVal =   51.054390    0.060480    0.476920   -12.902044
pDev =    8.6404054   0.0078864   0.0082692    0.1842718
```

The above implies

$$y(t) - y_{lin}(t) \approx 51\ \exp(0.06\,t) \cdot \cos(0.477\,t - 13)$$

The estimated standard deviations of the parameters are rather large, e.g. for the initial amplitude 51.1 ± 8.6 . Now we may generate Figure 2.28(b) .

Octave

```
yFit = f_exp_trig(t,p);

figure(3)
plot(t,y-yLin,'+-',t,yFit)
xlabel('t'); legend('y-yLin','yFit'); grid on
```

To verify the above result, we rerun `leasqr()` using the previously obtained parameters as starting values and asking for more accuracy. The result should not differ drastically from the above. This is confirmed by the following code and result.

Octave

```
[fr,p,kvg,iter,corp,covp,covr,stdresid,Z,r2] =...
    leasqr(t,t-tLin,pVal,'f_exp_trig',1e-8);
pVal = p'
pDev = sqrt(diag(covp))'
-->
pVal =   51.011746   0.06044   0.477038   -12.904584
pDev =    8.630768   0.00788   0.008269     0.184299
```

3. Now we have good estimates for all parameters and we are ready to rerun the original, fully nonlinear regression.

Octave

```
pNew = [p;pLin];  % combine the two parameter sets
[fr,p2,kvg,iter,corp,covp] = leasqr(t,y,pNew,'f_exp_trig_lin',1e-8);
p2Val = p2'
p2Dev = sqrt(diag(covp))'
-->
p2Val =   56.050   0.064194   0.48503   -13.162    550.00    0.83888
p2Dev =    7.962   0.006757   0.00781     0.177      1.54    0.05403
```

$$y = f(t) = 56 \cdot \exp(-0.064 \cdot t) \cdot \cos(0.485 \cdot t - 13.16) + 550 + 0.84 \cdot t$$

The result in Figure 2.29 is obviously superior to the naive attempt shown in Figure 2.27 .

Octave

```
yFit2 = f_exp_trig_lin(t,p2);
figure(4)
plot(t,y,'+-',t,yFit2)
xlabel('t'); legend('y','yFit2'); grid on
```

This example clearly illustrates that one of the most important aspect of nonlinear regression problems is to have good estimates for the parameters to be determined. If you start a fishing expedition in the dark for too many parameters, you will fail.

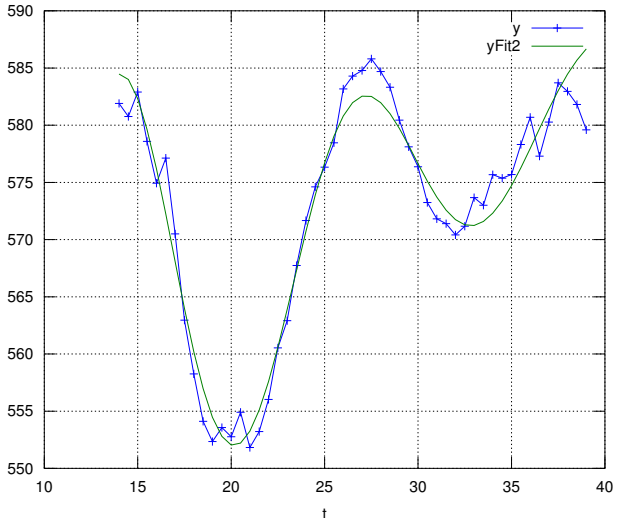


Figure 2.29: The optimal fit, using nonlinear regression

filename	function
`LinearRegression.m`	function to perform general linear regression
`LinearRegression1.m`	temporary code for linear regression
`testLine.m`	do a linear regression for a straight line
`NSHU550ALEDwide.pdf`	data sheet for an LED
`ReadGraph.m`	script file to grab data for LED from PDF file
`LEDdata.m`	script file with the intensity data for above LED
`FitLEDIntensity1.m`	first attempt to analyse intensity
`FitLEDIntensity2.m`	with rescaling
`FitLEDIntensity3.m`	even function with rescaling
`PfennigerData.m`	script file with the data on the linear motor
`Pfenniger1.m`	script file for a first regression
`Pfenniger2.m`	improved script file for the regression
`OrientationTest.m`	script file for calibration
`OrientationData.m`	data set 1 for the calibration
`OrientationData2.m`	data set 2 for the calibration
`SphrereRegression.m`	script file for radius of sphere
`SphereData.csv`	data file for radius of sphere
`Welter.m`	script file for the real world, nonlinear regression
`Readdata.m`	script file to read data for the above
`Matlab`	directory with `MATLAB` compatible files

Table 2.6: Codes and data files for section 2.2

2.2.13 List of codes and data files

In the previous section the codes and data files in Table 2.6 were used.

2.2.14 Exercises

The exercises

Exercise 2.2–1 Linear regression
If a straight line $y = a_0 + a_1\, x$ should pass through the points

$x =$	0.0	1.0	2.0	3.5	4.0
$y =$	-0.5	1.0	2.4	2.0	3.1

then one has to construct the matrix

$$\mathbf{X} = \begin{bmatrix} 1 & 0.0 \\ 1 & 1.0 \\ 1 & 2.0 \\ 1 & 3.5 \\ 1 & 4.0 \end{bmatrix} \quad \text{and} \quad \vec{y} = \begin{pmatrix} -0.5 \\ 1.0 \\ 2.4 \\ 2.0 \\ 3.1 \end{pmatrix}$$

and then solve the linear system

$$\mathbf{X}^T \cdot \mathbf{X} \begin{pmatrix} a_0 \\ a_1 \end{pmatrix} = \mathbf{X}^T \cdot \vec{y}$$

(a) Plot the given data points

(b) Construct the matrix $\mathbf{X}$ and the vector $\vec{y}$

(c) Solve for the parameters a_0 and a_1

(d) Generate a plot with the given data points and the regression by a straight line

Exercise 2.2–2 Example of linear regression by parabola
If a parabola $y = a_0 + a_1\, x + a_2\, x^2$ should pass through the points

$x =$	0.0	1.0	2.0	3.5	4.0
$y =$	-0.5	1.0	2.4	2.0	3.1

then one has to construct the matrix

$$\mathbf{F} = \begin{bmatrix} 1 & 0.0 & 0.0^2 \\ 1 & 1.0 & 1.0^2 \\ 1 & 2.0 & 2.0^2 \\ 1 & 3.5 & 3.5^2 \\ 1 & 4.0 & 4.0^2 \end{bmatrix} \quad \text{and} \quad \vec{y} = \begin{pmatrix} -0.5 \\ 1.0 \\ 2.4 \\ 2.0 \\ 3.1 \end{pmatrix}$$

and then solve the linear system

$$\mathbf{F}^T \cdot \mathbf{F} \begin{pmatrix} a_0 \\ a_1 \end{pmatrix} = \mathbf{F}^T \cdot \vec{y}$$

(a) Plot the given data points

(b) Construct the matrix $\mathbf{F}$ and the vector $\vec{y}$

(c) Solve for the parameters a_0 and a_1

(d) Generate a plot with the given data points and the regression by a parabola

Exercise 2.2–3 General linear regression by parabola
When trying to fit a parabola

$$y = p_1 \cdot 1 + p_2 \cdot x + p_3 \cdot x^2$$

through a given set of points $(x_i\,,\,y_i)$ for $1 \leq i \leq n$ we end up solving a system of linear equations

$$\mathbf{X} \cdot \vec{p} = \vec{b}$$

Determine the matrix $\mathbf{X}$ and the vector $\vec{b}$ as function of the given values x_i and y_i.

Exercise 2.2–4 Nova Energy
In 2004 the company **Nova Energy** was celebrating the event of 100 communities joining their program to conserve energy. Find the data below.

year	1994	1995	1996	1997	1998	1999	2000	2001	2002	2003
number of cities	1	3	5	11	20	35	48	67	84	102
number of people (1000)	7.5	51	177	299	512	870	1343	1530	1750	1950

Create graphical representations of

(a) the number of cities in the program as function of time

(b) the number of people in the program as function of time

(c) the average size of the cities in the program as function of time

Exercise 2.2–5 Nova Energy, linear
Assume that number of cities in exercise 4 is a linear function of time.

(a) Use linear regression to determine the equation of the straight line. It is advisable to choose the time $t = 0$ in the year 1994.

(b) Give a graphical representation of the data and the regression line.

(c) There are 2900 communities in Switzerland. Use the above straight line to predict by when all cities will have joined the program.

Exercise 2.2–6 Nova Energy, quadratic
Assume that number of cities in exercise 4 is a quadratic function of time.

(a) Use linear regression to determine the equation of the parabola. It is advisable to choose the time $t = 0$ in the year 1994.

(b) Give a graphical representation of the data and the regression parabola.

(c) There are 2900 communities in Switzerland. Use the above straight line to predict by when all cities will have joined the program.

Exercise 2.2–7 Nova Energy, exponential
Assume that number of cities in exercise 4 is an exponential function of time. Thus we find

$$\begin{aligned} \text{cities}(t) &= A\, e^{\alpha t} \\ \ln(\text{cities}(t)) &= \ln(A) + \alpha\, t \end{aligned}$$

(a) Compute the logarithm of the number of cities. Then use linear regression to determine the equation of the straight line, i.e. the values of $\ln(A)$ and α. It is advisable to choose the time $t = 0$ in the year 1994.

(b) Give a graphical representation of the data and the exponential curve.

(c) There are 2900 communities in Switzerland. Use the above straight line to predict by when all cities will have joined the program.

Exercise 2.2–8 Nova Energy, number of inhabitants
Redo the above three exercises, but use the number of inhabitants instead of the number of communities. Try to find an explanation for some of the striking differences. Assume that there are 7'000'000 inhabitants in Switzerland.

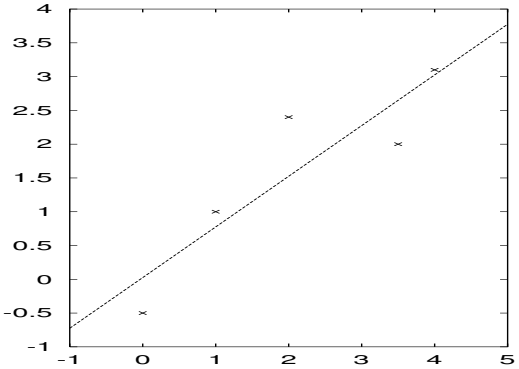
Exercise 2.2–9 Nonlinear Regression with `fsolve()`
Solve the nonlinear regression example in Section 2.2.11 with the help of `fsolve()`, i.e. use Section 2.2.11.

The answers

Exercise 2.2–1 Linear regression
The solution below is generated with *Octave*, the `MATLAB` solution is very similar. The correct values are $a_0 = 0.025$ and $a_1 = 0.75$.

Octave

```
x = [0.0   1.0   2.0   3.5   4.0]'
y = [-0.5   1.0   2.4   2.0   3.1]'
plot(x,y)

X = [ones(length(x),1) x]
a = (X'*X)\(X'*y)

xFit = linspace(-1,5,21)';
yFit = a(1)*ones(length(xFit),1)+a(2)*xFit;

plot(x,y,"+",xFit,yFit)
```



Exercise 2.2–2 Example of linear regression by parabola

The solution below is generated with *Octave*, the MATLAB solution is very similar. The correct values are $a_0 = -0.45298$, $a_1 = 1.74037$ and $a_2 = -0.24087$.

Octave

```
x = [0.0  1.0  2.0  3.5  4.0]'
y = [-0.5  1.0  2.4  2.0  3.1]'
F = [ones(length(x),1) x x.^2]
a = (F'*F)\(F'*y)

xFit = linspace(-1,5,21)';
yFit = a(1)*ones(length(xFit),1)+a(2)*xFit +a(3)*xFit.^2;

plot(x,y,"+",xFit,yFit)
```

Exercise 2.2–3 General linear regression by parabola

To examine is the system

$$\mathbf{X} \cdot p = \mathbf{F}^T \cdot \mathbf{F} \cdot \vec{p} = \mathbf{F}^T \cdot \vec{y}$$

where

$$\mathbf{F} = \begin{bmatrix} 1 & x_1 & x_1^2 \\ 1 & x_2 & x_2^2 \\ 1 & x_3 & x_3^2 \\ & \vdots & \\ 1 & x_n & x_n^2 \end{bmatrix}$$

Thus the result is given by

$$\begin{aligned} \mathbf{X} &= \mathbf{F}^T \cdot \mathbf{F} \\ &= \begin{bmatrix} 1 & 1 & 1 & \cdots & 1 \\ x_1 & x_2 & x_3 & \cdots & x_n \\ x_1^2 & x_2^2 & x_3^2 & \cdots & x_n^2 \end{bmatrix} \cdot \begin{bmatrix} 1 & x_1 & x_1^2 \\ 1 & x_2 & x_2^2 \\ 1 & x_3 & x_3^2 \\ & \vdots & \\ 1 & x_n & x_n^2 \end{bmatrix} \\ &= \begin{bmatrix} n & \sum_{i=1}^n x_i & \sum_{i=1}^n x_i^2 \\ \sum_{i=1}^n x_i & \sum_{i=1}^n x_i^2 & \sum_{i=1}^n x_i^3 \\ \sum_{i=1}^n x_i^2 & \sum_{i=1}^n x_i^3 & \sum_{i=1}^n x_i^4 \end{bmatrix} \\ &= \begin{bmatrix} n & S_x & S_{xx} \\ S_x & S_{xx} & S_{xxx} \\ S_{xx} & S_{xxx} & S_{xxxx} \end{bmatrix} \end{aligned}$$

and

$$\mathbf{F}^T \cdot \vec{y} = \begin{bmatrix} 1 & 1 & 1 & \cdots & 1 \\ x_1 & x_2 & x_3 & \cdots & x_n \\ x_1^2 & x_2^2 & x_3^2 & \cdots & x_n^2 \end{bmatrix} \cdot \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_n \end{pmatrix}$$

$$= \begin{pmatrix} \sum_{i=1}^{n} y_i \\ \sum_{i=1}^{n} x_i\, y_i \\ \sum_{i=1}^{n} x_i^2\, y_i \end{pmatrix} = \begin{pmatrix} S_y \\ S_{xy} \\ S_{xxy} \end{pmatrix}$$

Thus the system to be solved is

$$\begin{bmatrix} n & S_x & S_{xx} \\ S_x & S_{xx} & S_{xxx} \\ S_{xx} & S_{xxx} & S_{xxxx} \end{bmatrix} \cdot \begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix} = \begin{pmatrix} S_y \\ S_{xy} \\ S_{xxy} \end{pmatrix}$$

Exercise 2.2–5 Nova Energy, linear

(a) cities$(t) = -14.5 + 11.6\,t$ where $t =$ year $- 1994$

(b) a graphic

(c) at $t = 251$, i.e. in the year 2245

Exercise 2.2–6 Nova Energy, quadratic

(a) cities$(t) = 0.136 + 0.577\,t + 1.22\,t^2$ where $t =$ year $- 1994$

(b) a graphic

(c) at $t = 48$, i.e. in the year 2042

Exercise 2.2–7 Nova Energy, exponential

(a) $\ln(A) = 0.618$ and $\alpha = 0.502$. Thus cities$(t) = 1.85 + e^{0.502\,t}$.

(b) a graphic

(c) at $t = 14.6$, i.e. in the year 2008

Exercise 2.2–9 Nonlinear Regression with `fsolve()`

Octave

```
Ae = 1.5; ale = 0.1; omegae = 0.9 ; phie = 1.5;
noise = 0.1;
t = linspace(0,10,50)'; n = noise*randn(size(t));
function y = f(t,p)
  y = p(1)*exp(-p(2)*t).*cos(p(3)*t + p(4));
endfunction
y =  f(t,[Ae,ale,omegae,phie]) + n;
plot(t,y,'+;data;')

A0 = 2; al0 = 0; omega0 = 1; phi0 = pi/2;
% [fr,p]= leasqr(t,y,[A0,al0,omega0,phi0],'f',1e-10); p'
[p, fval, info, output] =  fsolve (@(p)(f(t,p)- y), [A0,al0,omega0,phi0]);
p
yFit = f(t,p);
plot(t,y,'+;data;', t,yFit,';fit;')
```

2.3 Regression with Constraints

2.3.1 Example 1: Geometric line fit

The Hessian form of the equation of a straight line is given by

$$n_1\, x + n_2\, y + d = \begin{pmatrix} n_1 \\ n_2 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} + d = \vec{n} \cdot \vec{x} + d = 0 \quad \text{where} \quad \|\vec{n}\| = 1$$

For a number of points $(x_i\,,\, y_i)$ for $1 \leq i \leq n$ the signed distance r_i of these points from the line is given by

$$r_i = \begin{pmatrix} n_1 \\ n_2 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} + d$$

Thus if we try to find the straight line such that the sum of the squared distances to the points is minimal we end of with the problem to minimize the length of the vector $\vec{r}$. This leads to the formulation in Figure 2.30.

minimize length of

$$\vec{r} \;=\; \begin{pmatrix} r_1 \\ r_2 \\ \vdots \\ r_n \end{pmatrix} = \begin{bmatrix} 1 & x_1 & y_1 \\ 1 & x_2 & y_2 \\ & \vdots & \\ 1 & x_n & y_n \end{bmatrix} \begin{pmatrix} d \\ n_1 \\ n_2 \end{pmatrix}$$

subject to the constraint $\|\vec{n}\|^2 = 1$

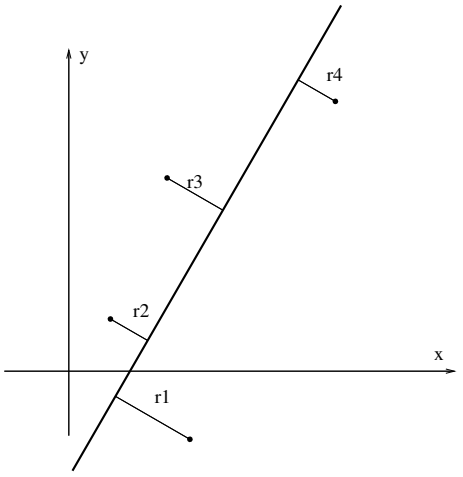


Figure 2.30: A straight line with minimal distance from a set of given points

We will first present a general approach to solve this type of problem and then come back to this example, with a solution.

2.3.2 An algorithm for minimization problems with constraints

Most of the results in this section are based on [GandHreb95, §6].

Description of the algorithm

For a $n \times m$ matrix $\mathbf{F}$ with $n > m$ minimize the length of the vector $\vec{r}$ where

$$\mathbf{F} \cdot \vec{p} = \vec{r} \quad \text{subject to} \quad \|\vec{n}\| = 1 \quad \text{where} \quad \vec{p} = \begin{pmatrix} \vec{d} \\ \vec{n} \end{pmatrix} \in \mathbb{R}^{m_1+m_2} \tag{2.2}$$

The algorithm is based on a QR factorization and one might consult Section 2.2.5.

$$\mathbf{F} \cdot \vec{p} = \mathbf{Q} \cdot \mathbf{R} \cdot \vec{p}$$

The matrix $\mathbf{R}$ may be written in the block form

$$\mathbf{R} = \begin{bmatrix} \mathbf{R}_u \\ \mathbf{0} \end{bmatrix} = \begin{bmatrix} \mathbf{R}_{1,1} & \mathbf{R}_{1,2} \\ \mathbf{0} & \mathbf{R}_{2,2} \\ \mathbf{0} & \mathbf{0} \end{bmatrix}$$

where $\mathbf{R}_{1,1}$ and $\mathbf{R}_{2,2}$ are upper triangular matrices. This leads to a new formulation of the minimization problem. For each of the expressions below the length of the vector on the RHS has to be minimized subject to the constraint $\|\vec{n}\| = 1$.

$$\begin{aligned} \mathbf{F} \cdot \vec{p} &= \mathbf{Q} \cdot \mathbf{R} \cdot \vec{p} = \vec{r} \\ \mathbf{R} \cdot \vec{p} &= \mathbf{Q}^T \cdot \vec{r} = \vec{z} \\ \begin{bmatrix} \mathbf{R}_u \\ \mathbf{0} \end{bmatrix} \cdot \begin{pmatrix} \vec{d} \\ \vec{n} \end{pmatrix} &= \begin{pmatrix} \vec{z}_u \\ \vec{z}_l \\ \vec{0} \end{pmatrix} \\ \begin{bmatrix} \mathbf{R}_{1,1} & \mathbf{R}_{1,2} \\ \mathbf{0} & \mathbf{R}_{2,2} \end{bmatrix} \cdot \begin{pmatrix} \vec{d} \\ \vec{n} \end{pmatrix} &= \begin{pmatrix} \vec{z}_u \\ \vec{z}_l \end{pmatrix} \end{aligned}$$

For a given vector $\vec{n}$ the first set of equations in

$$\begin{aligned} \mathbf{R}_{1,1} \cdot \vec{d} &= -\mathbf{R}_{1,2}\, \vec{n} + \vec{z}_u \\ \mathbf{R}_{2,2} \cdot \vec{n} &= \vec{z}_l \end{aligned}$$

can be solved such that $\vec{z}_u = \vec{0}$. Thus we have to minimize the length of $\vec{z}_l$ by finding the best vector $\vec{n}$. This subproblem can be solved with two different algorithms.

- Eigenvalue computation
  Examine the gradient of

  $$\|\vec{z}_l\|^2 = \langle \mathbf{R}_{2,2} \cdot \vec{n}\,,\, \mathbf{R}_{2,2} \cdot \vec{n} \rangle = \langle \mathbf{R}_{2,2}^T \cdot \mathbf{R}_{2,2} \cdot \vec{n}\,,\, \vec{n} \rangle$$

  to realize that the smallest eigenvalue of the symmetric matrix

  $$\mathbf{R}_{2,2}^T \cdot \mathbf{R}_{2,2}$$

  gives the minimal value for $\|\vec{z}_l\|^2$ and the corresponding eigenvector equals the vector $\vec{n}$ for which the minimum is attained.

- Singular value decomposition
  The matrix $\mathbf{R}_{2,2}$ can be decomposed as product of three matrices

  $$\mathbf{R}_{2,2} = \mathbf{U} \cdot \begin{bmatrix} \sigma_1 & & & \\ & \sigma_2 & & \\ & & \ddots & \\ & & & \sigma_k \end{bmatrix} \cdot \mathbf{V}^T \quad \text{where} \quad \sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_k > 0$$

  with orthogonal matrices $\mathbf{U}$ and $\mathbf{V}$. The smallest value σ_k in the diagonal matrix gives the minimal value of the function to be minimized and the last column of $\mathbf{V}$ equals the vector $\vec{n}$ for which the minimum is attained.

Using this vector $\vec{n}$ and

$$\mathbf{R}_{1,1} \cdot \vec{d} = -\mathbf{R}_{1,2}\, \vec{n}$$

we find the optimal solution of the problem in equation (2.2).

Weighted regression with constraint

The result in the previous section can be modified to take weight of the different points into account. Instaed of minimizing the standard norm

$$\|\vec{r}\|^2 = \sum_{i=1}^{n} r_i^2$$

we want to minimize the weighted norm

$$\|\mathbf{W} \cdot \vec{r}\|^2 = \sum_{i=1}^{n} \sqrt{w_i} r_i^2$$

Using the weight matrix $\mathbf{W}$ and the QR factorization of $\mathbf{W} \cdot \mathbf{F}$ the algorithm can me modified.

$$\begin{aligned}
\mathbf{F} \cdot \vec{p} &= \vec{r} \quad \text{weighted length to be minimized} \\
\mathbf{W} \cdot \mathbf{F} \cdot \vec{p} &= \mathbf{W} \cdot \vec{r} \quad \text{standard length to be minimized} \\
\mathbf{Q} \cdot \mathbf{R} \cdot \vec{p} &= \mathbf{W} \cdot \vec{r} \quad \text{standard length to be minimized} \\
\mathbf{R} \cdot \vec{p} &= \mathbf{Q}^T \cdot \mathbf{W} \cdot \vec{r} = \vec{z} \\
\begin{bmatrix} \mathbf{R}_{1,1} & \mathbf{R}_{1,2} \\ \mathbf{0} & \mathbf{R}_{2,2} \end{bmatrix} \cdot \begin{pmatrix} \vec{d} \\ \vec{n} \end{pmatrix} &= \begin{pmatrix} \vec{z}_u \\ \vec{z}_l \end{pmatrix}
\end{aligned}$$

The remaining part of the algorithm is unchanged. The final code can be found in Figure 2.31.

2.3.3 Example 1: continued

Now we use the presented algorithm to solve the problem of fitting a straight line through some given points.

The file `LineData.m` contains x and y values of a few points and with the code below we load the data and display the result.

Octave

```
LineData;
n = length(xi);
F1 = [ones(n,1) xi yi];
[p1,yvar,residual1orthogonal] = RegressionConstraint(F1,2);
p1   % display the optimal parameters
x = -2:0.1:2;
y = -(p1(1)+p1(2)*x)/p1(3);
plot(xi,yi,'*r',x,y,'g');
```

The equation of the line with minimal orthogonal distances is determined as

$$0.34978 + 0.70030\ x - 0.71385\ y = 0$$

or in the standard form

$$y = 0.49000 + 0.98101\ x$$

We can also perform a standard linear regression. It will minimize the sum of the squares of the **vertical** distances.

Octave

RegressionConstraint.m

```
function [p,y_var,r] = RegressionConstraint(F,nn,weight)

% [p,y_var,r] = RegressionConstraint(F,nn)
% [p,y_var,r] = RegressionConstraint(F,nn,weight)
% regression with a constraint
%
% determine the parameters p_j  (j=1,2,...,m) such that the function
% f(x) = sum_(i=1,...,m) p_j*f_j(x) fits as good as possible to the
% given values y_i = f(x_i), subject to the constraint that the norm
% of the last nn components of p equals 1
%
% parameters
% F  n*m matrix with the values of the basis functions at the support points
%    in column j give the values of f_j at the points x_i  (i=1,2,...,n)
% nn number of components to use for constraint
% weight  n column vector of given weights
%
% return values
% p     m vector with the estimated values of the parameters
% y_var estimated variance of the error
% r     residual  sqrt(sum_i (y_i- f(x_i))^2))

if ((nargin < 2)||(nargin>=4))
 usage('wrong number of arguments in RegressionConstraint(F,nn,weight)');
end

[n,m] = size(F);

if (nargin==2) % set uniform weights if not provided
  weight = ones(n,1);
end


[Q,R] = qr(diag(weight)*F,0);
R11 = R(1:m-nn,1:m-nn);
R12 = R(1:m-nn,m-nn+1:m);
R22 = R(m-nn+1:m,m-nn+1:m);
[u,l,v] = svd(R22);
p = [-R11\(R12*v(:,nn));v(:,nn)];

residual = F*p;                    % compute the residual vector
r = norm(diag(weight)*residual);   % and its norm
                                   % variance of the weighted y-errors
y_var = sum((residual.^2).*(weight.^4))/(n-m+nn);
```

Figure 2.31: Code for `RegressionConstraint()`

```
F2 = [ones(n,1) xi];
[p2,yvar,residual2vertical] = LinearRegression(F2,yi);
p2
x  = -2:0.1:2;
y2 = p2(1)+p2(2)*x;
plot(xi,yi,'*r',x,y,'b',x,y2,'g');
```

This optimal solution is given by the equation

$$y = 0.47547 + 0.91919\ x$$

or in the Hessian normal form

$$0.35006 + 0.67673\ x - 0.73623\ y = 0$$

Thus the straight line in Figure 2.32 with the slightly smaller slope minimizes the vertical distances to the given set of points.

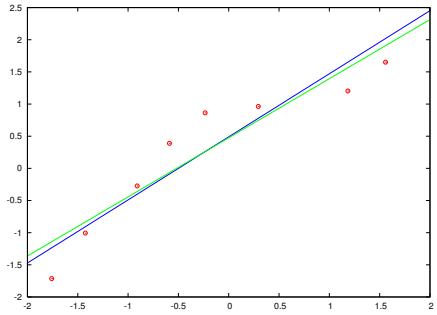


Figure 2.32: Some points with optimal vertical and orthogonal distance fit

The above two solutions should be compared, leading to the results in the table below.

Octave

```
y1new = -(p1(1)+p1(2)*xi)/p1(3);
residual1orthogonal
residual1vertical = sqrt(sum((yi-y1new).^2))

pp = [p2(1);p2(2);-1]/sqrt(1+p2(2)^2);
residual2vertical
residual2orthogonal = sqrt(sum((F1*pp).^2))
```

	orthogonal distance	vertical distance
optimized for orthogonal distance	0.787	1.103
optimized for vertical distance	0.799	1.085

This table confirms the results to be expected, e.g. when optimizing for orthogonal distance then the orthogonal distance is minimal.

2.3.4 Detect the best plane through a cloud of points

Assume we have a cloud of n points $(x_i, y_i, z_i)^T \in \mathbb{R}^3$. Then we seek the equation of the plane fitting best through the plane. This fits into the context of the previous section. Minimize the length of the vector $\vec{r}$

where

$$\vec{r} = \begin{pmatrix} r_1 \\ r_2 \\ \vdots \\ r_n \end{pmatrix} = \begin{bmatrix} 1 & x_1 & y_1 & z_1 \\ 1 & x_2 & y_2 & z_2 \\ & \vdots & & \\ 1 & x_n & y_n & z_n \end{bmatrix} \begin{pmatrix} d \\ n_1 \\ n_2 \\ n_3 \end{pmatrix}$$

subject to the constraint $\|\vec{n}\|^2 = 1$. This situation is similar to Figure 2.30 and thus we can use the command `RegressionConstraint()`. As a demo we first generate a clod of points almost on a plane and display the points in space in Figure 2.33.

Octave

```
nn = 100; % number of points
% generate and display the random points
A = [1 2 3;4 5 6; 7 8 10];
[V,lambda] =  eig(A'*A);
T = V*diag([1 3 0.1])*V';
points = randn(nn,3)*T;
x = points(:,1); y = points(:,2); z = points(:,3);
plot3(x,y,z,'b*')
xlabel('x'); ylabel('y'); zlabel('z');
```

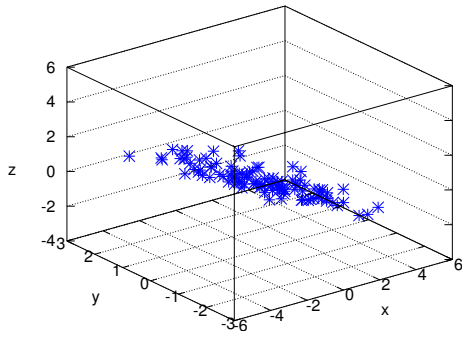


Figure 2.33: A cloud of points, almost on a plane

Now we determine the normal vector $\vec{n}$ and the distance d of the optimal plane from the origin.

Octave

```
p = RegressionConstraint([ones(nn,1),points],3);
p'
-->
0.0073459   -0.4681715   -0.5546819   -0.6878542
```

The above result implies

$$\vec{n} \approx \begin{pmatrix} -0.468 \\ -0.555 \\ -0.688 \end{pmatrix} \quad \text{and} \quad d \approx 0.0073$$

2.3.5 Identification of a straight line in a digital image

The above method of regression with constraint and weights can be used to identify the parameters of a straight line in a digital image. The basic idea is to use a weighted linear regression where dark points have a large weight and white spots will have no weight.

In Figure 2.34 find the photographs of two lines, a freehand version (left) and one generated with a ruler (right). The digital camera produces the images in the `jpg` format and with the command `convert` from the **ImageMagick** suite the high resolution photographs were transformed into 256×256 bitmaps, using the `bmp` format.

```
convert  Line1.jpg  -scale 256x256! Line1.bmp
convert  Line2.jpg  -scale 256x256! Line2.bmp
```

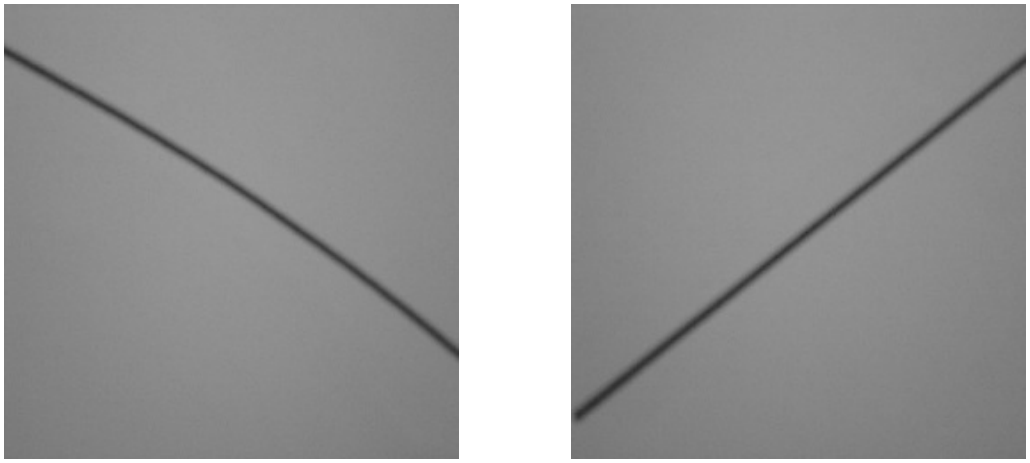


Figure 2.34: Two photographs of lines

Now we try to determine the obvious straight lines in those images.

- Read the file and display the result
  We use the command `imread` to get the data of the picture into *Octave*.

Octave

```
aa = imread('Line1.bmp');
aa = rgb2gray(aa);
colormap(gray);
imagesc(aa);
```

Since bright spots correspond to a high value we have to revert the scaling to obtain a high weight for the dark pixels. In addition we subtract the minimal value and chop all points below a given threshold.

Octave

```
a = 255-aa(:);      a = a-min(a(:));

pos = find(a>(0.4*max(a))); % select the points to be considered
a = double(a(pos));
numberOfPoints = length(a)  % number of points to be considered

[xx,yy] = meshgrid(1:256,1:256);
x = xx(:); x = x(pos);   y = yy(:); y = y(pos);
plot3(x,y,a)
-->
numberOfPoints =  1661
```

The resulting 3D graph clearly shows the points to be on a straight line.

- Regression with constraint
  Since we have to determine straight lines at all possible angles we use the method from Section 2.3.2 to determine the parameters of the straight line.

Octave
```
p = RegressionConstraint([ones(size(x)) x y],2,a)
-->
p =  17.02256
      0.55381
     -0.83264
```

  Thus the distance of the origin from the line is approximately 17 . Observe that the top left corner is the origin $(0\,,\,0)$ and the lower right corner corresponds to the point $(255\,,\,255)$. These values indicate that the straight line in the left part of Figure 2.34 is of the form

$$\begin{aligned} 0 &= 17.02256 + 0.55381\,x - 0.83264\,y \\ y &= 20.44404 + 0.66513\,x \end{aligned}$$

- Estimation of the variance of the parameters
  The command `RegressionConstraint()` does not give any information on the variance of the parameter $\vec{p}$. To obtain this information we rotate the straight line in a horizontal position and then apply standard linear regression, including the estimation of the variance of the parameters.

Octave
```
beta = pi/2 - atan2(p(3),p(2));
rotation = [cos(beta) -sin(beta);sin(beta) cos(beta)];
newcoord = rotation*[x';y'];
xn = newcoord(1,:)';  yn = newcoord(2,:)';
[p2,d_var,r,p2_var] = LinearRegression([ones(size(x)) xn],yn,a);
p2'
p2_var'
-->
p2'      = -1.7023e+01  -1.8148e-16
p2_var'  =  2.4450e-02   6.2699e-07
```

  The results of $\vec{p_2} \approx (-17\,,\,-1.8\cdot 10^{-16})$ confirm the distance from the origin and also show that the rotated line is in fact horizontal. The values of `p2_var` imply that the position of the line is determined with a standard deviation of $\sqrt{0.024} = 0.16$ and for the angle we obtain a standard deviation of $sqrt6.26\cdot 10^{-7} \approx 0.0008 \approx 0.05°$.

It is worth observing that we can determine the position of the straight line with a sub-pixel resolution, since we get some help from statistics.

All of the above code may be rerung in the image on the right in Figure 2.34. The only change is to replace the filename `Line1.bmp` by `Line2.bmp`.

2.3.6 Example 2: Fit an ellipse through some given points in the plane

Ellipse, axes parallel to coordinates

The equation of an ellipse with axes parallel to the coordinate axes and semi-axes of length a and b with center at $(x_0\,,\,y_0)$ can be given in different forms.

$$\frac{(x-x_0)^2}{a^2} + \frac{(y-y_0)^2}{b^2} = 1$$

$$\begin{aligned}\left\langle \begin{bmatrix} 1/a & 0 \\ 0 & 1/b \end{bmatrix} \begin{pmatrix} x-x_0 \\ y-y_0 \end{pmatrix}, \begin{bmatrix} 1/a & 0 \\ 0 & 1/b \end{bmatrix} \begin{pmatrix} x-x_0 \\ y-y_0 \end{pmatrix} \right\rangle &= 1 \\ \frac{1}{a^2}\,x^2 - \frac{2\,x_0}{a^2}\,x + \frac{1}{b^2}\,y^2 - \frac{2\,y_0}{b^2}\,y + \frac{x_0^2}{a^2} + \frac{y_0^2}{b^2} &= 1\end{aligned}$$

From the last form we may conclude that a the search for an ellipse passing through a set of given points might be formulated as a regression problem. Multiply the equation by a^2 and set $\gamma = \frac{a}{b}$ to find the equivalent equation

$$\begin{aligned}x^2 - 2\,x_0\,x + \frac{a^2}{b^2}\,y^2 - \frac{2\,a^2\,y_0}{b^2}\,y + x_0^2 + \frac{a^2\,y_0^2}{b^2} &= a^2 \\ x^2 - 2\,x_0\,x + \gamma^2\,y^2 - 2\,y_0\,\gamma^2\,y + x_0^2 + \gamma^2\,y_0^2 - a^2 &= 0\end{aligned}$$

We seek parameters $\vec{p} \in \mathbb{R}^4$ such that the length of the residual vector $\vec{r}$ is minimal, where

$$p_1\,x_i + p_2\,y_i^2 + p_3\,y_i + p_4 + x_i^2 = r_i$$

With standard linear regression we determine the optimal parameters $\vec{p}$. Then we have to solve for the parameters of the ellipse by solving the following system top to bottom.

$$\begin{aligned}-2\,x_0 &= p_1 \\ \frac{a^2}{b^2} = \gamma^2 &= p_2 \\ -2\,y_0\,\gamma^2 &= p_3 \\ x_0^2 + \gamma^2\,y_0^2 - a^2 &= p_4\end{aligned}$$

The *Octave* code below solves for the best ellipse where the points of the ellipse are stored in the file `EllipseData1.m`.

Octave

```
clf;
axis([-2 2 -2 2],'equal');
EllipseData1;
plot(xi,yi,'*r');

F = [xi yi.^2 yi ones(size(xi))];
[p,yvar,r] = LinearRegression(F,-xi.^2);

x0 = -p(1)/2
y0 = -p(3)/(2*p(2))
a  = sqrt( x0^2 + p(2)*y0^2 - p(4))
b  = sqrt(a^2/p(2))
```

With the computed parameters

$$x_0 = 0.15032 \quad , \quad y_0 = -0.17548 \quad , \quad a = 1.7109 \quad \text{and} \quad b = 0.79109$$

we can draw the ellipse, leading to the left half of Figure 2.35.

Octave

```
phi = (0:5:360)'*pi/180;
x = x0+a*cos(phi);
y = y0+b*sin(phi);
plot(xi,yi,'*r',x,y,'b');
```

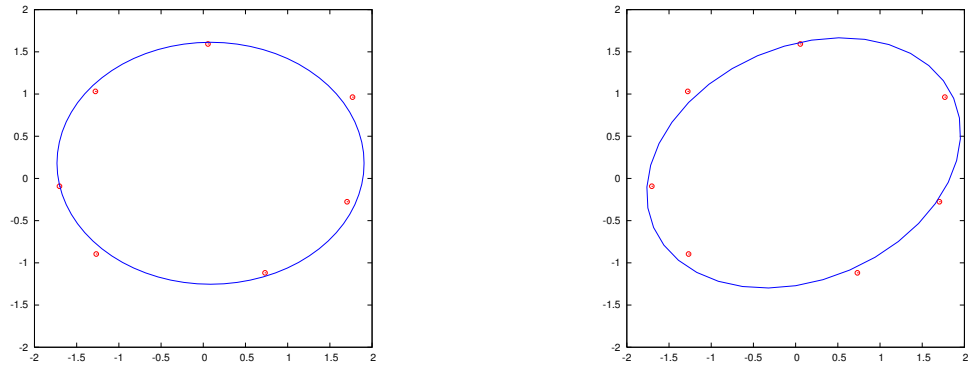


Figure 2.35: Some points and best fit ellipses, parallel to axes and general

General ellipse

As a starting point we consider the equation for an ellipse with semi–axes (parallel to coordinates) of length a and b in the matrix form

$$\langle \begin{bmatrix} 1/a & 0 \\ 0 & 1/b \end{bmatrix} \begin{pmatrix} x - x_0 \\ y - y_0 \end{pmatrix} , \begin{bmatrix} 1/a & 0 \\ 0 & 1/b \end{bmatrix} \begin{pmatrix} x - x_0 \\ y - y_0 \end{pmatrix} \rangle = 1$$

Rotating a vector by an angle α can be written as a matrix multiplication

$$\begin{bmatrix} \cos\alpha & -\sin\alpha \\ \sin\alpha & \cos\alpha \end{bmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{bmatrix} n_1 & -n_2 \\ n_2 & n_1 \end{bmatrix} \begin{pmatrix} x \\ y \end{pmatrix}$$

Thus we can write down the equation of a general ellipse with the help of

$$\mathbf{M} = \begin{bmatrix} 1/a & 0 \\ 0 & 1/b \end{bmatrix} \cdot \begin{bmatrix} n_1 & -n_2 \\ n_2 & n_1 \end{bmatrix} = \begin{bmatrix} \frac{n_1}{a} & \frac{-n_2}{a} \\ \frac{n_2}{b} & \frac{n_1}{b} \end{bmatrix}$$

in the form

$$\begin{aligned} 1 &= \langle \mathbf{M} \cdot \begin{pmatrix} x - x_0 \\ y - y_0 \end{pmatrix} , \mathbf{M} \cdot \begin{pmatrix} x - x_0 \\ y - y_0 \end{pmatrix} \rangle \\ &= \langle \begin{pmatrix} x - x_0 \\ y - y_0 \end{pmatrix} , \begin{bmatrix} \frac{n_1^2}{a^2} + \frac{n_2^2}{b^2} & \frac{-n_1 n_2}{a^2} + \frac{n_1 n_2}{b^2} \\ \frac{-n_1 n_2}{a^2} + \frac{n_1 n_2}{b^2} & \frac{n_2^2}{a^2} + \frac{n_1^2}{b^2} \end{bmatrix} \begin{pmatrix} x - x_0 \\ y - y_0 \end{pmatrix} \rangle \\ &= \langle \begin{pmatrix} x - x_0 \\ y - y_0 \end{pmatrix} , \mathbf{A} \cdot \begin{pmatrix} x - x_0 \\ y - y_0 \end{pmatrix} \rangle \\ &= \langle \begin{pmatrix} x \\ y \end{pmatrix} , \mathbf{A} \cdot \begin{pmatrix} x \\ y \end{pmatrix} \rangle - 2 \langle \begin{pmatrix} x_0 \\ y_0 \end{pmatrix} , \mathbf{A} \cdot \begin{pmatrix} x \\ y \end{pmatrix} \rangle + \langle \begin{pmatrix} x_0 \\ y_0 \end{pmatrix} , \mathbf{A} \cdot \begin{pmatrix} x_0 \\ y_0 \end{pmatrix} \rangle \end{aligned}$$

With the help of the symmetric matrix

$$\mathbf{A} = \begin{bmatrix} a_{1,1} & a_{1,2} \\ a_{1,2} & a_{2,2} \end{bmatrix}$$

we can compute a residual r_i for each given point $(x_i\,,\,y_i)$

$$\begin{aligned} r_i &= a_{1,1}\,x_i^2 + 2\,a_{1,2}\,x_i\,y_i + a_{2,2}\,y_i^2 - 2\,(a_{1,1}\,x_0\,x_i + a_{1,2}\,(x_0\,y_i + y_0\,x_i) + a_{2,2}\,y_0\,y_i) \\ &\quad + a_{1,1}\,x_0^2 + 2\,a_{1,2}\,x_0\,y_0 + a_{2,2}\,y_0^2 - 1 \\ &= a_{1,1}\,x_i^2 + 2\,a_{1,2}\,x_i\,y_i + a_{2,2}\,y_i^2 - 2\,(a_{1,1}\,x_0 + a_{1,2}\,y_0)\,x_i - 2\,(a_{2,2}\,y_0 + a_{1,2}\,x_0)\,y_i \\ &\quad + a_{1,1}\,x_0^2 + 2\,a_{1,2}\,x_0\,y_0 + a_{2,2}\,y_0^2 - 1 \end{aligned}$$

Dividing this expression by $a_{1,1}$ leads us to a least square problem with modified residuals

$$\frac{r_i}{a_{1,1}} = x_i^2 + p_1\,x_i\,y_i + p_2\,y_i^2 + p_3\,x_i + p_4\,y_i + p_5$$

This is now a standard linear regression problem for the vector $\vec{p} \in \mathbb{R}^5$. Knowing the optimal values of $\vec{p}$ we have to compute the parameters of the ellipse with the help of the equations.

$$\begin{aligned} a_{1,1}\,p_1 &= 2\,a_{1,2} \\ a_{1,1}\,p_2 &= a_{2,2} \\ a_{1,1}\,p_3 &= -2\,(a_{1,1}\,x_0 + a_{1,2}\,y_0) \\ a_{1,1}\,p_4 &= -2\,(a_{1,2}\,x_0 + a_{2,2}\,y_0) \\ a_{1,1}\,p_5 &= a_{1,1}\,x_0^2 + 2\,a_{1,2}\,x_0\,y_0 + a_{2,2}\,y_0^2 - 1 \end{aligned}$$

Using the first two equations in the last 3, divided by $a_{1,1}$ we conclude

$$\begin{aligned} p_3 &= -2\,x_0 - p_1\,y_0 \\ p_4 &= -p_1\,x_0 - 2\,p_2\,y_0 \\ p_5 &= x_0^2 + p_1\,x_0\,y_0 + p_2\,y_0^2 - \frac{1}{a_{1,1}} \end{aligned}$$

The first two equations are linear with respect to the unknowns x_0 and y_0 .

$$\begin{bmatrix} 2 & p_1 \\ p_1 & 2\,p_2 \end{bmatrix} \cdot \begin{pmatrix} x_0 \\ y_0 \end{pmatrix} = -\begin{pmatrix} p_3 \\ p_4 \end{pmatrix}$$

Thus we know the values for x_0 and y_0. Now the last equation can be solved for the only remaining unknown $a_{1,1}$ since

$$\frac{1}{a_{1,1}} = x_0^2 + p_1\,x_0\,y_0 + p_2\,y_0^2 - p_5$$

Now we know all values in the matrix $\mathbf{A}$. The eigenvalues and eigenvectors of $\mathbf{A}$ give the lengths a and b of the semi-axis and the angle of rotation α.

$$\begin{aligned} \mathbf{A} &= \begin{bmatrix} n_1 & n_2 \\ -n_2 & n_1 \end{bmatrix} \cdot \begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix} \cdot \begin{bmatrix} n_1 & -n_2 \\ n_2 & n_1 \end{bmatrix} \\ &= \begin{bmatrix} \cos\alpha & -\sin\alpha \\ \sin\alpha & \cos\alpha \end{bmatrix} \cdot \begin{bmatrix} \frac{1}{a^2} & 0 \\ 0 & \frac{1}{b^2} \end{bmatrix} \cdot \begin{bmatrix} \cos\alpha & -\sin\alpha \\ \sin\alpha & \cos\alpha \end{bmatrix} \end{aligned}$$

The above algorithm is implemented in *Octave* and the graphical result can be found in the right half of Figure 2.35.

Octave

```
EllipseData1;
plot(xi,yi,'*r');

F = [xi.*yi yi.^2  xi yi ones(size(xi))];
p = LinearRegression(F,-xi.^2);

m   = [2 p(1);p(1) 2*p(2)];
x0  = -m\[p(3);p(4)]
a11 =1/(x0(1)^2+p(1)*x0(1)*x0(2)+p(2)*x0(2)^2-p(5));

[V,la] = eig(a11*m/2);
alpha = atan(V(2,1)/V(1,1))*180/pi
a = 1/sqrt(la(1,1))
b = 1/sqrt(la(2,2))

np = 37; phi = linspace(0,2*pi,np);

xx = V*([a*cos(phi); b*sin(phi)])+x0*ones(1,np);
x = xx(1,:); y = xx(2,:);

plot(xi,yi,'*r',x,y,'b'); grid on
```

Observations about the fitting of ellipses

The algorithm in the previous section only yields good results if the points to be examined are rather close to an ellipse. If we run the algorithm on a set of random points we can not expect reasonable results. Often we will obtain no result at all, since the values of a^2 or b^2 turn out to be negative.

Also observe that we **do not minimize the distance to the ellipse**, since the residuals r_i used in the algorithm correspond not exactly to the distance of a point $(x_i\,,\,y_i)$ from the ellipse. The precise minimal distance problem is considerably harder to solve and leads to a nonlinear regression problem. One of the subproblems to be solved is how to determine the distance of a point from an ellipse.

We illustrate the above remarks with a simulation. First choose the parameters of an ellipse, then generate a set of points rather close to this ellipse. The values are stored in the column vectors `xi` and `yi`.

Octave

```
ain = 1.2; bin = 0.8; alphain = 15*pi/180;  x0in = 0.1 ; y0in = -0.2;
np = 15; sigma = 0.05;

phi = linspace(0,2*pi,np)';
xi  = x0in+ain*cos(phi)+sigma*randn(size(phi));
yi  = y0in+bin*sin(phi)+sigma*randn(size(phi));

xynew = [cos(alphain) -sin(alphain); sin(alphain) cos(alphain)]*[xi,yi]';
xi = xynew(1,:)'; yi=xynew(2,:)';
```

Then we fit an ellipse with axes parallel to the coordinates to those points and display the parameters of the ellipse.

Octave

```
%% fit ellipse parallel to axis
F = [xi yi.^2 yi ones(size(xi))];
[p,yvar,r] = LinearRegression(F,-xi.^2);

x0 = -p(1)/2
y0 = -p(3)/(2*p(2))
```

```
a  = sqrt( x0^2 + p(2)*y0^2 - p(4))
b  = sqrt(a^2/p(2))

phi = (0:5:360)'*pi/180;
x = x0+a*cos(phi);   y = y0+b*sin(phi);
figure(1);
plot(xi,yi,'*r',x,y,'b');
```

Then redo the fitting for a general ellipse, display the parameters and create Figure 2.36.

Octave

```
%% fit general ellipse
F = [xi.*yi yi.^2  xi yi ones(size(xi))];
p = LinearRegression(F,-xi.^2);

m  = [2 p(1);p(1) 2*p(2)];
x0 = -m\[p(3);p(4)]
a11 = 1/(x0(1)^2+p(1)*x0(1)*x0(2)+p(2)*x0(2)^2-p(5));
[V,la] = eig(a11*m/2);

alpha = atan(V(2,1)/V(1,1))*180/pi
a = 1/sqrt(la(1,1))
b = 1/sqrt(la(2,2))

np  = 37;
phi = linspace(0,2*pi,np);
xx  = V*([a*cos(phi); b*sin(phi)])+x0*ones(1,np);

xg = xx(1,:);  yg = xx(2,:);

figure(2);
plot(xi,yi,'*r',x,y,'b',xg,yg,'r'); grid on
```

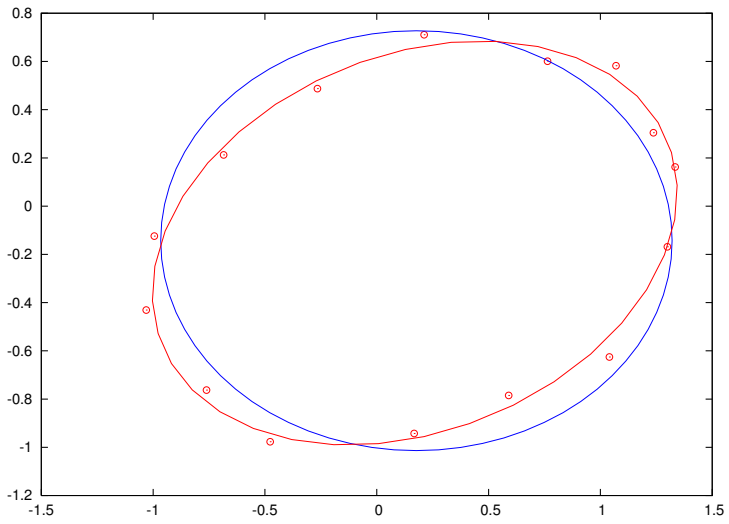


Figure 2.36: Some random points and a best fit ellipses, parallel to axes and general

If exactly 4 points are given then an ellipse parallel to the axis is uniquely determined. If exactly 5 points are given then an ellipse parallel to the axis is uniquely determined. But not all combination of points

will admit solutions. The above algorithm will obtain a negative number for b^2 and thus fail to produce an ellipse. This can be illustrated with the code below. The instructions are as follows:

1. Start the script and it will first pause for 2 seconds.
2. Mark the x and y scale on the screen. Read the on-screen instruction.
3. Use the left button of the mouse to mark the points. Give at least 5 points, approximately on an ellipse.
4. Click on the right button to terminate the collection of data points.
5. Determine the parameters of a horizontal ellipse.
6. Determine the parameters of a general ellipse.
7. Draw both ellipses and the chosen points.

Observe that the call of the function `ginput()` assumes that *Octave* is used on a X Window System. This command has to be modified when using `MATLAB` and it might not work at all with *Octave* on Windows.

Octave

```
pause(2); % wait 2 seconds
[xi,yi] = ginput([-2 2 -2 2])
axis('equal');

%% fit ellipse parallel to axis
F = [xi yi.^2 yi ones(size(xi))];
[p,yvar,r] = LinearRegression(F,-xi.^2);

x0 = -p(1)/2
y0 = -p(3)/(2*p(2))
a  = sqrt( x0^2 + p(2)*y0^2 - p(4))
b  = sqrt(a^2/p(2))


phi = (0:5:360)'*pi/180;
x = x0+a*cos(phi);   y = y0+b*sin(phi);

%% fit general ellipse
F = [xi.*yi yi.^2  xi yi ones(size(xi))];
p = LinearRegression(F,-xi.^2);

m  = [2 p(1);p(1) 2*p(2)];
x0 = -m\[p(3);p(4)]
a11 = 1/(x0(1)^2+p(1)*x0(1)*x0(2)+p(2)*x0(2)^2-p(5));
[V,la] = eig(a11*m/2);

alpha = atan(V(2,1)/V(1,1))*180/pi
a = 1/sqrt(la(1,1))
b = 1/sqrt(la(2,2))

np  = 37;
phi = linspace(0,2*pi,np);
xx  = V*([a*cos(phi); b*sin(phi)])+x0*ones(1,np);

xg = xx(1,:);   yg = xx(2,:);

figure(1);
plot(xi,yi,'*r',x,y,'b',xg,yg,'r');
```

2.3.7 List of codes and data files

In the previous section the codes and data files in Table 2.7 were used.

filename	function
`RegressionConstraint.m`	function to perform regression with constraint
`LineFitOrthogonal.m`	regression for a straight line
`LineData.m`	data file for a line fit
`ImageLine.m`	script file to determine a line in an digital image
`Line1.bmp`	image data for a first line
`Line2.bmp`	image data for a second line
`Ellipse1.m`	fit a parallel ellipse to data
`Ellipse2.m`	fit a general ellipse to data
`EllipseData1.m`	data file for an ellipse
`EllipseCompare.m`	script file to comapre the two methods
`EllipseClick.m`	script file to read points with mouse and fit ellipses

Table 2.7: Codes and data files for section 2.3

2.3.8 Exercises

The exercises

Exercise 2.3–1 Repeat the analysis in Section 2.3.5 for the line in the right part of Figure 2.34. The file is stored in `Line2.bmp`.

Exercise 2.3–2 Circle, center at origin
Find an algorithm to fit a circle with radius R and center at the origin through a given set of points $(x_i\,,\,y_1)$ where $1 \leq i \leq n$.

Exercise 2.3–3 Circle, aritrary center
Find an algorithm to fit a circle with radius R and center at $(x_0\,,\,y_0)$ through a given set of points $(x_i\,,\,y_1)$ where $1 \leq i \leq n$.

The answers

Exercise 2.3–2 Circle, center at origin
The equation of a circle with radius R is given by $x^2 + y^2 - R^2 = 0$. Thus we consider a linear regression problem for the residuals

$$(x_i^2 + y_i^2)\; p_1 - 1 = r_i$$

where the parameter p corresponds to $p = \frac{1}{R^2}$. For this regression problem we can find the optimal solution explicitly.

$$\begin{aligned} \text{minimize} \quad \|\vec{r}\|^2 &= \sum_{k=1}^{n} \left((x_k^2 + y_k^2)\, p - 1 \right)^2 = \sum_{k=1}^{n} \left((x_k^2 + y_k^2)^2\, p^2 - 2\,(x_k^2 + y_k^2)\, p + 1 \right) \\ \frac{\partial}{\partial p} \|\vec{r}\|^2 = 0 &= \sum_{k=1}^{n} \left(2\,(x_k^2 + y_k^2)^2\, p - 2\,(x_k^2 + y_k^2) \right) \end{aligned}$$

$$\begin{aligned} p &= \frac{\sum_{k=1}^{n}(x_k^2+y_k^2)}{\sum_{k=1}^{n}(x_k^2+y_k^2)^2} \\ R^2 &= \frac{\sum_{k=1}^{n}(x_k^2+y_k^2)^2}{\sum_{k=1}^{n}(x_k^2+y_k^2)} \end{aligned}$$

Exercise 2.3–3 Circle, arbitrary center
The equation of a circle with radius R is given by

$$\begin{aligned} (x-x_0)^2+(y-y_0)^2-R^2 &= 0 \\ x^2+y^2-2\,x_0\,x-2\,y_0\,y+x_0^2+y_0^2-R^2 &= 0 \end{aligned}$$

Consider this as a regression problem with residuals

$$p_1\,x_i+p_2\,y_i+p_3+x^2+y^2=r_i$$

where the parameters $\vec{p}$ are related to the circle by

$$p_1=-2\,x_0 \quad , \quad p_2=-2\,y_0 \quad \text{and} \quad p_3=+x_0^2+y_0^2-R^2$$

Thus we try to minimize the length of

$$\begin{bmatrix} x_1 & y_1 & 1 \\ x_2 & y_2 & 1 \\ & \vdots & \\ x_n & y_n & 1 \end{bmatrix} \cdot \begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix} + \begin{pmatrix} x_1^2+y_1^2 \\ x_2^2+y_2^2 \\ \vdots \\ x_n^2+y_n^2 \end{pmatrix} = \begin{pmatrix} r_1 \\ r_2 \\ \vdots \\ r_n \end{pmatrix}$$

Now a standard regression problem will give the optimal values of the parameters $\vec{p}$ and thus the circle.

2.4 Computing Angles on an Embedded Device

In this section[8] we illustrate how to use *Octave* to design an algorithm and its implementation on a micro controller with limited hardware resources. A particular example is examined very carefully, but the methods and results are applicable to a wide variety of problems.

2.4.1 Arithmetic operations on a micro controller

On most micro controllers only the integer operations for addition, subtraction and multiplication are implemented directly. We use integer data types `int16` or `int32` to examine the results of the algorithms. The use of *Octave* to design an integer algorithm has some obvious advantages:

- *Octave* code is easier to develop than code in C, do not even think of the trouble with assembler code.
- Using the data types `int16` in *Octave* will automatically take care of overflow and underflow and make rounding problems visible.
- We can compare the results of an integer computation with a similar floating point computations and thus determine approximation errors.
- We can use all the graphical power of *Octave* to visualize results and approximation errors.
- Once the integer computation algorithm is developed and tested in *Octave* we can translate to C code or even assembler.

General observations

Typical micro controllers have either 8–bit or 16–bit integer arithmetic, but lack any floating point commands. Emulating floating point operations with the help of a library leads to a huge computational overhead and should be avoided if possible. Most often software is written in C, occasionally in assembler.

Most micro controllers provide a set of arithmetic operations with a given resolution. Precise information can be found on the manuals of the micro controllers.

- 8-bit micro controller, e.g. 8051, Cygnal
  - Signed integer numbers have to be between -128 and 127.
  - Unsigned integer numbers have to be between 0 and 255.
  - 8-bit add/subtract 8-bit leads to 8-bit result.
  - 8-bit multiply 8-bit leads to 16-bit result.
  - 8-bit divide by 8-bit leads to 16-bit result, 8-bit integer part, 8-bit remainder.
  - 16-bit additions and subtracions are not very difficult to implement.

  Based on the above commands one can implement fast 16-bit additions and subtraction and also 8 bit multiplications
- 16-bit micro controller (e.g. Cyan)
  - Signed integer numbers have to be between -2^{15} and $2^{15}-1$.
  - Unsigned integer numbers have to be between 0 and $2^{16}-1$.
  - 16-bit add/subtract 16-bit leads to 16-bit result.
  - 16-bit multiply 16-bit leads to 32-bit result.

[8] Currently (2006) this section is based on *Octave*, due to some internal limitations `MATLAB` can not run the code in this section.

  - 32-bit divide by 16-bit leads to 32-bit result, 16-bit integer part, 16-bit remainder.

  Based on the above commands one can implement fast 16-bit additions and subtraction and also 16-bit multiplications/divisions

When writing arithmetic code for a micro controller the following facts should be kept in mind:

- Multiplication by 2^k are easy to implement as shifts of binary representation. Multiplications and division by 2^8 have not be be computed at all, since they result in shifts by complete bytes.
- When implementing the algorithm one may apply shifts to make full use of the 16 bit resolution.
- When adding two numbers $z = x + y$ we find the error estimations

$$\begin{aligned} z &= x + y \\ \Delta z &\approx \Delta x + \Delta y \end{aligned}$$

  Thus the absolute errors are to be added and the final error is dominated by the largest error of the arguments.

- Multiplication is also susceptible to loss of accuracy. Examine the error analysis.

$$\begin{aligned} z &= x \cdot y \\ \Delta z &\approx y\,\Delta x + x\,\Delta y \\ \frac{\Delta z}{z} &\approx \frac{\Delta x}{x} + \frac{\Delta y}{y} \end{aligned}$$

  Thus the relative errors are to be added. If one argument has a large relative error, then the result has a large relative error.

> As a consequence we should design algorithms that use the full accuracy of the hardware.

A sample computation with `int8` and `int16` data types

As an example we want to compute $y = f(x) = 1 - 0.8\,x^2$ for $0 \le x \le 2$ on an 16-bit processor, assuming that for x and y we need an 8-bit resolution. The code is developped with *Octave* and we first generate a graph of the function.

Octave

```
x = linspace(0,2,1001);
function y = f(x)  % test function
  y = 1-0.8*x.^2;
endfunction

y = f(x);
plot(x,y);
title('original function');
xlabel('x'); ylabel('y = 1-0.8*x*x'); grid on
```

Now we want to perform the arithmetic operations for

$$y = 1 - 0.8 \cdot x^2 = 1 - 0.8 \cdot (x \cdot x)$$

keeping track of the effects of the 16-bit arithmetic.

- For the return values y we know $-3 \le y \le 1$ and this domain should be represented with the data range for `int8`, i.e. between -128 and +127. Thus we aim for $y8 = y \cdot 2^5$ as results.
- The true values of x are $0 \le x \le 2$. To use an 8-bit resolution we pass the values $x8 = x \cdot 2^6 = x \cdot 64$. We the know $0 \le x8 \le 127$ and thus we use it as an `int8` data type.

Octave

```
x8 = int8(x*2^6);
```

- As a first intermediate result we compute $r1 = x8 * x8 = x^2 \cdot 2^{12}$. The result will be a 16-bit integer. We verify that the data range is respected.

Octave

```
r1 = uint16(int16(x8).*int16(x8));  % r1 = x^2*2^(6+6) = x^2*2^12
limr1 = [min(r1),max(r1)]  % verify the limits, maximal value 2^15
-->
limr1 =  0   16129
```

- The next step is to multiply the previous result by 0.8 with an integer multiplication. Since $0.8 \cdot 256 \approx 204.8$ we use the factor 205. But before multiplying $r1$ by 205 we have to divide $r1$ by 2^{-8}, otherwise the data range is not respected. The result is rescaled, such that it may be treated as an 8-bit integer.

Octave

```
%  0.8*2^8 approximately 205
r2 = int16(205*(r1*2**-8));  % r2=0.8*x^2*2^12
r3 = int8(bitshift(r2,-7));  % rescale, r3 = 0.8*x^2*2^5
limr3 = [min(r3),max(r3)]    % verify the limits, maximal value 2^7
-->
limr3 = 0   100
```

- Now we have to subtract the previous result $r3$ from 1, respectively from $2^5 = 32$.

Octave

```
r4 = int8(1*2^5-r3);        % r4 =(1-0.8*x^2)*2^5
limr4 = [min(r4),max(r4)]  % verify the limits
-->
limr4 =  -68   32
```

The results equals $y \cdot 2^5$ and thus we may plot the exact function $y = 1 - 0.8 \cdot x^2$ and the 8-bit approximation.

Octave

```
r5 = single(r4)/2^5;
plot(x,y,x,r5)
xlabel('x'); ylabel('1-0.8*x*x'); grid on
```

To examine the error we plot the difference of the exact and approximate function.

Octave

```
figure(2);
plot(x,r5-y)
title('arithmetic error')
xlabel('x'); ylabel('error'); grid on
relErr = max(abs(r5-y))/max(abs(y))
bitError = log2(relErr)
bitErrorMean = log2(mean(abs(r5-y))/max(abs(y)))
-->
relErr =  0.040962
bitError = -4.6096
bitErrorMean = -6.0771
```

2.4.2 Computing the angle based on xy information

A pair of sensors might give the x and y component of a point in the plane. The expression to be measured is the angle α. On a pure mathematical level the answer is given with the formulas in Figure 2.37, but for a good impementation in an actual device some further aspect have to be taken into account.

$$\begin{aligned} \tan\alpha &= \frac{y}{x} \\ \alpha &= \arctan\frac{y}{x} \end{aligned}$$

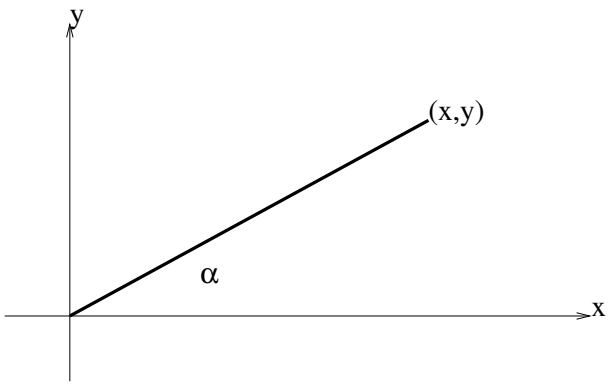


Figure 2.37: The angle α as function of x and y

- The values of x and y are given with errors Δx and Δy. The error $\Delta\alpha$ has to be controlled and minimized.
- The evaluation of the formulas has to be implemented on a micro controller and thus should require as little computational resources as possible.
- The evaluation has to be reliable and fast.

2.4.3 Error analysis of $\arctan$–function

Use the derivative $\frac{\partial}{\partial u}\arctan u = \frac{1}{1+u^2}$ and a linear approximation for the function $f(x,y) = \arctan\frac{y}{x}$.

$$\begin{aligned} \Delta\alpha &\approx \frac{\partial f}{\partial x}\,\Delta x + \frac{\partial f}{\partial y}\,\Delta y \\ &= \frac{1}{1+(y/x)^2}\,\frac{-y}{x^2}\,\Delta x + \frac{1}{1+(y/x)^2}\,\frac{1}{x}\,\Delta y \\ &= \frac{-y}{x^2+y^2}\,\Delta x + \frac{x}{x^2+y^2}\,\Delta y \\ &= \frac{1}{r^2}\,(-y\,\Delta x + x\,\Delta y) \end{aligned}$$

If the errors are randomly given, with variance $V(x) = \sigma_x^2$ (resp. $V(y) = \sigma_y^2$), we use the law of error propagation to conclude

$$\begin{aligned} V(\alpha) &= \frac{1}{r^4}\,\left(y^2\,V(x) + x^2\,V(y)\right) \\ \sigma_\alpha &= \frac{1}{r^2}\,\sqrt{y^2\,\sigma_x^2 + x^2\,\sigma_y^2} \end{aligned}$$

If the standard deviations for the angles are of equal size ($\sigma_x = \sigma_y = \sigma$) this simplifies to

$$V(\alpha) = \frac{1}{r^2}\,\sigma^2 \quad \text{or} \quad \sigma_\alpha = \frac{\sigma}{r}$$

The error contributions Δx and Δy are determined by the hardware (e.g. resolution of AD converters) and might be determined by statistical methods, see also Section 2.2.9.

2.4.4 Clever evaluation of arctan–function

The formula $\alpha = \arctan \frac{y}{x}$ might lead to an unnecessary division by zero. Thus we divide the plane in 8 different sectors and use a slightly different formula for each sector in Figure 2.38 .

No	conditions			result
1	$x > 0$	$y \geq 0$	$y \leq x$	$\alpha = \arctan \frac{y}{x}$
2	$x \geq 0$	$y > 0$	$x \leq y$	$\alpha = \frac{\pi}{2} - \arctan \frac{x}{y}$
3	$x \leq 0$	$y > 0$	$\lvert x\rvert \leq y$	$\alpha = \frac{\pi}{2} + \arctan \frac{-x}{y}$
4	$x < 0$	$y \geq 0$	$y \leq \lvert x\rvert$	$\alpha = \pi - \arctan \frac{y}{-x}$
5	$x < 0$	$y \leq 0$	$\lvert y\rvert \leq \lvert x\rvert$	$\alpha = -\pi + \arctan \frac{-y}{-x}$
6	$x \leq 0$	$y < 0$	$\lvert x\rvert \leq \lvert y\rvert$	$\alpha = -\frac{\pi}{2} - \arctan \frac{-x}{-y}$
7	$x \geq 0$	$y < 0$	$\lvert x\rvert \leq \lvert y\rvert$	$\alpha = -\frac{\pi}{2} + \arctan \frac{x}{-y}$
8	$x > 0$	$y \leq 0$	$\lvert y\rvert \leq \lvert x\rvert$	$\alpha = -\arctan \frac{-y}{x}$

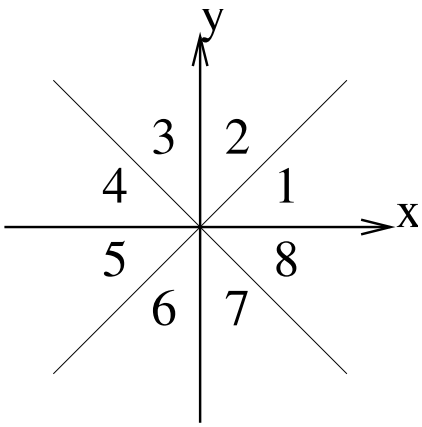


Figure 2.38: The eight sectors used to compute $\tan \alpha = \frac{y}{x}$

Using the table in Figure 2.38 we see that the arctan–function only has to be evaluated for arguments $0 \leq z \leq 1$. As additional effort we have to distinguish the eight sectors. All good mathematical packages offer this type of function. As typical example consider the result of the command `help atan2` from *Octave*.

Octave

```
help atan2
.
atan2 is a built-in function

 -- Mapping Function:  atan2 (Y, X)
     Compute atan (Y / X) for corresponding elements of Y and X.  The
     result is in range -pi to pi.
```

The algorithms in the next section thus only have to compute values of $y = \arctan z$ for $0 \leq z \leq 1$ leading to results $0 \leq y \leq \frac{\pi}{4}$. This is suitable for a Chebyshev approximation. On larger intervals polynomials of higher degree would be necessary.

2.4.5 Implementations of the arctan–function on micro controllers

Thus we are left with the task to compute the function $f(z) = \arctan z$ for arguments $0 \leq z \leq 1$. We assume that x and y are measured and then digitalized with a 10-bit AD converter. The values of x and y vary between $-r$ and $+r$. Thus we can expect at best a relative error of $\frac{\Delta x}{x} \approx 2^{-9} \approx \frac{1}{500} = 0.02$. Based on the result of the previous section we can not hope for a better accuracy for α. The only operations to be used on a micro controller are the basic arithmetic operations.

Taylor series approximation

A standard Taylor series (with error estimate) leads to the formula

$$\arctan z \sum_{k=0}^{n} \frac{(-1)^k}{2\,k+1}\, z^{2\,k+1} + R_n$$

where the approximation error is $|R_n| \approx \frac{1}{2\,k+3}\,z^{2\,k+3}$. Since we examine $0 \leq z \leq 1$ we would need $2\,k+3 \approx 500$, that is $k \approx 250$ terms. Obviously there have to be better solutions than this.

Chebyshev polynomial of degree 2

Any good book on numerical analysis has a section on Chebyshev polynomials and as an application one can verify that the polynomial

$$\begin{aligned} \arctan z &\approx -0.003113205848 + 1.073115615\,z - 0.283642707\,z^2 \\ &= -0.003113205848 + z\,(1.073115615 - z\,0.283642707) \end{aligned}$$

is an approximation with a maximal error of 0.003 on $0 \leq z \leq 1$. For sake of completeness a very brief explanation is given in Section 2.4.6. This error is comparable to the error contribution from the 10–bit resolution of the AD converters. The number of given digits is too large and using the Horner scheme we may simplify the expression to

$$\arctan z \approx -0.0031 + z\,(1.0731 - z\,0.2836) \quad \text{for} \quad 0 \leq z \leq 1$$

This requires only 2 additions and multiplications to compute the value of $\arctan z$. The computational sequence is given by

1. Multiply z by 0.2836
2. Subtract this result from 1.0731
3. Multiply the result by z
4. Subtract 0.0031 from the result

A few plots let you recognize that all intermediate results are positive for all $0 \leq z \leq 1$. The goal is to implement these calculations on a micro controller using the following arithmetic operations with integer numbers. Since all expressions are positive we use the data type unsigned integers.

- Addition of 16-bit unsigned integers leading to a 16-bit integer result
- Multiplication of 8-bit unsigned integers leading to a 16-bit integer result
- Multiplications by 2^k to be implemented with arithmetic shifts.

All of the above operations are suited for an 8-bit micro controller. For each intermediate step we check for under- and overflow. Since we also aim for accuracy we have to assure that the arguments of the multiplications are as close as possible to the maximal number 2^8.

Prepare the computations by storing the precomputed constants $0.2836 \cdot 2^8$, $1.0731 \cdot 2^{15}$ and $0.0031 \cdot 2^{16}$ and also define the Chebyshev approximation to the $\arctan$–function for comparative purposes.

Octave

```
a0 = 0.283642707;      i0 = uint16(a0*2**8)
a1 = 1.073115615;      i1 = uint16(a1*2**15)
a2 = 0.003113205848;   i2 = uint16(a2*2**16)

function  res = myatan(z)
  res= -0.003113205848 + z.*( 1.073115615  - z*0.283642707);
end
```

Then for a given value $0 \leq z \leq 1$ compute $z \cdot 2^8$ as a 16-bit unsigned integer. The algorithm below requires 2 multiplications, 2 additions and a few shifts.

Octave

```
z = 0:0.001:1;
zi = uint16(z*2**8);
```

1. Multiply z by 0.2836
   - Compute $(z \cdot 2^8) \cdot (0.2836 \cdot 2^8)$
   - The intermediate result is modified by a factor of 2^{16}

   Octave
   ```
   r1 = uint16(zi.*i0);
   limits1 = [min(r1) max(r1)]
   ```

2. Subtract this result from 1.0731
   - Divide the previous result by 2
   - Subtract it from $1.0731 \cdot 2^{15}$
   - The intermediate result is modified by a factor of 2^{15}

   Octave
   ```
   r2 = uint16(i1-r1/2);
   limits2 = [min(r2) max(r2)]
   ```

3. Multiply the result by z
   - Divide the previous result by 2^7. It might be faster to divide by 2^8 and then multiply by 2 .
   - Multiply it with $z \cdot 2^8$
   - The intermediate result is modified by a factor of 2^{16}

   Octave
   ```
   r3 = uint16(zi.*bitshift(r2,-7));
   limits3 = [min(r3) max(r3)]
   ```

4. Subtract 0.0031 from the result
   - Subtract $0.0031 \cdot 2^{16}$ from the result
   - The intermediate result is modified by a factor of 2^{16}

   Octave
   ```
   r4 = uint16(r3-i2);
   limits4 = [min(r4) max(r4)]
   ```

This result is converted back to floats and then Figure 2.39 can be generated. The graph shows that the error is smaller than 0.005 which corresponds to $0.29°$. Considering that the possible results range from $0°$ to $45°$ we find an accuracy of 7.5 bit ($\log_2(45*4)$). This is quite good since we started with 8-bit accuracy for the input z . Figure 2.39 also show that the contributions form the Chebyshev approximation and the integer arithmetic are both of the same size.

Octave
```
res = single(r4)/2**16;
plot(z,res-atan(z),'r;int16;',z,myatan(z)-atan(z),'b;float;')
grid on; legend('show')
```

This can all be crammed into one lengthy formula

$$\arctan z \approx 2^{-16}\left(-0.0031 \cdot 2^{16} + (z \cdot 2^8) \cdot (2^{-7}(1.0731 \cdot 2^{15} - 2^{-1}(z \cdot 2^8) \cdot (0.2836 \cdot 2^8)))\right)$$

but for an implementation it is wise to use the above description.

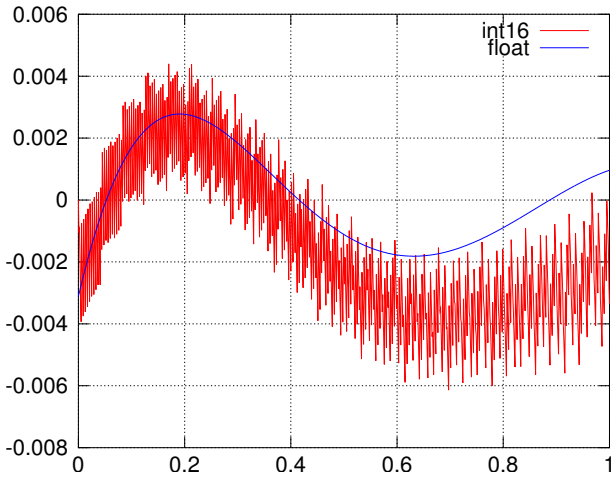


Figure 2.39: Comparison of errors for a Chebyshev approximation and its integer implementation

Improvements and implementation in C

The approximation error in the previous section can be improved by choosing a higher order approximation and by using better integer arithmetic. Exercise 1 shows a modified, improved version of the above solution, using a micro controller with more powerful arithmetic commands. In Exercise 2 the algorithm is implemented in C .

Look up tables, 8-bit

Another approach might be to use a look-up table for the values of the $\arctan$–function. For easy and fast processing we choose a table of 256 equally spaced values for z. Thus we use $z_i = \frac{i-1}{255}$ as midpoints of the intervals and compute the corresponding values $y_i = \arctan z_i$. Then we scale those values to use the full range of a 8-bit resolution and we choose to round to the closest integer. We are lead to the tabulated values $T_i = \text{round}\left(\frac{255 \cdot 4}{\pi}\, y_i\right)$. These 256 values have to be computed once and then stored on the device.

Octave

```
zc = linspace(0,1,256);
atantab = round(atan(zc)*255*4/pi);
```

For a given value of $0 \le z \le 1$ we then perform the following steps to find an approximated values of the $\arctan$ function:

- Round $255\, z$ to the closest integer. This is equivalent to the integer part of $255\, z + 0.5$.
- Add 1 to the above index, since in *Octave* and MATLAB indexes are 1–based. Use this index to acces the number on the above table of precomputed values.

Octave

```
z = 0:0.001:1;

res = zeros(size(z));
for k = 1:length(z)
  res(k) = atantab(single(255*z(k)+0.5)+1)/255*pi/4;
endfor

figure(1);
plot(z,res-atan(z),'r;error;')
grid on; legend('show')
```

The resulting Figure 2.40 shows a maximal error of approximately 0.003, which corresponds to $0.17°$.

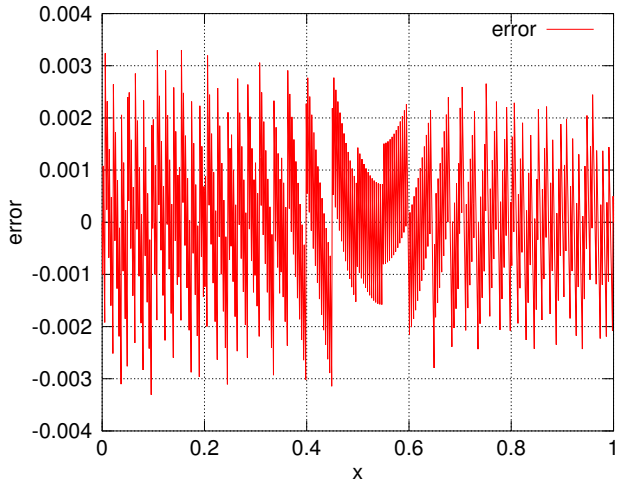


Figure 2.40: The errors for a tabulated approximation of the $\arctan$–function

Piecewise linear interpolation

Lets us divide the interval $0 \le z \le 1$ into $n-1$ subintervals of length $h = \frac{1}{n}$. Then we tabulate the values of the function at the n points $z_i = i\,h$ for $i = 0,\ 1,\ 2,\ \ldots\ n$. For values of z between the points of support we use piecewise linear interpolation to estimate the value of the function $\arctan z$. According to Figure 2.41 the interpolated value is given by

$$f(z_i + \Delta z) \approx f(z_i) + \frac{f(z_{i+1}) - f(z_i)}{z_{i+1} - z_i}\,\Delta z = f(z_i) + m_i \cdot \Delta z \tag{2.3}$$

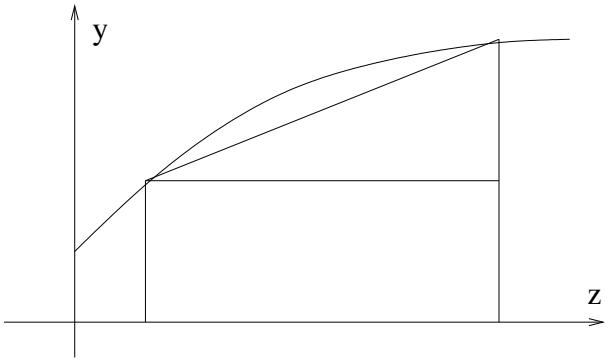


Figure 2.41: Linear interpolation of a function

Using calculus one verifies that on an interval of length h the error of a linear interpolation using the left and right endpoint is estimated by

$$|\text{error}| \le \frac{1}{8}\,M_2\,h^2$$

where M_2 is the maximal absolute value of the second derivative of the function. For our function $f(z) = \arctan z$ with $0 \le z \le 1$ we have to determine M_2 by the calculations below.

$$f''(z) \quad = \quad \frac{-2\,z}{(1+z^2)^2}$$

$$\begin{aligned} f'''(z) &= \frac{-2\,(1+z^2)^2 + 8\,z^2\,(1+z^2)}{(1+z^2)^2} = 2\,\frac{-1-z^2+4\,z^2}{(1+z^2)} = 0 \\ z_m &= \frac{1}{\sqrt{3}} \\ M_2 &= |f''(1/\sqrt{3})| = \frac{2/\sqrt{3}}{(1+1/3)^2} = \frac{3\,\sqrt{3}}{8} \approx 0.64 < 1 \end{aligned}$$

If we divide the interval $0 \le z \le 1$ into $2^5 = 32$ subintervals of equal length we find $h = \frac{1}{32}$ and thus

$$|\text{error}| \le \frac{1}{8}\,M_2\,h^2 \le \frac{1}{8 \cdot 32^2} \approx 1.3 \cdot 10^{-4}$$

Since $\log_2 \frac{1.3 \cdot 10^{-4}}{\pi/4} \approx -12.6$ we conclude that we have at least 12-bit accuracy with this algorithm.

To understand the following computations we have to examine the binary representation of numbers. As example consider the number $z = 0.3$. The code

Octave

```
bin = dec2bin(round(0.33*2^15))
-->
bin = 010101000111101
```

implies that

$$z = 0.33 \approx \frac{1}{2^2} + \frac{1}{2^4} + \frac{1}{2^6} + \frac{1}{2^{10}} + \frac{1}{2^{11}} + \frac{1}{2^{12}} + \frac{1}{2^{13}} + \frac{1}{2^{15}}$$

and we decompose the number into the 5 leading digits of the binary representation and the remainder

$$z \approx 0.\underbrace{01010}_{\text{zint}=10}\,\underbrace{1000111101}_{\text{zfrac}=573} = \text{zint} \cdot 2^{-5} + \text{zfrac} \cdot 2^{-15} = z_i + \Delta z$$

Using the linear interpolation formula (2.3) we conclude

$$\begin{aligned} \arctan(z) &\approx \arctan(z_i) + m_i \cdot \Delta z = \arctan(\text{zint} \cdot 2^{-5}) + m_i \cdot \text{zfrac} \cdot 2^{-15} \\ \arctan(z) \cdot 2^{31} &\approx \arctan(\text{zint} \cdot 2^{-5}) \cdot 2^{31} + m_i \cdot 2^{16} \cdot \text{zfrac} \end{aligned}$$

The above idea leads to the following algorithm:

1. Precompute the integer parts $y_i = \arctan(\frac{i}{2^5}) \cdot 2^{15}$ for $i = 0,\, 1,\, \ldots 31$ and store these 32 values. These 16-bit values will be used as the upper half of 32-bit values. This hides a multiplication by 2^{16} .

2. Precompute the integer parts of

$$s_i = m_i \cdot 2^{16} = \frac{\arctan(\frac{i+1}{2^5}) - \arctan(\frac{i}{2^5})}{2^{-5}} \cdot 2^{16} = (\arctan(\frac{i+1}{2^5}) - \arctan(\frac{i}{2^5})) \cdot 2^{21}$$

   for $i = 0,\, 1,\, \ldots 31$ and store these 32 values. These are 16-bit values.

3. Use the 5 bits on positions 10 through 14 of $z \cdot 2^{15}$ as integer index $i = \text{zint}$ into the table entries y_i and s_i.

4. Consider bits 0 through 10 of $z \cdot 2^{15}$ as integer zfrac and compute

$$y_i \cdot 2^{16} + s_i \cdot \text{zfrac}$$

   The result is a good approximation of $\arctan(z) \cdot 2^{31}$.

The only computationally demanding task in the above algorithm are one multiplication of 16-bit numbers, with 32-bit results and one 32-bit addition[9]. The code below is one possible implementation and leads to Figure 2.42. The maximal error of $1.2 \cdot 10^{-4}$ leads to a value of `bitaccuracy`≈ -12.7 and thus we find at least 12-bit resolution of this implementation.

Octave

```
nn = 5; zc = linspace(0,1,2^nn+1);
atantab = int16(round(atan(zc)*(2^(15))));      % 16-bit values tabulated
%%  errorest=1/8*zc./(1+zc.^2).^2*2^(-2*nn);
%%  atantab=int16(round((atan(zc)+errorest)*(2^(15))));
atantab = int32(int32(atantab)*(2^(16)));       % move to upper half of 32-bit

datantab = int32(round(diff(atan(zc))*2^(16+nn))); % 16-bit unsigned

z = 0:0.001:1-1e-10;

zint  = uint8(floor(z*2^nn));           % integer part
zfrac = int32(mod(z*2^15,2^(15-nn)));   % fractional part

res = zeros(size(z)); res2 = res;
for k = 1:length(z);
  ind = zint(k)+1;
  res(k) = int32(atantab(ind) + zfrac(k)*datantab(ind));
endfor

res = res/2^(31);

figure(1);
plot(z,res-atan(z),'r;error;')
grid on
accuracybits = log(max(abs(res-atan(z))*4/pi))/log(2)
```

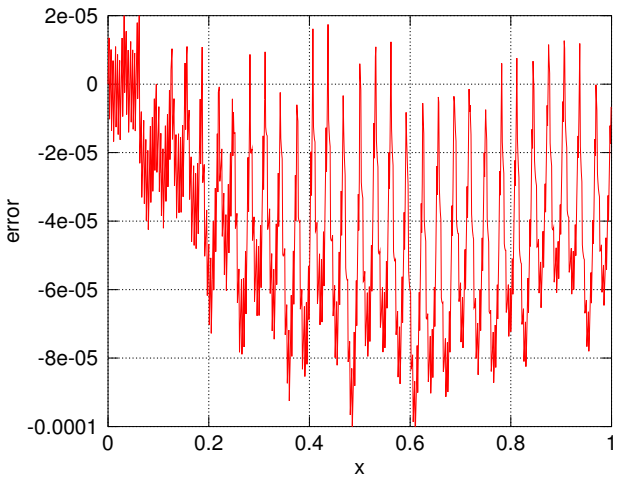


Figure 2.42: The errors for a piecewise linear approximation of the arctan–function

Figure 2.41 and the graph of $\arctan z$ explain why the piecewise linear interpolation is below the actual function. Thus the error in Figure 2.42 is everywhere negative. Since we have an estimate for the maximal

[9]This author developed a modification that uses only one 8-bit multiplication, with a 16-bit result, and one 16-bit addition. The resolution is slightly better than 12-bit. It requires 96 Bytes to store lookup tables. This might be a good solution for a 8-bit controller and moderate accuracy requirements. The result is given in the next section.

error on each subinterval given by

$$\frac{1}{8}\, f''(z)\, h^2 = \frac{-2\,z}{8\,(1+z^2)^2}\ \frac{1}{32^2}$$

we can try to correct this error. This is implemented by the commented out section in the above code. When using this modification we find a maximal absolute error of 0.00006 and `accuracybits`≈ -13.4 and thus we have a slightly improved result.

Standard C code for a piecewise linear interpolation

The above mentioned algorithm using piecewise linear interpolation with one 8-bit multiplication and one 16-bit addition can be implemented in the programming language **C**. The code below will, when called with an unsigned 16-bit integer z ($0 \le z \le 2^{16}-1 = 65535$), return an integer value y ($0 \le y \le 2^{15}-1 = 32767$), giving a good approximation of

$$y \approx (2^{15}-1)\ \arctan\left(\frac{z}{2^{16}-1}\right)$$

Observe that the computations of the integer part and the factional part are implemented with bit operations only and thus very fast.

C

```
unsigned short atan16(unsigned short z){
  static unsigned short atantab[]=
    {    4, 1026, 2048, 3065, 4077, 5081, 6076, 7059, 8030, 8987, 9928,
     10852,11760,12648,13518,14367,15197,16006,16793,17560,18306,19034,
     19740,20425,21090,21734,22360,22969,23557,24129,24683,25219};
  static unsigned char datantab[]=
     {255,255,254,253,251,249,246,243,239,235,231,227,222,217,212,207,
      202,197,192,187,182,176,171,166,161,157,152,147,143,138,134,130};
  unsigned char zint;
  unsigned char zfrac;
  zint = z>>11;
  zfrac=(z&4095)>>3;
  return  atantab[zint] + (zfrac*datantab[zint])>>6;
}
```

Comparison of the previous algorithms

In Table 2.8 find some essential information on the algorithms developed in this section. If you are to choose an algorithm for a concrete application the following points should be taken into consideration.

- If 7-bit accuracy is sufficient then choose between a Chebyshev polynomial of degree 2 and a 8-bit lookup table.
  - The lookup table is the fastest algorithm and rather easy to implement, but it uses some memory.
  - The Chebyshev polynomial requires less memory, but takes longer to evaluate.
- If you need 12-bit accuracy choose between the other two options in Table 2.8 or use Exercises 1 and 3.
  - The Chebyshev polynomial of degree 4 in Exercise 3 requires very little storage, but a couple of 16-bit arithmetic operations.

  - The improved linear interpolation method in Table 2.8 needs fewer arithmetic operations, but 96 Bytes of additional memory.
  - A full 16-bit lookup table is possible and would be very fast, but requires a prohibitive amount of memory.

- If you need even higher accuracy you want to consider polynomials of higher degree or a lookup table with quadratic interpolation, see Exercise 4.

	Chebyshev, degree 2	table look-up, 8-bit	interpolation 1	interpolation 2
absolute error	0.005	0.003	0.00006	0.00001
resolution	7 bit	7 bit	13 bit	12 bit
multiplications	2 (8-bit)	0	1 (16-bit)	1 (8 -bit)
additions	2 (16-bit)	0	1 (32-bit)	1 (16 bit)
memory for lookup	6 Bytes	256 Bytes	128 Bytes	96 Bytes
table look ups	0	1	2	2

Table 2.8: Comparisons of the algorithms for the arctan–function

2.4.6 Chebyshev approximations

The goal of this section is to present the formulas necessary to determine the values of the optimal coefficients c_n for the approximation by Chebyshev polynomials

$$f(x) \approx \frac{c_0}{2} + \sum_{n=1}^{N} c_n \, T_n(x)$$

Determine the coefficient of the Chebyshev polynomials

The Chebyshev polynomials on the interval $[-1\,,\,1]$ are defined by

$$T_n(x) = \cos(n \, \arccos(x))$$

Using the trigonometric identity $\cos(\alpha+\beta) = \cos(\alpha)\,\cos(\beta) - \sin(\alpha)\,\sin(\beta)$ and with $\alpha = \arccos(x)$ we find a recursion formula for the polynomials.

$$\begin{aligned}
\cos(+\alpha + n\,\alpha) &= \cos(\alpha)\,\cos(n\,\alpha) - \sin(\alpha)\,\sin(n\,\alpha) = x\,T_n(x) - \sin(\alpha)\,\sin(n\,\alpha) \\
\cos(-\alpha + n\,\alpha) &= \cos(-\alpha)\,\cos(n\,\alpha) + \sin(\alpha)\,\sin(n\,\alpha) = x\,T_n(x) + \sin(\alpha)\,\sin(n\,\alpha) \\
T_{n+1}(x) + T_{n-1}(x) &= 2\,x\,T_n(x) \\
T_{n+1}(x) &= 2\,x\,T_n(x) - T_{n-1}(x)
\end{aligned}$$

This leads to

$$\begin{aligned}
T_0(x) &= \cos(0) = 1 \\
T_1(x) &= \cos(\arccos(x)) = x \\
T_2(x) &= 2\,x\,(x) - 1 = 2\,x^2 - 1 \\
T_3(x) &= 2\,x\,(2\,x^2 - 1) + x = 4\,x^2 - 3\,x \\
T_4(x) &= 2\,x\,(4\,x^2 - 3\,x) - 2\,x^2 + 1 = 8\,x^4 - 8\,x^2 + 1 \\
&\vdots
\end{aligned}$$

The above recursive algorithm can be used to write *Octave* code to compute the coefficients of these Chebyshev polynomials.

Chebyshev.m

```
function pn = Chebyshev(n)
% compute coefficients of the n'th order Chebyshev polynomial of the first kind
pA = [1];  pB = [1 0];

if n==0
  pn = [1];
elseif n==1;
  pn = [1,0];
else
  for i=2:n
    pn = (2*[pB,0] - [0,0,pA]);
    pA = pB;     pB = pn;
  endfor
endif
```

The code below will generate the graphs of the first few Chebyshev polynomials in Figure 2.43.

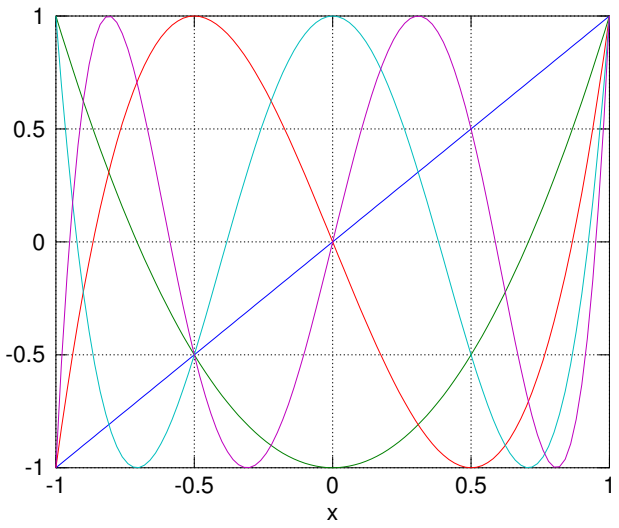


Figure 2.43: Graphs of the first 5 Chebyshev polynomials

Octave

```
nn = 5;    x = -1:0.02:1;
y = zeros(nn,length(x));

for n = 1:nn
  y(n,:) = polyval(Chebyshev(n),x);
endfor
plot(x,y)
```

Orthogonality of the Chebyshev polynomials

These polynomials are orthogonal on the interval $[-1\,,\,1]$ with respect to the integration weight $1/\sqrt{1-x^2}$.

$$\langle T_n(x)\,,\,T_m(x)\rangle \;=\; \int_{-1}^{1} T_n(x)\,T_m(x)\,\frac{1}{\sqrt{1-x^2}}\,dx$$

$$
\begin{aligned}
&= \int_{-1}^{1} \cos(n \cdot \arccos(x))\ \cos(m \cdot \arccos(x))\ \frac{1}{\sqrt{1-x^2}}\ dx \\
\text{substitution} \qquad & \cos\phi = x \quad , \quad -\sin(\phi)\,\frac{d\phi}{dx} = 1 \quad , \quad \sqrt{1-x^2} = \sqrt{1-\cos^2(\phi)} = \sin(\phi) \\
&= \int_{\pi}^{0} \cos(n\,\phi)\ \cos(m\,\phi)\ \frac{-\sin(\phi)}{\sin(\phi)}\ d\phi \\
&= \int_{0}^{\pi} \cos(n\,\phi)\ \cos(m\,\phi)\ d\phi = 0 \quad \text{if } n \neq m \\
\langle T_n(x)\,,\, T_n(x)\rangle \quad &= \int_{0}^{\pi} \cos(n\,\phi)\ \cos(n\,\phi)\ d\phi = \frac{\pi}{2} \quad \text{if } n \geq 1
\end{aligned}
$$

Compute the coefficients

The idea is to use the polynomials $T_n(x)$ and approximate an arbitrary function $f(x)$ in terms of $T_n(x)$. This is similar to the Fourier series, where the arbitrary function is rewritten in terms of functions $\cos(n\,x)$ and $\sin(n\,x)$. One can verify that the Chebyshev polynomials give almost the best possible uniform approximation on the interval $[-1\,,\,1]$. The result can at most be improved by a constant factor, but the Chebyshev polynomial readily be determined. As one possible reference consider [Rivl69, Theorem 2.2].

For a function $f(x)$ defined on the interval $[-1,\ 1]$ compute the coefficients

$$
\begin{aligned}
\frac{\pi}{2}\,c_n \quad &= \int_{-1}^{1} f(x)\ T_n(x)\ \frac{1}{\sqrt{1-x^2}}\ dx \\
&= \int_{-1}^{1} f(x)\ \cos(n \cdot \arccos(x))\ \frac{1}{\sqrt{1-x^2}}\ dx \\
\text{substitution} \qquad & \cos\phi = x \quad , \quad -\sin(\phi)\,\frac{d\phi}{dx} = 1 \quad , \quad \sqrt{1-x^2} = \sqrt{1-\cos^2(\phi)} = \sin(\phi) \\
&= \int_{\pi}^{0} f(\cos(\phi))\ \cos(n\,\phi)\ \frac{-\sin(\phi)}{\sin(\phi)}\ d\phi \\
&= \int_{0}^{\pi} f(\cos(\phi))\ \cos(n\,\phi)\ d\phi
\end{aligned}
$$

Then the Chebyshev approximation is given by

$$
f(x) \approx \frac{c_0}{2} + \sum_{n=1}^{N} c_n\ T_n(x) = \frac{c_0}{2} + \sum_{n=1}^{N} c_n\ \cos(n\ \arccos(x))
$$

A function $g(z)$ defined on an interval $[a\,,\,b]$ has to be transformed onto the interval $[-1\,,\,1]$ by the transformations

$$
\begin{aligned}
z \quad &= \quad -1 + 2\,\frac{x-a}{b-a} \qquad a \leq x \leq b \\
x \quad &= \quad a + \frac{1}{2}\,(z+1)\,(b-a) = \frac{a+b}{2} + z\,\frac{b-a}{2} \\
g(z) \quad &= \quad f(\frac{a+b}{2} + z\,\frac{b-a}{2}) \qquad -1 \leq z \leq 1
\end{aligned}
$$

and then the coefficients for this new function $g(z)$ have to be computed. We find

$$
f(x) = g(z) = \frac{c_0}{2} + \sum_{n=1}^{N} c_n\ T_n(z) = \frac{c_0}{2} + \sum_{n=1}^{N} c_n\ T_n(-1 + 2\,\frac{x-a}{b-a}) \tag{2.4}
$$

Octave code

The above results are readily inplemented in *Octave* for the exemplary function $f(x) = \arctan(x)$ on the interval $A = 0 \leq x \leq 1 = B$.

Octave

```
%% compute the Chebyshev approximation of order n of the function fun
n = 2;
accuracy = 1e-8;
global k;    % order of approximation polynom
global A B   % have to be global variables
A = 0;       % left endpoint
B = +1;      % right endpoint

function y = fun(x)
  y = atan(x);
endfunction
```

The remaining parts of the code remain unchanged if we were to examine another function. First the function to be integrated over the standard interval $[-1\,,\,1]$ has to be defined. Then we compute the coefficients using an integration with `quad()`. With `Chebyshev()` we then determine the coefficients of the Chebyshev approximation.

Octave

```
function y = newFun(x)
  global A;
  global B;
  y = feval('fun',A+0.5*(x+1)*(B-A));
endfunction

function y = intfun(p)
  global k;
  y = feval('newFun',(cos(p)))*cos(k*p);
endfunction

c = zeros(n+1,1); k = 0;
c(1) = quad('intfun',0,pi,accuracy)*1/pi;
for k = 1:n
  c(k+1) = quad('intfun',0,pi,accuracy)*2/pi;
endfor

coeff = zeros(n+1,n+1);
for i = 1:n+1;
  coeff(i,n-i+2:n+1) = Chebyshev(i-1);
endfor

newPol = coeff'*c
```

The vector `newPol` contains the coefficients for the modified function $g(z)$ in the previous section. To apply the transformation we use equation (2.4) and seek the coefficients p_k such that

$$y_i = g(-1 + i\,\frac{2}{n}) = p(x_i) = p(A + i\,\frac{B-A}{n}) = \sum_{k=0}^{n} p_k\, x_i^k \quad \text{for} \quad i = 0, 1, 2, 3, \ldots, n$$

This can be regarded as a system of $n+1$ linear equations with a Vandermonde matrix.

$$\begin{bmatrix} x_0^n & x_0^{n-1} & x_0^{n-2} & & 1 \\ x_1^n & x_1^{n-1} & x_1^{n-2} & \cdots & 1 \\ x_2^n & x_2^{n-1} & x_2^{n-2} & & 1 \\ & \vdots & & \ddots & \vdots \\ x_n^n & x_n^{n-1} & x_n^{n-2} & \cdots & 1 \end{bmatrix} \cdot \begin{pmatrix} p_n \\ p_{n-1} \\ p_{n-2} \\ \vdots \\ p_0 \end{pmatrix} = \begin{pmatrix} y_0 \\ y_1 \\ y_2 \\ \vdots \\ p_n \end{pmatrix}$$

This is easily implemented in *Octave*.

Octave

```
y = polyval(newPol,linspace(-1,1,n+1))';
F = vander(linspace(A,B,n+1)');
p = F\y
```

Then the results can be visualized. A part of the result is shown in Figure 2.39.

Octave

```
x  = linspace(A,B,101);
y1 = fun(x);
y2 = polyval(p,x);
figure(2);  plot(x,y2-y1)
figure(1);  plot(x,y1,x,y2)
```

2.4.7 List of codes and data files

In the previous section the codes and data files in Table 2.9 were used.

filename	function
`atanInteger.m`	function $\arctan z$ using integer operations
`Chebyshev2.m`	Chebyshev approximation of degree 2
`Lookup8bit.m`	Approximation by an 8-bit look-up table
`LinearInterpol.m`	Approximation by a piecewise linear interpolation
`Chebyshev.m`	function the determine the coefficients of $T_n(x)$
`ChebyshevApproximation.m`	script file to determine the Chebyshev approximation
`Chebyshev3.m`	Chebyshev approximation of degree 3, Exercise 1
`atan32.c`	Chebyshev approximation of degree 3, C code for Exercise 2
`Chebyshev4.m`	Chebyshev approximation of degree 4 for 12 bit resolution, Exercise 3

Table 2.9: Codes and for section 2.4

2.4.8 Exercises

The exercises

Exercise 2.4–1 Chebyshev polynomial of degree 3
Use the Chebyshev approximation

$$\begin{aligned} \arctan z &\approx -0.0011722644 + 1.038178669\, z - 0.1904775175\, z^2 - 0.06211012633\, z^3 \\ &= -0.0011722644 + z\,(1.038178669 + z\,(-0.1904775175 - z\,0.06211012633)) \end{aligned}$$

with the maximal error approximately 0.001 and a 16-bit micro controller to compute the $\arctan$–function. Implement these calculations using the following arithmetic operations.

- Addition of 16-bit signed integers leading to a 16-bit integer result
- Multiplication of 16-bit signed integers leading to a 32-bit integer result.
- Multiplications by 2^k to be implemented with arithmetic shifts.

Determine the approximation error of your implementation and its resolution (how many bits?). Complete Table 2.8 with the information on this algorithm.

Exercise 2.4–2 Chebyshev polynomial of degree 3, C code
Write C–code for a function to compute the $y = \arctan(z)$ for $0 \le z \le 1$. Use the algorithm from the previous Exercise 1. Work with the data type `int`, i.e. with 32 bit. The header of the function might be given by

C
```
//  for x=z*2^15 the value of y=2^15 * arctan(z) will be computed
int atan32(int z)
```

Exercise 2.4–3 12-bit AD converters
Many AD converters have a resolution of 12 bit. The Chebyshev approximation

$$\begin{aligned}\arctan z \;\approx\; & -0.0000771717602306579 5 + 0.0031357062620350346\, z - 0.015262708673125458\, z^2 \\ & -0.34245381909783135\, z^3 + 0.14017184670506358\, z^4\end{aligned}$$

shows a maximal error of 0.0001 for $0 \le z \le 1$. Since $\log_2\left(\frac{0.0001 \cdot 4}{\pi}\right) \approx -13$ this approximations allows to keep the 12-resolution of the AD converter.

- Develop an algorithm for a 16-bit micro controller to determine the angle with a 12-bit resolution.
- Count the number of necessary multiplications and additions in your above solution.
- Estimate the memory necessary to achieve the same resolution with a pure lookup table.
- Complete Table 2.8 with the information on this algorithm.

Exercise 2.4–4 Piecewise quadratic interpolation
Use a piecweise quadratic interpolation for the function $f(z) = \arctan z$ on the intervall $0 \le z \le 1$ with 32 subintervals of equal length. The interpolation error ist estimated by

$$|\text{error}| \le \frac{1}{6}\, M_3\, h^3$$

where M_3 is the maximal absolute value of the third derivative of the function.
Determine the resolution (in bits) of this interpolation method.

Exercise 2.4–5 Approximation of $\sin$–function
Find the Chebyshev approximation of order 4 of the function $y = \sin(x)$ on the interval $[0\,,\, \pi/2]$. Use the results and codes in Section 2.4.6.

(a) Determine the coefficients of the approximating polynomial.

(b) Generate a plot of the difference of the approximating polynomial and the function $y = \sin(x)$. Estimate the size of the maximal error.

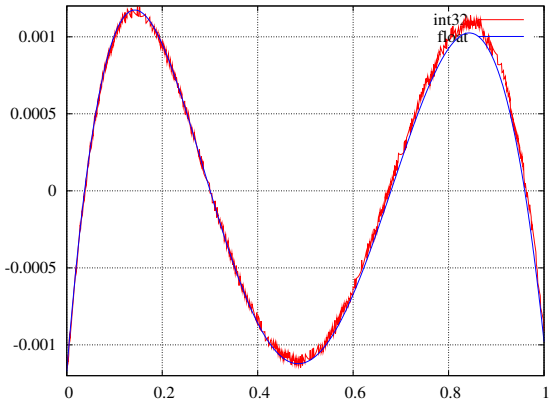
The answers

Exercise 2.4–1 Chebyshev polynomial of degree 3

Octave

```
a0 = -0.06211012633; i0 = int32(a0*2^16)
a1 = -0.1904775175;  i1 = int16(a1*2^16)
a2 = +1.038178669 ;  i2 = int32(a2*2^14)
a3 = -0.0011722644;  i3 = int16(a3*2^14)

function  res = myatan(z)
  res = -0.0011722644 +z.*(1.038178669 + z.*(-0.1904775175-z*0.06211012633));
end

z  = 0:0.001:1;
zi = int32(z*2**15);

r1 = int32(zi.*i0);        %% 15+16
limits1 = [min(r1) max(r1)]

r2 = int16(i1+int16(bitshift(r1,-15)));  %% 16
limits2 = [min(r2) max(r2)]

r3 = int32(zi.*int32(bitshift(r2,-2)));  %%16-2+15=29
limits3 = [min(r3) max(r3)]

r4 = int16(bitshift(r3,-15)+i2);         %% 29-15 =14
limits4 = [min(r4) max(r4)]

r5 = int32(zi.*int32(r4));         %% 14+15 =29
limits5 = [min(r5) max(r5)]

r6 = int16(bitshift(r5,-15))+i3; %% 29-15
limits6 = [min(r4) max(r4)]

res = single(r6)*2**-14;

plot(z,res-atan(z),'r;int32;',z,myatan(z)-atan(z),'b;float;')
grid on; legend('show')
```

The graph below shows that the error of approximately 0.001 is largely dominated by the Chebyshev approximation. Thus using a polynomial of higher degree will improve the accuracy. With this solution we have 9-bit accuracy.



Exercise 2.4–2 Chebyshev polynomial of degree 3, C code
One possible solution is

C

```
//  for x=z*2^15 the value of y=2^15 * arctan(z) will be computed
int atan32(int z){
    static int i0 = -4070;
    static int i1 = -12483;
    static int i2 =  17009;
    static int i3 = -19;

    int r;
    r = i1+((i0*x)>>15);
    r = i2+((x*(r>>2))>>15);
    r = i3+((x*r)>>15);
  return  r<<1;
}
```

A very crude measurement indicated that the above algorithm required approximately 25 CPU cycles to compute one value.

Exercise 2.4–3 12-bit AD converters

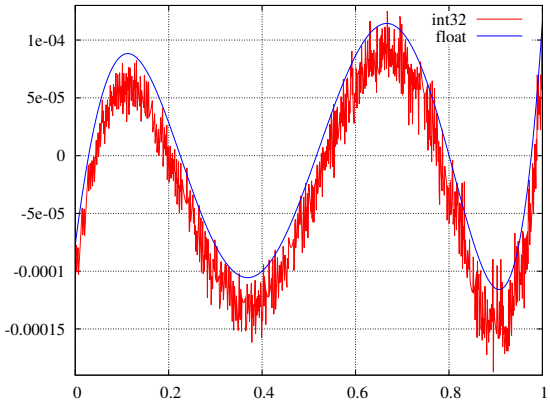
- One possible solution is given by

Octave

```
a0 =  0.14017184670506358;     i0 = int32(a0*2^15)
a1 = -0.34245381909783135;     i1 = int16(a1*2^15)
a2 = -0.015262708673125458;    i2 = int16(a2*2^15)
a3 =  1.0031357062620350346;   i3 = int16(a3*2^14)
a4 = -0.00007717176023065795; i4 = int16(a4*2^15)

function  res = myatan(x)
  res =  -0.00007717176023065795 +   1.0031357062620350346*x ...
    -   0.015262708673125458*x.^2 -  0.34245381909783135*x.^3 ...
    +  0.14017184670506358*x.^4;
end

z  = 0:0.001:1;
zi = int32(z*2**15);

r1 = int32(zi.*i0);       %% 15+16=30
limits1 = [min(r1) max(r1)]

r2 = int16(int16(bitshift(r1,-15))+i1);  %% 30-15=15
limits2 = [min(r2) max(r2)]

r3 = int32(zi.*int32(r2));  %%15+15=30
limits3 = [min(r3) max(r3)]

r4 = int16(int16(bitshift(r3,-15))+i2);      %% 30-15 =15
limits4 = [min(r4) max(r4)]

r5 = int32(zi.*int32(r4));    %% 15+15 =30
limits5 = [min(r5) max(r5)]
```

```
r6 = int16(int16(bitshift(r5,-16))+i3); %% 30-16=14
limits6 = [min(r6) max(r6)]

r7 = int32(zi.*int32(r6));     %% 14+15 =29
limits5 = [min(r7) max(r7)]

r8 = int16(int16(bitshift(r7,-14))+i4); %% 29-14=15
limits6 = [min(r8) max(r8)]

res  =single(int32(r8))*2**-15;

plot(z,res-atan(z),'r;int32;',z,myatan(z)-atan(z),'b;float;')
grid on ; legend('show')

bitaccuracy = log2(1.4e-4/pi*4)
```

leading to the result the figure below. The value of `bitaccuracy`≈ -12.5 shows that we achieved the desired 12-bit resolution. The graph also shows that the maximal error of approximately 0.00014 is largely dominated by the Chebyshev approximation.



- The above code shows 4 necessary 16-bit multiplications (for `r1`, `r3`, `r5` and `r7`) and also 4 additions (for `r2`, `r4`, `r6` and `r8`).
- For 12-bit resolution we have to store at least $2^{12} = 4096$ numbers. Since we have to store 16-bit numbers we need $2^{13} = 8192 = 8$ K bytes of memory. Adding one more bit of resolution would double the memory requirement.

Exercise 2.4–4 Piecewise quadratic interpolation
First compute $M_3 = 2$ and then

$$|\text{error}| \leq \frac{1}{6}\, M_3\, h^3 = \frac{2}{6 \cdot 32^3} \approx 10^{-5}$$

Then the bit resolution is given by

$$\log_2(\frac{4}{\pi}\, 10^{-5}) = \frac{\ln(\frac{4}{\pi}\, 10^{-5})}{\ln 2} \approx -16.2$$

and thus we find a 16-bit resolution.

Exercise 2.4–5 Approximation of $\sin$**–function**

(a) The code in Section 2.4.6 can be used with minor modifications. We find

$$\sin(x) \approx 2.8566\,10^{-2}\,x^4 - 2.0312\,10^{-1}\,x^3 + 1.9516\,10^{-2}\,x^2 + 9.9629\,10^{-1}\,x + 1.1389\,10^{-4}$$

(b) The maximal error is approximately 10^{-4}.

2.5 Analysis of Stock Performance, Value of a Stock Option

In many situation one needs to extract information from a file generated by another code. In this section we illustrate a flexible method by analyzing the value of a given stock over an extended time. The file `IBM.csv` contains data for the stock price of IBM from 1990 through 1999[10].

2.5.1 Reading the data from the file, using `dlmread()`

The data retriefed from the internet is stored in a file, whose first few lines are shown below.
The first few lines in the file `IBM.csv` are shown below.

IBM.csv

```
Date,Open,High,Low,Close,Volume
31-Dec-99,108.671,108.982,106.121,107.365,2870300
30-Dec-99,109.169,109.977,108.049,108.236,3435100
29-Dec-99,109.915,109.977,108.236,108.485,2683300
28-Dec-99,109.044,110.226,108.547,109.293,4083100
27-Dec-99,109.169,109.48,107.614,109.231,3740700
...
```

The easy way to go is to use the command `dlmread()` to extract the needed information. In this example we only want the second column.

IBMscriptDLM.m

```
data = dlmread('IBM.csv',',');  % read all the data
indata = data(:,2)';              % use second column only
k = length(data)-1;
indata = fliplr(indata(2:k+1));  % reverse the order of the stock values
disp(sprintf('Number of trading days from 1990 to 1999 is %i',k))

plot(indata)
xlabel('days'); ylabel('value of stock');
axis([0, k, 0, max(indata)]);
grid on
```

2.5.2 Reading the data from the file, using formatted reading

Instead of the above short code we can also use formatted reading. We use this simple example to illustrate the general procedure:

1. open the file for reading
2. read one item of information at a time and store the useful items
3. close the file

Due to the structure of the file the following operations have to be performed:

- open the file for reading
- read the title line and ignore it
- allocate memory for all the data to be read
- read a first line
- for each line in the file

[10]The results were found at `http://finance.yahoo.com` trough `http://chart.yahoo.com/d/`

  - determine the location of the first comma and then only use the trailing string
  - read the first number in the string and store it properly
  - read the next line

- close the file
- adjust the size of the resulting matrix and rearrange it to have early values first. Then display the number of trading days and plot the value of the stock. Find the result in Figure 2.44.

IBMscript.m

```
indata = zeros(1,365*10);          % allocate storage for the data

infile = fopen('IBM.csv','rt');  % open the file text for reading
tline  = fgetl(infile);            % read the title line

k = 0;                             % a counter
inline = fgetl(infile)             % read a line
while (~isscalar(inline))          % test for end of input file (Octave)
  counter=find(inline==',');       % find the first ','
                                   % then consider only the rest of the line
  newline = inline(counter(1)+1:length(inline));
                                   % read the numbers
  A = sscanf(newline,'%f%c%f%c%f%c%f%c%f');
  k = k+1;
  indata(k) = A(1);                % store only the first number
  inline = fgetl(infile);          % get the next input line
end
fclose(infile);                    % close the file

disp(sprintf('Number of trading days from 1990 to 1999 is %i',k))

indata = fliplr(indata(1:k));      % reverse the order of the stock values
plot(indata)
xlabel('days'); ylabel('value of stock');
axis([0, k, 0, max(indata)]);
grid on
```

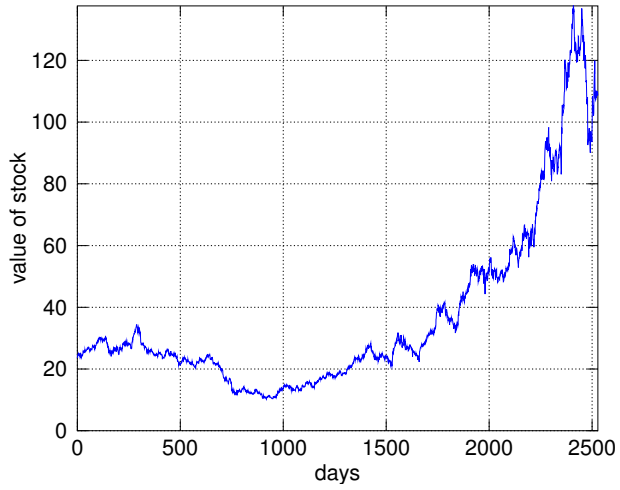


Figure 2.44: The price of IBM stock from 1990 to 1999

2.5.3 Analysis of the data

Moving averages

The value of the stock has a rather high volatility. To visualize this we might compare the actual value of the stock with the average value over a few days. The code below achieves just this and the result is shown in Figure 2.45.

IBMaverage.m

```
% the array indata contains the value of the stock
k = length(indata);

% find the range of trading days for each year
y1 = 1:253;
y2 = 254:506;
y3 = 507:760;

% choose the length of the averaging period
avg = 20;

% create the data
avgdata = indata;
for i = 1:avg
  avgdata(i) = mean(indata(1:i));
end
% average over last avg days for the remaining time period
for i = avg+1:k
  avgdata(i) = mean(indata(i-avg:i));
end

% plot results for the third year
plot(y3,indata(y3),y3,avgdata(y3))
grid on
title('Value of IBM stock and its moving average in 1992')
xlabel('Trading day'); ylabel('Value')
text(510,15,'moving average over 20 days')
```

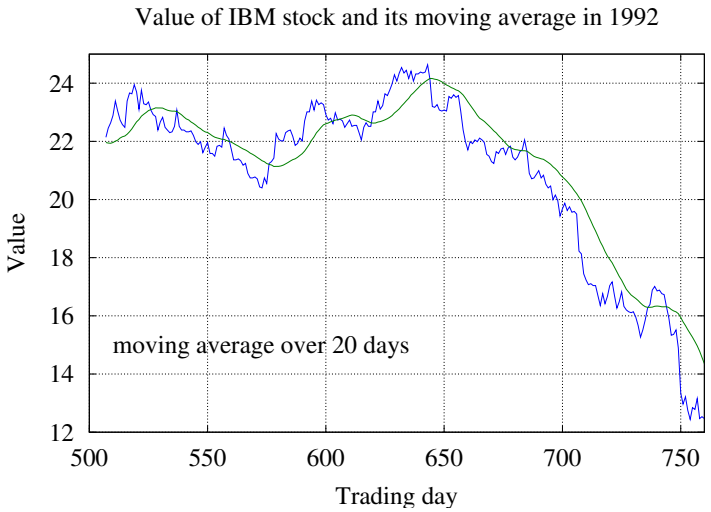


Figure 2.45: The price of IBM stock from 1992 and its average value over 20 days

Daily interest rates

Using the above data we can compute a daily (per trading day) interest rate r by

$$S(n) = S(0)\, e^{n\,r}$$

where r is the interest per day and $S(n)$ the value of the investment after n days. If one year has N trading days then the annual interest rate can be computed by

$$e^{N\,r} - 1 \approx N\,r \quad \text{if} \quad N\,r \ll 1$$

Based of this we can compute the interest rate by using the starting and final value of the stock

$$\begin{aligned} S(n) &= S(0)\, e^{n\,r} \\ e^{n\,r} &= \frac{S(n)}{S(0)} \\ r &= \frac{1}{n}\,\ln\frac{S(n)}{S(0)} \end{aligned}$$

The code below implements this formula

Octave

```
n = length(indata);
rcomp = log(indata(n)/indata(1))/(n-1)
-->
rcomp = 0.00060481
```

This interest rate can be compared to the average of the daily interest rates, i.e. the average of the expressions

$$r(j) = \ln\left(\frac{S(j)}{S(j-1)}\right)$$

This will be a set of daily interest rates and we may consider the statistical distribution of the values.

Octave

```
% mean value and standard deviation of daily interest rate
rates = log(indata(2:n)./indata(1:n-1));
rmean = mean(rates)
rstd  = std(rates)
-->
rmean = 0.00060481
rstd  = 0.019396
```

As one would expect the average of the daily interest rates (computed day by day) coincides with the average daily interest rate (computed by using initial and final value only).

To illustrate the distribution of the daily interest rates a histogram can be used, as shown in Figure 2.46.

Octave

```
dr = 0.005;
edges = [-inf,-0.1:dr:0.1,inf];
histdata = hist(rates,edges);
nn = length(edges);
figure(1);
bar(edges(2:nn-1)-dr/2,histdata(2:nn-1));
axis([-0.1,0.1,0,400]); grid on
xlabel('rate'); ylabel('# of cases')
```

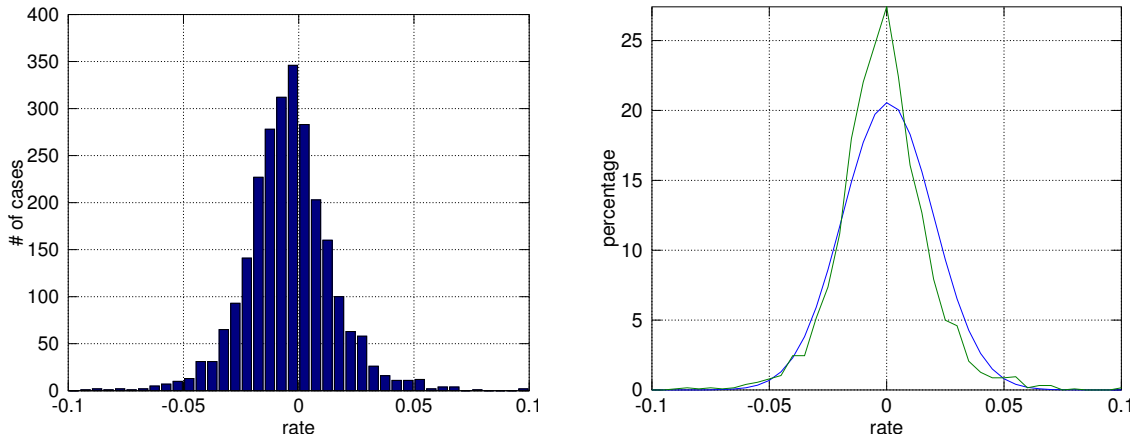


Figure 2.46: Histogram of daily interest rate of IBM stock

It is possible to approximate the distribution of interest rates by a normal distribution with the mean value and standard deviation from above. To do this a function `gauss` given by

$$\text{gauss}(x) = \frac{1}{\sigma\sqrt{2\,\pi}}\, e^{-\dfrac{(x-\bar{x})^2}{2\,\sigma^2}}$$

can be defined by (the code has to be stored in a file `gauss.m`)

gauss.m

```
function res = gauss(x,mean,stddev)
% find the value of a Gauss function  at argument x
% with mean value MEAN and standard deviation STDDEV
  res = exp(-1/2*(x - mean).^2/stddev^2)*1/(sqrt(2*pi)*stddev);
```

Then this function is used to generate the right part in Figure 2.46.

Octave

```
figure(2);
y = gauss(edges(2:nn-1),rmean,rstd);
factor = sum(histdata(2:nn-1))*dr;
histnew = histdata(2:nn-1)/factor;
plot(edges(2:nn-1),[y;histnew])
axis([-0.1,0.1,0,max(histnew)]); grid on
xlabel('rate'); ylabel('percentage')
```

One might use the correlation coefficient of two vectors to obtain a numerical criterion on how similar the shape of the functions is. For two vectors $\vec{a}$ and $\vec{b}$ the correlation coefficient is given by

$$\cos\alpha = \frac{\langle \vec{a}\,,\,\vec{b}\rangle}{\|\vec{a}\|\,\|\vec{b}\|} = \frac{\sum_i a_i\,b_i}{\sqrt{\sum_i a_i^2}\,\sqrt{\sum_i b_i^2}}$$

where α is the angle between the two vectors. If the vectors are generated by discretizing two functions then a correlation coefficient close to 1 implies that the graphs of the two functions are of similar shape. For the two functions (resp. vectors) in Figure 2.46 we obtain

Octave

```
y = gauss((edges(2:nn-2)+edges(3:nn-1))/2,rmean,rstd);
correlation = histdata(2:nn-2)*y'/(norm(histdata(2:nn-2))*norm(y))
-->
correlation = 0.9812
```

Thus in this example the distribution of the daily interest rates is quite close to a normal distribution.

2.5.4 A Monte Carlo Simulation

Since we found an average daily interest rate and its standard deviation we can use random numbers to simulate the behavior of stock values. We generate random numbers for the daily interest rates with the known average value and standard deviation. Then we use these interest rates to compute the behavior of the value of the stock when those interest rates are applied. We can even run multiple of those simulations to extract information on an *average performance*.

Simulation of one year

We assume that the initial value of the stock is $S(0) = 1$ and one year has 250 trading days. Then we generate a vector of random numbers with the mean and standard deviation of the daily interest rate of the above IBM stock. The command `randn(1,days)` will create normally distributed random numbers with average 0 and standard deviation 1 . Thus we have to multiply these numbers with the desired standard deviation and then add the average value. We assume that the value of the stock is given by $S(0) = 1$ on the first trading day. For subsequent days we use

$$S(k) = S(k-1) \cdot e^{r(k)}$$

to find the value $S(k)$ on the k-th day. Then we plot the values of the stock to arrive at the left part in Figure 2.47.

IBMsimulation.m

```
days = 250;                          % number of trading days to be simulated
values = ones(1,days);               % value of stock
rates = randn(1,days)*rstd + rmean;  % daily interest rates
for k = 2:days                       % loop to compute new value of stock
  values(k) = values(k-1)*exp(rates(k));
end

plot(values); grid on
xlabel('trading day'); ylabel('relative value')
```

Please observe that repeated runs of the same code will **not** produce identical results, due to the random nature of the simulation. Running the script a few times will convince you that the value of the stock can either move up or move down. The result of one or multiple runs are shown in Figure 2.47. Observe that most final results are rather close together, but individual runs may show a large deviation. This indicates that one might to examine the statistical behavior of the final value of the stock.

Multiple runs of the simulation

The above simulation can be run many times and the final value of the stock can be regarded as the outcome of the simulation. If the simulation is run many times the outcome can be drastically different, as illustrated by the right part of Figure 2.47. Thus we can run this simulation many times and consider the final value after one year as the result. We will obtain a probability distribution of values of the stock after one year. This function can be shown as a histogram. The code below does just this.

- Generate the random data.

Octave

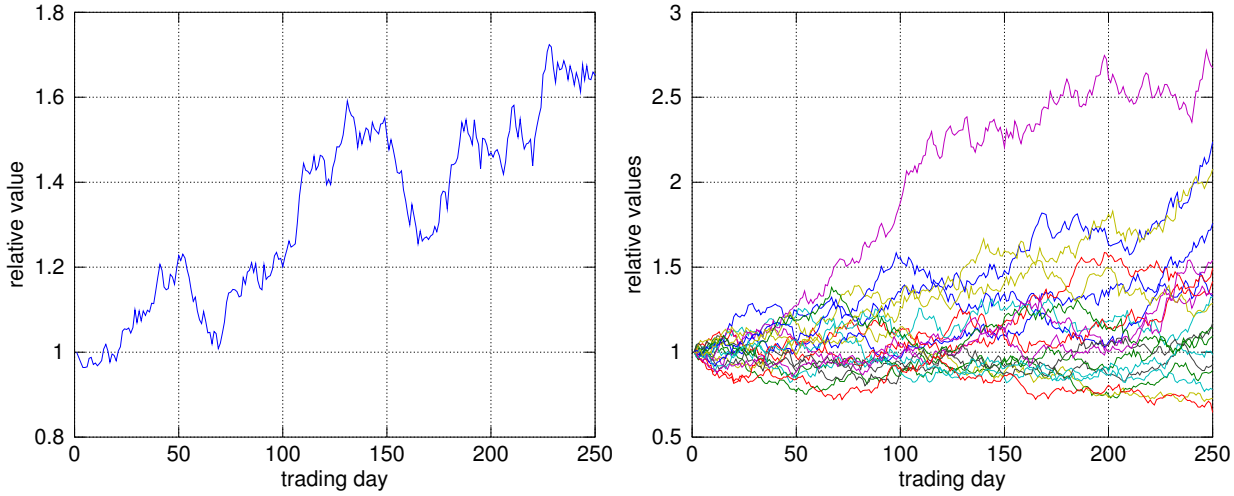


Figure 2.47: Simulation of annual performance of IBM stock

```
days = 250;        % number of trading days to be simulated
runs = 1000;       % number of trial runs

finalvalues = zeros(1,runs);

for rr = 1:runs
  values = ones(1,days);                  % value of stock
  rates = randn(1,days)*rstd + rmean;     % daily interest rates
  for k = 2:days
    values(k) = values(k-1)*exp(rates(k));
  end
  finalvalues(rr) = values(days);
end

MeanValue = mean(finalvalues)
StandardDeviation = std(finalvalues)
LogMeanValue = mean(log(finalvalues))
LogStandardDeviation = std(log(finalvalues))
```

One specific run of the above code lead to the numerical values below. Be aware that the numbers change from one run to the next, as they depend on the random simulation.

Octave

```
MeanValue = 1.2167
StandardDeviation = 0.37752
LogMeanValue = 0.14898
LogStandardDeviation = 0.30962
```

- Create the histogram of the final values.

Octave

```
dr = 0.1;  edges = [-inf,0:dr:3,inf];
histdata = histc(finalvalues,edges)/runs;

figure(1);
nn = length(edges);
bar(edges(2:nn-1)-dr/2,histdata(2:nn-1));
```

```
title('Histogram of probability')
xlabel('value of stock')
axis([0 3 0 0.15]);
grid on
```

- Create the histogram of the final logarithmic values.

Octave

```
dr = 0.1;  edges = [-inf,-1:dr:1,inf];
histdata = histc(log(finalvalues),edges)/runs;

figure(2);
nn = length(edges);
bar(edges(2:nn-1)-dr/2,histdata(2:nn-1));
title('Histogram of probability')
xlabel('logarithm of value of stock');
axis([-1 1 0 0.15]);
grid on
```

The numerical results are shown above and the graphs are given in Figure 2.48 . One should realize that the logarithm of the final values are given by a normal distribution, whereas the distribution of the values is not even symmetric.

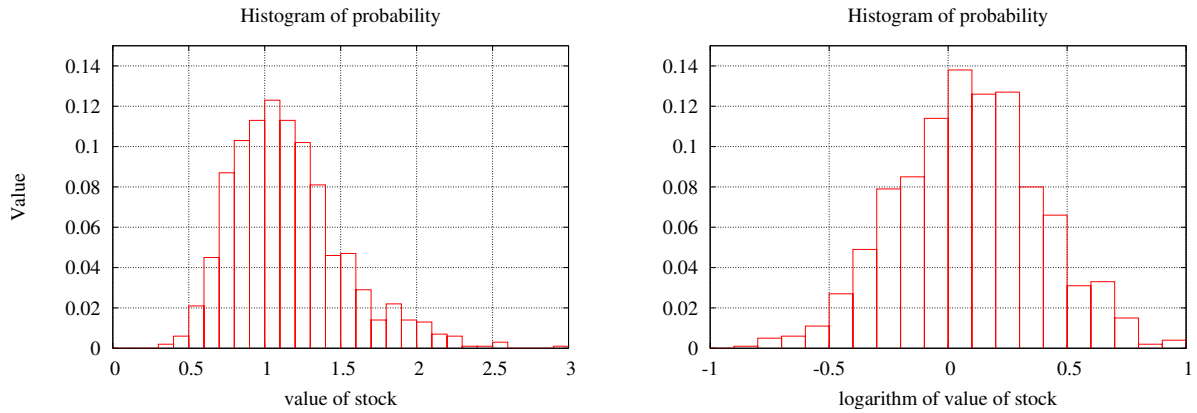


Figure 2.48: Final values of annual performance of IBM stock

If the daily interest rate has a mean value of r and a standard deviation of σ then the logarithm of the values of the stock after N days should be given by a normal distribution with mean value $N\,r$ and standard deviation $\sigma\,\sqrt{N}$. Thus the probability density function of the logarithm of the value of the stock is given by

$$\mathrm{PDF}(z) = \frac{1}{\sigma\,\sqrt{N}\,\sqrt{2\,\pi}}\; e^{-\dfrac{(z-N\,r)^2}{2\,\sigma^2\,N}}$$

Thus the probability that $\ln S(N)$ is between z and $z+\Delta z$ is given by $\mathrm{PDF}(z)\,\Delta z$, as long as Δz is small.

$$\mathrm{P}(z \le \ln S(N) \le z+\Delta z) \approx \mathrm{PDF}(z)\cdot\Delta z$$

With the above numbers $r = 6.0481\cdot 10^{-4}$, $\sigma = 0.0194$ and $N = 250$ we obtain

$$r\,N = 0.1512 \quad \text{and} \quad \sigma\,\sqrt{N} = 0.3067$$

Thus the predicted values are very close to the simulation results LogMeanValue = 0.1490 and LogStandardDeviation = 0.3096 of the above simulation.

2.5.5 Value of a stock option : Black–Scholes–Merton

The question

Assume that today's value of IBM stock is $S_0 = 1$. A trader is offering the option to buy this stock one year from today for the fixed strike price of $C = 1.05$. Assume you acquire a few of these options. Your action taken one year from now will depend on the value S_1 of the stock.

- If $S_1 \leq C$ you will not use your right to buy, since it would be cheaper to buy at the stock market.
- If $S_1 > C$ you will certainly use the option and buy, as you will make a profit of $S_1 - C$.

This option has some value to you. You can not loose on the option, but you might win if the actual value after one year is larger than C.

What is a fair value (price) for this option?

Assumptions

To determine the value of this option the following assumptions can be used:

- The value of the stock is a random process, as simulated by the computations in the previous section.
- The probability for the value S_1 to satisfy $z \leq \ln S_1 \leq z + \Delta z$ is given by

$$\mathrm{PDF}(z) \cdot \Delta z = \frac{1}{\sigma \sqrt{N} \sqrt{2\,\pi}}\, e^{-\dfrac{(z - N\,r)^2}{2\,\sigma^2\,N}} \cdot \Delta z$$

  with $r = 6.0481 \cdot 10^{-4}$, $\sigma = 0.0194$ and $N = 250$.

- The fair value p of the option is determined by the condition that the expected value of the payoff should equal the price.

The answer

The probability for the value S_1 of the stock after one year to satisfy $\ln C \leq z \leq \ln S_1 \leq z + \Delta z$ for Δz small is given by

$$\mathrm{PDF}(z) \cdot \Delta z = \frac{1}{\sigma \sqrt{N} \sqrt{2\,\pi}}\, e^{-\dfrac{(z - N\,r)^2}{2\,\sigma^2\,N}} \cdot \Delta z$$

The graph of this function is shown in Figure 2.49. The figure has to be compared with the left part in Figure 2.48.

With the help of this probability function we can compute the probability for certain events. To find the probability that the value of the stock is larger than twice its original value we compute

$$\int_{\ln 2}^{\infty} \mathrm{PDF}(z)\; dz = \frac{1}{\sigma \sqrt{N} \sqrt{2\,\pi}} \int_{\ln 2}^{\infty} e^{-\dfrac{(z - N\,r)^2}{2\,\sigma^2\,N}}\; dz \approx 0.039$$

Thus there is only a 4% chance to double the value within one year. The integral

$$\int_{\ln 1}^{\infty} \mathrm{PDF}(z)\; dz = \frac{1}{\sigma \sqrt{N} \sqrt{2\,\pi}} \int_{\ln 1}^{\infty} e^{-\dfrac{(z - N\,r)^2}{2\,\sigma^2\,N}}\; dz \approx 0.69$$

indicates that there is a 69% chance of the value of the stock to increase. These probabilities have to be taken into account when estimating the value of the option.

If the value of the stock after one year is given by S_1 then the payoff is

$$\max\{0, S_1 - C\}$$

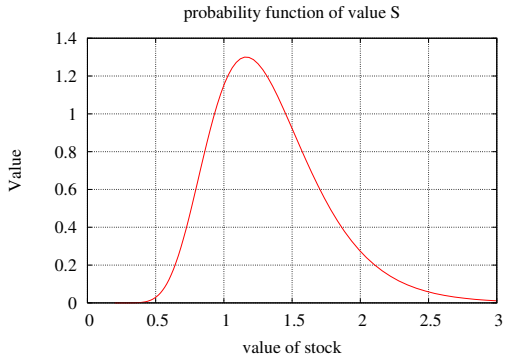


Figure 2.49: Probability density function of final values

- If $S_1 \leq C$ then there is no payoff
- If $\ln C \leq z \leq \ln S_1 \leq z + \Delta z$ then the payoff is approximately $S_1 - C = e^z - C$. Since the probability for this is given by $\mathrm{PDF}(z) \cdot \Delta z$ we find

$$\text{payoff of } e^z - C \quad \text{with probability} \quad \mathrm{PDF}(z) \cdot \Delta z = \frac{1}{\sigma \sqrt{N} \sqrt{2\,\pi}}\, e^{-\dfrac{(z - N\,r)^2}{2\,\sigma^2\,N}} \cdot \Delta z$$

To examine the expected payoff we plot the product of the payoff with the probability density function. The result is shown in Figure 2.50 . Observe the following

- You can not expect any payoff if the value of the stock will fall below $C = 1.05$.
- Values of S_1 slightly larger than C are very likely to occur, but the payoff $S_1 - C$ will be small.
- Very high values of S_1 are unlikely to happen. Thus the large payoff $S_1 - C$ is unlikely to occur.
- Most of the return from this option will occur for values of S_1 between 1.3 and 2.0 .

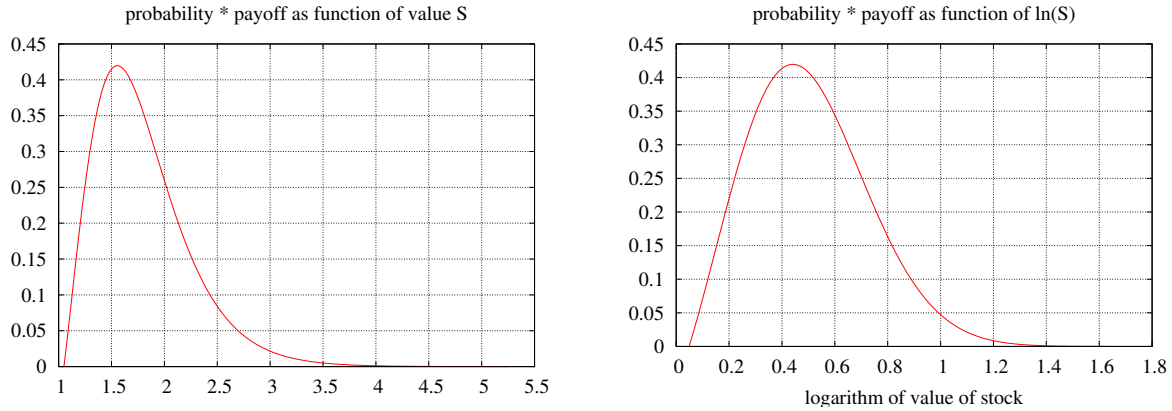


Figure 2.50: Product of payoff with probability density function

All those possible contributions to the payoff have to be taken into account. The possible values for S_1 are $0 < S_1 < \infty$ and thus $-\infty < z = \ln S_1 < \infty$. By adding up, resp. integrating the above payoff we

arrive at an expected value of the payoff (and thus the price of the option) of

$$\begin{aligned} p &= \lim_{\Delta z_i \to 0} \left(\sum_{z_i = \ln C}^{\infty} (e^{z_i} - C)\ \mathrm{PDF}(z_i)\ \Delta z_i \right) \\ &= \int_{\ln C}^{\infty} (e^z - C)\ \mathrm{PDF}(z)\ dz = \frac{1}{\sigma\sqrt{N}\sqrt{2\,\pi}} \int_{\ln C}^{\infty} (e^z - C)\ e^{-\frac{(z - N\,r)^2}{2\,\sigma^2\,N}}\ dz \approx 0.23887 \end{aligned}$$

Thus the fair value of the option is $p \approx 0.24$.

The above computations can be repeated for multiple values of the strike price C . This might generate Figure 2.51 .

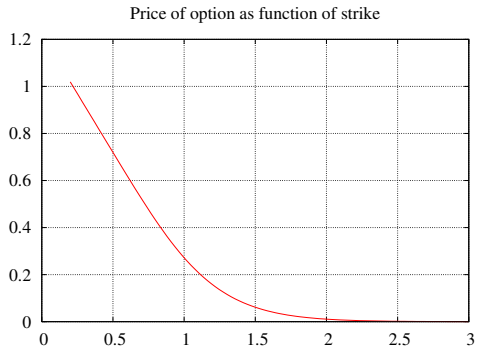


Figure 2.51: Price of the option as function of the strike price C

The *Octave*–code

The result of the previous sections were computed with the help of the following *Octave*–code.

- Give the basic data and plot the probability density function.

Octave

```
rmean = 6.0481e-4       % mean of the daily interest rate
rstd  = 0.0194          % standard deviation of the daily interest rate
N  = 250                % number of trading days in a year
C  = 1.05               % strike price
NN = 100;
zval = linspace(log(0.2),log(3),NN);
Prob = gauss(zval,N*rmean,rstd*sqrt(N));
figure(1);
plot(exp(zval),Prob)
title('probability function of value S')
grid on
```

- Compute the probabilities for the value of the stock to double or at least increase.

Octave

```
zval  = linspace(log(1),log(6),NN);
Prob  = gauss(zval,N*rmean,rstd*sqrt(N));
prob1 = trapz(zval,Prob)
zval  = linspace(log(2),log(6),NN);
Prob  = gauss(zval,N*rmean,rstd*sqrt(N));
prob2 = trapz(zval,Prob)
```

- Compute the value of the stock option.

Octave

```
maxVal = 5*C;
zval = linspace(log(C),log(maxVal),NN);
Prob = gauss(zval,N*rmean,rstd*sqrt(N));
payoffProb = (exp(zval)-C).*Prob;

figure(2);
plot(zval,payoffProb)
title('probability * payoff as function of ln(S)')
grid on

figure(3);
plot(exp(zval),payoffProb)
title('probability * payoff as function of value S')
grid on
OptionValue = trapz(zval,payoffProb)  % use builtin trapezoidal rule
```

- Examine different values for the strike price C .

Octave

```
NN    = 100;
cval  = linspace(0.2,3,100);
price = zeros(size(cval));
for k = 1:length(cval)
  zval = linspace(log(cval(k)),log(6),NN);
  Prob = gauss(zval,N*rmean,rstd*sqrt(N));
  payoffProb = (exp(zval)-cval(k)).*Prob;
  price(k) = trapz(zval,payoffProb);
end
figure(4);
plot(cval,price)
title('Price of option as function of strike')
grid on
```

Nobel Price in Economics

This observation is used as a foundation for the famous Black–Scholes formula to find the value of stock options. Further effects have to be taken into account, e.g. interest rates and other types of options. The theory was developed by Fischer Black, Myron Scholes and Robert Merton in 1973. Since then their results are extensively used. The 1997 Nobel Prize in Economics was awarded to Merton and Scholes (Black died earlier). Further information on this interesting topic can be found in [Seyd00] and [Wilm98].

2.5.6 List of codes and data files

In the previous sections the codes and data files in Table 2.10 were used.

Script file	task to perform
IBMscriptDLM.m	csv read the data and create basic plot
IBMscript.m	formatted scanning of the data and create basic plot
IBM.csv	data file with the value of IBM stock
IBMaverage.m	compute daily interest rates
IBMhistogram.m	create histogram with interest rates
IBMsimulation.m	simulation for value of stock during one year
IBMsimulationMultiple.m	multiple runs of above simulation
IBMsimulationHist.m	histogram for multiple runs of above simulation
gauss.m	compute the value of a Gauss function
IBMBlackScholes.m	find the value of a stock option

Table 2.10: Codes and data files for section 2.5

2.6 Vibration Analysis of a Circular Disk

2.6.1 Description of problem

A circular disk (watch) is submitted to a shock acceleration and thus will start to move. The vertical displacement is measured at several points along the perimeter. The resulting movement should be visualized. The typical situation at a given time is shown in Figure 2.52.

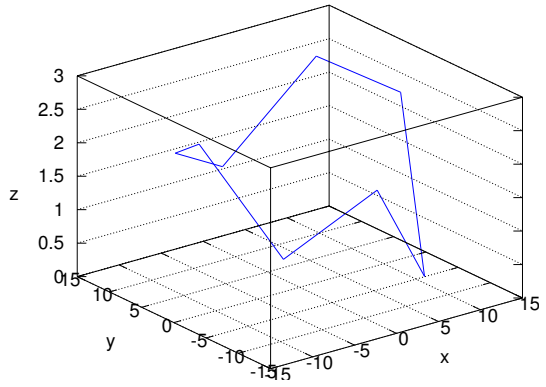


Figure 2.52: Deformed circle for a given time

2.6.2 Reading the data

The first task is to read all the data files. Each data file contains about 4460 data points. The plan is to read one out of 5 points and ignore the other measurements. Thus we read only 345 points. On the circle 8 different points were examined.

- First we create matrices big enough to contain all data.

Octave

```
%% nt number of points to be read
 nt = 345;
%% skip number of frames to be ignored before the next image is created
 skip = 5;
%% lineskip number of lines to be ignored for the header
 lineskip = 1;
%% nt*skip < number of points to be measured
%% Npts number of measurement points on caliber
 Npts = 8;

%% define the matrices for the coordinate data of points
 x = zeros(Npts+1,nt);
 y = zeros(Npts+1,nt);
 t = zeros(Npts+1,nt);
 h = zeros(Npts+1,nt);
```

- First we define the horizontal position of each point, given by the x and y coordinates. We copy the first point to the 9^{th}, to close the circle.

Octave

```
x(1,:) = -12.0; %% first line of x
x(2,:) = -8.4;
x(3,:) = 0;
x(4,:) = 8.4;
x(5,:) = 12;
x(6,:) = 8.4;
x(7,:) = 0;
x(8,:) = -8.4;
x(9,:) = -12.0; %% copy of the first line

y(1,:) = 0;   %% first line of y
y(2,:) = -8.4;
y(3,:) = -12;
y(4,:) = -8.4;
y(5,:) = 0;
y(6,:) = 8.4;
y(7,:) = 12;
y(8,:) = 8.4;
y(9,:) = 0; %% copy of the first line
```

- Each of the files `cg*a.txt` contains two columns of data. The first number indicates the time and the second the vertical displacement.

cg1a.txt

```
   temps          chemin
-4.02E-7       6.66173E-3
1.551E-6       -7.02712E-2
3.504E-6       -5.89382E-2
5.457E-6       1.47049E-2
7.41E-6        9.04202E-3
9.363E-6       2.95391E-2
1.1316E-5      3.40761E-2
1.3269E-5      5.05111E-2
...
```

The entries on each line are separated by a TAB character. We use the command `dlmread()` to read the data files. This allows to skip the first row[11], use `help dlmread`.

ReadDataDLM.m

```
row = 1;
data = dlmread('cg1a.txt','\t',1,0);
t(row,1:nt) = data(skip*[1:nt],1);
h(row,1:nt) = data(skip*[1:nt],2);

row = 2;
data = dlmread('cg10a.txt','\t',1,0);
t(row,1:nt) = data(skip*[1:nt],1);
h(row,1:nt) = data(skip*[1:nt],2);

%%%%% followed by a few similar sections of code
```

- Another option is to first open the file for reading (`fopen()`), then read each line by `fgets()` and use formatted scaning (`sscanf()`) to extract the two numbers.

ReadData.m

[11] This does **not** work with the `MATLAB` version of `dlmread()`.

```
row = 1;
fid = fopen('cg1a.txt','r');
for ii = 1:lineskip
  tline = fgets(fid);
end
for ii = 1:nt
  for s = 1:skip tline = fgets(fid);end
  res = sscanf(tline,'%e %e');
  t(row,ii) = res(1);
  h(row,ii) = res(2);
end
fclose(fid);

row = 2;
fid = fopen('cg10a.txt','r');
for ii = 1:lineskip
  tline = fgets(fid);
end
for ii = 1:nt
  for s = 1:skip tline = fgets(fid);end
  res = sscanf(tline,'%e %e');
  t(row,ii) = res(1);
  h(row,ii) = res(2);
end
fclose(fid);

%%%%% followed by a few similar sections of code
```

- The new last point has to be created as a copy of the first point. This will close the cricle.

Octave

```
% copy first point to last point
t(9,:) = t(1,:);
h(9,:) = h(1,:);
```

With the above preparation one can now create the picture in Figure 2.52.

Octave

```
k = 20;
plot3(x(:,k),y(:,k),h(:,k));
xlabel('x'); ylabel('y'); zlabel('z');
grid on
```

2.6.3 Creation of movie

By creating pictures similar to Figure 2.52 for each time slice we can now create a movie and display it on the screen. The code below does just this with the switch `movie=0`. If we set `movie=1` then the images are written to the subdirectory `pngmovie` in a bitmap format (png) and an external command (`mencoder`) is used to generate a movie file `Circle.avi` to be used without *Octave*. The command is composed of two strings, for them to fit on one display line. Subsequently the directory is cleaned up.

MovieAVI.m

```
movie = 0; %% switch to generate movie 0: no movie, 1: movie generated
cd pngmovie
k = 1;
plot3(x(:,k),y(:,k),h(:,k));
```

```
xlabel('x'); ylabel('y'); zlabel('h');
axis([-14 14 -14 14 -360 80])
grid on
for k = 1:nt
   plot3(x(:,k),y(:,k),h(:,k));
   xlabel('x'); ylabel('y'); zlabel('h');
   axis([-14 14 -14 14 -360 80])
   grid on
   drawnow();
if movie
   filename = ['movie',sprintf('%03i',k),'.png'];
   print(filename,'-dpng')
 endif
end

if movie
  c1 = 'mencoder mf://*.png -mf fps=5 -ovc lavc -lavcopts vcodec=mpeg4';
  c2 = ' -o Circle.avi';
  system([c1,c2]);
  system('rm -f *.png');
endif
cd ..
```

To generate the move we may use the program `mencoder` on a Linux system. To generate WMV files I used

```
mencoder mf://*.png -mf fps=5 -ovc lavc -lavcopts vcodec=wmv1 -o movie.avi
```

and for MPEG files accordingly

```
mencoder mf://*.png -mf fps=5 -ovc lavc -lavcopts vcodec=mpeg4 -o movie.avi
```

To play the movie you may use any movie player, e.g. `vlc` or `xine`.

2.6.4 Decompose into displacement and deformation

The movement of the circle can be decomposed into four different movements:

1. moving the center of the circle up and down
2. rotating the circle about the y axis
3. rotating the circle about the x axis
4. internal deformation of the circle

Using linear regression we want to visualize the above movements and deformation. To determine the movement and rotations we search for coefficients p_1, p_2 and p_3 such that for any given time t the plane

$$z(t, x, y) = p_1(t) + p_2(t) \cdot x + p_3(t) \cdot y$$

describes the location of the circle a good as possible, in the least square sense. Thus for a given time t we have the following problem:

- Given:
  - location of points $(x_i\,,\, y_i)$ for $1 \leq i \leq m$

  - measured height z_i for $1 \leq i \leq m$

- Search parameters $\vec{p}$ such that $p_1 \cdot 1 + p_2 \cdot x_i + p_3 \cdot y_i$ is as close as possible to z_i .

We use linear regression (see Section 2.2) to find the optimal parameters. We introduce a matrix notation.

$$\mathbf{X} = \begin{bmatrix} 1 & x_1 & y_1 \\ 1 & x_2 & y_2 \\ 1 & x_3 & y_3 \\ & \vdots & \\ 1 & x_n & y_n \end{bmatrix} \quad \text{and} \quad \vec{z} = \begin{pmatrix} z_1 \\ z_2 \\ z_3 \\ \vdots \\ z_n \end{pmatrix}$$

Now we can use the command `LinearRegression()` to determine the parameters and then create Figure 2.53. In Figure 2.53(a) find the height as function of time. The down an up movement of the circle is clearly recognizable. In Figure 2.53(b) the two slopes of the circle in x and y direction are displayed.

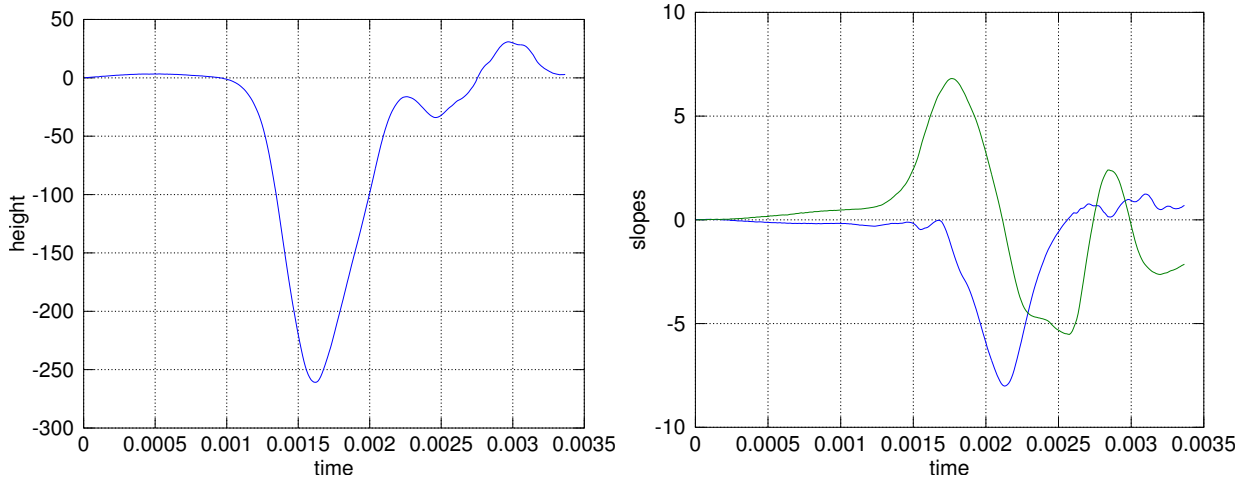
regress.m

```
X = [ones(1,8);x(1:8,1)';y(1:8,1)']';
% nt=345;
par = zeros(3,nt);

for kk = 1:nt
  p = LinearRegression(X,h(1:8,kk));
  par(:,kk) = p;
end

figure(3);
plot(t(1,:),par(1,:));
grid on; axis([t(1,1), max(t(1,:)), -300, 50])
xlabel('time'); ylabel('height'); grid on

figure(4);
plot(t(1,:),par(2:3,:));
grid on; axis([t(1,1), max(t(1,:)), -10, 10])
xlabel('time'); ylabel('angles');
```

As a next step we create a movie with the movement and rotations of the plane only. First we compute the position of the planes and then reuse the code from the previous section to generate a movie.

MovieLinear.m

```
hlinear = X*par;
hlinear(9,:) = hlinear(1,:);
horiginal = h;
hdeform = h-hlinear;

figure(5);
hdisp = hlinear;

movie = 0; %% switch to generate movie
cd pngmovie
k = 1;
plot3(x(:,k),y(:,k),hdisp(:,k));
xlabel('x'); ylabel('y'); zlabel('h');
axis([-14 14 -14 14 -360 80])
grid on
for k = 1:nt
```



(a) height as function of time

(b) the two slopes as function of time

Figure 2.53: Height and slopes of the moving circle

```
    plot3(x(:,k),y(:,k),hdisp(:,k));
    xlabel('x'); ylabel('y'); zlabel('h');
    axis([-14 14 -14 14 -360 80])
    grid on
    drawnow()
if movie
    filename = ['movie',sprintf('%03i',k),'.png'];
    print(filename,'-dpng')
end

if movie
  c1 = 'mencoder mf://*.png -mf fps=25 -ovc lavc -lavcopts vcodec=mpeg4';
  c2 = ' -o movieLinear.avi';
  system([c1,c2]);
  system('rm -f *.png');
endif
cd ..
```

Then the internal deformations can be displayed too. Since the amplitudes are smaller we have to change the scaling to be used.

MovieDeform.m

```
hlinear = X*par;
hlinear(9,:) = hlinear(1,:);
horiginal = h;
hdeform = h-hlinear;

figure(5);
hdisp = hdeform;

movie = 0; %% switch to generate movie
cd pngmovie
k = 1;
plot3(x(:,k),y(:,k),hdisp(:,k));
xlabel('x'); ylabel('y'); zlabel('h');
axis([-14 14 -14 14 -50 50])
```

```
grid on
for k = 1:nt
   plot3(x(:,k),y(:,k),hdisp(:,k));
   xlabel('x'); ylabel('y'); zlabel('h');
   axis([-14 14 -14 14 -50 50])
   grid on
   drawnow
if movie
   filename = ['movie',sprintf('%03i',k),'.png'];
   print(filename,'-dpng')
 endif
end

if movie
  c1 = 'mencoder mf://*.png -mf fps=25 -ovc lavc -lavcopts vcodec=mpeg4';
  c2 = ' -o movieDeform.avi';
  system([c1,c2]);
  system('rm -f *.png');
endif
cd ..
```

2.6.5 List of codes and data files

In the previous sections the codes and data files in Table 2.11 were used.

Script file	task to perform
`cg*a.txt`	data files
`ReadDataDLM.m`	read all data files, using `dlmread()`
`ReadData.m`	read all data files, using `sscanf()`
`MovieAVI.m`	display movie and create `Circle.avi`
`regress.m`	do the linear regression and plot the graphs
`MovieLinear.m`	display and create movie of the linear movements
`MovieDeform.m`	display create movie of the internal deformations
`Circle.avi`	movie of the complete movement
`movieLinear.avi`	movie of the linear movement
`movieDeform.avi`	movie of the deformations

Table 2.11: Codes and data files for section 2.6

2.7 Analysis of a Vibrating Cord

The diploma thesis of Andrea Schüpbach examined vibrating cord sensors, produced by DIGI SENS AG. A sample is shown in Figure 2.54. An external force will lead to an increase in tension on a vibrating string whose frequency is used to determine the force. For further developments DIGI SENS needs to examine the frequency and quality factor of this mechanical resonance system. An electronic measurement system was developed and tested. In this section the data analysis for this project will be presented.

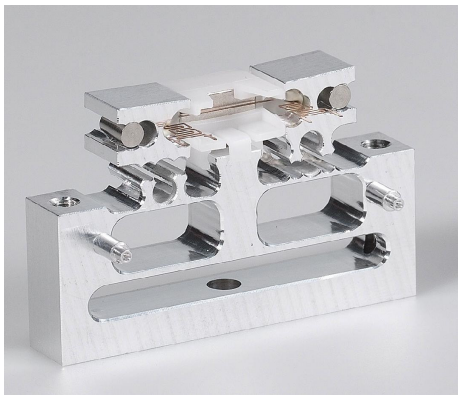


Figure 2.54: A vibrating cord sensor produced by DIGI SENS AG

2.7.1 Design of the basic algorithm

The raw signal of a sensor is measured with `LabView` and the data then written to a file. A typical result is shown in Figure 2.55. At first the cord is vibrating with a constant amplitude and the the amplitude seems to converge to zero, exponentially. Thus we find functions of the form

$$\text{first:} \quad y(t) = A\,\cos(\omega\,t) \qquad \text{then:} \quad y(t) = A\,e^{-\alpha(t-t_0)}\,\cos(\omega\,t)$$

To characterize the behavior of the sensor the initial amplitude A and the decay exponent α have to be determined reliably.

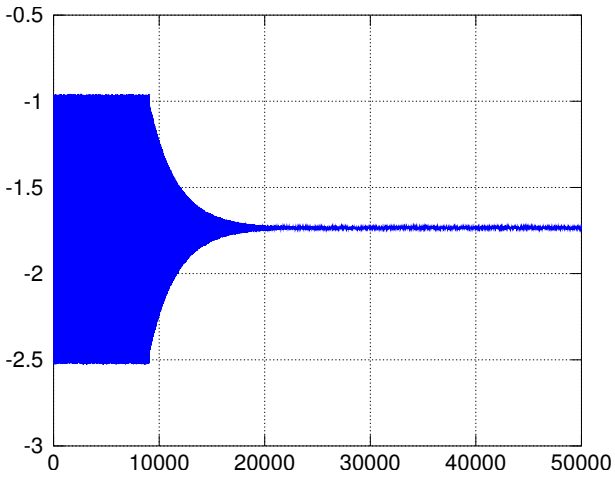


Figure 2.55: The signal of a vibrating cord sensor

The essential steps to be taken to arrive at the desired data are:

- Read the data from a file and display.
- Subtract the average value to have the signal oscillate about 0 .
- Take the average of the absolute value to arrive at an amplitude signal.
- Use linear regression of the logarithmic data to determine the decay exponent.

The goal of this section is to obtain code for the above algorithm to be applied to data in a file. The result is a *Octave* function `automatic.m` that will analyze a data set, generate the graphs and display the results. An example is given by

Octave

```
[amplitude,factor] = automatic('m4')
-->
Slope: -18.3789, Variance of slope: 0.00337408, relative error:0.000183584
amplitude = 0.49640
factor = -0.054410
```

Thus the body of the function is given by

automatic.m

```
function [amp,fact] = automatic(filename)

write your code here

endfunction
```

Reading the data

The sensor is examined with the help of a DAQ card and LabView. The result are files with the data below.

m4

```
waveform          [0]
t0        03.10.2007   15:36:19.
delta t  2.080000E-5

time      Y[0]
03.10.2007   15:36:19.    -1.275252E+0
03.10.2007   15:36:19.    -1.294272E+0
03.10.2007   15:36:19.    -2.469335E+0
03.10.2007   15:36:19.    -1.826837E+0
03.10.2007   15:36:19.    -9.730251E-1
03.10.2007   15:36:19.    -2.076841E+0
...
```

The data consists of 5 header lines and then the actual data lines, in this case 50000 lines. Since there are many data lines the scanning of the data will take time. The same data set will have to be analyzed many times, to determine the optimal parameters. Thus once the data is read from the file (e.g. from `m4`) a new binary file (e.g. `m4.bin`) is generated. On subsequent calls of this function the binary file will be read, leading to sizable time savings[12].

- We use the fact that the sampling rate is 48 kHz.
- If a file with binary data exist, read it with the help of the command `load()`.

[12] On this authors PC the time was cut from 12 seconds to 1 second.

- Otherwise use the tools from Section 1.2.8 to read and scan the data file. After reading generate the file with the binary data.
- Generate a graph with the raw data for visual inspection.

Octave

```
dt = 1/48000; %% set the sampling frequency
Nmax = 50000; %% create arrays large enough to contain all data
x = zeros (Nmax, 1 ) ; y = x;
%% read the binary file, if it exists
%% otherwise read the original file and write binary file
if (exist([filename,'.bin'],'file')==2)
  eval(['load ',filename,'.bin'])
else
  inFile = fopen(filename ,'rt' ) ; %% read the information from the file
  for k = 1:5
    inLine = fgetl(inFile);
  end
  k = 1;
  for j = 1:Nmax
    inLine = fgetl(inFile);
    counter = find(inLine=='E');
    y(j) = sscanf(inLine(counter-9:length(inLine)) ,'%f');
  end
  fclose(inFile) ;
  eval(['save -binary ',filename,'.bin y'])
end

figure(1);
plot(y) %% plot the raw data
grid on
```

Determine the amplitude as function of time

The result of the above code is shown in Figure 2.55. Now we aim for the amplitude as a function of time and first subtract the average value of the result. Thus we arrive at oscillations about 0. Then we take the absolute value of the result. With the measurements we sample a function $y = \mathrm{abs}(\sin(\omega\, t))$ at equidistant times, as shown in Figure 2.56. This figure indicates that the mean value of the sampled amplitudes should be equal to the average height h of the function $\sin(t)$ on the interval $[0, \pi]$, i.e.

$$h = \frac{1}{\pi}\int_0^\pi \sin(t)\; dt = \frac{\cos(t)}{\pi}\Big|_{y=0}^{\pi} = \frac{2}{\pi}$$

Thus the average value of a larger sample with constant amplitude has to be multiplied by $\pi/2$ to obtain the correct amplitude. Since the instrument has to be calibrated we might as well ignore the factor $\pi/2$. One has to be careful though. The cords are vibrating with frequencies of 14-18 kHz and the sampling frequency is only 48 kHz. Thus we only find about 3 points in one period. This may cause serious discretization problems. By using 100 points the algorithm proved to be robust. A first implementation of the above idea is given by

Octave

```
y2 = abs(y-mean(y)); % subtract average value
FilterLength = 100+1; % average over some points
t0 = cputime();
y3 = zeros(Nmax-FilterLength,1);
for k = 1:Nmax-FilterLength
```

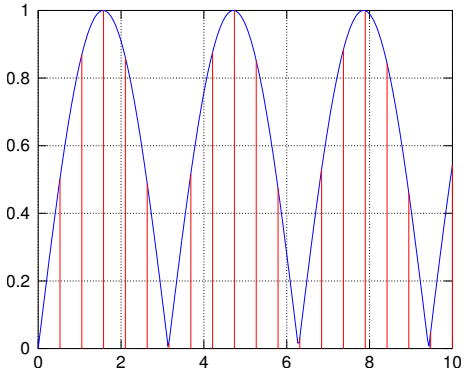


Figure 2.56: A function $y = \mathrm{abs}(\sin(\omega\, t))$ and a sampling

```
    y3(k) = mean(y2(k:k+FilterLength));
  endfor
  tt = cputime-t0
```

leading to an excessive computation time of 35 seconds. The *Octave* command `conv()`, short for convolution, leads to a much faster implementation with a computation time of less than one tenth of a second. The algorithm used in `conv()` is based on FFT.

Octave

```
y2 = abs(y-mean(y));  % subtract average value
FilterLength = 100+1; % average over some points
Filter = ones(FilterLength,1)/FilterLength;
y3 = conv(Filter,y2(1:end-FilterLength+1))';
y3 = y3(FilterLength:end);
N = length(y3);
```

The results are shown in Figure 2.57, generated by

Octave

```
figure(2);
t = linspace(0,(N-1)*dt,N)';
plot(t,log(y3));  grid on
```

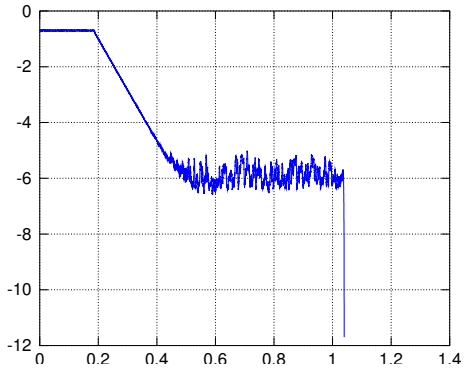


Figure 2.57: The logarithm of the amplitude as function of time

In Figure 2.57 we clearly recognize the constant amplitude in the first sector and then a straight line segment. This is caused by

$$A = A_0\, e^{-\alpha\, t} \qquad \Longrightarrow \qquad \ln A = \ln A_0 - \alpha\, t$$

The wild variations on the right part in Figure 2.57 are caused by the almost 0 values. The resolution of the involved instruments do not allow to determine small amplitudes reliably. They will have to be ignored.

Compute the initial amplitude and the decay exponent

As full amplitude A_0 we use the average of the first 200 values. Then we choose an upper and a lower cutoff value.

- Determine the first data point below the upper cutoff value.
- Determine the first data point below the lower cutoff value.
- Examine only data points between the above two points.

Octave

```
amplitude = mean(y3(1:200));
topcut = 0.8; lowcut = 0.4;  %% choose the cut levels on top and bottom
Nlow  = find(y3<topcut*amplitude)(1);
Nhigh = find(y3<lowcut*amplitude)(1);

y4 = log(y3(Nlow:Nhigh));
N  = length(y4);
t  = linspace(0,(N-1)*dt,N)';
```

On this reduced data set we use linear regression (see Section 2.2) to determine the slope of the straight line and the estimated standard deviation of the slope.

Octave

```
%% run the linear regression
F = ones(N,2); F(:,2) = t;
[p,y_var,r,p_var] = LinearRegression(F,y4');
yFit = F*p;

figure(3);
plot(t,y4,t,yFit)  % display the real data and the regression line
grid on

fprintf('Slope: %g, Variance of slope: %g, relative error:%g\n',...
        p(2), sqrt(p_var(2)), -sqrt(p_var(2))/p(2));
factor = 1/p(2);
```

The numerical result and Figure 2.58 clearly indicate that we have **one exponential function** on the decaying section of the signal. Based on the above results the algorithm was implemented in `LabView` and graphs of the amplitude and quality factor as function of the frequency are generated on screen.

2.7.2 Analyzing one data set

The above basic algorithm is used to make one measurement of data. For each frequency multiple measurements should be made, to estimate the variance of the results. These measurements have to be repeated for many different frequencies and a usefull graph has to be generated, to be included in reports on the development of new sensors. A possible result is given in Figure 2.59. Graphs of this type can not be generated directly by *Octave* and thus we will use *Gnuplot*. Currently (Nov 2009) *Octave* can not generate graphs with two different vertical axis.

We expect the following features for the final graphics:

- For each frequency the average value of all the measurements is shown and and error lines at a distance of one standard deviation are drawn.

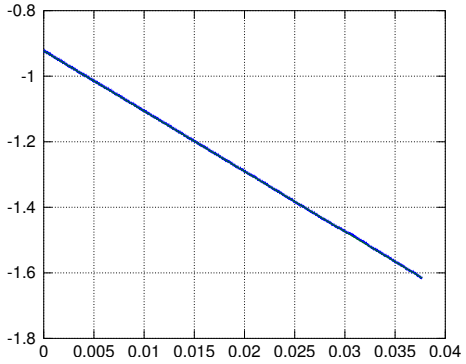


Figure 2.58: The result of linear regression

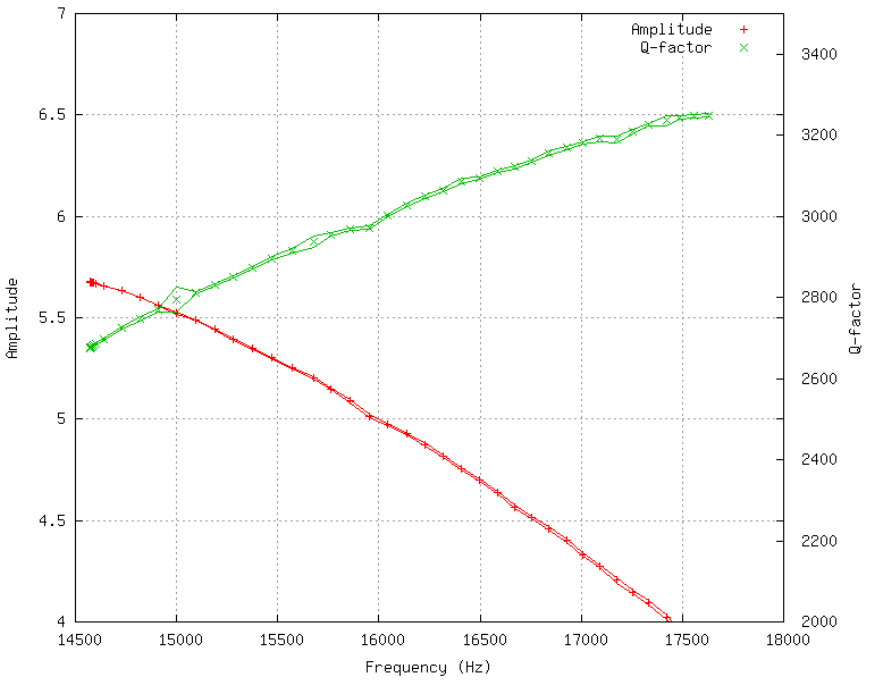


Figure 2.59: Amplitude and Q-factor as function of frequency, including error

- The labeled axis for the amplitude is shown on the left edge of the graph.
- The labeled axis for the Q-factor is shown on the right edge of the graph.
- The scales shall not change from one data set to another. Thus it is easier to compare two different graphs.
- The graphics should be generated in a format that can be used by most text processing software. We choose PNG. The resolution and size of this bitmap format have to be well chosen, since rescaling bitmaps is a very bad idea.
- A simpler graph without the error estimates should be generated to.
- Create a graph with the temperature as a function of the frequency.

The `LabView` program generates data files in a specified format, shown in the example below. The header lines contain information on the total number of measurements and the number of repetitions for one fixed frequency.

Elektro22.data

```
01.12.2007 12:13
42 Messungen
22 Wiederholungen



Amplitude Frequenz Q–Faktor Strom Temperatur

5.684363        14571.520000    2676.159581     0.000000        24.750000
5.685096        14572.430000    2675.312131     0.000000        24.750000
5.684854        14573.010000    2677.640868     0.000000        24.750000
5.684326        14573.550000    2678.034266     0.000000        24.750000
5.684079        14573.900000    2677.439599     0.000000        24.750000
5.684086        14574.140000    2679.226273     0.000000        24.750000
...
```

The *Octave* code to be written has to:

- Open the file with the measured data for reading and a open a data file `gnu.dat` for writing the data to be used by *Gnuplot*. `gnu.dat` for the data to be used by *Gnuplot*.
- Read all the data for one frequency f.
- Compute the average amplitude A and estimate the variance ΔA.
- Compute the average Q-factor Q and estimate the variance ΔQ.
- Write one data line with the data to be displayed, i.e. write f, A, $A-\Delta A$,$A+\Delta A$, Q, $Q-\Delta Q$ and $Q+\Delta Q$.
- Within *Octave* a system call to *Gnuplot* has to generate the graphs.

A sample call is shown below.

Octave

```
[freq,freqS,amp] = WriteData('Elektro22.data');
-->
mean STDEV frequency 3.804698e+00, maximal STDEV frequency 6.416919e+01
mean STDEV amplitude 5.145861e-03, maximal STDEV amplitude 1.269707e-02
mean STDEV Q-factor 4.76711, maximal STDEV Q-factor 31.0231
mimimal temperature 24.8455, maximal temperature 42.1364
```

If a data file `gnu.dat` contains the data in the above format *Gnuplot* can generate Figure 2.59 with the commands below. For most of the lines one can guess the effect of the command. Otherwise reading the manual of *Gnuplot* might be necessary.

- The line `set terminal` allows to chose the type of output format and the size of the resulting graphics.
- `Set output` sets the name of the output file.
- The labels for the different axis have to be set.
- The range for the two vertical scales have to be set with `set yrange` and `set y2range`.
- Finally **one** plot command will use different columns in the data file `gnu.dat` to create the 6 different graphs in one image.

AmpQ.gnu

```
set terminal png large size 800,600
set output 'AmpQ2.png'
set y2tics border
set xlabel "Frequency (Hz)"
set ylabel "Amplitude"
set y2label "Q-factor"
set grid
set xrange [14500:18000]
set yrange [4:7]
set y2range [2000:3500]
plot 'gnu.dat' using 1:2 with points lt 1 title 'Amplitude' axes x1y1,\
     'gnu.dat' using 1:3 with lines lt 1 notitle axes x1y1,\
     'gnu.dat' using 1:4 with lines lt 1 notitle axes x1y1,\
     'gnu.dat' using 1:5 with points lt 2 title 'Q-factor' axes x1y2,\
     'gnu.dat' using 1:6 with lines lt 2 notitle axes x1y2,\
     'gnu.dat' using 1:7 with lines lt 2 notitle axes x1y2
```

The *Octave* file `WriteData.m` fullfills the above requirements[13]. The tools used are again found in Section 1.2.8. The last line of code uses a system call to use *Gnuplot* and the above command file `AmpQ.gnu` to generate the graphic files in the current directory.

WriteData.m

```
function [freq,freqS,amp,ampS,quali,qualiS,curr,currS,temp,tempS]...
   = WriteData(filename)

% function to write data for the DigiSens sensor
%
% WriteData(filename)
% [freq,freqS,amp,ampS,quali,qualiS,curr,currS,temp,tempS] = WriteData(filename)
%
% when used without return arguments  WriteData(filename) will analyze data
```

[13] On Win* system the last line should be replaced by `system('pgnuplot AmpQ.gnu');`

```
% in filename and then write to the new file 'gnu.dat'. Then a system call
% 'gnuplot AmpQ.gnu' is made to generate graphs in the files
% AmpQ.png AmpQ2.png and Temp.png
%
% when used with return arguments the consolidated data will be returned
% and may be used to generate graphs, e.g.
% [freq,freqS,amp] = WriteData('test1.dat');
% plot(freq,amp)
%

if ((nargin !=1))
  usage('give filename in WriteData(filename)');
end

calibrationFactor = 11.2; % factor for amplitudes, ideal value is 1.0
calibrationFactor = 1.0;

infile = fopen(filename,'rt');

tline = fgetl(infile); % dump top line
tline = fgetl(infile); % read number of measurements
meas  = sscanf(tline,'%i');
tline = fgetl(infile); % read number of repetitions
rep   = sscanf(tline,'%i');

freq = zeros(meas,1); freqS=freq; freqT=zeros(rep,1);
curr = freq; currS = freq; currT = freqT;
quali = freq; qualiS=freq; qualiT = freqT;
amp = freq; ampS = freq; ampT = freqT; temp = freq;

for k = 1:8;   % read the headerlines
  tline = fgetl(infile);
endfor

for im = 1:meas;
  for ir = 1:rep
    tline = fgetl(infile);
    t = sscanf(tline,'%g %g %g %g %g');
    ampT(ir) = calibrationFactor*t(1);
    freqT(ir)  = t(2);
    qualiT(ir) = t(3);
    currT(ir)  = t(4);
    tempT(ir)  = t(5);
  endfor
  amp(im)   = mean(ampT);   ampS(im)   = sqrt(var(ampT));
  freq(im)  = mean(freqT);  freqS(im)  = sqrt(var(freqT));
  quali(im) = mean(qualiT); qualiS(im) = sqrt(var(qualiT));
  curr(im)  = mean(currT);  currS(im)  = sqrt(var(currT));
  temp(im)  = mean(tempT);  tempS(im)  = sqrt(var(tempT));
endfor
fclose(infile);

printf('mean STDEV frequency %3e, maximal STDEV frequency %3e\n',mean(freqS),max(freqS));
printf('mean STDEV amplitude %3e, maximal STDEV amplitude %3e\n',mean(ampS),max(ampS));
printf('mean STDEV Q-factor %3g, maximal STDEV Q-factor %3g\n',mean(qualiS),max(qualiS));
printf('mimimal temperature %3g, maximal temperature %3g\n',min(temp),max(temp))

outfile = fopen('gnu.dat',"wt");
```

```
fprintf(outfile,'# Freq Amp amp-STDEV amp+STDEV Q Q-STDEV Q+STDEV temp\n');
for im = 1:meas;
  fprintf(outfile,"%g %g %g %g %g %g %g %g\n",...
        freq(im),amp(im),amp(im)-ampS(im),amp(im)+ampS(im),...
           quali(im),quali(im)-qualiS(im),quali(im)+qualiS(im),temp(im));
endfor
fclose(outfile);

system('gnuplot AmpQ.gnu');
endfunction
```

With very similar tools the results in Figure 2.60 are generated. The file `AmpQ.gnu` will create all three graphs in this section.

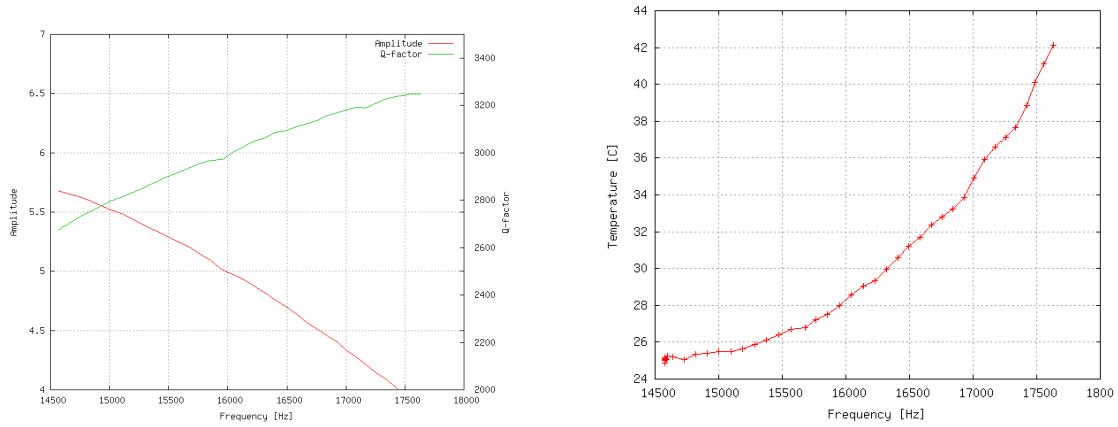


Figure 2.60: Amplitude, Q-factor and temperature as function of frequency

2.7.3 Analyzing multiple data sets

To compare different sensors or the influence of external parameters it is necessary to display the results of multiple measurements in one graph. As example consider the three Figures 2.61, 2.62 and 2.63. They are created by

Octave

```
WriteDataAll('Elektro',[1:5],'.data')
-->
estimated temperature dependence of amplitude: -0.047083 um/C
estimated temperature dependence of Q-factor: -10.0248 /C
```

In this section we will examine the code carefully. The documentation of this command is contained at the top of the function file `WriteDataAll.m`.

WriteDataAll.m

```
function  WriteDataAll(basename,numbers,ext)

% function to analyze data for a series of Digi Sens sensor
%
% WriteDataAll(basename,numbers,ext)
%
% will analyze data given in files and then generate graphs
% and files AmpAll.png and QAll.png
% It will also display the estimated dependencies of amplitude
```

```
% and Q-factor on the temperature
%
% sample calls:
%   WriteDataAll('elektro',[1:5],'.data')
%   WriteDataAll('elektro',[1, 2, 4, 5],'.data')
```

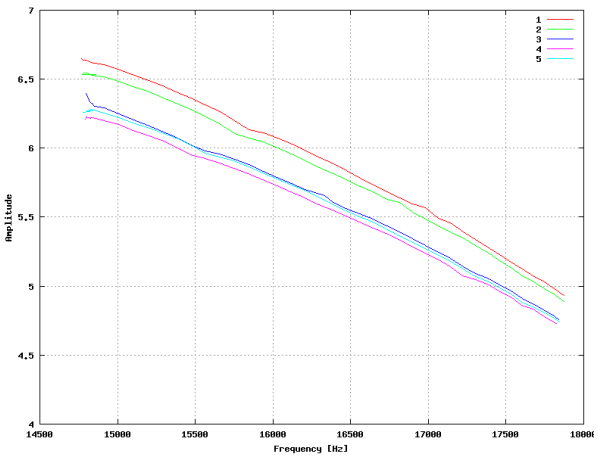


Figure 2.61: Amplitude for multiple measurements

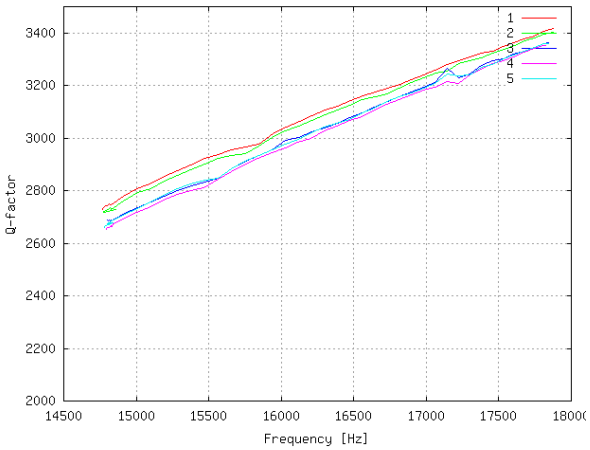


Figure 2.62: Q-factor for multiple measurements

The the code in `WriteDataAll()` uses some special tricks to generate the graphs and some lines of code of require comments. You might want to read the comments shown after the code.

WriteDataAll.m

```
function  WriteDataAll(basename,numbers,ext)

% function to analyze data for a series of Digi Sens sensor
%
% WriteDataAll(basename,numbers,ext)
%
% will analyze data given in files and then generate graphs
% and files AmpAll.png and QAll.png
% It will also display the estimated dependencies of amplitude
```

```
% and Q-factor on the temperature
%
% sample calls:
%   WriteDataAll('elektro',[1:5],'.data')
%   WriteDataAll('elektro',[1, 2, 4, 5],'.data')
%

if ((nargin !=3))
  usage('give filenames in WriteDataAll(basename,numbers,ext)');
end

%calibrationFactor = 11.2; % factor for amplitudes, ideal value is 1.0
calibrationFactor = 1.0;

freqA = []; ampA = []; qualiA = []; tempA = [];
cmd1 = ['plot('']; cmd2 = cmd1;
for sensor = 1:length(numbers)
  filename = [basename,num2str(numbers(sensor)),ext];
  infile   = fopen(filename,'rt');

  tline = fgetl(infile); % dump top line
  tline = fgetl(infile); % read number of measurements
  meas  = sscanf(tline,'%i');
  tline = fgetl(infile); % read number of repetitions
  rep   = sscanf(tline,'%i');

  freq = zeros(meas,1); freqS = freq; freqT = zeros(rep,1);
  curr = freq; currS = freq; currT = freqT;
  quali = freq; qualiS = freq; qualiT = freqT;
  amp = freq; ampS = freq; ampT = freqT; temp = freq;
  for k = 1:8;   % read the headerlines
    tline = fgetl(infile);
  endfor

  for im = 1:meas;
    for ir = 1:rep
      tline = fgetl(infile);
      t = sscanf(tline,'%g %g %g %g %g');
      ampT(ir) = calibrationFactor*t(1);
      freqT(ir)  = t(2);
      qualiT(ir) = t(3);
      currT(ir)  = t(4);
      tempT(ir)  = t(5);
    endfor % rep
    amp(im)   = mean(ampT);   ampS(im)   = sqrt(var(ampT));
    freq(im)  = mean(freqT);  freqS(im)  = sqrt(var(freqT));
    quali(im) = mean(qualiT); qualiS(im) = sqrt(var(qualiT));
    curr(im)  = mean(currT);  currS(im)  = sqrt(var(currT));
    temp(im)  = mean(tempT);  tempS(im)  = sqrt(var(tempT));
  endfor  % meas
  freqA = [freqA;freq]; ampA = [ampA;amp];
  qualiA = [qualiA;quali]; tempA = [tempA;temp];
  fclose(infile);

  key = num2str(numbers(sensor));
  freqn = ['freq',key,'=freq;']; eval(freqn);
  ampn  = ['amp',key,'=amp;']; eval(ampn);
  qualin = ['quali',key,'=quali;']; eval(qualin);
```

```
  cmd1 = [cmd1,'freq',key,',amp',key,',\'',num2str(sensor),';',key,';\',''];
  cmd2 = [cmd2,'freq',key,',quali',key,',\'',num2str(sensor),';',key,';\',''];
endfor  % loop over all files


figure(1);
clf;
cmd1 = cmd1(1:end-1);cmd1 = [cmd1,');'];
eval(cmd1)
grid on
axis([14500 18000 4 7]);
legend('show')
xlabel('Frequency [Hz]'); ylabel('Amplitude')
%%print('AmpAll.png','-S800,600');
print('AmpAll.png');

figure(2);
clf;
cmd2 = cmd2(1:end-1); cmd2 = [cmd2,');'];
eval(cmd2);
grid on
axis([14500 18000 2000 3500]);
legend('show')
xlabel('Frequency [Hz]'); ylabel('Q-factor')
print('QAll.png');

NN = length(freqA);
F = ones(NN,3);
F(:,1) = freqA; F(:,2) = tempA;
[p,y_var,r,p_var] = LinearRegression(F,ampA);
printf('estimated temperature dependence of amplitude: %g um/C\n',p(2))
[p,y_var,r,p_var] = LinearRegression(F,qualiA);
printf('estimated temperature dependence of Q-factor: %g /C\n',p(2))

figure(3); clf; axis();
plot3(freqA,tempA,ampA,'+')
endfunction
```

- At first empty matrices are created to contain the data for all frequencies, amplitudes, quality factors and temperatures.

  Octave
  ```
  freqA=[]; ampA=[]; qualiA=[]; tempA=[];
  ```

- When the function is called by `WriteDataAll('Elektro',[1,3,5],'.data')` the data files `Elektro1.data`, `Elektro3.data` and `Elektro5.data` have to be analyzed. The code uses a loop of the form

  Octave
  ```
  for sensor = 1:length(numbers)
    ...
  endfor
  ```

  to read each of the requested files and constructs the file names within the loop by

  Octave

```
filename = [basename,num2str(numbers(sensor)),ext];
```

- Each data file is scanned using the tools from Section 1.2.8. Once the data is read named variables will be generated. As example consider the case `key='3'`. Then the commands

Octave

```
key   = num2str(numbers(sensor));
freqn = ['freq',key,'=freq;']; eval(freqn);
```

will generate the string `'freq3=freq;'` and then evaluate this command. The variable `freq3` contains the frequencies from the data file `Elektro3.data`.

- The plot command to generate Figure 2.61 is constructed step by step. Examine the patches of code.

Octave

```
cmd1 = ['plot('];
for sensor = 1:length(numbers) % lop over all data files
  key  = num2str(numbers(sensor));
  cmd1 = [cmd1,'freq',key,',amp',key,',\'',num2str(sensor),';',key,';\','];
endfor
cmd1 = cmd1(1:end-1); cmd1 = [cmd1,');'];
eval(cmd1)
```

If the function is called by `WriteDataAll('Elektro',[1 3 5],'.data')` then the string `cmd1` will have the final value

```
plot(freq1,amp1,'1;1;',freq3,amp3,'2;3;',freq5,amp5,'3;5;');}
```

and thus `eval(cmd1)` will generate the graphics with standard *Octave* commands. With the help of `grid`, `axis()`, `legend()`, `xlabel()`, `ylabel()` the appearance of the grapics is modified.

- Finally a call of `print('AmpAll.png'` will generate the graphics in the PNG format. With recent versions of *Octave* the resolution may be given by `print('AmpAll.png','-S800,600');`.

- When comparing different measurements one realizes that the amplitude can not depend on the frequency only, but the temperature might be important too. This is verified by Figure 2.63, generated by

Octave

```
figure(3); clf;  axis()
plot3(freqA,tempA,ampA,'+')
```

- By rotating Figure 2.63 one might come up with the idea that all measured points are approximately on a plane, i.e. the amplitude A depends on the frequency f and the temperature T by a linear function

$$A(f,T) = c_f\, f + c_T\, T + c_0$$

The optimal values for the coefficients can be determined by linear regression.

Octave

```
NN = length(freqA);
F  = ones(NN,3);
F(:,1) = freqA;F(:,2)=tempA;
[p,y_var,r,p_var] = LinearRegression(F,ampA);
printf('estimated temperature dependence of amplitude: %g um/C\n',p(2))
```

As a result we find that the amplitude A decreases by 0.047 μm per degree of temperature increase.

- A similar computation shows that the Q-factor is diminished by 10 units per degree of temperature increase.

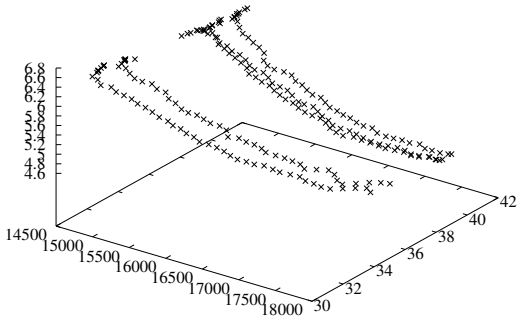


Figure 2.63: Amplitude as function of frequency and temperature

2.7.4 Calibration of the device

The electronic device to be calibrated with the help of a vibrometer, which can measure absolute amplitudes A_a of the vibrating cord. The electronic device built by Andrea Schüpbach lead to a voltage signal with amplitude A_e. Using linear regression an optimal choice of the calibration parameter α such that

$$A_a = \alpha\, A_e$$

was determined and then built into the Labview code. The device now used by DIGI SENS yields amplitudes in micro meters.

2.7.5 List of codes and data files

In the previous section the codes in Table 2.12 were used.

filename	function
`automatic.m`	function file to examine test data
`m4`	sample data file
`Readm4.m`	script file to read the raw data
`WriteData.m`	function file to analyse one data set
`AmpQ.gnu`	command file for *Gnuplot*
`WriteDataAll.m`	function file to analyse multiple data sets
`Elektro*.data`	sample data files

Table 2.12: Codes and data files for section 2.7

2.8 An Example for Fourier Series

A beam is clamped on both sides. Stroke the beam with a hammer and measure the acceleration of the hammer and the acceleration of one point of the bar. Analyze the collected data.

2.8.1 Reading the data

To read the collected data we first examine the content of the file.

SC1007.TXT

```
LECROYLT364L,73
Segments,1,SegmentSize,10002
Segment,TrigTime,TimeSinceSegment1
#1,03-Jun-2002 15:28:33,0
Time,Ampl
-0.0060034,0.001875
-0.0059934,0.001875
-0.0059834,0.001875
-0.0059734,0.001875
-0.0059634,-0.00125
...
```

- Since the data is given in a comma separated value format we can use the command `dlmread()` to read and display the data. A possible result is shown in Figure 2.64.

ReadDataDLM.m

```
filename1 = 'SC1001.TXT';
indata = dlmread(filename1,',',5,0); % read data, starting row 6
k = length(indata);
disp(sprintf('Number of datapoints is %i',k))
timedataIn = indata(:,1); ampdataIn = indata(:,2);

TimeIn = timedataIn(k)-timedataIn(1)
FreqIn = 1/(timedataIn(2)-timedataIn(1))
figure(1);
plot(timedataIn,ampdataIn)
title('Amplitude of input'); grid on

dom = 1070:1170; % choose the good domain by zooming in
figure(3);
plot(timedataIn(dom),ampdataIn(dom))
title('Amplitude of input'); grid on

%%%% similar code to read the acceleration of a point on the vibrating bar
```

- Since `MATLAB`'s version of `dlmread()` is not as flexible one has to read line by line and scan for the desired values. Proceed as follows
  - give the name of the files to be read
  - create an matrix of zeros large enough to store all data to be read
  - open the file to be read
  - read 5 lines, then ignore them
  - for each of the following lines

    - read a string with the line
    - extract the first number (time), the comma and the second number (amplitude)
    - store time and amplitude in a vector
  - close the file and display the number of data points read

ReadData.m

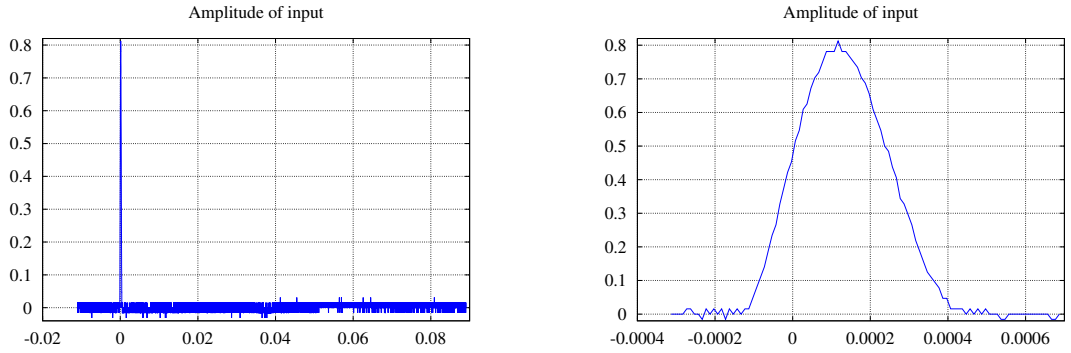
```
filename1 = 'SC1001.TXT';
indata = zeros(2,10007);        % allocate storage for the data

infile = fopen(filename1,'r');   % open the file for reading
for k = 1:5
  tline = fgetl(infile);         % read 5 lines of text
end

k = 0;                           % a counter
inline = fgetl(infile);          % read a line
%%while inline >= 0              % test for end of input file (Matlab version)
while !is_scalar(inline)         % test for end of input file (Octave)
  A = sscanf(inline,'%f%c%f');   % read the two numbers
  k = k+1;
  indata(1,k) = A(1);            % store only the time
  indata(2,k) = A(3);            % store only the amplitude
  inline = fgetl(infile);        % get the next input line
end
fclose(infile);                 % close the file

disp(sprintf('Number of datapoints is  %i',k))
```

Once the information is available to *Octave* the basic data has to be extracted and displayed

- store the time and amplitudes in separate vectors
- determine the total time of the measurement and the sampling frequency
- create a graph of the amplitude as function of time for a graphical verification. A possible result is shown in Figure 2.64.
- to examine the behavior of the driving stroke by the hammer one might enlarge the section where the excitation does not vanish.

Octave

```
timedataIn = indata(1,1:k);
ampdataIn  = indata(2,1:k);
TimeIn = timedataIn(k)-timedataIn(1)
FreqIn = 1/(timedataIn(2)-timedataIn(1))

figure(1);
plot(timedataIn,ampdataIn)
title('Amplitude of input'); grid on

dom = 1070:1170;
plot(timedataIn(dom),ampdataIn(dom))
title('Amplitude of input'); grid on
```



(a) the complete time domain

(b) zoomed ito the strike area

Figure 2.64: Acceleration of the hammer

2.8.2 Further information

- **Time of contact**
  The result in Figure 2.64(b) shows that the time of contact can be computed. We have to choose a threshold for accelerations. If the measured acceleration is above this limit we decide that contact occurs. In this example we chose 0.05 as threshold.

Octave

```
contact = ampdataIn>0.05;   % find all points with acceleration above the
                            % threshold of 0.05
ContactTimes = sum(contact) % compute the number of timepoints above treshold
timeOfContact = sum(contact)/FreqIn % time of contact
-->
ContactTimes =  48
timeOfContact =  4.8000e-04
```

Thus we find that the hammer contacted the bar for 0.48 msec .

- **Initial speed of hammer**
  Since the signal is proportional to the acceleration $a(t)$ of the hammer we can compute the difference of the velocity of the hammer before and after contact by

$$v_2 - v_1 = \int_{t_1}^{t_2} a(t)\, dt$$

With *Octave* we can use two slightly different codes, leading to very similar results.

  - The first version uses all points with an acceleration larger than the above specified threshold of 0.05.
  - The second version integrates over the time domain specified in Figure 2.64(b).

Octave

```
speed1 = trapz(timedataIn,ampdataIn.*contact)
speed2 = trapz(timedataIn(dom),ampdataIn(dom))
-->
speed1 =  2.2515e-04
speed2 =  2.2812e-04
```

The resulting number is not equal to the actual speed, since we do not know the scale factor between the signal and the acceleration. The device would have to be calibrated to gain this information.

2.8.3 FFT

The data file with the acceleration of the point on the bar has to be read in a similar fashion. To analyze the data we proceed as follows:

- Decide on the number of data points to be analyzed. It should be a power of 2 , we use 2^{N2} points. Thus `N2` decides on the artificial period T of the signal. The periodicity is introduced by the Fourier analysis. With the period T we also choose the base frequency $1/T$. Due to the Nyquist effect we will at best be able to analyze frequencies up to $2^{N2-1}/T$.
- Choose the number `Ndisp` of frequencies to be displayed. We will create a graph with frequencies up to `Ndisp`$/T$.
- Apply the FFT (Fast Fourier Transform) to the data.
- Plotting the absolute value of the coefficients as function of the corresponding frequencies will give a spectrum of the signal. The results are shown in Figure 2.65 .

Fourier.m

```
N2 = 12;      % analyze 2^N2 points
Ndisp = 200;  % display the first Ndisp frequency contributions

tdata = timedataIn(1:2^N2);
adata = ampdataIn(1:2^N2);
PeriodIn = timedataIn(2^N2)-timedataIn(1)
frequencies = linspace(1,Ndisp,Ndisp)/PeriodIn;

fftIn = fft(adata);
figure(1);
plot(frequencies,abs(fftIn(2:Ndisp+1)))
title('spectrum of input amplitude'); grid on

tdata = timedataOut(1:2^N2);
adata = ampdataOut(1:2^N2);
PeriodOut = timedataOut(2^N2)-timedataOut(1)
fftOut = fft(adata);

figure(2);
plot(frequencies,abs(fftOut(2:Ndisp+1)))
title('spectrum of output amplitude');   grid on
```

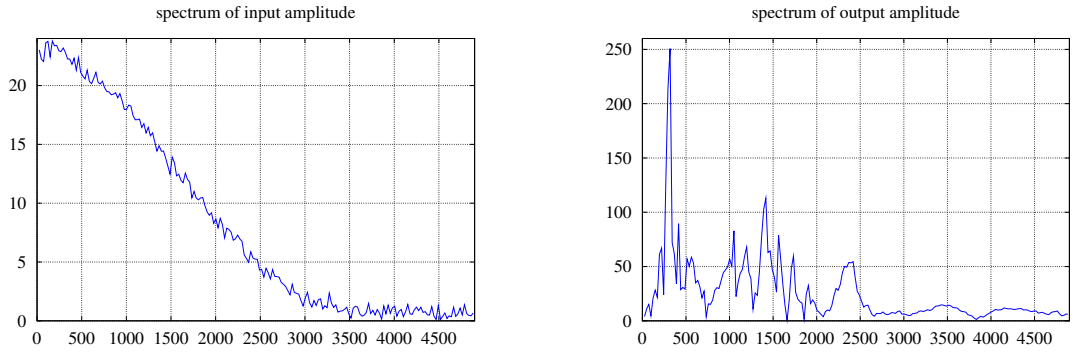
The results in Figure 2.65 show that

- The input has no significant contribution for frequencies beyond 3000 Hz .
- The spectrum of the output has some significant peaks. These might correspond to eigenmodes of the vibrating beam.

2.8.4 Moving spectrum

Instead of analyzing the signal over the full time span we may also consider the spectrum on shorter sections of time. We proceed as follows:

- Examine slices of $2^{11} = 2048$ data points, thus 0.1 sec at different starting times. Here we choose starting times from 0 to 0.5 sec in steps of 0.1 sec . The starting time in the code below is chosen by setting the variable `level`. The value of `level` tells *Octave* at which point to start.



(a) spectra of hammer acceleration

(b) spectra of beam acceleration

Figure 2.65: Spectra of the accelerations of hammer and bar

- The graphs of the above 6 computations are shown in Figure 2.66 . Observe that the scales vary from one picture to the next. Obviously the spectrum changes its shape as function of time, but some features persist.

SpectrumSlice.m

```
% set level before calling this script, e.g. by level=100
N2 = 11;      % analyze 2^N2 points
Ndisp = 50;  % display the first Ndisp contributions

PeriodIn = timedataIn(2^N2)-timedataIn(1);
frequencies = linspace(1,Ndisp,Ndisp)/PeriodIn;

adata  = ampdataOut(level:level+2^N2-1);
fftOut = fft(adata);
spectrum = abs(fftOut(2:Ndisp+1));

figure(1);
plot(frequencies,spectrum)
```

Another option would be to consider even more starting times and generate a 3D–graph. The code below[14] does just this. The result in Figure 2.67 allows to discuss the behavior of the amplitudes as functions of time and frequency.

MovingFourier.m

```
N2 = 11;      % analyze 2^N2 points
Ndisp = 50;  % display the first Ndisp contributions

levels = 1:200:1800;
levels = 1:250:5000;

spectrum = zeros(length(levels),Ndisp);
PeriodIn = timedataIn(2^N2)-timedataIn(1);
frequencies = linspace(1,Ndisp,Ndisp)/PeriodIn;

for kl = 1:length(levels)
  adata  = ampdataOut(levels(kl):levels(kl)+2^N2-1);
  fftOut =fft(adata);
```

[14] Recently your author learned about the command `specgram()` which applies a similar procedure.

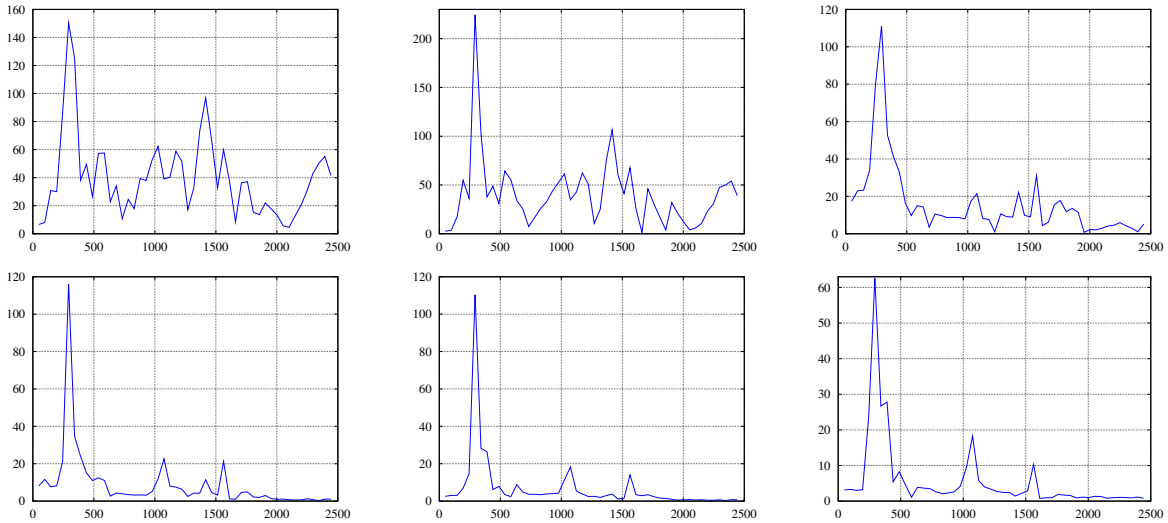


Figure 2.66: Spectra at different times

```
    spectrum(kl,:) = abs(fftOut(2:Ndisp+1));
end
figure(3);
mesh(frequencies,levels,spectrum)
xlabel("frequency");ylabel("starting time");
title("spectrum as function of starting time");
view(15,30)
```

2.8.5 Transfer function

If we consider the acceleration of the hammer as input and the acceleration of the point on the bar as output we can examine the transfer function.

Octave

```
figure(3);
plot(frequencies,abs(fftOut(2:Ndisp+1))./abs(fftIn(2:Ndisp+1)))
title('Transfer Function')
xlabel('Frequency'); ylabel('Output/Input'); grid on
```

Expect the result to be highly unreliable for frequencies above 2500 Hz . This is based on the fact that the amplitude of input and output are small and thus minor deviations can have a drastic influence on the result of the division. Thus the large values of the transfer function for the highest frequencies in the left part of Figure 2.68 should not be taken too seriously. The right part of the figure examines only smaller frequencies. This result might be useful. It is generated by the code below.

Octave

```
nn = sum(frequencies <2500);
plot(frequencies(1:nn),abs(fftOut(2:nn+1))./abs(fftIn(2:nn+1)))
title('transfer function')
xlabel('Frequency'); ylabel('Output/Input'); grid on
```

2.8.6 List of codes and data files

In the previous section the codes and data files in Table 2.13 were used.

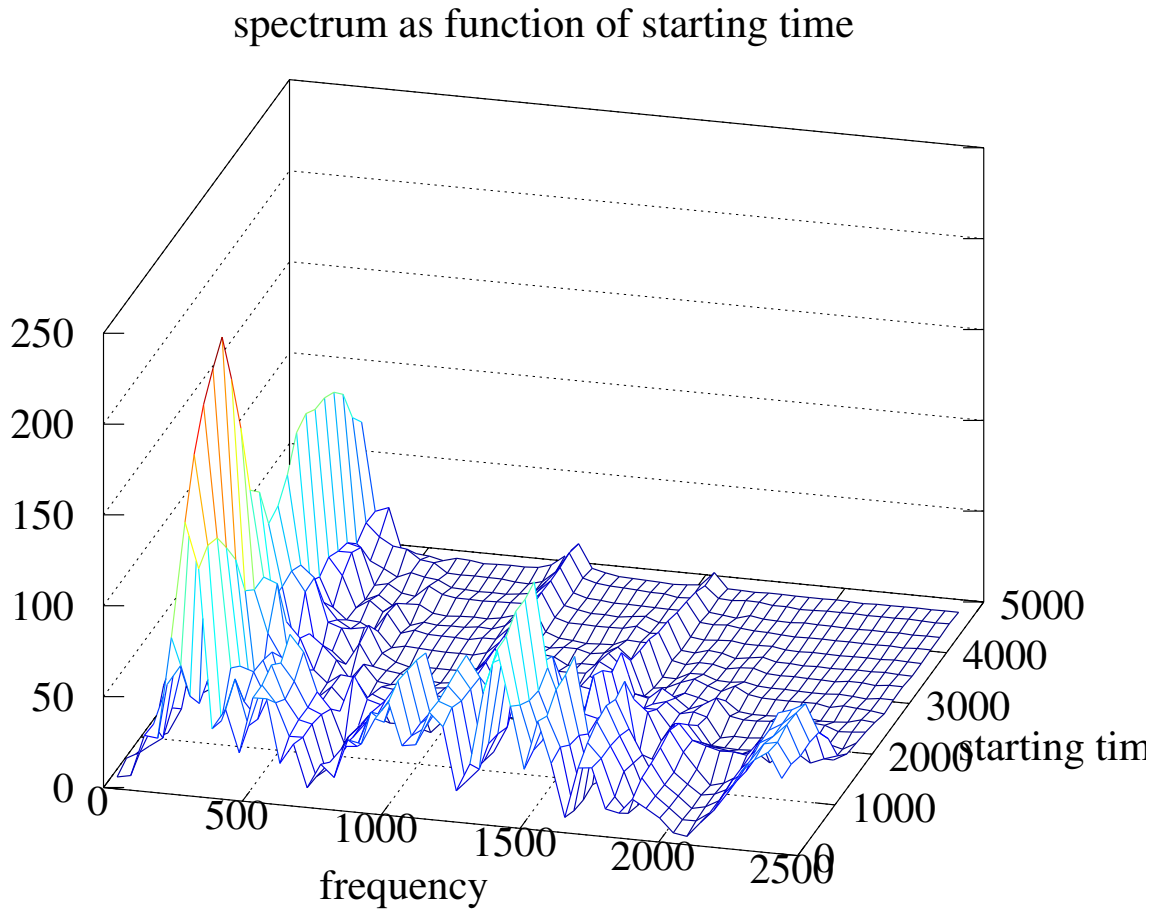
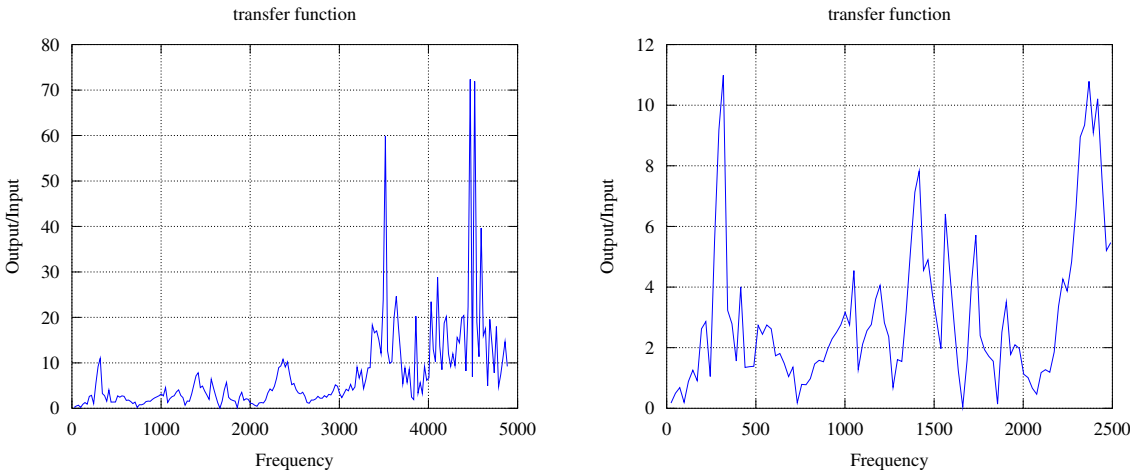


Figure 2.67: Spectra at different times as 3d graph



(a) full frequency domain

(b) smaller frequency domain

Figure 2.68: Transfer function for the acceleration of hammer and bar

filename	function
`ReadDataDLM.m`	read the basic data from files, short version
`ReadData.m`	read the basic data from files, long version
`Fourier.m`	determine the spectra and the transfer function
`SpectrumSlice.m`	find the spectrum over subsection of the time interval
`MovingFourier.m`	create 3d graph of spectrum
`SC1001.TXT`	first data file with amplitude of hammer
`SC2001.TXT`	first data file with amplitude of point on bar
`SC1002.TXT`	second data file with amplitude of hammer
`SC2002.TXT`	second data file with amplitude of point on bar
`SC1003.TXT`	third data file with amplitude of hammer
`SC2003.TXT`	third data file with amplitude of point on bar
`SC1007.TXT`	fourth data file with amplitude of hammer
`SC2007.TXT`	fourth data file with amplitude of point on bar

Table 2.13: Codes and data files for section 2.8

2.9 Reading Information from the Screen and Spline Interpolation

In this section we

- first show to read data from the any section of the screen with the help of mouse clicks. This only works with *Octave* on a Linux system.
- Then we examine how to read data from an *Octave* graphics window with the help of the mouse. This should work with *Octave* and MATLAB on any operations system.

2.9.1 Create `xinput()` to replace `ginput()`

On recent version of *Octave* the command `ginput()`, to be used below, is now compatible with MATLAB. As a consequence a very useful feature is lost: one can not read to screen coordinates any more, but only coordinates within the active graphics window. Since *Octave* is an open source project we can use the old code of the commands and keep this feature. If the instruction in the sections below do not allow you to read from the screen, then use the following steps to save the situation (might not work on Win* systems).

- Assure that you have copies of the files `xinput.m` and `grab.cc` in the current directory.
- Compile the code `grab.cc` using the instructions in the file, i.e. use a shell and run
  `mkoctfile -L/usr/X11R6/lib -lX11 -I/usr/X11R6/include/ grab.cc`
  With this command the C++ file `grab.cc` is compiled and the binary file `grab.oct` is generated. This file is then loaded by *Octave* when calling `grab()`. If you desire to do, you can also examine the source code.
- Now you can use the command `xinput()` instead of `ginput()` to use the previously available functionality.
- With the files created above the commands `grab()` and `xinput()` will be available when working in this directory. To make this feature generally available you have to copy the files `xinput.m` and `grab.oct` location in the path of *Octave*. This author uses a directory `~/octave/site` and then uses the command `addpath (genpath ('~/octave/site'));` in the startup file `~/.octavrerc` to make the directory known to *Octave*. See also Section 1.1.1 (page 8).

The above is a good illustration of the advantages of Open Source software. On Linux systems the independent program `g3data` might be useful for the same purpose.

2.9.2 Reading an LED data sheet with *Octave*

In Figure 2.69 you find data for an LED (Light Emitting Diode). We will closely examine the intensity of the emitted light as a function of the angle. For this we want to read the data into *Octave*[15]. The command `xinput()` allows to read the screen coordinates of any point on the screen, even in the window covered by other applications. Thus we can launch an PDF reader (e.g. `acroread`) on a command line or through the GUI of the operating system to display the file `NSHU550ALEDwide.pdf`. Locate the page shown in Figure 2.69. Then we read the data of the left part in the graph in the lower right corner.

- The first click determines the location of $x = 0$ and $y = 0$.
- The second click determines the location of $x = 90$ and $y = 1$.
- Subsequent clicks with the left mouse button specify the points to be collected.
- A click with the right button will terminate the data collection, where this last location will not be stored.
- Display the result. A possible answer is shown in Figure 2.70(a).

[15] With MATLAB this is unfortunately not possible, and *Octave* on Win?? systems seems to be problematic too.

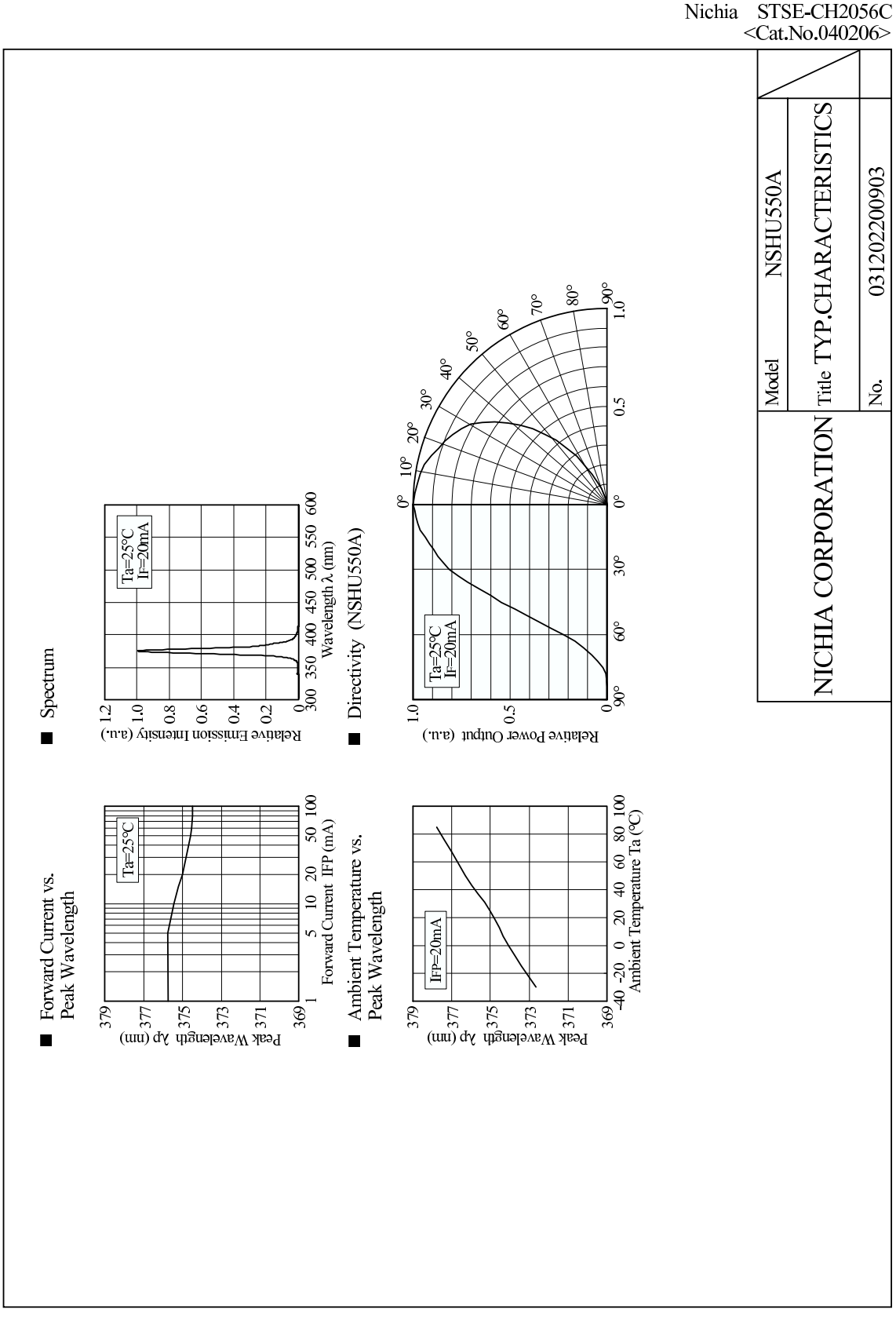
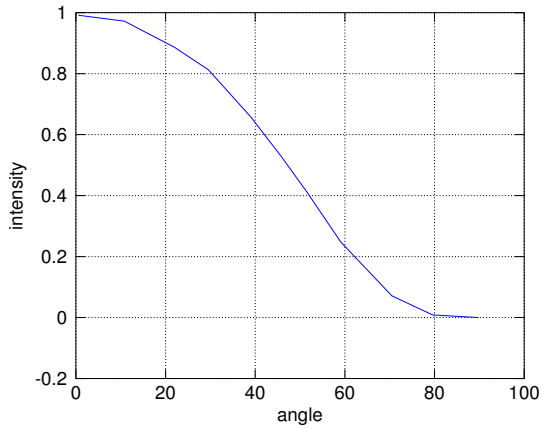


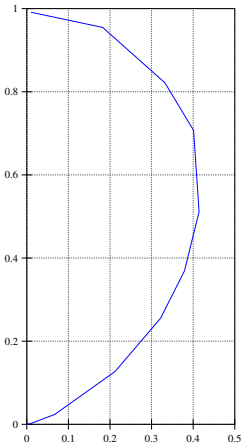
Figure 2.69: Data sheet for an LED

LEDread.m

```
more off
% show messages for the user
disp('Left mouse button picks points.')
disp('Right mouse button to quit.')
pause(2);  % give the user some time to get the graph in the foreground
[xi,yi] = xinput([0 90 0 1])        % read the points
figure(1);
plot(xi,yi);
grid on; axis('normal');
xlabel('angle'); ylabel('intensity');
```



(a) the intensity as function of the angle



(b) polar coordinates

Figure 2.70: Light intensity data for an LED

Using the data collected above we want to generate the polar plot of the intensity as a function of the angle. Thus we have to transform the data. Find the result in Figure 2.70(b).

Octave

```
figure(2);
polar(pi/2-xi/180*pi,yi)
axis([0 0.5 0 1],'equal')
```

In section 2.2.4 (page 127) the above information is used as input for linear regression to determine the intensity as a function of the angle.

With very similar code we can try to read the information from the polar plot in Figure 2.69.

- Click on the corner with angle 0° and radius 1 .
- Click on the corner 90° and radius 1 .
- Collect the (x, y) coordinates for the LED by clicking on the points along the polar section of the graph.
- Transform the (x, y) information into angles and intensities.
- Plot the result. The graph should be similar to Figure 2.70(a).

LEDreadPolar.m

```
more off
% show messages for the user
disp('Left mouse button picks points.')
disp('Right mouse button to quit.')
disp('first click on the corner r=1 at angle 90')
disp('then click on the corner r=1 at angle 0')
pause(2);  % give the user some time to get the graph in the foreground
[xi,yi] = xinput([0 1 0 1]);        % read the points
figure(1);
xi = 1-xi;
plot(xi,yi);

al = pi/2-atan2(yi,xi);
Intensity = sqrt(xi.^2 + yi.^2);
figure(2);
plot(al*180/pi,Intensity),
grid on
axis('normal');
```

2.9.3 Interpolation of data points

The aim of this section is to develop code to collect the coordinates of a few data points with the mouse as input device. We only read points in graphics window generated by *Octave*. Then the points should be visualized. We will use different type of interpolation to construct a curve connecting the points:

- Spline interpolation. This will lead to a smooth curve. With the help of a numerical integration, we determine the area between this curve and the horizontal axis.
- Piecewise linear interpolation. The function is tabulated at a regular set of grid points. Using the representation we compute and visualize the derivative of the function.

Getting the data, using the mouse as input device

The code below is organized as follows:

1. Initialize the graphics window and number and coordinates of the points to be collected.
2. Show a message to the user with the information on how to proceed.
3. Use the command `ginput()` (graphical input) to obtain the coordinates of the points to be used. Plot the data while it is collected.
4. Store the data in vector with the x and y components of the points

The code below is stored in a file `GetData.m`. Run this command in *Octave* or `MATLAB` and you will find two vectors xi and yi containing the coordinates of the points. If the data is generated by different methods, this section of the code has to be adapted.

GetData.m

```
figure(1);                  % write to the first graphic window
clf
axislimits = [0 2 0 1];     % x values from 0 to 2 and y values from 0 to 1
axis(axislimits)            % fixed axis for the graphs
x = []; y = [];             % initialise the empty matrix of values

% show messages for the user
```

```
disp('Use the left mouse button to pick points.')
disp('Use the right mouse button to pick the last point.')
but = 1;                        % boolean variable to indicate the last point
while but == 1                  % while loop, picking up the points.
    [xi,yi,but] = ginput(1);    % get coodinates of one point
    x = [x,xi]; y = [y,yi];
    plot(x,y,'ro')              % plot all points point
    axis(axislimits);           % fix the axis
end
```

Spline Interpolation

MATLAB and *Octave* provide the command `spline()` to compute the interpolating spline polynomial for a given set of points.

SplineInterpolation.m

```
% Interpolate with a spline curve and finer spacing.
% the code in GetData.m must be run first
n = length(x);
t  = 1:n;                       % integers from 1 to n
ts = 1: .2: n;                  % from 1 to n, stepsize 0.2
xys = spline(t,[x;y],ts);       % do the spline interpolation
xs = xys(1,:);  ys = xys(2,:);  % extract the components

% Plot the interpolated curve.
figure(1);                      % plot in the first graphics window
plot(xs,ys,x,y,'*-');
xlabel('x'); ylabel('y')
grid on

figure(2);                      % write to second window
% Plot the two components of the spline curve separately  show the labels
plot([1:length(xs)],xs,'g-',[1:length(ys)],ys,'b-')
legend('x values','y values')
xlabel('numbering'); ylabel('values')
grid on
```

After having computed many points on the curve we now attempt to compute the integral of the function, i.e. for $a \leq x \leq b$ we try to determine

$$F(x) = \int_a^x f(s)\, ds$$

Based on Figure 2.71 we use a trapezoidal integration rule, i.e.

$$\int_{x_0}^{x_5} f(x)\, dx \approx (x_1 - x_0)\, \frac{y_0 + y_1}{2} + (x_2 - x_1)\, \frac{y_1 + y_2}{2} + (x_3 - x_2)\, \frac{y_2 + y_3}{2} + (x_4 - x_3)\, \frac{y_3 + y_4}{2}$$

Based on this idea we can integrate step by step, adding the area of the new rectangle at each step. This is implemented in the script file `Integration.m` shown below.

Integration.m

```
% use the data generated by GetData and SplineInterpolation
integral = zeros(size(xs));  % create vector of correct size

% perform a numerical integration by adding the contributions
% use a trapezoidal integration
for k = 2:length(xs)
    integral(k) = integral(k-1) + (xs(k)-xs(k-1))*(ys(k-1)+ys(k))/2;
```

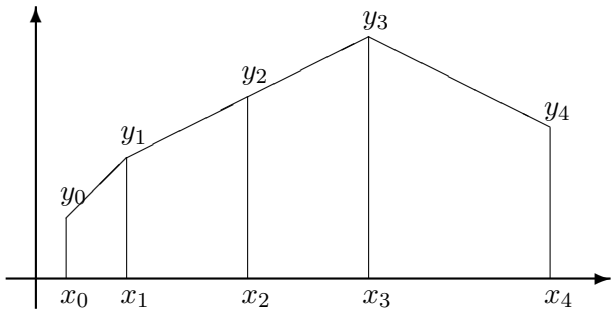


Figure 2.71: Trapezoidal integration

```
endfor
figure(3);
axis(axislimits)
plot(xs,ys,";function;",xs,integral,";integral;")
```

The identical result can be obtained by the command `cumtrapz()`, short for cummulative trapezoidal rule.

```
integral = cumtrapz (xs,ys);
```

Piecewise linear interpolation

Since the data points were collected with the help of the mouse, the values of x are not necessarily sorted. If y is supposed to be a explicit function of x the graph may not 'swing back'. This requires that the values of x and y be renumbered properly, as illustrated in Figure 2.72. With the sorted values we then call the function

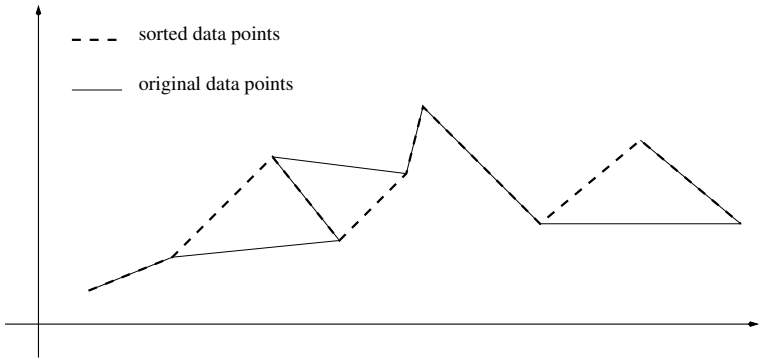


Figure 2.72: Data points in original order and sorted

`interp1()` to determine the values of the piecewise linear interpolating function at a set of regularly spaced grid points. A plot is easily generated.

LinearInterpolation.m

```
% Interpolate with a piecewise linear curve
% GetData must be run first
nx   = 51;                          % number of grid points
xlin = linspace(min(x),max(x),nx);  % uniformly distributed points
% sort x and y values, based on the order of the x values
xysort = sortrows([x;y]',1);
```

```
% compute the values of y at the given points xlin
ylin = interp1(xysort(:,1),xysort(:,2),xlin);

% Plot the interpolated curve.
figure(3);
plot(x,y,'*', xlin,ylin);
legend('given points','interpolation')
grid on

% compute the derivatives at the midpoints
dy = diff(ylin)./diff(xlin);
% compute the midpoints of the intervals
xmid = xlin(2:length(xlin))-diff(xlin)/2;
hold on
plot(xmid,dy,'r')
legend('given points','interpolation','derivative')
hold off
```

A finite difference approximation was used above to find a numerical derivative of the given function.

2.9.4 List of codes and data files

In the previous section the codes and data files in Table 2.14 were used. The codes should be run in the given order.

filename	function
`LEDread.m`	read the LED data from screen, generate plot
`LEDreadPolar.m`	read the LED data from polar plot
`NSHU550ALED.pdf`	Data sheet for an LED
`GetData.m`	read the basic data from screen using mouse
`SplineInterpolation.m`	perform a spline interpolation and show the results as graph of the two components and as one curve
`Integration.m`	apply a trapezoidal integration rule and show the function and its integral
`LinearInterpolation.m`	perform a piecewise linear interpolation and show the results as graph of the function and its derivative
`xinput.m`	script file as replacement for `ginput.m`, (*Octave* only)
`grab.cc`	C++ source for the command `grab()`, (*Octave* only)

Table 2.14: Codes and data files for section 2.9

2.10 Intersection of Circles and Spheres

Intersection points of circles may be used to determine a position from distances to known points. Te Global Positioning System (GPS) uses intersection points of spheres to compute the current position.

The following examples will show you how to implement mathematical operations in MATLAB or *Octave*. We consider a problem from geometry, solved by algebraic methods.

2.10.1 Intersection of two circles

As can be seen in Figure 2.73 the two points of intersection (if they exist) of two circles determine a straight line. To compute those points of intersection we may first determine the equation of this straight line and then intersect with one of the circles. The code below shows how this idea can be implemented.

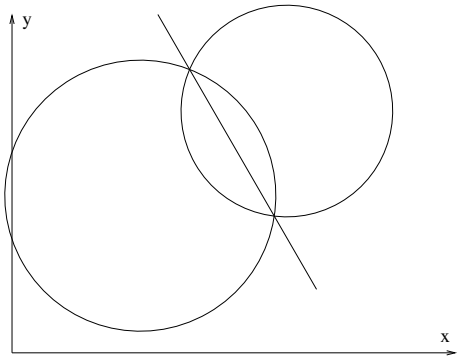


Figure 2.73: Intersection of two circles

A circle with center at $\vec{x}_m = (x_1\,,\, y_1)^T$ and radius r_1 corresponds to the solution of the equation

$$\|\vec{x} - \vec{x}_m\|^2 = (x - x_1)^2 + (y - y_1)^2 = r_1^2$$

and a possible parametrization of this circle is given by

$$\begin{pmatrix} x(t) \\ y(t) \end{pmatrix} = \begin{pmatrix} x_1 \\ y_1 \end{pmatrix} + r_1 \begin{pmatrix} \cos(t) \\ \sin(t) \end{pmatrix} \quad \text{for} \quad 0 \le t \le 2\,\pi$$

First choose the parameters for the first circle

Octave

```
xlm = 2; ylm = 3;        % coordinates of the center
r1  = 1.5;               % radius
```

then create the graph.

Octave

```
t  = linspace(0,2*pi,51);   % values of all angles, 51 steps
x1 = xlm+r1*cos(t);         % x coordinates of all points
y1 = ylm+r1*sin(t);         % y coordinates of all points
plot(x1,y1);                % create the plot
axis([0,5,0,5],"equal")     % choose a domain
```

A second circle is plotted using similar code.

Octave

```
x2m = 4; y2m = 2;          % coordinates of the center
r2 = 2;                    % radius
x2 = x2m+r2*cos(t);        % x coordinates of all points
y2 = y2m+r2*sin(t);        % y coordinates of all points
plot(x1,y1,x2,y2);         % create the plot with both circles
```

For two given circles we try to solve for the points of intersection and arrive at the system of quadratic equations

$$\begin{aligned} x^2 - 2\,x\,x_1 + x_1^2 + y^2 - 2\,y\,y_1 + y_1^2 &= r_1^2 \\ x^2 - 2\,x\,x_2 + x_2^2 + y^2 - 2\,y\,y_2 + y_2^2 &= r_2^2 \end{aligned}$$

Subtracting the two equations we find the equation for a straight line on which both points of intersection have to be.

$$-2\,x\,(x_1 - x_2) + x_1^2 - x_2^2 - 2\,y\,(y_1 - y_2) + y_1^2 - y_2^2 = r_1^2 - r_2^2$$

By choosing $x = 0$ we find the point

$$\vec{x}_p = \begin{pmatrix} x_p \\ y_p \end{pmatrix} = \begin{pmatrix} 0 \\ \frac{r_1^2 - r_2^2 - y_1^2 + y_2^2 - x_1^2 + x_2^2}{-2\,(y_1 - y_2)} \end{pmatrix}$$

and

$$\vec{v} = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = \begin{pmatrix} y_1 - y_2 \\ -x_1 + x_2 \end{pmatrix}$$

is a vector pointing in the direction of the straight line. Thus

$$\vec{x}(t) = \vec{x}_p + t\,\vec{v} \quad \text{with} \quad t \in \mathbb{R}$$

is a parametrization of this straight line.

Octave

```
xp = [0; (-r1^2+r2^2+x1m^2-x2m^2+y1m^2-y2m^2)/(2*(y1m-y2m))];
v  = [y1m-y2m; -x1m+x2m];
```

Then use this parametrization in the equation for the first circle to find

$$\begin{aligned} r_1^2 = \|\vec{x}(t) - \vec{x}_m\|^2 &= \langle \vec{x}(t) - \vec{x}_m\,,\, \vec{x}(t) - \vec{x}_m \rangle \\ &= \langle t\,\vec{v} + \vec{x}_p - \vec{x}_m\,,\, t\,\vec{v} + \vec{x}_p - \vec{x}_m \rangle \\ &= \|\vec{v}\|^2\,t^2 + 2\,\langle \vec{v}\,,\, \vec{x}_p - \vec{x}_m \rangle\,t + \|\vec{x}_p - \vec{x}_m\|^2 \end{aligned}$$

This is a quadratic equation for the unknown parameter t with the two solutions

$$t_{1,2} = \frac{-b \pm \sqrt{b^2 - 4\,a\,c}}{2\,a} = \frac{-2\,\langle \vec{v}\,,\, \vec{x}_p - \vec{x}_m \rangle \pm \sqrt{D}}{2\,\|\vec{v}\|^2}$$

where the discriminant D is given by

$$D = 4\,(\langle \vec{v}\,,\, \vec{x}_p - \vec{x}_m \rangle)^2 - 4\,\|\vec{v}\|^2\,\|\vec{x}_p - \vec{x}_m\|^2$$

Octave

```
a = v'*v;
b = 2*v'*(xp-[x1m;y1m]);
c = norm(xp-[x1m;y1m])^2-r1^2;
D = b^2-4*a*c;  % discriminant

% compute the two solutions
t1 = (-b+sqrt(D))/(2*a);
t2 = (-b-sqrt(D))/(2*a);
```

Then the two points of intersection are

$$\vec{x}_p + t_1\,\vec{v} \quad \text{and} \quad \vec{x}_p + t_2\,\vec{v}$$

Octave

```
p1 = xp + t1*v
p2 = xp + t2*v
```

If the discriminant $D < 0$ is negative, then there are no points of intersection.

With the above algorithm and resulting codes we have all building blocks to determine the intersection points of two general circles in a plane.

2.10.2 A function file to determine intersection points

All the above computation can be put in one function file `IntersectCircles.m`

Octave

```
function res = IntersectCircles(x1m,y1m,r1,x2m,y2m,r2)
% draw the graph of two circles and find the intersection points

t = linspace(0,2*pi,51);     % values of all angles, 51 steps

x1 = x1m+r1*cos(t);          % x coordinates of all points
y1 = y1m+r1*sin(t);          % y coordinates of all points
x2 = x2m+r2*cos(t);          % x coordinates of all points
y2 = y2m+r2*sin(t);          % y coordinates of all points
plot(x1,y1,x2,y2);           % create the plot with both circles

% find the parameters for the straight line
xp = [0; (-r1^2+r2^2+x1m^2-x2m^2+y1m^2-y2m^2)/(2*(y1m-y2m))];
v  = [y1m-y2m;-x1m+x2m;];
% determine coefficients of the quadratic equation
a = v'*v;    b = 2*v'*(xp-[x1m;y1m]);    c = norm(xp-[x1m;y1m])^2-r1^2;
D = b^2-4*a*c;  % discriminant
% compute the two solutions
t1 = (-b+sqrt(D))/(2*a);
t2 = (-b-sqrt(D))/(2*a);

res = [xp + t1*v,xp + t2*v];
```

Then one single *Octave* command will draw the circles and determine the intersection points.

Octave

```
InterPoints = IntersectCircles(2,3,1.5,4,2,2)
-->
InterPoints =  3.2368   2.0632
               3.8487   1.5013
```

2.10.3 Intersection of three spheres

When the three pairs of double beams in Figure 2.74 are move the central point will move too. Its position is determined by the fact, that the distances of the points of attachment have known values. To determine the position of the central point in the lower part of the section as function of the position of the three guiding beams in the upper part we have to determine the intersection point of three spheres in space. A robot of this type was constructed by Sebastien Perroud in 2004, to be used as a pick and place robot. At the CSEM Sebastien did develop the concept and the results are PoketDelta and MicroDelta robots.

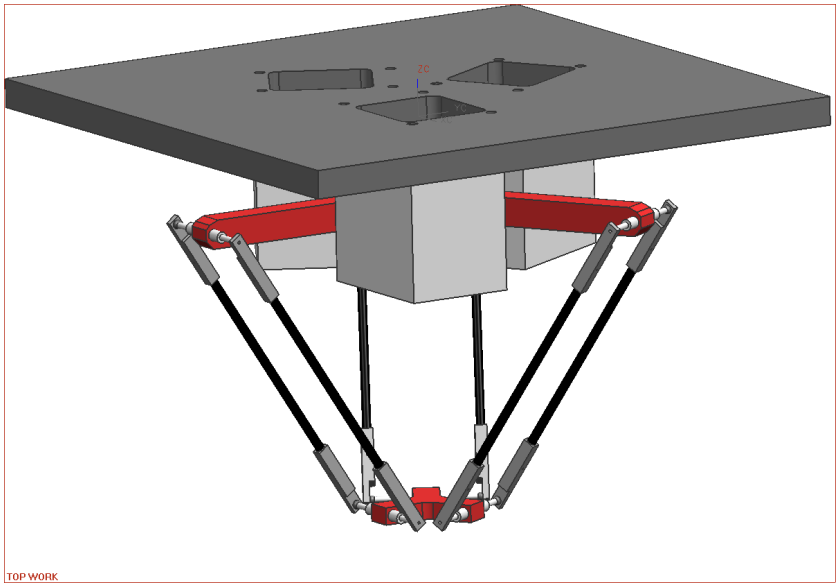


Figure 2.74: A Delta Robot

To determine the points of intersection we use the following geometric facts.

- The intersection of two spheres is typically a circle, which lies in a plane.
- The intersection of two of the above planes determines a straight line.
- With the help of this line and one of the spheres we can determine the points of intersection of the three spheres.

The code below shows how this idea can be implemented.

To find the intersection points of three spheres the following set of quadratic equations have to be solved for x, y and z.

$$\begin{aligned}(x-x_1)^2+(y-y_1)^2+(z-z_1)^2 &= r_1^2\\ (x-x_2)^2+(y-y_2)^2+(z-z_2)^2 &= r_2^2\\ (x-x_3)^2+(y-y_3)^2+(z-z_3)^2 &= r_3^2\end{aligned}$$

By subtracting these equations we find a linear system of two equations for three unknowns.

$$\begin{aligned}-2(x_1-x_2)\,x \quad -2(y_1-y_2)\,y \quad -2(z_1-z_2)\,z &= r_1^2-x_1^2-y_1^2-z_1^2-r_2^2+x_2^2+y_2^2+z_2^2\\ -2(x_2-x_3)\,x \quad -2(y_2-y_3)\,y \quad -2(z_2-z_3)\,z &= r_2^2-x_2^2-y_2^2-z_2^2-r_3^2+x_3^2+y_3^2+z_3^2\end{aligned}$$

Using matrix notation we find

$$-2 \begin{bmatrix} x_1 - x_2 & y_1 - y_2 & z_1 - z_2 \\ x_2 - x_3 & y_2 - y_3 & z_2 - z_3 \end{bmatrix} \cdot \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} r_1^2 - x_1^2 - y_1^2 - z_1^2 - r_2^2 + x_2^2 + y_2^2 + z_2^2 \\ r_2^2 - x_2^2 - y_2^2 - z_2^2 - r_3^2 + x_3^2 + y_3^2 + z_3^2 \end{pmatrix}$$

or equivalently

$$2 \begin{bmatrix} \vec{M}_2 - \vec{M}_1 \\ \vec{M}_3 - \vec{M}_2 \end{bmatrix} \vec{x} = \begin{pmatrix} r_1^2 - \|\vec{M}_1\|^2 - r_2^2 + \|\vec{M}_2\|^2 \\ r_2^2 - \|\vec{M}_2\|^2 - r_3^2 + \|\vec{M}_3\|^2 \end{pmatrix}$$

where

$$\vec{M}_i = (x_i\,,\, y_i\,,\, z_i)$$

With the definitions for $\mathbf{A}$ and $\vec{b}$ we obtain an inhomogeneous system of two linear equations for three unknowns.

$$\mathbf{A} \cdot \vec{x} = \vec{b}$$

The general solution of this system can be parametrized with the help of a particular solution $\vec{x}_p$ and the solution of the homogeneous problem $\vec{v}$.

$$\vec{x}_p = \mathbf{A} \backslash \vec{b} \quad \text{and} \quad \vec{v} = \ker(\mathbf{A})$$

All solutions of the linear system are of the form

$$\vec{x}(t) = \vec{x}_p + t\ \vec{v}$$

and this expression can be used with the equation of the first sphere to find a quadratic equation for the parameter $t \in \mathbb{R}$.

$$\begin{aligned} \|\vec{x} - \vec{M}_1\|^2 - r_1^2 &= 0 \\ \|t\,\vec{v} + \vec{x}_p - \vec{M}_1\|^2 - r_1^2 &= 0 \\ t^2\,\|\vec{v}\|^2 + t\ 2\,\langle \vec{v}\,,\, \vec{x}_p - \vec{M}_1 \rangle + \|\vec{x}_p - \vec{M}_1\|^2 - r_1^2 &= 0 \\ a\,t^2 + b\,t + c &= 0 \\ t_{1,2} &= \frac{-b \pm \sqrt{b^2 - 4\,a\,c}}{2\,a} \end{aligned}$$

where $\vec{M}_1 = (x_1\,,\, y_1\,,\, z_1)^T$. The two intersection points are then given by

$$\vec{x}_p + t_1\ \vec{v} \quad \text{and} \quad \vec{x}_p + t_2\ \vec{v}$$

This algorithm can be implemented in *Octave* or `MATLAB`.

2.10.4 List of codes and data files

In the previous section the codes in Table 2.15 were used.

filename	function
`twocircles.m`	script file to determine intersection points
`IntersectCircles.m`	function file to compute intersection points

Table 2.15: Codes and data files for section 2.10

2.10.5 Exercises

Exercise 2.10–1 Write a function `IntersectSpheres()` in *Octave* or `MATLAB` to determine the intersection points of three spheres.

The answers

Exercise 2.10–1

Octave

```
function res = IntersectSpheres(M1,r1,M2,r2,M3,r3)
% find the intersection points of three spheres
% Mi is a row vector with the three components of the center of the i-th circle
% ri is the radius of the i-th sphere

% create the matrix and vector for the linear system
A = 2*[M2-M1;M3-M2];
b = [r1^2-norm(M1)^2-r2^2+norm(M2)^2;r2^2-norm(M2)^2-r3^2+norm(M3)^2];

% determine a particular solution xp and the homogeneous solution v
xp = A\b
v  = null(A)

% determine coefficients of the quadratic equation
a = v'*v;
b = 2*v'*(xp-M1');
c = norm(xp-M1')^2-r1^2;

% solve the quadratic equation
D = b^2-4*a*c;  % discriminant
if (D<0)
  sprintf('no intersection points')
  res = [];
else
  % compute the two solutions
  t1  = (-b+sqrt(D))/(2*a);
  t2  = (-b-sqrt(D))/(2*a);
  res = [xp + t1*v,xp + t2*v];
end
```

As a simple test run the following commands

Octave

```
M1 = [3  -0.1   0]; r1=3;
M2 = [0   3     0]; r2=3;
M3 = [0   0.35  4]; r3=4;
IntersectSpheres(M1,r1,M2,r2,M3,r3)
```

with the result

Octave

```
2.4652e+00   1.7077e-03
2.3841e+00   3.9699e-05
1.5948e+00   1.5339e-02
```

2.11 Scanning a 3–D Object with a Laser

A solid is put on a plate and then scanned with a laser from a certain angle. An CCD camera is recording the laser spot on the solid, thus one can compute the height of the solid at this points. This should lead to a 3–D picture of the solid. The aim is to show this solid in a graphic. The laser scan is performed according to the following scheme:

- For a fixed x position of the laser, move it stepwise in the y direction and detect the resulting x position of the laser spot on the solid. Compute the height z of the solid at this spot. Store the values of x, y and z.
- Advance the laser in the x direction by a fixed step size and repeat the above procedure.

2.11.1 Reading the data

The first task is to read the numbers in those files and store them in matrices. The code below does just this for the x values. Similar code will read the other matrices. The comments indicate the function of each line of code.

ReadData.m

```
% with Octave you you might want to call
% graphics_toolkit fltk
% for performance reasons
%
% read each of the three data files
x = load('Xmatnew1.txt');
y = load('Ymatnew1.txt');
z = load('Zmatnew1.txt');
[nstep,npix] = size(x);

figure(1);
mesh(x,y,z);
view(50,30);
xlabel('x'); ylabel('y'); zlabel('z');

% read the rotated data
xR = load('Xmatnew2.txt');
yR = load('Ymatnew2.txt');
zR = load('Zmatnew2.txt');
```

As a result each row in the matrices `x`, `y` and `z` contains the values of the coordinates along one line in x direction, where the value of y is fixed. A sample is shown in Figure 2.75, generated by the code below.

Octave

```
kk = 175; plot(x(:,kk),z(:,kk))
xlabel('x'); ylabel('z');
```

In Figure 2.76 find a visualization of this fact. Obviously the x values will not be uniformly spaced. It is in fact this nonuniform distribution of points that allows to compute the height of the solid.

With the commands `mesh(x(1:25,1:30))` and `mesh(y(1:25,1:30))` we obtain the results in Figure 2.77. This figure shows that the y values are very regularly spaced, while the x coordinate of the laser spot varies, due to the changing height of the solid, as illustrated in Figure 2.76.

The command `mesh(x,y,z)` will create Figure 2.78, a first try of a picture of the solid. On the left in this figure the traces of the shadow lines are clearly visible. In this section the shape of the solid is not correctly represented, the laser beam can not "see" this part of the solid. Thus appropriate measures have to be taken. We will scan the same object and then try to match the two pictures.

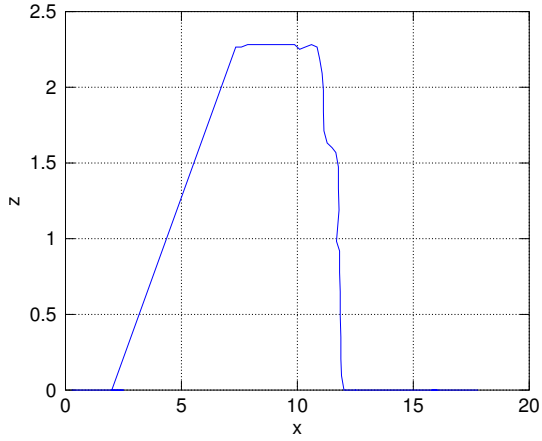


Figure 2.75: Cross section in x direction

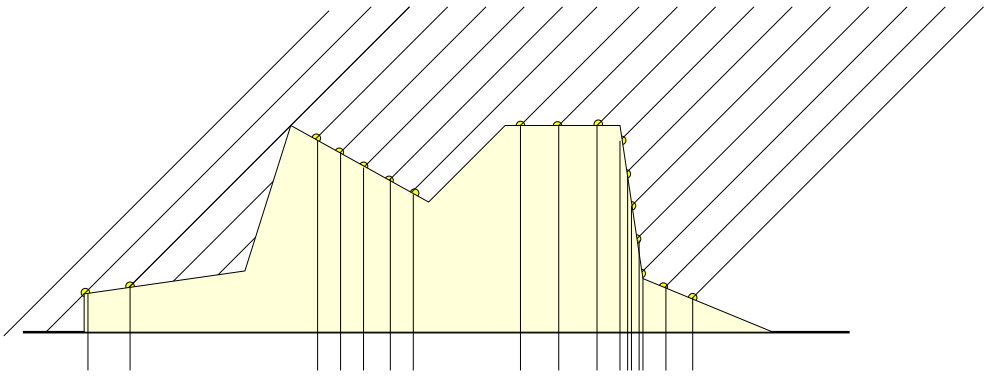


Figure 2.76: Location of laser spot, varied in x direction

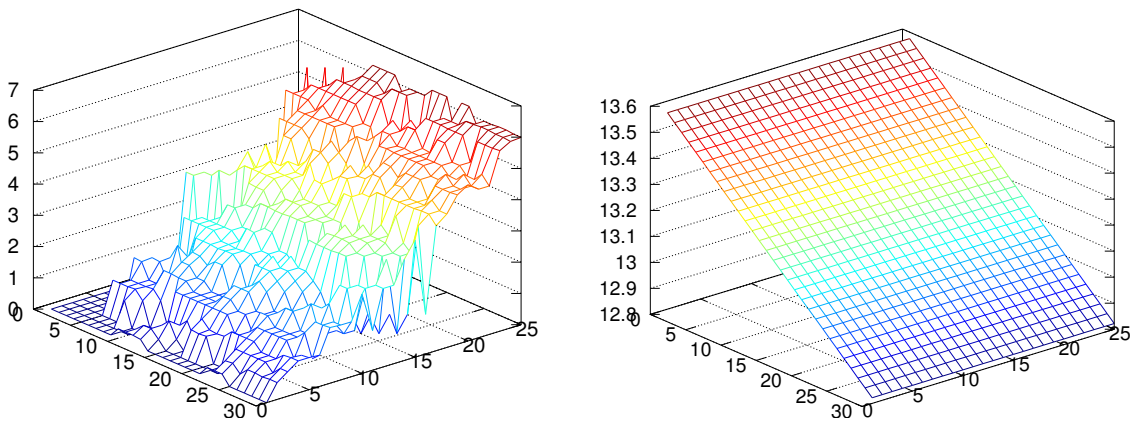


Figure 2.77: Values of x and y coordinates of points

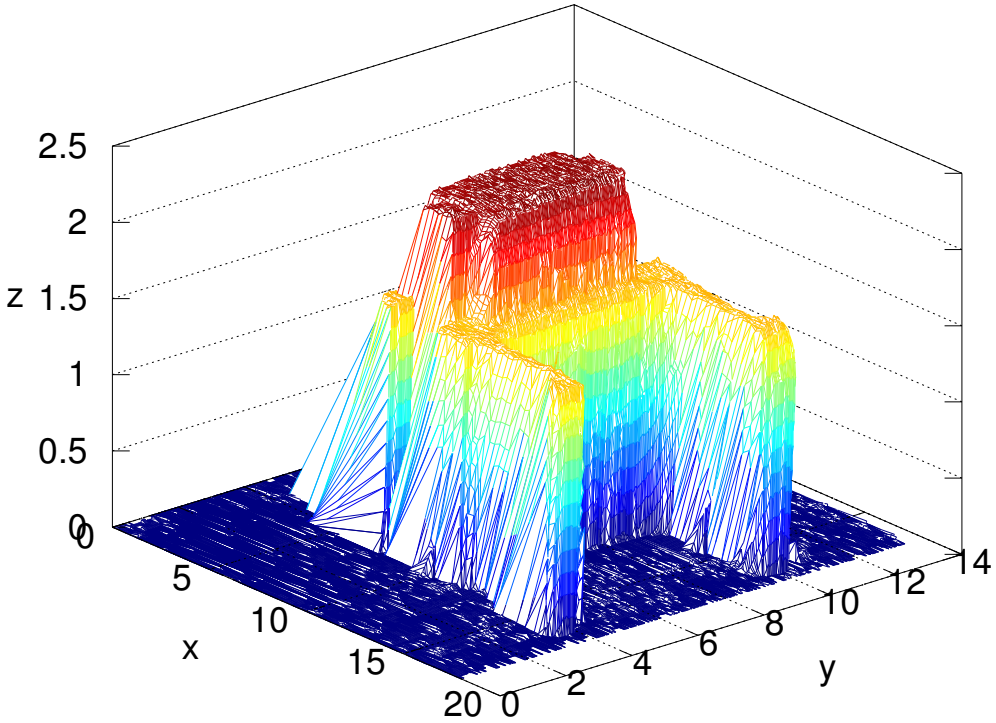


Figure 2.78: 3–D scan of solid from one direction

2.11.2 Display on a regular mesh

For subsequent calculations it is advantageous to compute the (measured) height on a regular grid. To achieve this goal we

1. choose the number of grid points in either direction.
2. along each line in x direction (see Figure 2.75) we compute the height with the help of a piecewise linear interpolation. The command `interp1()` will perform this operation.
3. The above process has to be applied to each line in x direction.

Octave

```
nx   = 200;       % number of grid points in x direction
xmin = 0.5;       % minimal and maximal value of x
xmax = 16;
xlin = linspace(xmin,xmax,nx);
zlin = zeros(nx,npix);

for k = 1:npix
  xt = x(:,k)';                 % values of x and z in this row
  zt = z(:,k)';
  aa = sortrows([xt;zt]',1);    % sort with the x values as criterion
  xt = aa(:,1);
  xt = xt+(1:length(xt))'*1e-8; % tag on a minimal slope to prevent identical values
  zt = aa(:,2);
  t = interp1(xt,zt,xlin);      % perform a linear interpolation
  zlin(:,k) = t';               % store the result in the matrix
end

xlin = xlin'*ones(1,npix);      % create the uniformly spaced x and y values
```

```
ylin = ones(1,nx)'*y(1,:);

% plot the interpolated data
figure(2);
mesh(xlin,ylin,zlin)
xlabel('x'); ylabel('y'); zlabel('z');
```

As a next task we try to decide which points are on a shadow line in the plot. For the given data we know that the angle of the laser beam is $\alpha = 30° = \pi/6$ an thus the slope of the shadow is given by $\tan\alpha = 0.5$. With a comparison operator we determine all points where the slope deviates less than 0.1 from the ideal value of 0.5 . The plot generated by the code below represents the shadowed area.

Octave

```
dx = xlin(2,1)-xlin(1,1);    dz = diff(zlin);

tip = abs(dz./dx-0.5)<0.1;        % mark the shadowed area
tip(nx,1:npix) = zeros(1,npix);  % no shadows on last row
figure(3);
mesh(xlin,ylin,1.0*tip)
xlabel('x'); ylabel('y'); zlabel('shadow');
```

2.11.3 Rescan from a different direction and rotate the second result onto the first result

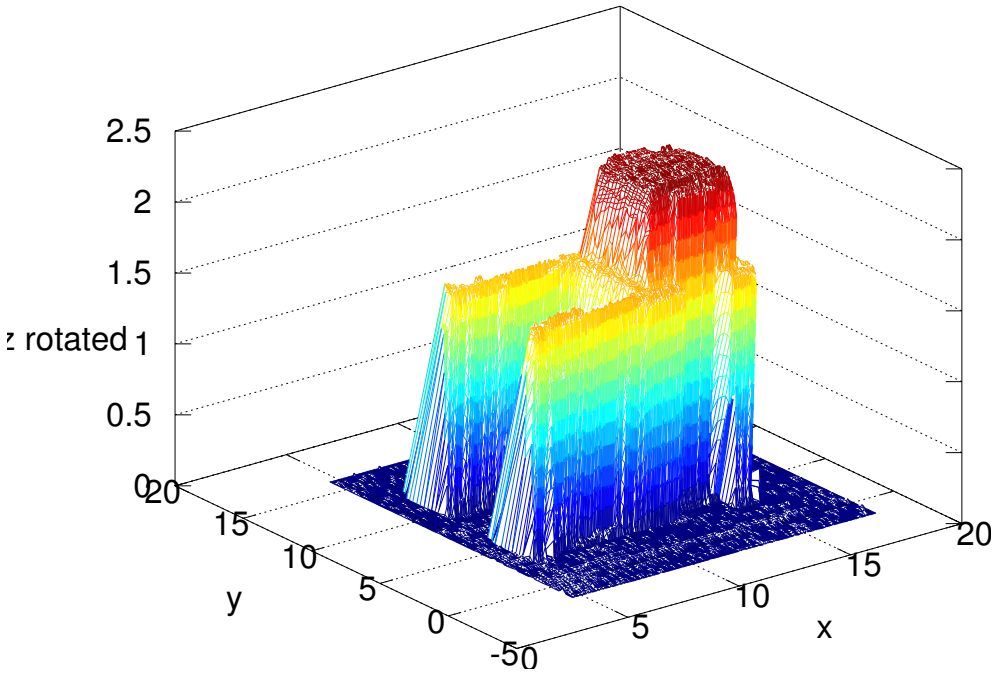


Figure 2.79: 3–D scan of solid from a second direction

Now the solid is rotated by $90°$ on the mounting plate and a second scan generates independent results, shown in Figure 2.79. The result has to be compared with Figure 2.78. The shadows are now falling in a different direction. The goal is to combine the two pictures by the following algorithm:

1. Rotate the second graph such that the two pictures should coincide.
2. If a point in Figure 2.78 is in a shadowed area, replace the height by the result form Figure 2.79.

3. Plot the new, combined picture.

Consider the affine mapping

$$\begin{pmatrix} x \\ y \end{pmatrix} \mapsto \begin{pmatrix} +y + x_0 - y_0 \\ -x + x_0 + y_0 \end{pmatrix}$$

The direction of the two axis will be interchanged and since

$$\begin{pmatrix} x_0 \\ y_0 \end{pmatrix} \mapsto \begin{pmatrix} +y_0 + x_0 - y_0 \\ -x_0 + x_0 + y_0 \end{pmatrix} = \begin{pmatrix} x_0 \\ y_0 \end{pmatrix}$$

we have a rotation about the fixed point $(x_0, y_0)^T$. Thus the code below will create the picture of the solid in the original direction, but the laser will now throw its shadows into another direction.

Octave

```
x0 = 10.508;  y0 =  5.897;
xn = -yR +y0+x0;
yn = -xR +x0+y0;

figure(4);
mesh(xn,yn,zR)
xlabel('x'); ylabel('y'); zlabel('z rotated');
```

The next task is to compute the height of the "new" solid at the regular grid points of the first scan. This leads to an interpolation problem for a function of two variables. The algorithm is rather elaborate, implemented as `griddata()`. Then we use the matrix `tip` to construct the combined height.

- If `tip=0` then `(1-tip) * A + tip * B = A` and the first value is used.
- If `tip=1` then `(1-tip) * A + tip * B = B` and the second value is used.

The result is shown in Figure 2.80.

Octave

```
zInt = griddata(xn,yn,zR,xlin,ylin,'nearest');
znew = (1-tip).*zlin + tip.*zInt;

figure(5);
mesh(xlin,ylin,znew)
xlabel('x'); ylabel('y'); zlabel('z combined');  view(50,60)
```

2.11.4 List of codes and data files

In the previous sections the codes and data files in Table 2.16 were used. The following sequence of commands in *Octave* or `MATLAB` should reproduce the results in this section. Use `ReadData` to read all data files and generate a first plot. Then use `UniformMesh` to examine the solid on a uniform mesh and determine the shadow areas. Finally the two scans are combined with the help of `RotateShape`.

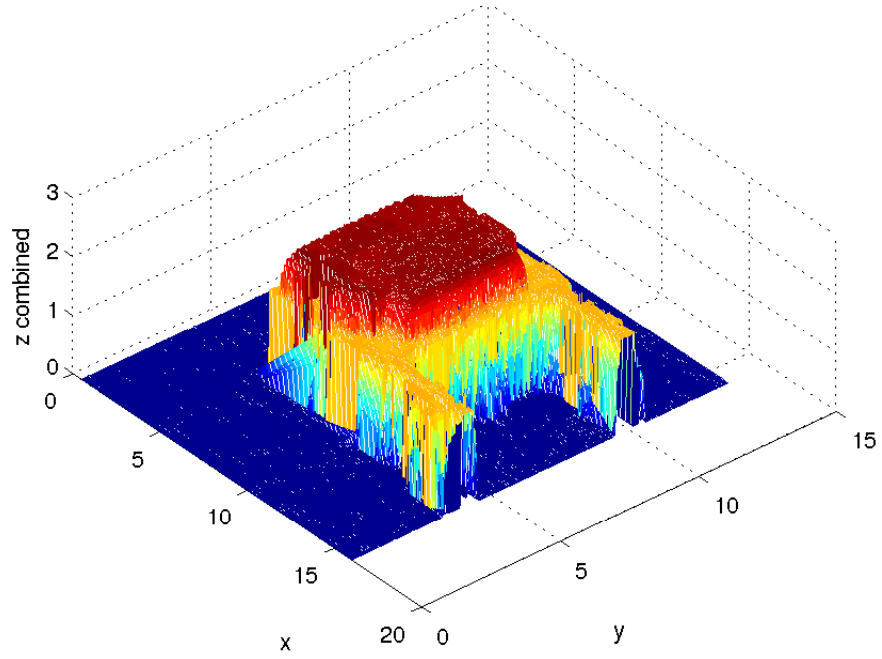


Figure 2.80: Combination of the two scans

filename	function
`ReadData.m`	read the basic data from files, including plot
`UniformMesh.m`	interpolate on a uniform mesh, determine shadow
`RotatedShape.m`	rotate the second scan and combine the two graphs
`?newmat1.txt`	data for the first scan
`?newmat2.txt`	data for the second scan

Table 2.16: Codes and data files for section 2.11

2.12 Transfer function, Bode and Nyquist plots

For control applications the behavior of many systems can be described by their transfer function. Bode and Nyquist plots are tools often used in connection with transfer functions. In this section we show how to create those plots

- with code of our own
- using a MATLAB toolbox
- the commands provided by *Octave*

2.12.1 Create the Bode and Nyquist plots of a system

Consider the transfer function

$$G(s) = \frac{4 + 4.8\,s}{5.5 + 17.5\,s + 14.5\,s^2 + 3.5\,s^3 + s^4}$$

By writting a script function and storing it in a file `mytf.m`

Matlab

```
function res=mytf(s);
  res=(4+4.8*s)./(5.5+17.5*s+14.5*s.^2 + 3.5*s.^3 + s.^4);
```

we can then compute the result $G(2)$ by calling `mytf(2)`, with the result 0.0954 . Since the function file uses element wise operations we may compute the values of the function for multiple arguments by passing a vector as argument to a single call of the function, e.g.

Matlab

```
mytf([0 1 2 3 4 5])
.
ans =    0.7273    0.2095    0.0954    0.0505    0.0295    0.0184
```

By using the above code we can compute the values of this transfer function along the positive imaginary axis and then generate the plot. We choose to examine the domain $10^{-2} \leq \omega \leq 10^5$. The code below will generate one half of the Nyquist plot of this transfer function, as shown in Figure 2.81.

Matlab

```
% generate the Nyquist plot of a transfer function
w=logspace(-2,5,200);
z=mytf(i*w);
plot(z)
grid on; axis equal
```

A very similar call will generate the Bode plots of $G(s)$.

Matlab

```
% generate the Bode plots of a transfer function
semilogx(w,20*log10(abs(z)))
semilogx(w,angle(z)*180/pi)
```

2.12.2 Create the Bode and Nyquist plots of a system with the MATLAB–toolbox

The built-in command `nyquist()` in MATLAB will generate Figure 2.82 . This function needs the coefficients or the numerator and denominator polynomial as arguments. The frequency domain will be chosen automatically. Similarly the command `bode()` will create the Bode plots in Figure 2.83. Unfortunately both commands are part of a toolbox of MATLAB and thus have to be purchased separately. Consult the on-line help for more information.

Matlab

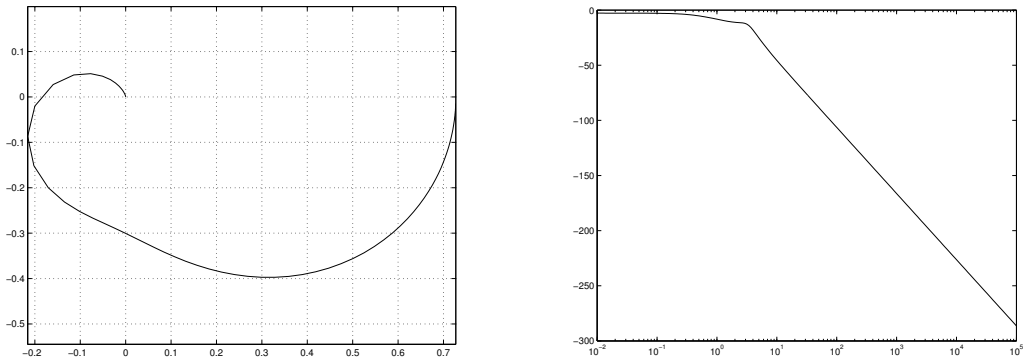


Figure 2.81: Nyquist and Bode plots of the system, programmed with MATLAB

```
num   = [4.8  4];
denum = [1  3.5  14.5  17.5  5.5];
nyquist(num,denum);
bode(num,denum);
```

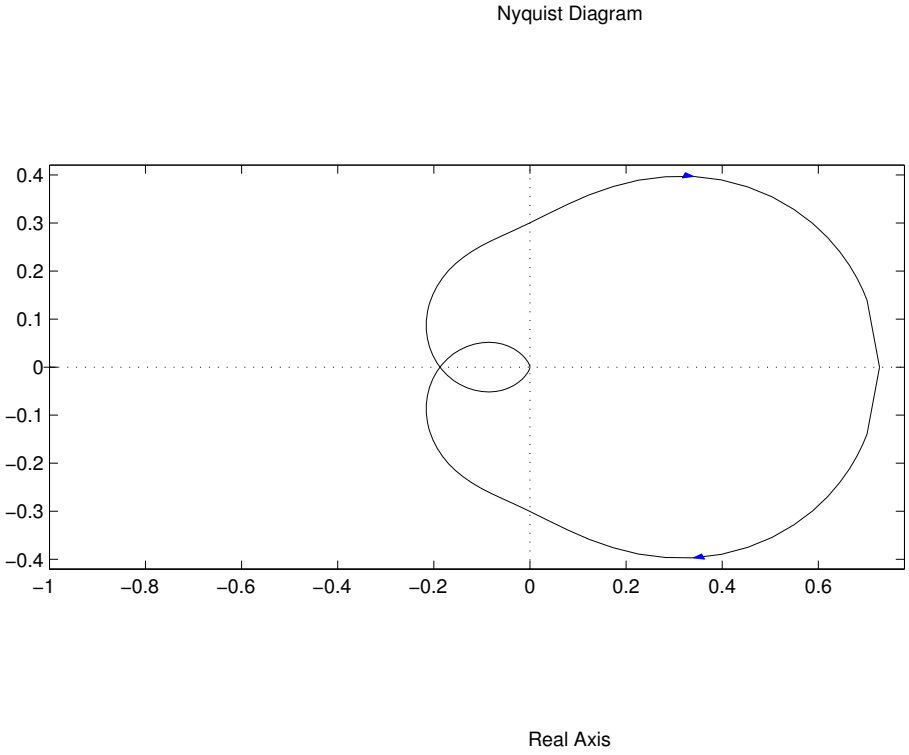


Figure 2.82: Nyquist plot of the system, with control toolbox of MATLAB

2.12.3 Create the Bode and Nyquist plots of a system with *Octave* commands

The SourceForge package `control` of *Octave* provides a set of commands for control theory, including Bode and Nyqist plots. The code below leads to the Figures 2.84 and 2.85. You may want to consult the online help on the commands `tf()`, `bode()` and `nyquist()`.

Octave

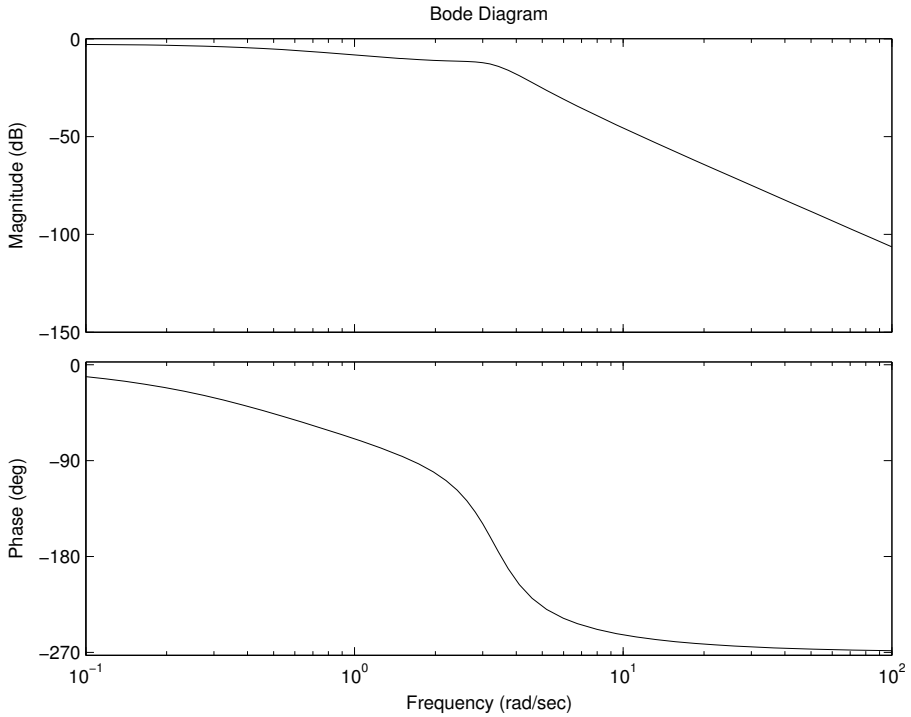


Figure 2.83: Bode plots of the system, with control toolbox of MATLAB

```
mysys = tf([4.8 4],[1 3.5 14.5 17.5 5.5]);
figure(1);  bode(mysys);
figure(2);  nyquist(mysys);
```

2.12.4 Eliminate artificial phase jumps in the argument

In Figure 2.85 the argument jumps by 360°. This does not create a problem for this figure, but might be troublesome in another application. Thus we seek to eliminate this artificial jump in the phase. The function `fixangles()` does take a vector of angle values as argument an returns the adjusted angles, such that no 2π jumps appear. The used algorithm is rather elementary:

- Start out with no correction `k=0` . Take the known angles (`angles`) and the compute the difference between subsequent angles by `da=diff(angles)` .
- For each step in the angles determine what number of 2π–steps is closest to the actual change in the angle. This is done by the command `k -= round(da(i)/(2*pi))` . For most steps the values of k will not change.
- Then add the correct numbers of steps to the angle by `res(i+1)+=k*2*pi` .

fixangles.m

```
function res = fixangles(angles)
%% res = fixangles(angles) eliminates the 2*pi jumps in a vector of angle values

n   = length(angles);
res = angles;
k   = 0;
da = diff(angles);
for i = 1:n-1;
```

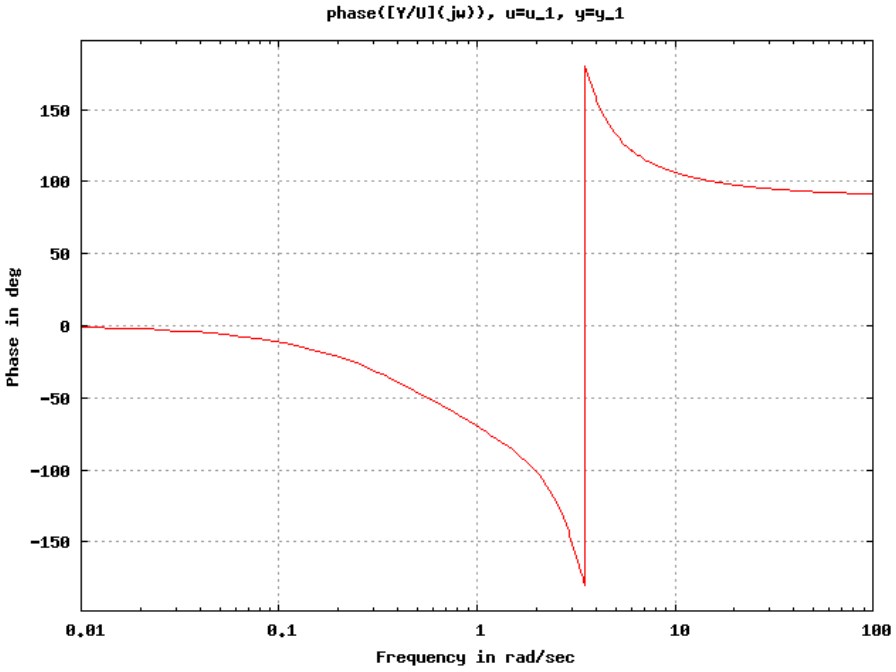


Figure 2.84: Nyquist plot of the system, created by *Octave*

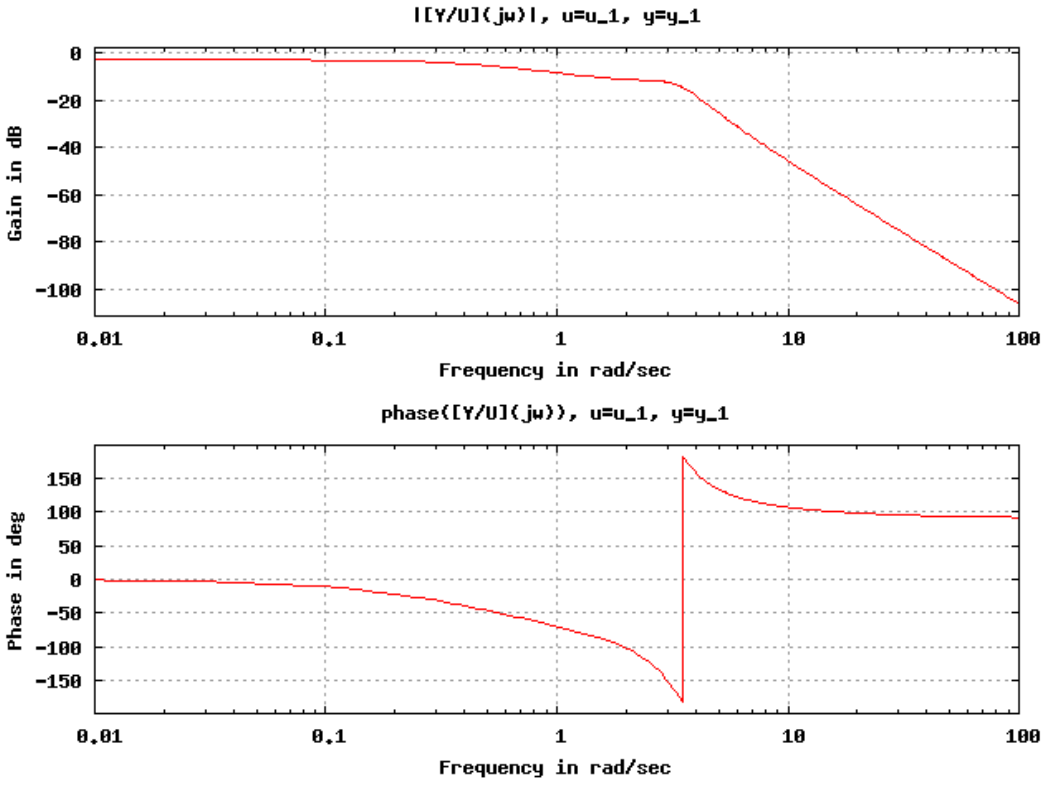


Figure 2.85: Bode plots of the system, created by *Octave*

```
    k -= round(da(i)/(2*pi));
    res(i+1) += k*2*pi;
  end
```

The code below is an elementary test of the function `fixangle()` .

Octave

```
mysys = tf([4.8 4],[1 3.5 14.5 17.5 5.5]);

[mag,phase,w] = bode(mysys);

semilogx(w,phase/180*pi)
hold on
phase2 = fixangles(phase/180*pi);
semilogx(w,phase2)
hold off
```

2.12.5 The SourceForge commands for control theory

Octave has a sizable number of commands to operate on control systems. The documentation should be included with the distribution. It is also available through this authors home page. An abbreviated list of commands is shown below.

- `tf()` build system data structure from transfer function format data
- Find the description of `bode()` and `nyquist()` above
- `sysout()` print out a system data structure in desired format

As an elementary example we determine the pole of the above transfer function.

Octave

```
mysys=tf([4.8 4],[1 3.5 14.5 17.5 5.5]);
sysout(mysys,'zp')
.

Input(s)       1: u_1

Output(s):     1: y_1

zero-pole form:
4.8 (s + 0.8333)
-------------------------------------------------
  (s + 0.5) (s + 1) (s + 1 - 3.162i) (s + 1 + 3.162i)
```

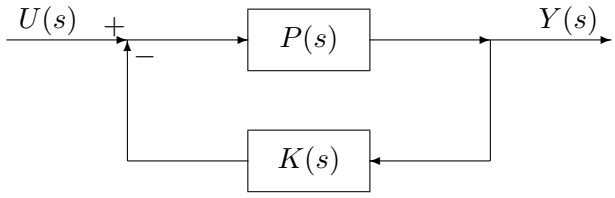
The result shows that the system is in fact stable, since all poles (zeros of the denominator) have negative real part.

There are some demos of the specialized commands, all documented in the section `OCST demos` of the SourceForge documentation. Below find a noncomplete list of demos.

- `DEMOcontrol` or `controldemo` Launch the demos
- `bddemo` Block Diagram Manipulations demo
- `rldemo` Root Locus demo
- `frdemo` Frequency Response demo
- `moddemo` Model Manipulations demo

32 Example : As an example we consider a feedback system where the individual transfer functions are given by

$$K(s) = \frac{s+1}{s} \quad \text{and} \quad P(s) = \frac{1}{s+2}$$



Standard results for transfer functions imply that the transfer function for this feedback system is given by

$$T(s) = \frac{P(s)}{1 + K(s)\,G(s)} = \frac{\frac{1}{s+2}}{1 + \frac{s+1}{s}\frac{1}{s+2}} = \frac{s}{s^2 + 3\,s + 1}$$

The command `feedback` will combine the given systems P and K to a new system. Then `sys2tf()` and `sys2zp()` will determine the transfer function and its zeros and poles for the feedback system.

Octave

```
nump = 1; denp = [1 2];
P = tf(nump,denp,0,"plant input","plant output");

numk = [1 1]; denk = [1 0];
K = tf(numk, denk,0,"controller input","controller output");

FeedbackSys = feedback(P,K);

[num,den] = sys2tf(FeedbackSys)
[z,p] = sys2zp(FeedbackSys)
```

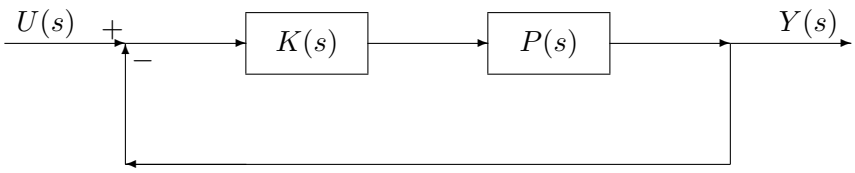
The results of the above code are given by

Octave

```
num =  1  0
den =  1  3  1

z = 0
p =  -2.61803  -0.38197
```

This confirms the numerator and denominator of the transfer function $T(s)$ and its poles $p_{1,2} = \frac{1}{2}\,(-3 \pm \sqrt{3^2 - 4})$ at $p_1 \approx -2.6$ and $p_2 \approx -0.38$. ♢

33 Example : A very similar example is examined in the demo `bddemo -> Design Examples`. We use the same functions for $G(s)$ and $K(s)$ as in the previous example.



Some algebraic operations lead to the transfer function of this feed back system

$$Y(s) \;=\; K(s)P(s)\,(U(s) - Y(s))$$

$$\begin{aligned}(1+K(s)P(s))\,Y(s) &= K(s)P(s)\,U(s)\\ Y(s) &= \frac{K(s)P(s)}{1+K(s)P(s)}\,U(s)\\ &= \frac{\frac{s+1}{s^2+2\,s}}{1+\frac{s+1}{s^2+2\,s}}\,U(s) = \frac{s+1}{s^2+3\,s+1}\,U(s)\end{aligned}$$

Detailed explanations of the code below are beyond the scope of these notes.

Octave

```
%%   step 1: create systems P and K
nump = 1; denp = [1 2];
P = tf(nump,denp,0,"plant input","plant output");

numk = [1 1]; denk = [1 0];
K = tf(numk, denk,0,"controller input","controller output");

%%   step 2: group P and K together
PK = sysgroup(P,K);

%%   step 3: create a summing junction
%%   Step 3a: duplicate controller input: (input 2 of PK)
PK = sysdup(PK,[],2);

%%   step 3b: scale input 3 by -1
PK = sysscale(PK,[],diag([1, 1, -1]));

%%   step 4: connect outputs to respective inputs
%%Step 4: connect:
%%   y(t) (output 1) to the negative sum junction (input 3)
%%   u(t) (output 2) to plant input (input 1)
%%   and prune extraneous inputs/outputs (retain input 2, output 1)
out_connect = [1, 2]
in_connect  = [3, 1]
PK0 = sysconnect(PK, out_connect, in_connect);

%%   step 5: prune the desired i/o connections
PK0 = sysprune(PK0,1,2);
[num,den] = sys2tf(PK0)
[z,p] = sys2zp(PK0)
```

You find the source code of the above, and other demos, in the file `bddemo.m` on yous system as part of the *Octave* distribution. ♢

2.12.6 A root locus problem

Examine one given system

Now we examine the location of the poles of the feedback system. First define numerator and denominator of the system and create the Nyquist plot. Then the system is converted to the `MATLAB` form and the poles of the transfer function are located. The result implies that the open loop system is stable.

- Define numerator and denominator of the transfer function with the help of the coefficient of the polynomials.
- The command `nyquist()` will then create a Nyquist plot of the system with the given transfer function.

- With `tf()` the polynomial coefficients are converted to a `MATLAB` objet of the type transfer function.
- With `pole()` the poles of the above transfer function are computed.

Octave

```
num   = [4.8  4];
denum = [1  3.5  14.5  17.5  5.5];
figure(1);
mysys = tf(num,denum);
nyquist(mysys);
[z,p] = sys2zp(mysys);
p
```

The result should be Figure 2.82 and the poles are given by

Octave

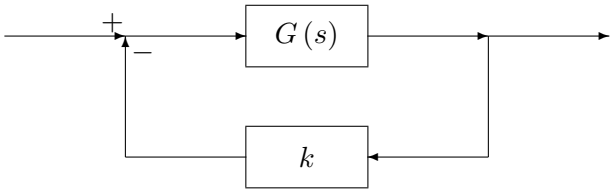
```
-1.0000 + 3.1623i
-1.0000 - 3.1623i
-1.0000
-0.5000
```

With *Octave* the command `sys2zp()` determines to zeros and poles of the transfer function. Since all real parts of the poles are negative we conclude that the open loop system is stable.

Consult the on-line help for information on the commands `nyquist()`, `tf()` and `sys2zp()`. For `MATLAB` the command `[z,p]=sys2zp(mysys)` has to be replaced by `pole(mysys)`.

A parameter dependent system

Next generate all the values of the amplification factors for different values of the parameter k. The Nyquist plot in Figure 2.82 implies that the feedback system should be stable for the amplification factor $-1.3 < k < 5$. With a loop construct the transfer function of the closed loop system and compute the poles. They are stored in the variable `poles`, sorted by their real part.



- Create a vector with 50 equidistant values of the parameter k between -1.3 and 5.
- A variable `poles` is created, with the correct size to store all poles of the systems for all parameter values. It is initialized with zeros.
- Then for each value of the parameter k the following commands are executed:
  - With `backsys=tf(kvalues(j),1);` the feedback part of the system is created. The amplification factor given by `kvalues(j)`. Then with `FeedbackSys=feedback(mysys,backsys);` the feedback system is computed.
  - Using `sys2zp()` all poles of the system are computed and then stored in `poles` .

Octave

```
num = [4.8 4]; denum = [1 3.5 14.5 17.5 5.5]; mysys=tf(num,denum);
kvalues = linspace(-1.3,5,50);

for j = 1:length(kvalues)
  backsys = tf(kvalues(j),1);
  FeedbackSys = feedback(mysys,backsys);
  [z,p] = sys2zp(FeedbackSys);
  poles(j,:) = p';
endfor
```

Now create a graph with all the poles marked. Figure 2.86 shows that all poles are in the in the left half plane for values of $-1.3 \leq k \leq 5$ and thus the closed loop system will be stable.

Octave

```
rr = real(poles);
ri = imag(poles);
figure(2);
grid on
axis([-3,1,-4,4])
plot(rr,ri,'b+');
title('All poles'); xlabel('Real');  ylabel('Imaginary')
```

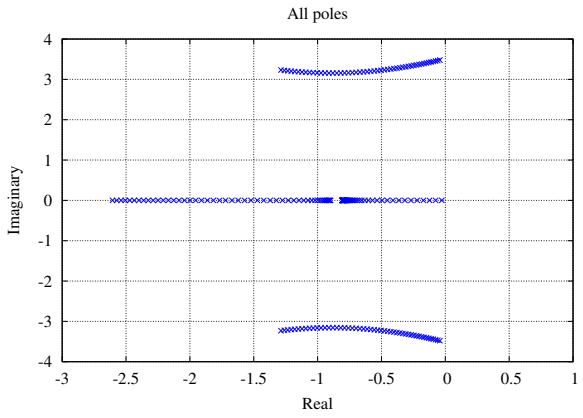


Figure 2.86: Pole location of the closed loop system

2.12.7 List of codes and data files

In the previous section the codes in Table 2.17 were used.

filename	function
`fixangles.m`	function file to eliminate artificial phase jumps
`mybode.m`	a modified version of the command `bode()`
`mybodeTest.m`	a test for the above modification
`feedbackdemo1.m`	an elementary demo for the OCST commands
`feedbackdemo2.m`	a second elementary demo for the OCST commands
`rootlocus.m`	script file to compute pole locations

Table 2.17: Codes and data files for section 2.12

2.13 Planed Topics

- Rewrite the section on Transfer Functions, Bode and Nyquist
- Integrate the image processing with Fourier from Fourier lecture notes: Zielfilm.
- Use the playerc code `spectrum_analyser.m` to modify a graph.
- Filter design, using a heart beat analysis by Josef Götte, well done by Annie Zoss. A filter design interface might be nice.
- Present PCA, using my notes in `Correlation.tex`, [GlovJenkDone11]
- Finite difference methods to solve BVP and IBVP, use lecture notes from Numerical Methods. Makes extensive use of sparse matrices.
- Sparse matrix operations, use `LinearSystems.tex` and the test provided in that directory.
- Present my solution of KdV, using the conservation law
- Add and index with the keywords.
- Terminal interaction by `input()`, `menue()`, `yes_or_no()`, `kbhit()`

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