

Octave and MATLAB for Engineers

Andreas Stahel, Bern University of Applied Sciences, Switzerland

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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 *Octave* and you will still find sections to be adapted to MATLAB. The current version is available at web.sha1.bfh.science/Labs/PWF/Documentation/OctaveAtBFH.pdf.

Wherever possible I attempted to provide code working with both *Octave* and MATLAB . Most of the codes are available at web.sha1.bfh.science/Labs/PWF/Codes .

The notes consist of two chapters.

- The first chapter is an introduction to the basic *Octave/MATLAB* commands and data structures. The goal is to provide simple examples 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 MATLAB/*Octave*. In each section the question or problem is formulated and then solved with the help of *Octave/MATLAB*. This small set of applications with solutions shall help you to solve **your** engineering problems. In class I choose a few of those topics and present them to the students.

Starting in 2015 our students have legal access to MATLAB and thus I have to take this into account in class and most instructions and codes work with both *Octave* and MATLAB!

There is no such thing as “*the perfect lecture notes*” and improvements are always possible. I welcome feedback and constructive criticism. Please let me know if you use/like/dislike the lecture notes. Please send your observations and remarks to Andreas.Stahel@bfh.ch .



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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 types.
- Create basic graphics and manipulate images.
- Solve ordinary differential equations. Include C++ code in *Octave*.

1.1 Starting up *Octave* or **MATLAB** and First Steps

The goal of this section is to get the students started 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. *Octave*¹ is very similar to **MATLAB**. If you master *Octave* then **MATLAB** is easy too. *Octave* is developed and maintained on Unix systems, but can be used on Mac and Win* systems too. There is a number of excellent additional packages for *Octave* available on the internet at *Octave Forge*².

For most tasks **MATLAB** and *Octave* are equivalent

The home page of this author³ [[www:sha](#)] gives more information and also information on *Octave* for different operating systems.

References

- For quick consulting there is a reference card for *Octave*. It should come with your distribution of *Octave*.
- David Griffiths from the University of Dundee prepared an excellent set of short 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 web page [web.sha1.bfh.science/Octave.html](#) (part of this autors web page at [[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.
 - The *Octave* packages are documented on the web site of Octave Forge at <http://octave.sourceforge.net/>

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. As an introduction to **MATLAB** and some of its extensions you might consider [[HuntLipsRose14](#)].
- On the *Octave* web page there is a Frequently Asked Questions (FAQ) page:
<http://www.gnu.org/software/octave/FAQ.html>

¹ <http://www.gnu.org/software/octave/>

² <http://octave.sourceforge.net/>

³ <https://web.sha1.bfh.science>

- Find a wiki for *Octave* at <http://wiki.octave.org/> with useful information.
- There is an active mailing list for *Octave*. Access the mailing list through the main *Octave* page using the entry Support. The mailing list is also available at <dir.gmane.org/gmane.comp.gnu.octave.general>. Starting in August 2016 the site `gmane.org` was not available any more, the maintainer suffered to many networks attacks. You can also use Nabble to be found at <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.

- 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 arrow string `-->`, short for “leading to”.

Octave

```
code
-->
results
```

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

1.1.1 Starting up Octave

Working with the Octave GUI

Starting with version 4.0.0 of *Octave* has a GUI (Graphical User Interface) as interface, see Figure 1.1. To start *Octave* with the GUI use

your mouse to click the menu entry on your desktop environment, e.g. Xfce, Gnome, Mac OS*, Win*

type `octave &` in a terminal with versions 4.0 and 4.2

type `octave --gui &` in a terminal with version 4.4 and 5.1

Within one window frame you can

- execute commands and observe their results in the **Command Window**.
- edit code segments and run them directly from the **Editor** window with one key stroke (F5).
- gather information on all variables in the current workspace in the **Workspace** window.
- work with the built-in **File Browser**.
- read the standard Octave documentation in the **Documentation** window.
- read and change the current directory in the top line of the GUI.
- Starting with version 4.4.0 Octave has a **Variable Editor**. By clicking on a variable in the workspace the name and the value(s) will be displayed in the variable editor, where you can display and change the value(s). To show and modify the variable *a* use the command `openvar('a')`.

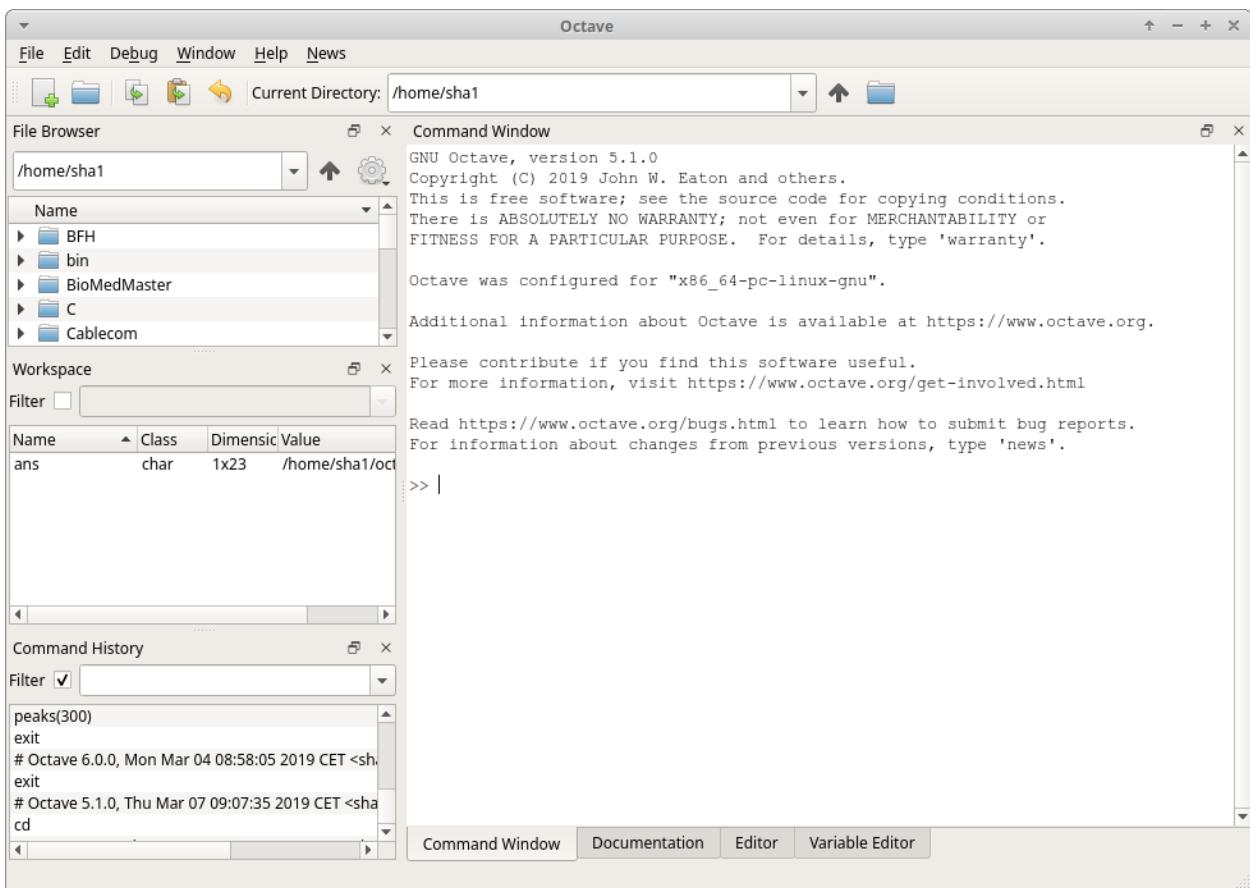


Figure 1.1: The Octave GUI

Figure 1.1 shows a typical screenshot of the Octave GUI. There are several advantages using the GUI:

- The built in editor has good highlighting and syntax checking of Octave code.
- In the editor you can set break points and step through your code line by line.
- You can detach some windows from the main frame. I most often use the editor in a separate window.
- You can move in the directory tree with the top line of the GUI.
- Graphics generated by Octave will always show up in separate windows.

Working with the CLI (Command Line Interface) of Octave

If you want to use *Octave* without the GUI then use the command

```
type octave --no-gui in a terminal with versions 4.0 and 4.2
```

```
type octave in a terminal with version 4.4 and 5.1
```

A working CLI 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 you might want to try *gedit*.
 - For WIN* systems the editor *notepad++* might be a good choice.
3. Possibly a browser to access the documentation.
4. Possiblly one or more graphics windows.

Thus a working screen might look like Figure 1.2. Your window manager (e.g. Xfce, KDE or GNOME) will allow you to work with multiple, virtual screens. This is very handy to avoid window cluttering on one screen.

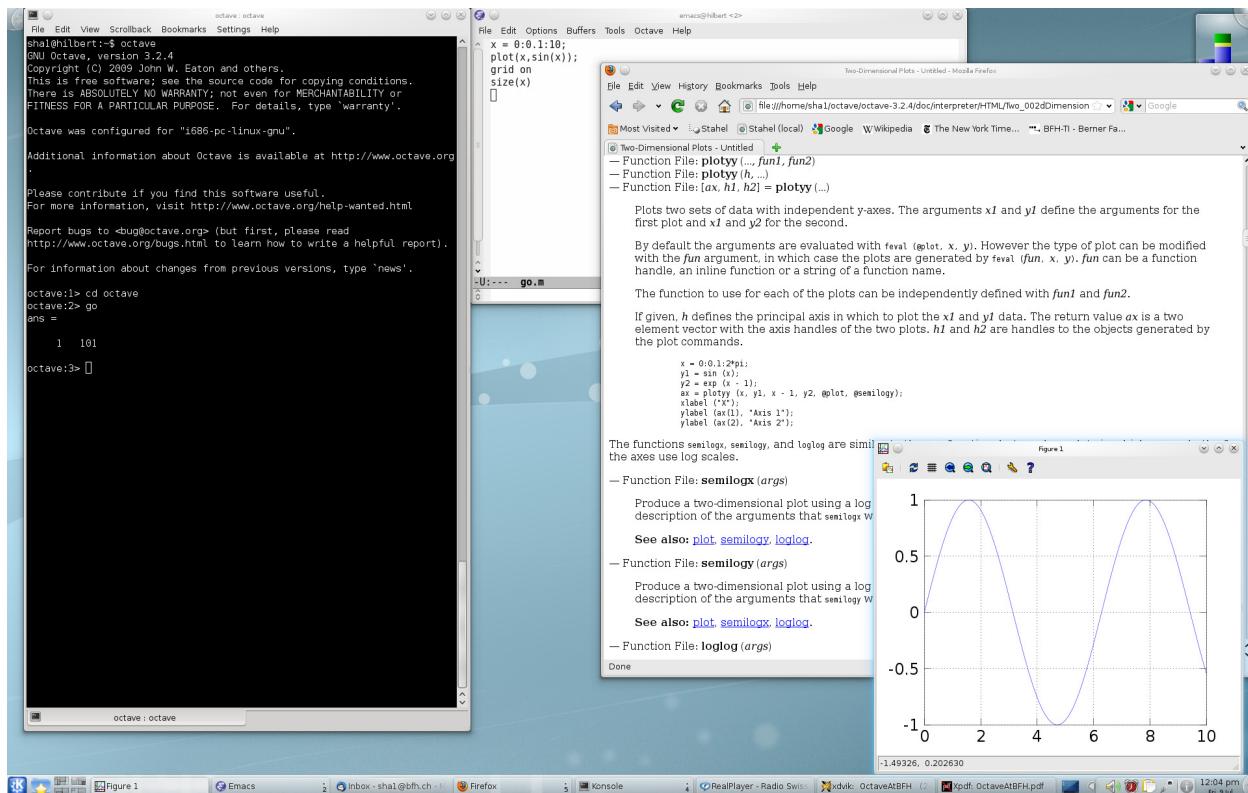


Figure 1.2: Screenshot of a working CLI *Octave* setup

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

- Open a shell and change to the directory in which you want to work. Use `cd` to change into the desired directory.
- Type `octave --no-gui` (4.0, 4.2) or `octave` (4.4, 5.1) for the CLI, For a setup with GUI use `octave &` (4.0, 4.2) and `octave --gui&` (4.4, 5.1) .
- You may also use the currently installed windowing system user interface. Locate the menu entry 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 files with *Octave* code is `*.m` .

There are many command line options to be used. Type `octave --help` or examine Section 2.1.1 Command Line Options in the *Octave* manual.

The startup file `.octaverc`

On startup *Octave* will read a file `.octaverc` in the current users home directory⁴. In this file the user can give commands to *Octave* to be applied at each startup. You can add a directory to the current search path by adding to the variable `path`. Then *Octave* will search in this directory and all its subdirectories for commands. Thus the user can place his/her script and function files in this directory and *Octave* will find these commands, independent of the current directory. My current version of the startup file is

`.octaverc`

```
pkg prefix ~/octave/forge ~/octave/forge;
% capitalization of letters is ignored
addpath(genpath('~/octave/site'))
set(0,'DefaultTextFontSize',20)
set(0,'DefaultAxesFontSize',20)

set(0,'DefaultAxesXGrid','on')
set(0,'DefaultAxesYGrid','on')
set(0,'DefaultAxesZGrid','on')

set(0,'DefaultLineWidth',2)
more off
```

With this initialization file I configure *Octave* to my desire:

- The packages are installed and searched for in the directory `~/octave/forge` .
- *Octave* will always search in the directory `~/octave/site` and its sub-directories for commands, in addition to the standard search path.
- I choose larger default fonts for the text and axis in graphics.
- For any graphics I want the grid lines on by default.
- I choose a larger line width by default for lines in graphics.
- The pager `more` is turned off by default.

If you want to ignore your startup file for some special test you can use a command line option, i.e. launch *Octave* by `octave --no-init-file` .

⁴On a Windows10 system in 2017 the file `octaverc` was located in the directory `C:\Octave\Octave-4.0.3\share\octave\site\m\startup` . On your system it might be in a similar directory.

1.1.2 Packages for Octave

As an essential addition to *Octave* a large set of additional packages⁵ is freely available on the internet at <https://octave.sourceforge.io/>. An extensive documentation is given by the option `Packages` on that web page. If you find a command in those packages and want to make it available to your installation you have to install the package once and then load it into your *Octave* environment.

How to install and use packages provided by the distribution

On Win* systems

- On a recent (2017) win* system with *Octave* 4.0.3 many packages came with the distribution. You have to make the prebuilt packages available. To be done once: launch the command `pkg rebuild` to make the packages available.
- The Win* package for *Octave* 4.2.1 has many packages prebuilt and installed.
- Use `pkg list` to generate a list of all packages. Those marked by * are already loaded and ready to be used.
- Use `pkg load image` to load the image package and similar for other packages.

On Linux/Unix systems Most Linux distributions provide *Octave* and the most of *Octave Forge* with their distribution. We illustrate the use of the package manager by Debian, also used by Ubuntu and its derivatives.

- To install *Octave* use a shell and type `sudo apt-get octave`.
- Use `sudo apt-get install octave-doc octave-info octave-html-doc` to install most of the documentation.
- To install a few packages (image, IO, optimization and statistics) use `sudo apt-get install octave-image octave-io octave-optim octave-statistics`.
- If you plan to compile the packages on your system (see below) you also need the header files and some libraries. To install those use a shell and `sudo apt-get install liboctave-dev`.
- To list the installed packages use the *Octave* prompt and type `pkg list`. Those marked by * are already loaded and ready to be used.
- Use `pkg load image` to load the image package and similar for other packages.

How to install a package from Octave Forge

On the web page <https://octave.sourceforge.io/> current versions of the packages are available and can be installed manually.

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

Octave

⁵For MATLAB you do not have packages, but toolboxes. They are installed when you install your version of MATLAB.

```
pkg prefix ~/octave/forge ~/octave/forge
```

Since the tilde character `~` is replaced by the current users (in this case `sha1`) home directory the packages will be setup in the directory `/home/sha1/octave/forge` and its sub-directories. This command can and should be integrated in your `.octaverc` file.

- To be done for each package:

As example we consider the image package, aiming for the command `edge()`. There are different options to install the image package, containing this command:

- It might already be installed, try `help edge`. If Octave knows about the command, the package is installed and probably loaded. If it is not loaded yet, type `pkg load image`.
- On a Linux installation use your favorite package manager to install the image package of Octave, e.g. Synaptic or `apt-get ...`
- Let Octave try to download, compile and install the package.

Octave

```
pkg install --forge image
```

- You can download, compile and install step by step, as outlined below.
- Go to the web page <https://octave.sourceforge.io/> and choose the option Packages. Then search for the package `image` 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 image-2.10.0.tar.gz
```

From now on the commands provided by the package are available. To use them you still have to load the package, e.g. `pkg load image`.

- You may also locate the source for the command `edge.m` by

Octave

```
which edge
→
'edge' is a function from the file /home/sha1/octave/forge/image/edge.m
```

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

- Loading a package: if a package is installed it will show up with the command `pkg list`, but it is not loaded yet. To load a package use `pkg load image`, then the package `image` will be loaded and listed with a star.

Octave

```
pkg load image
pkg list
→
Package Name | Version | Installation directory
control      | 3.1.0   | /home/sha1/octave/forge/control-3.1.0
financial    | 0.5.3   | /home/sha1/octave/forge/financial-0.5.3
general      | 2.1.0   | /home/sha1/octave/forge/general-2.1.0
image        *| 2.10.0  | /home/sha1/octave/forge/image-2.10.0
io           | 2.4.12  | /home/sha1/octave/forge/io-2.4.12
```

miscellaneous	1.2.1	/home/sha1/octave/forge/miscellaneous - 1.2.1
optim	1.5.3	/home/sha1/octave/forge/optim - 1.5.3
signal	1.4.0	/home/sha1/octave/forge/signal - 1.4.0
splines	1.3.2	/home/sha1/octave/forge/splines - 1.3.2
statistics	1.4.0	/home/sha1/octave/forge/statistics - 1.4.0
struct	1.0.15	/home/sha1/octave/forge/struct - 1.0.15

- Commands to maintain the packages:

- To show a list of all packages use

```
Octave
pkg list
```

- To make the additional commands unavailable you may unload a package, e.g.

```
Octave
pkg unload image
```

- You can load an already installed package, e.g.

```
Octave
pkg load image
```

- To update all installed packages using the Octave Forge site.

```
Octave
pkg update
```

1.1.3 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 resulting maximal array size of $2.1475 \cdot 10^9 \approx 2^{31}$ is a consequence of 32-bit integers being used to index arrays.

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

```
Octave
uname()
→
ans = scalar structure containing the fields:
    sysname = Linux
    nodename = hilbert
    release = 4.15.0-46-generic
    version = #49-Ubuntu SMP Wed Feb 6 09:33:07 UTC 2019
    machine = x86_64
```

- With `version()` the currently used version of Octave is displayed, e.g. 4.4.0.

Octave

```
version()
→
ans = 4.4.0
```

With the command `ver()` the versions of all installed packages are displayed.

Octave

```
>> ver()
```

```
GNU Octave Version: 5.1.0 (hg id: d05d6eebde10)
GNU Octave License: GNU General Public License
Operating System: Linux 4.15.0-46-generic #49-Ubuntu SMP
                  Wed Feb 6 09:33:07 UTC 2019 x86_64
```

Package Name	Version	Installation directory
control	3.1.0	/home/sha1/octave/forge/control-3.1.0
financial	0.5.3	/home/sha1/octave/forge/financial-0.5.3
general	2.1.0	/home/sha1/octave/forge/general-2.1.0
image *	2.10.0	/home/sha1/octave/forge/image-2.10.0
io	2.4.12	/home/sha1/octave/forge/io-2.4.12
miscellaneous	1.2.1	/home/sha1/octave/forge/miscellaneous-1.2.1
optim	1.5.3	/home/sha1/octave/forge/optim-1.5.3
signal	1.4.0	/home/sha1/octave/forge/signal-1.4.0
splines	1.3.2	/home/sha1/octave/forge/splines-1.3.2
statistics	1.4.0	/home/sha1/octave/forge/statistics-1.4.0
struct	1.0.15	/home/sha1/octave/forge/struct-1.0.15

The star on the line `image` indicated that the package `image` is not only installed, but also loaded.

- With the commands `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 currently 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.

1.1.4 Starting up MATLAB

A working environment for MATLAB consists of

- a command line shell with MATLAB to launch the commands
- an editor to write the code

3. possibly a browser to access the documentation
4. possibly one or more graphics windows

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

- Open a shell or terminal
- Change to the directory in which you want to work, use `cd .`
- If you type `matlab &` then MATLAB will launch with the flashy Java interface. By using the ampersand `&` you can later launch other commands in the same shell.
- Type `matlab -nojvm &` to launch MATLAB. The option `-nojvm` launches MATLAB without the flashy Java interface and thus uses a lot less memory, which might be a precious resource your system. On newer versions of MATLAB some of the MATLAB features are not available without the Java interface, this concerns mainly the handling of graphics.
- You may also use the GUI of your operating system, locate the menu entry 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 will 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. Often it is in `~/Documents/MATLAB/`. In this file the user can give commands to MATLAB to be applied at each startup.

1.1.5 Calling the operating system and using basic Unix commands

Within Octave or MATLAB it is possible to launch programs of the operating system. This can be very useful, e.g. to call external image processing tools, see page 87. The details for the functions obviously depend on the underlying operating system.

- `system()` : execute a shell command and return the status and result of the command. As a simple example call the command `whoami` which returns the current users name.

	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

```
unix('whoami');
→
sha1
```

- `unix()` : execute a system command if running under a Unix-like operating system, otherwise do nothing. `dos()` : execute a system command if running under a Dos or Windows-like operating system, otherwise do nothing.

With MATLAB the three commands `system()`, `unix()` and `dos()` are interchangeable. With *Octave* their result depends on the operating system. It is a good idea to use the command `system()` only.

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

1.1.6 How to find out whether you are working with MATLAB or Octave

There are still very few occasions when the codes for *Octave* or MATLAB differ slightly. Thus it might be useful to have a command telling you whether you work with *Octave* or MATLAB. The command `IsOctave()` returns 1 if *Octave* is running and 0 otherwise. Copy the file below in directories where MATLAB/*Octave* will find it, e.g. `~/Documents/Matlab` and `~/octave/site/`.

```
isOctave.m
function result = IsOctave()
% Returns true if this code is being executed by Octave.
% Returns false if this code is being executed by MATLAB, or any other MATLAB
% variant.
%
% usage: result = isOctave()

persistent octaveVersionIsBuiltIn;
if (isempty(octaveVersionIsBuiltIn))
    octaveVersionIsBuiltIn = (exist('OCTAVE_VERSION', 'builtin') == 5);
    % exist returns 5 to indicate a built-in function.
end
result = octaveVersionIsBuiltIn;
% If OCTAVE_VERSION is a built-in function, then we must be in Octave.
% Since the result cannot change between function calls, it is cached in a
% persistent variable. isOctave cannot be a persistent variable, because it
```

```
% is the return value of the function, so instead the persistent result must
% be cached in a separate variable.

end
```

1.1.7 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));
title ('quiver plot')

quiver example 2:
clf;
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, 0.4);
axis equal tight;
hold on; plot (x,y,'r'); hold off;
title ('quiver() with scaled arrows');
```

By calling `demo quiver` the examples will be executed and you can examine code and results.

- Most of the *Octave* code is given as script file. You can look at the source. As it is Open Source code you can copy the file in your directory and modify the code perform the desired operation. To locate the source code for the command `quiver` use which.

Octave

```
which quiver
→ 'quiver' is a function from the file
/usr/local/share/octave/4.0.0/m/plot/draw/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 4.2.0 is also available on my web site at <http://web.sha1.bfh.science/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 hopefully these notes too.
 - For the Octave packages the site <http://octave.sourceforge.net/> provides documentation.

1.1.8 Vectors and matrices

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

- A matrix is enclosed in square brackets ([]) and is a rectangular set of numbers (real or complex).
- Different rows are separated by semicolons (;).
- Within 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. Octave does distinguish between row and column vectors, for beginners often a stumbling block.

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]', % create a column vector by transposing a row vector
x = [1; 2; 3; 4; 5] % create the column vector directly
```

- 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 known we can generate the vector more efficiently using colons (:). Examine the results of the elementary code below.

Octave

```
% x = begin:step:end
x2 = 1:10      % all integer numbers from one to 10
x1 = 1:0.5:10  % all numbers from 1 to 10, with stepsize 0.5
```

- 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) % creates a 2 by 3 matrix filled with zeros
x1 = zeros(5,1) % creates a column vector with 5 zeros
y1 = ones(10,6) % creates a 10 by 6 matrix filled with ones
```

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%for
a
```

The result is generated more efficiently by using vectorized code, as shown below.

Octave

```
a = [1:10].^2
```

Vector operations

Addition and multiplication of matrices and vectors follows strictly (almost, except for broadcasting, see Section 1.1.9) 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 , but watch out for automatic broadcasting
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 $y(x) = |\cos(x)|$ 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%for
plot(x,y);
```

This code is correct, but very inefficient. It 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 1.3.

Octave

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

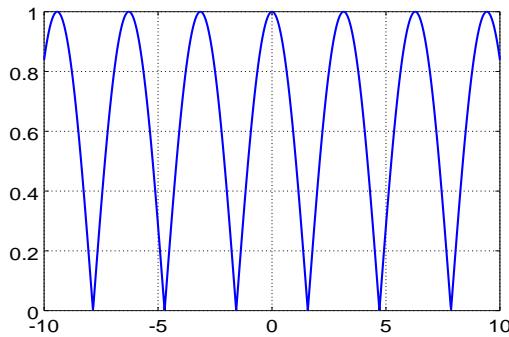


Figure 1.3: Graph of the function $|\cos(x)|$

1 Example : Speed of vectorized code

The three sections of code below compute the values of $\sin(n)$ for $n = 1, 2, 3, \dots, 100000$. One might expect similar computation times.

Octave

```
clear
N = 100000;

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

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

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

On a sample run we found

$$\text{timer1} = 48 \text{ sec} \quad \text{timer2} = 2.4 \text{ sec} \quad \text{timer3} = 0.013 \text{ sec}$$

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

- **preallocation of vectors**⁶

For the second and third code the resulting vector x was first created with the correct size and then the

⁶Newer version of Octave use an improved memory allocation scheme and thus the first loop will be considerably faster.

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 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 use vectorized code whenever possible and preallocate the memory for large vectors and matrices.



Examine the example on page 96 using vectorized code. 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 1.3 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 use loops. Vectorization is one of the main speed advantages of *Octave* over other programs. It should be used whenever possible. Use `tic()` and `toc()` (see Section 1.1.10) to 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));
end%for
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%for
end%for
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 $n = 1, 2, \dots, 10$ we can use a loop

Octave

```

for n = 1:10
    x(n) = n*sin(n);
end%for

```

or the faster vectorized code

Octave

```

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

```

Matrices

Octave obviously has many commands for operations with matrices. Only very seldom loops have to be used for matrix operations.

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 $x=\mathbf{A}\backslash\mathbf{b}$, i.e. we ‘divide’ the vector \mathbf{b} from the left by the matrix \mathbf{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 \mathbf{A} is not invertible the command `null (A)` will give more information about the solvability of the linear system.

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 (\mathbf{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 for this system of over-determined equations:

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 \mathbf{x} with residual vector \mathbf{r} of smallest length, i.e. the best possible solution.

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

This can be a rather useful feature⁷, but also create a problems if the user is not aware of what MATLAB or Octave are actually computing.

1.1.9 Broadcasting

In newer versions of *Octave* broadcasting is applied to some operations and then the computational rules for matrix operations are not strictly respected. As an example consider the subtraction

$$\begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{bmatrix} - \begin{bmatrix} 1 \\ 2 \end{bmatrix}$$

which is mathematical nonsense. With broadcasting *Octave* will automatically subtract the vector from each column of the matrix, but not without a warning.

Octave

```
A = [1 2 3; 4 5 6]; b = [1;2];
r1 = A-b
->
warning: operator -: automatic broadcasting operation applied
r1 =
  0   1   2
  2   3   4
```

If you do not want to see the warning (unwise) you may turn it off by the command `warning('off', 'Octave:broadcast')`⁸. To turn it back on use `warning('error','Octave:broadcast')`.

MATLAB does not know about broadcasting⁹. Both *Octave* and MATLAB have the broadcasting function `bsxfun()`, used below to achieve the same result.

Octave

⁷This can be used to solve linear regression problems, see Section 2.2.

⁸In version 4.0.0 the broadcasting warning has been removed. You may use another warning to indicate broadcasting, i.e. `warning('on','Octave:language-extension')`.

⁹The most recent version of MATLAB (R2016b) seems to use broadcasting too.

```
r2 = bsxfun(@minus,A,b)
```

Use `doc bsxfun` to find out which operations can be broadcasted. If you want to assure compatibility with MATLAB you can force Octave to spot broadcasting as an error and stop the execution of the code.

Octave

```
warning ("error", "Octave:broadcast");
r1 = A-b
->
error: operator -: automatic broadcasting operation applied
```

1.1.10 Timing of code and using a profiler

Timing with `tic()`, `toc()` and `cputime()`

In the above code we used `tic()` and `toc()` to determine the run-time of the loops. The resolution of this timer 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()`.
- Some commands (e.g. `fft()`, `fft2()`) automatically use multithreaded libraries and `cputime()` will add up all the time consumed in the threads, thus you might end up with more CPU time than wall time!

Using the profiler

Octave has a powerful profiler. It will analyze where your code is consuming time. Here is a simple example.

Octave

```
clear *
profile on % turn the profiler on
n = 1000;
for jj = 1:100
    a = rand(n);
    b = exp(cos(a));
end%for

T = profile('info');
profile off % turn the profiler off
profshow(T) % examine the result
```

and the results might look like

#	Function Attr	Time (s)	Time (%)	Calls
3	exp	1.530	42.13	100
2	cos	1.286	35.40	100
1	rand	0.816	22.47	100
4	profile	0.000	0.00	1
6	binary !=	0.000	0.00	1
5	nargin	0.000	0.00	1
7	--profiler_data--	0.000	0.00	1

Thus the above code called the function `exp()` 100 times and this consumed 1.5 sec of CPU time to evaluate the `exp` functions. This is not too bad, as each call actually computed a million¹⁰ values of the exponential function. Thus it only took $0.015 \mu\text{s}$ to compute one value. Compare this to the result of the code below and act accordingly!

```
n = 1000;
for ii = 1:n
    for jj = 1:100
        a = rand(1);
        b = exp(cos(a));
    end%for
end%for
```

1.1.11 Debugging your code

There are different options to debug *Octave/MATLAB* code.

- In the editor window you can set a breakpoint. When running the code execution will stop at this point and you can use the command line to examine the current content variables, modify them, or continue with the execution of the program.
- To continue the running program type `dbcont`. Execution of the current function will continue. With `dbquit` the remaining part of the current function will not be executed, but *MATLAB/Octave* returns to the calling function.
- The GUI editor allows to single step through the code, step into sub-functions, or run the code to the next breakpoint.
- With the command `dbstop` you can set break point from the command line, e.g. `dbstop myfunction 17` will set a breakpoint in the function `myfunction()` on line 17. With `dbclear` you can clear the breakpoint.
- You may also use the function `keyboard()` to interrupt running code on a selected line and the use the command line to examine the current values of the variables.

1.1.12 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`.

¹⁰`rand(n)` generates a $n \times n$ matrix of random values. With $n = 1000$ this leads to a million values.

- Write a **function file**

Functions to be used repeatedly can be written 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 a common 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`. If working with the editor of the *Octave-GUI* you may use the F5 key to save the file and run the code.

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

$$\text{mean} = \mu = \frac{1}{n} \sum_{k=1}^n x_k$$

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

stat.m

```
function [mean,stdev] = stat(x)
% STAT Interesting statistics. This documentaion is displayed by the command
% help stat
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])
```

There are a few differences between MATLAB and *Octave* concerning script and function files.

- MATLAB¹¹ 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.

¹¹Starting with Version 2016b MATLAB allows definition of functions within script files too. The functions within a script file have to be at the end of the script.

- 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.

1.1.13 Local and global variables, nested functions

In Octave/MATLAB the visibility of variables has to be taken into account. A variable declared in the workspace is not visible inside a function, unless you pass it as an argument.

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
```

If you really desire a variable to be visible inside a function (usually a bad idea) you can force Octave to do so by the keyword `global`, as illustrated by the code below.

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 value is 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
```

An important deviation from the above visibility of variable is given by nested functions. If a variable is declared in a function file, then it is visible inside all of the nested function in the same file.

TestNest.m

```
function TestNest()
a = 17    % set the value of a in this function

function res = modify_a(x)
    % the variable a from the outer function is visible
    a = 2; % the outer variable a is overwritten by 2
    res = a*x;
endfunction
```

```
a2 = modify_a(a) % display 34, the result of the function
a % displays 2, modified by the function modify_a
endfunction
```

Since MATLAB allows nested functions, the above idea can be used to define many functions in one file. But observe that the functions defined within another function body will **not** be visible outside of the function. In addition nested functions can not be used inside program control statements e.g. `switch/case`, `if/else, while, ...`

Persistent variables

1.1.14 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 1.4.

Octave

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

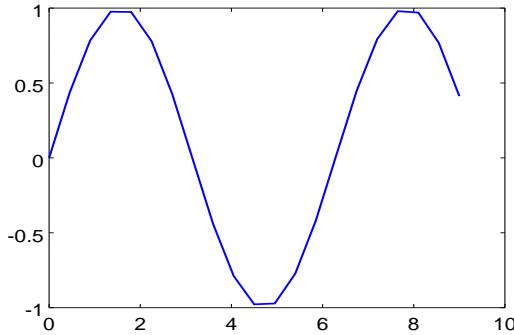


Figure 1.4: Elementary plot of a function

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))
```

1.1.15 A breaking needle problem

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 are given by a normal distribution with mean value μ_p and standard deviation σ_p . The values of F_b are 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.

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

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 a function in our script file to compute the value of this function for a vector of arguments.

Octave

```
mup = 2.0; sigmap = 0.5; mub = 4.5; sigmab = 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 1.5.

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);
```

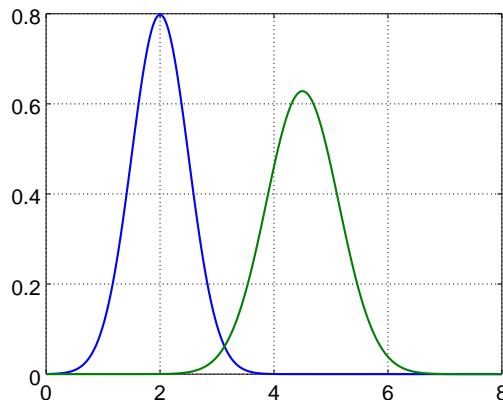


Figure 1.5: Probability of needles to penetrate, or to break

To be determined is the probability that 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 penetrates 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 penetrating at a force f is thus given by the probability density function.

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

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 1.6 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 with a loop
%for k = 2:length(pb)
%    p2(k) = p2(k-1)+pb(k)*df;
%end%for
p2 = cumsum(pb); % the same integration with a single command

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

trapz(f, pfail)
```

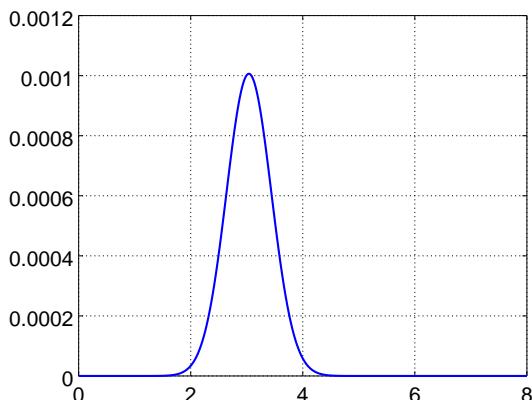


Figure 1.6: Probability distribution of needles to break before penetration

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** $\text{erf}(z)$, defined by

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

Using the definition of the normal distribution¹²

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

¹²MATLAB and Octave have many and powerfull commands to examine statistical questions of this type, see e.g. [Stah16].

and basic calculus we find

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

Thus for the above problem we may equivalently write

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

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 the 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

```

1.1.16 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 pointwise 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 = flip1r(1:(length(pp)-1));
    p3(k) = p3(k+1) + pp(k)*df;
end%for

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

1.2 Programming with *Octave*

This short section cannot and will not cover all aspects of programming with MATLAB or Octave. You certainly have to consult the online documentation and other references, e.g. [Grif01] or [BiraBrei99]. The amount of available literature is enormous, free and nonfree. It is the goal of this section to get you started and point out some important aspects of MATLAB/Octave. It is assumed that you are familiar with a procedural programming language, e.g. C, C++, Java, ...

1.2.1 Displaying results and commenting code

If a line of code is not terminated by a semicolon (;) the results will be displayed in the command window with the name of the variable, followed by a new line. If you do not want to see the result, add the semicolon. With the command `disp()` you can display the result. One can use formatted output to add information, see Section 1.2.4

```
x = exp(pi)
disp(x)
disp(sprintf('the value of exp(pi) is %g',x))
fprintf('the value of exp(pi) is %g\n',x)
→
x = 23.141
23.141
the value of exp(pi) is 23.1407
the value of exp(pi) is 23.1407
```

An essential feature of good code is a readable documentation. For 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
```

There is no feature in MATLAB or Octave to comment out complete sections, you have to do line by line. Many editors provide function to comment and uncomment sections.

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

By far most the 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 expect at best 15 decimal digits to be correct. The exact values are given by the variables `realmin`, `realmax`, and `eps`, respectively. The information about your system can be obtained 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 with real or complex entries.¹³ Complex numbers are described by their real and imaginary parts. All arithmetic operations and most mathematical functions 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
```

Observe that the simplified syntax $2i$ is equivalent to $2*i$.

Octave also provides the data type **single**, i.e. single precision floating point numbers. Its main advantage is to use less memory, the disadvantage is a smaller range and resolution.

Octave

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

You can convert between single and double variables with the commands `single()` and `double()`. The command `whos` will display all current variables, their size, memory foot print and their class.

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
```

Octave has **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.

type	int8	uint8	int16	uint16	int32	uint32	int64	uint64
min	-128	0	-32'768	0	-2'147'483'648	0	-9.2e+18	0
max	+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 illustrated by an elementary example.

Octave

¹³For many years a matrix of floating point numbers was the **only** data type in MATLAB.

```
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 -11 255]
```

When applied to floating point numbers the commands `int8()`, `int16()`,... do not return the integer part, but use rounding.

Integer data types with a prescribed resolution may be used to develop code for micro controllers, as shown in Section 2.4, starting on page 209.

Observe that there are considerable differences in how the programming language C and MATLAB/Octave handle integers.

- In Octave calculations are truncated to their range, e.g. `int8(100) + 30` leads to the result 127.
- Operations with different integer types are not allowed, e.g. `int8(10) + int16(70)` will generate an error message.
- Operations with integer and floating types are allowed and lead to integer results, again truncated to their domain.

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. You can subtract and add letters, or add numbers to letters, for the computations the ASCII codes are used.

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

Building on the basic data types Octave can work with a variety of structured data types: vectors, matrices, strings, structures, cell arrays, lists.

Strings

Octave also works with strings, consisting of a sequence of characters, enclosed in either single-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.¹⁴

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 used in many codes. Consider the trivial example below.

Octave

```

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
}

```

¹⁴In MATLAB you will have to use the function `str2mat()`.

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 be used as a counter in a loop.

Octave

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

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 access individual entries use three indices, e.g. $A(2, 1, 4)$. As an example we compute for each position the average along the height, leading to a 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 commands 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 may lead to a few surprises.

Functions with scalar arguments

- **trigonometric functions:** `sin()`, `cos()`, `tan()`, `atan()`, `asin()`, `acos()`, `atan()`, `atan2()`
Observe that all trigonometric functions compute in radians, and not degrees. There are a few functions with a version 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 results as `atan(y/x)`, while the calls `atan2(-y, -x)` and `atan2(y, x)` yield different results.

- **exponential functions:** `exp()`, `cosh()`, `sinh()`, `tanh()`, `pow2()`. For most of the exponential functions the corresponding inverse functions are also available: `log()`, `log2()`, `log10()`, `acosh()`, `asinh()`, `atanh()`. The only possible surprise 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

```
a1 = 0.2;
[exp(i*a1), cos(a1), sin(a1)]
→
ans = 0.98007 + 0.19867i 0.98007 + 0.00000i 0.19867 + 0.00000i
```

- **generating 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
```

One often needs random numbers with a normal distribution, i.e. the command `randn()`. 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.

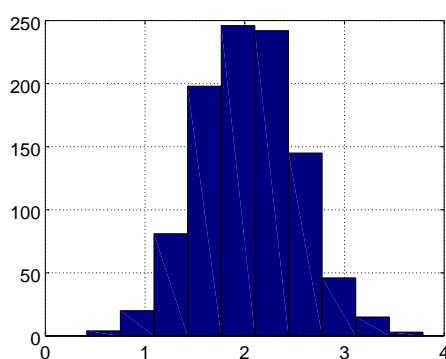


Figure 1.7: Histogram of random numbers with mean 2 and standard deviation 0.5

- `rand()` : uniformly distributed in $[0, 1]$.
- `randi()` : integer random numbers.
- `randn()` : normal distribution with mean 0 and variance 1.
- `rande()` : exponentially 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 1.8. There are many other special functions, e.g `airy()`, `beta()`, `bincoeff()`, `erf()`, `erfc()`, `erfinv()`, `gamma()`, `legendre()`. A good reference for special functions and their basic properties is [AbraSteg] or its modern version [DLMF15], freely accessible on the internet at DLMF.nist.gov.

Octave

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

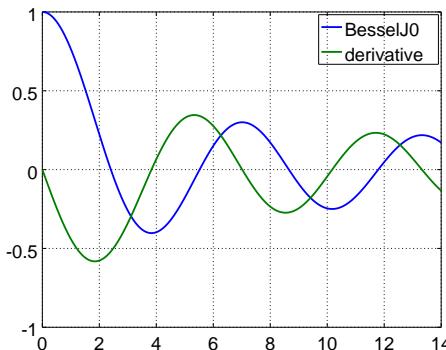


Figure 1.8: Graph of the Bessel function $J_0(x)$ and its derivative

Functions with matrix and vector arguments

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

Octave

```
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 : Element wise 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 yields 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 of the same size.



4 Example : A few possible implementations 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 codes 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. \diamond

5 Example : Matrix exponential

There are also functions that behave differently. The solution of the linear system of differential equations

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

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

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

Unfortunately this is 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()` (**matrix exponential**). 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 the result is different from `sqrt(B)`. ◊

Formatted input and output functions

When reading or writing data one often has to insist on 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.

<code>printf()</code>	formatted output to <code>stdout</code> , not in MATLAB
<code>sprintf()</code>	formatted output to a string
<code>fprintf()</code>	formatted output to a stream (file) or <code>stdout</code>
<code>sscanf()</code>	formatted input from a string
<code>fscanf()</code>	formatted input from a stream (file)
<code>disp()</code>	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) % in Matlab use sprintf()
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
```

<code>%i</code> or <code>%d</code>	signed integer
<code>%ni</code> or <code>%nd</code>	signed integer in a field of length n , no leading zeros
<code>%0ni</code> or <code>%0nd</code>	signed integer in a field of length n , with leading zeros
<code>%u</code>	unsigned integer
<code>%f</code>	regular floating point number
<code>%8.3f</code>	in field of width 8 with precision 3
<code>%e</code>	floating point number with exponential notation
<code>%10.5e</code>	in field of width 10 with precision 5
<code>%g</code>	floating point number in normal or exponential format
<code>%s</code>	string, will stop at white spaces
<code>%c</code>	one or multiple characters

Table 1.4: Some output and input conversion templates

6 Example : Generating numbered file names

Assume that you want to number your files with a three digit integer, e.g. `data001.dat`, `data002.dat`, `data003.dat`, ... This requires that you translate the integer number into a string, including the leading zeros. The name is composed of three sections.

- The first four characters are `data`.
- Then we use formatted printing into a string (`sprintf()`) to generate the string containing the 3 digit number, including the leading zeros. Use the format '`%03d`'.
- The tail of the file name is given by its extension `.dat`. Since strings are vectors of characters we can combine the three segments.

Here is one possibility to do so.

Octave

```
numbers = [ 0 1 2 3 115]; % numbers to be considered
for n = numbers
    filename = [ 'data' , sprintf('%03d',n) , '.dat' ]
end
→
filename = data000.dat
filename = data001.dat
filename = data002.dat
filename = data003.dat
filename = data115.dat
```

If using the simpler format '`%d`', then the length of the file names might change, see below.

Octave

```
numbers = [ 0 1 2 3 115]; % numbers to be considered
for n = numbers
    filename = [ 'data' , sprintf('%d',n) , '.dat' ]
end
→
filename = data0.dat
filename = data1.dat
filename = data2.dat
filename = data3.dat
filename = data115.dat
```

In a real example you will obviously perform other operations in the loop too!



7 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 may 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()`¹⁵ : 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

¹⁵Currently MATLAB does not provide the function `tosacii()`, but you may obtain a similar by using the function `int16()`.

```
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 be used too, 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.¹⁶

- Locating 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/3.6.4/m/general/logspace.m
```

Using the location of the source file you can copy it into a directory of yours and adapt the code. This is a very 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 too, e.g.

Octave

```
which cosh
→
'cosh' is a built-in function from the file libinterp/corefcn/mappers.cc
```

- To just look at the code you can also use `type logspace` and Octave or MATLAB will display the source code of the function.
- The source to many (Octave only) functions have built-in tests and you can call those with the command `test`.

Octave

¹⁶One has to be careful when redistributing modified code. With MATLAB it is forbidden and with Octave you have to respect the GPL license.

```
test logspace
→
PASSES 6 out of 6 tests
```

- The source for many (*Octave* only) 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.¹⁷

Loops generated by `for`

The general form is given by

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

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

```
Octave
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 numbers 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
```

¹⁷If 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. This author considers the *Octave* version to be more readable. A possible workaround is to use a well placed comment sign, e.g `end%for` or `end%while`. I have adapted this notation in most places and it is working just fine.

```

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;             % Octave only
  %   vec(k) = vec(k) -50;     % Matlab and Octave
  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 on the size of the numbers 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 on whether the number is smaller or larger than 50.

Octave

```
vec = round(rand(1,10)*100)
for k = 1:10
  if (vec(k) >= 50)
    vec(k) += -50; % with Matlab use vec(k) = vec(k) - 50
  else
    vec(k) += +50; % with Matlab use vec(k) = 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 `continue` statement appears within 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 that we do **not** leave the loop completely, but only ignore the remaining command for the current run through the loop. It is the `break` statement that will leave the loop completely. The code below will display the numbers, until encountering a value 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` statement

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

Octave

```
switch EXPRESSION
  case LABEL
    COMMANDLIST
  case LABEL
    COMMANDLIST
  ...
  otherwise
    COMMANDLIST
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 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
```

8 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 illustrate 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 = counter+1;
  end%if
end%for
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
```

There is a shortcut version of the above commands. You may also use an array of logical values to select elements. In the code below we generate a vector with numbers from 1 through 12. Then we select and display only the numbers between 5 and 8.7 . There is no need for the command `find()` . On some occasions this might be slightly faster.

Octave

```
x = 1:0.5:12; % all numbers from 1 to 12 in steps of 0.5
ind = (x>=5)&(x<8.7)
x(ind)
—> 0 0 0 0 0 0 1 1 1 1 1 1 1 0 0 0 0 0 0 0 0
      5.0000 5.5000 6.0000 6.5000 7.0000 7.5000 8.0000 8.5000
```



1.2.8 Reading from and writing data to files

With *Octave* you have different options 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.

<code>load()</code> <code>save()</code>	load <i>Octave</i> variables save <i>Octave</i> variables
<code>dlmread()</code>	read all data from a file
<code>dlmwrite()</code>	write data to a file
<code>textread()</code>	read data from a file
<code>strread()</code>	read data from a string
<code>fopen()</code>	open a stream (file)
<code>fclose()</code>	close a stream
<code>fgetl()</code>	read one line from the file
<code>sscanf()</code>	scan a string for formated data

Table 1.5: Reading and writing with files

Loading and saving *Octave* variables

With the command `save()` you can save some, or all, variables to 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 to a file. Then all variables in *Octave* are cleared and the matrix is reloaded.

Octave

```

clear *
aMat = rand(2);      % create a random matrix
save data.mat aMat  % save this matrix to a file
clear                % clear the variables
aMat                 % try to access the matrix, should fail
load data.mat        % load the variable
aMat
→
'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*. By using flags one can choose which format should be used, e.g. `save -v6 MyVariable.mat` will save the data on a MATLAB Version 6 specific format, which can be used by *Octave* and MATLAB.

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. **Comma Separated Values**. 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 2.2.12.

Using `textread()`

With the command `textread()` a file can be scanned line by line, and a format string can be provided. As example examine the following file with data in a csv format.

FuelConsumption.csv

```

Toyota Auris Hybrid – Fuel Consumption
Date,km=reading,km driven,km driven, gas [1],cost [CHF],1/100km
,,calculated,manual,,
01/17/15,10800,,,
02/20/15,11368,568,568,34.62,47.75,6.10
03/12/15,11987,619,619,34.56,51.50,5.58
04/01/15,12754,767,767,38.93,57.60,5.08
04/25/15,13506,752,752,38.26,56.60,5.09
...

```

This data is now used in the code `FuelConsumption.m`, leading to Figure 1.9. The essential function `textread()` takes a few arguments:

- The string '`'FuelConsumption.csv'`' lists the name of the file with the data.
- The format string '`'%s %f %f %f %f %f'`' gives the format of the available data: first a string, then a sequence of 6 numbers. All numbers are read as data type double, even if integer would be possible. This is to avoid undesired type conversions in subsequent computations.
- The strings '`'delimiter',''`' indicate the the data is separated by commas.
- The last argument '`'headerlines', 4`' informs `textread` that the first 4 lines are header lines and should be ignored.

The first data entry is a string in a date format, e.g. '`'02/20/15'`'. This has to be converted to a number of days of using this car. This is performed by `Day = datenum(datevec(Date))`; . The first function `datevec` converts this string into a serial number corresponding to this date, e.g. `[2015, 2, 20, 0, 0, 0]`. Then the command `datenum` is used to convert this into a number of days since the start of the current year minus 50, e.g. `736015`. Using `Day = Day - Day(1)` arrive at the days of usage of this car by the current user. To finish the code two graphics are generated, see Figure 1.9,

- The fuel used for 100 km as function of the days of usage.
- A histogram of the fuel usage of this car.

FuelConsumption.m

```

% Fuel Consumption Auris 2018
[Date ,Status_km ,Distance ,DistanceManual ,FuelUsed ,Price ,Gasfor100km] = ...
    textread('FuelConsumption.csv','%s %f %f %f %f %f' ,...
        'delimiter ','' , 'headerlines ',4);
Day = datenum(datevec(Date)); Day = Day-Day(1);

FuelFor100km = 100*FuelUsed ./ Distance;

figure(1)
plot( Day,FuelFor100km ,'+')
xlabel('Day'); ylabel('Fuel used [1/100km]')

figure(2)
hist(FuelFor100km)
xlabel('Fuel used [1/100km]')

```

Scanning a file, line by 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:

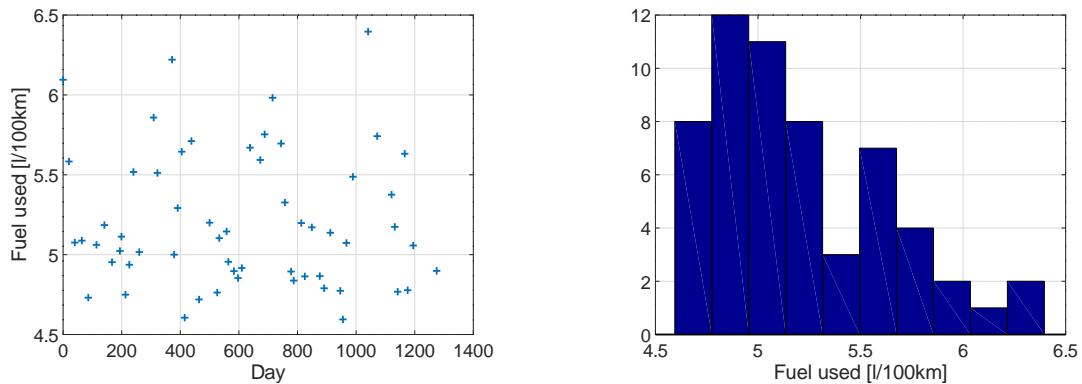


Figure 1.9: Fuel consumption for a hybrid car

- 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; % preallocate 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 ischar(tline))
    % if tline not character, 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
```

```

end%while

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 .

The above file can also be read by using command `textread()`, as shown below.

```

[letters , num1, num2] = textread('Sample.txt','%s %f %u','headerlines ',3)
→
letters = {
    [1,1] = a
    [2,1] = b
    [3,1] = c
    [4,1] = d
    [5,1] = e }
num1 = 4.0300e+00 -5.8000e+00 1.0000e+03 -4.7000e-06 0.0000e+00
num2 = 5 4 3 2 1

```

Internally `textread()` is using `strread()` . Consult `help strread` to find out about the different formats supported.

Some applications 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, it may serve as a starting point. There are many other types of very important problems to be solved that are 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 2.2.14, 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()	constrained minimization with respect to one variable
fmins()	minimization, one or multiple variables
fminsearch()	minimization, one or multiple variables
fminunc()	unconstrained minimization, one or multiple variables

Table 1.6: Commands to solve equations and optimization

1.3.1 Systems of linear equations

Since the 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

9 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

$$\left[\begin{array}{ccc} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 10 \end{array} \right] \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}$$

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

$$\mathbf{A} \cdot \vec{x} = \vec{b} \quad \Leftrightarrow \quad \vec{x} = \mathbf{A} \setminus \mathbf{A} \cdot \vec{x} = \mathbf{A} \setminus \vec{b}$$

In Octave and MATLAB 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 use the operator \ many times. One may either use a matrix for the right hand side or use the LU factorization presented in the two examples below. If you want to solve 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.

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

- \mathbf{L} is a lower triangular matrix
- \mathbf{U} is an upper triangular matrix
- \mathbf{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

$$\mathbf{A} \vec{x} = \vec{b} \iff \mathbf{L} \mathbf{U} \vec{x} = \mathbf{P} \mathbf{A} \vec{x} = \mathbf{P} \vec{b} \iff \begin{cases} \mathbf{L} \vec{y} = \mathbf{P} \vec{b} \\ \mathbf{U} \vec{x} = \vec{y} \end{cases}$$

Instead of solving $\mathbf{A} \vec{x} = \vec{b}$ directly, 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 systems 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. \diamond

10 Example : Solving linear systems is a n^3 process

According to results you have seen in your class on linear algebra the 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

$$\text{CPU} \approx c n^3$$

$$\log(\text{CPU}) \approx \log(c) + 3 \log(n)$$

On a doubly logarithmic scale we expect a straight line with slope 3. This is confirmed by the code below and the resulting Figure 1.10¹⁸.

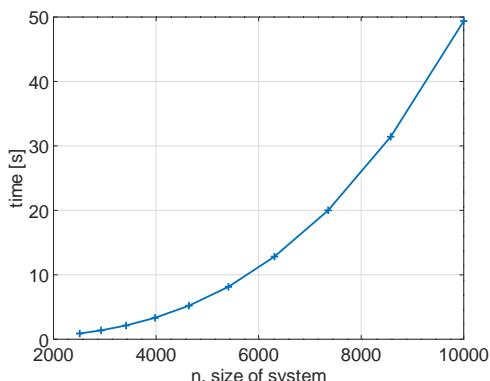
Octave

```
nlist = floor(logspace(3.4,4,10));
timer = zeros(size(nlist));
for k = 1:length(nlist)
    n = nlist(k);
    A = rand(n)-0.5 + n*eye(n);
    f = rand(n,1);
    t0 = cputime();
    x = A\f;
    timer(k) = cputime() - t0;
end%for

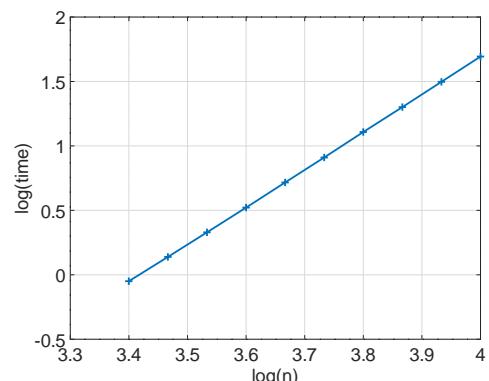
MFlops = 1/3*nlist.^3./timer/1e6

figure(1)
plot(nlist,timer,'+-')
xlabel('n, size of system'); ylabel('time [s]'); grid on

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



(a) linear scales



(b) logarithmic scales

Figure 1.10: 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 $8n^2$ bits 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 for systems $\mathbf{A} \vec{x} = \vec{b}$ without unique solution the backslash operator will lead to a result.

- Even if a linear system is over-determined and has no solution, Octave and MATLAB will give an answer. In this case the result will be the solution of a linear regression problem, see Section 2.2. The answer \vec{x} is determined such that the norm of the residual vector $\vec{r} = \mathbf{A} \vec{x} - \vec{b}$ is minimal.

¹⁸Most of the time for this simulation is used up for generating the random numbers. But only the solving time is measured by calling `cputime()`.

- If the system is under-determined and has infinitely many solutions, the backslash operator \ will give one answer. It will return the solution — \vec{x} with minimal norm. You have to use linear algebra to be able to generate all solutions.

11 Example : A linear system without solution

This will be even more useful if there are no unique solutions. The system

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

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

Then 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 system $\mathbf{U}\vec{x} = \vec{y}$ turns into

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

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
→
warning: 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 warning, but a very different 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 your linear algebra book for details. The system has (nonunique) solutions 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 the command `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 $\mathbf{A}\vec{x} = \vec{b}$. \diamond

12 Example : Solving an over-determined system of linear equations

With the system of four equations

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

we only have two unknowns. The system is **over-determined**. 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 2.2.6. ◇

13 Example : Solving an under-determined system of linear equations

The linear system of 2 equations

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

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, or faster.

14 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 sequence of systems with triangular matrix.

$$\mathbf{A} \vec{x} = \vec{b} \quad \iff \quad \mathbf{R}^T \mathbf{R} \vec{x} = \vec{b} \quad \iff \quad \begin{cases} \mathbf{R}^T \vec{y} = \vec{b} \\ \mathbf{R} \vec{x} = \vec{y} \end{cases}$$

To examine the system

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

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. Use `help chol` to find out more. \diamond

15 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' % display 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. $n = 100'000$. Working with full matrices you would run out of memory. ◇

16 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\(\mathbf{R}'\backslash 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

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

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 $x = A \setminus b$, 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

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

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 1.11.

```
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
xlabel('x'); ylabel('y = 1+2*x+3*x^3')
```

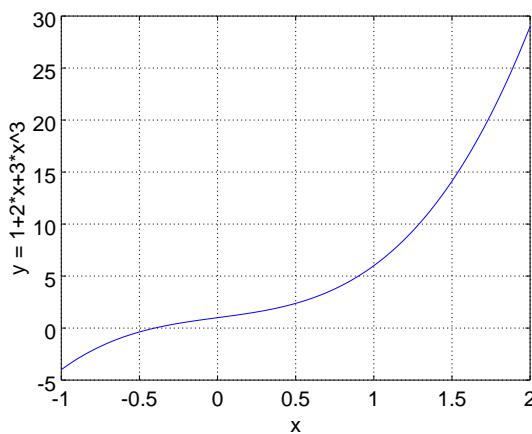


Figure 1.11: Graph of the polynomial $1 + 2x + 3x^3$

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
```

The command `fzero()` is very reliable at solving one single equation for one unknown. In particular if you can bracket the solution, i.e. you have one value with $f(a) < 0$ and another with $f(b) > 0$, then there is a solution in the interval between a and b .

Octave

```
format long
x0 = fzero(@(x) sin(x),[3,3.2])
difference = x0-pi
→
x0 = 3.14159265358979
difference = -1.33226762955019e-15
```

17 Example : Zero of a Bessel function

Examine Figure 1.8 (page 43) 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 `help fsolve`. \diamond

18 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 that one can pass a function 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 evaluations¹⁹ 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);
    disp([x,y]) % display value and derivative 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';

[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  3.2470e-16
```

We observe that the number of correct digits is doubled for each iteration. We needed only 5 iterations to arrive at the desired accuracy. \diamond

19 Example : Options of `fsolve()`²⁰

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 $1.5 \cdot 10^{-8}$.

¹⁹Without any further measures the function will be called twice for each step, which is not necessary. Read `help fsolve` to learn how to avoid this double evaluation.

²⁰Specific for *Octave*.

- `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 prompt to find the exact location of the source file and then examine the file with your favourite editor. As an 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 over-determined systems of equations and may be used for nonlinear regression problems, see Section 2.2.14.

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

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

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 Newton's Algorithm

As a first example of an extended function we develop code for Newton's algorithm to solve systems of equations.

The main tool to solve a system of nonlinear equations of the form $\vec{f}(\vec{x}) = \vec{0}$ is Newton's 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 over-determined systems too (see Section 2.2.14).

All 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

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

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 already solved 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 $\frac{\partial f(x)}{\partial x}$ the above codes uses finite difference approximations of the form

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

1.3.4 Optimization

In this section we will use some commands from the optimization package at SourceForge²¹. Thus have a quick look at the package, resp. its documentation. If the package is not installed on your system (hint: `pkg list`) you will have to download, install and load the package, using the instructions in Section 1.1.2 (page 12).

20 Example : The function $f(x) = \sin(2x)$ 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

```

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%)

```

²¹In MATLAB with the Optimization toolbox installed you may use the function `fminsearch()` instead of `fmins()`. In Octave both are available.

```

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 the 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

```

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

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

we seek a minimum of $-f(x, y)$. Examine the graph of $f(x, y)$ in Figure 1.12.

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

```

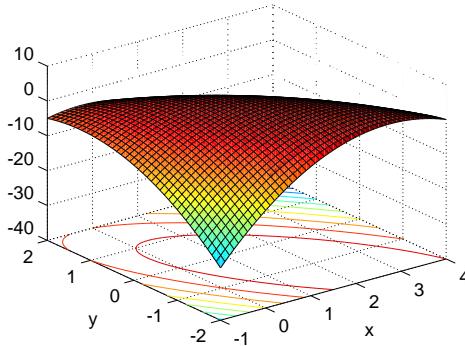


Figure 1.12: Graph of a function $h = f(x, y)$, with contour lines

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
```



22 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

$$f(a, b, c) = \max_{0.5 \leq x \leq 1} \left| \frac{1}{x} - ax^2 - bx - c \right|$$

As a starting guess for our parabola we use the straight line through the points $(0.5, 2)$ and $(1, 1)$. Another option would be to generate the Chebyshev approximating polynomial of degree 2, see Section 2.4.6 on page 221.

To improve accuracy and reliability we repeat the call of `fmins()` until the result stabilizes.

Octave

```
x = linspace(0.5,1,1001);
format long % display (too) many digits
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 = 2.74516598909596 -6.05887449195935 4.32842712578459
pOptim = 2.74516598880275 -6.05887449156216 4.32842712566662
```

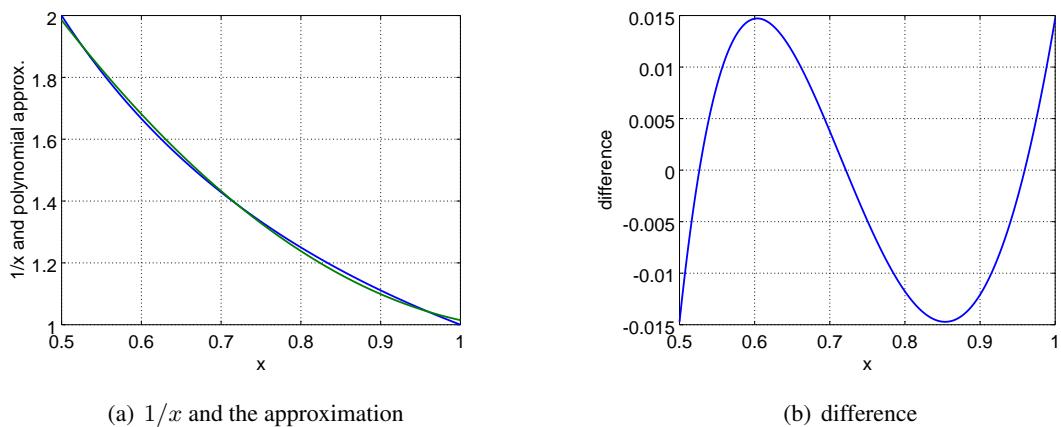
The result can be verified visually by the code below and the resulting Figure 1.13. Obviously we have an excellent approximation of $1/x$ by a second order polynomial.

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')
```



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 Section 2.2.14 for nonlinear regression problems.

Figure 1.13: $1/x$ and a polynomial approximation of degree two

1.4 Basic Graphics

For the graphics commands there are only some small differences between MATLAB and Octave. 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 multiple graphics windows, using the command `figure()`.
- Within a graphics window you can use the mouse to zoom, move or rotate the picture.
- 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.
 - `qt` : this toolkit is used with Octave 4.0.1 and allows for interactive modifications of the figure.
 - `gnuplot` : this was 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 possible. Close all graphics windows with `close all` and then change the graphics toolkit, e.g. with the command below.

Octave

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

- With MATLAB there is only one graphics toolkit, thus there is nothing to choose.

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 1.14(a).

Octave

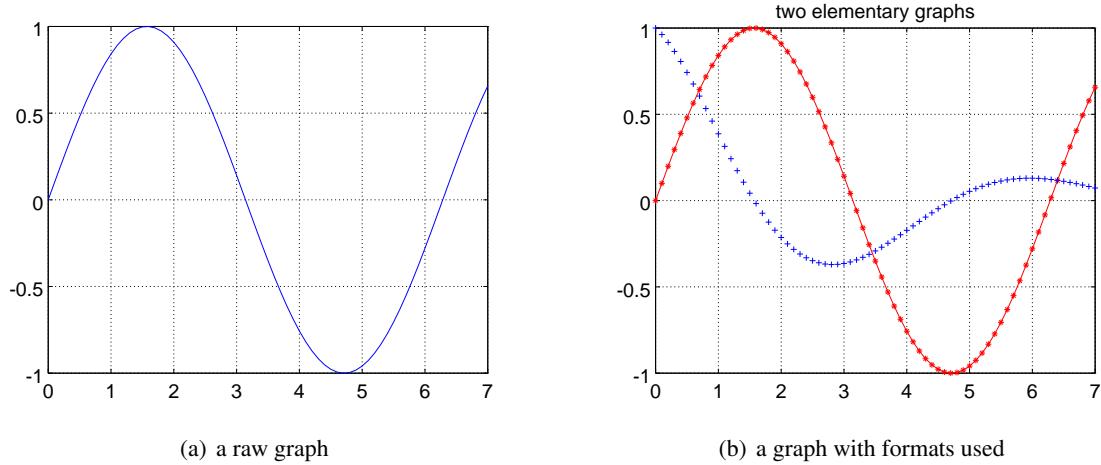


Figure 1.14: Elementary graphs of functions

```
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 how to connect the points.

- The command `plot()` can only²² display points and straight line connections between them. Thus you have to compute the coordinates of the points first and then generate the graphics.
 - The command `plot()` with one argument only will use the numbering of the given values for the horizontal coordinate and the values for the vertical coordinates.
 - The command `plot()` with two arguments requires the values of the x coordinates as the first argument and the y components as the second argument.
 - A third argument of `plot()` may be a format string, specifying how `plot()` has to display and connect the individual points. There are many options:
 - * Choose a lines style: – lines, . dots, ^ impulses, L steps
 - * Choose the color by a letter: k (black), r (red), g (green), b (blue), m (magenta), c (cyan), w (white)
 - * Use +, *, o or x in combination with the lines style to choose the point style
 - In Octave you can set the text for the legend with '`;key text;`'.
 - In Octave and MATLAB you can set the text for the legend by `legend('key text')`.
- 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 1.14(b).

Octave

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

²²We knowingly ignore the command `ezplot()`, `fplot()` and its friends. They are of very limited use and you are better off using the Octave/MATLAB way to generate figures: first compute the data, then display the data.

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

Table 1.7: Generating 2D plots

Options and additions to `plot()`

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 these options with the result shown in Figure 1.15(a).

- To generate a PDF (Portable Document Format) use `print -dpdf` (MATLAB and Octave). This will lead to a full PDF page. You will have to crop the large margins of the graphics if you only need the picture and there are many tools achieve this, e.g. the command `pdfcrop` to be used outside of MATLAB.. With Octave you may use `print -dpdfwrite` to generate the cropped graphics directly. This file is suitable to be included in L^AT_EX documents when using PDF as graphics format, e.g. by `pdflatex`.
- An 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 L^AT_EX documents when using EPS as graphics format, e.g. by `latex`.
- For LibreOffice 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.
- Observe that with MATLAB a command `print('myPic.png')` will print directly to the printer of your system, and not write the graphics to a file. If you want the file specify the device explicitly, e.g. `print('myPic.png',' -dpng')` .
- There are many more formats available, see `help print` or examine Section 1.4.2.

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 ')
% Matlab is slightly different
print('graph3.pdf',' -dpdfwrite ') % Octave only
print('graph3.png',' -S600,400') % in Matlab slightly different
%% to obtain a 4 by 3 inches picture with a resolution of 200dpi use
%% the code below. The resulting PNG file will contain a 800x600 picture
% set(gcf,'PaperUnits','inches','PaperPosition',[0 0 4 3])
% print('graph3.png',' -dpng ',' -r200 ')

```

Octave

```

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

```

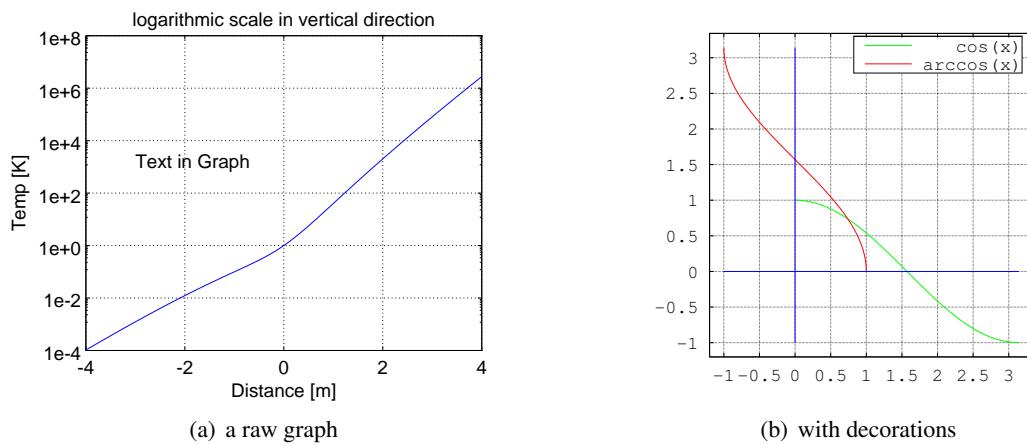


Figure 1.15: Two graphs without and with some decorations

With `subplot()` one can generate multiple graphs in one figure. The code on the last two lines generates a title over all subfigures.

Octave

```
x = linspace(-2*pi,2*pi,200);
clf
axis('normal');
axis() % leave the scaling up to Octave/Matlab
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));
ha = axes('Position',[0 0 1 1],'Xlim',[0 1],'Ylim',[0 1],...
    'Box','off','Visible','off','Units','normalized','clipping','off');
text(0.4, 0.95,'Titel Over all Subplots')
```

Find another example in Figure 1.28 on page 100.

Interactive manipulations

With MATLAB and new versions of Octave you can manipulate properties of graphics interactively.

- You can zoom in and out.
- Rotate a 3D graph. Works with 2D graphs too!!
- You can add text at any position in the picture.
- Label and rescale the axis.
- You can turn the grid on and off.
 - With Matlab choose the small arrow in the menu line of the graphics to edit the plot. Then click in the graph and use the right mouse button to obtain the menu with the options to choose.
 - With Octave click on the graph and either hit the key “G” (Gnuplot toolkit) or use the menu item in the top line.

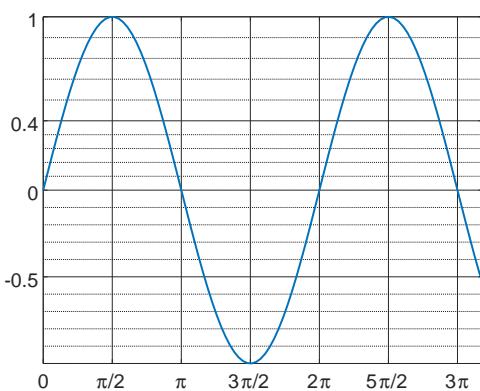
Grid lines and tick marks

One can modify the tick marks and the grid lines in a plot by setting properties of the axis object. With the code below we generate figure 1.16(a).

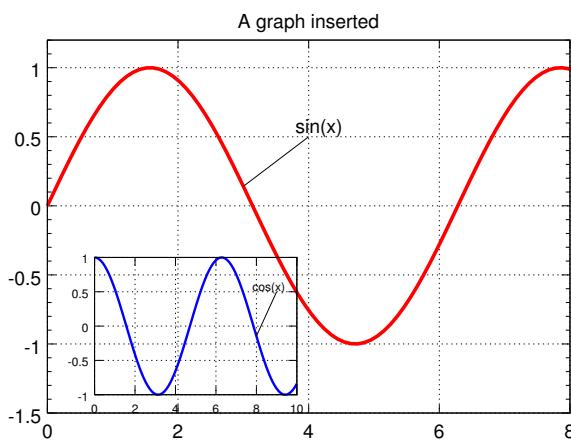
- With the command `set()` the properties of the current axis are modified. The function `gca()` returns a handle to the current axis.
- On the x-axis the tick marks are shown at multiples of $\pi/2$ and labeled accordingly.
- On the y-axis the labels are unevenly spaced, but more grid lines are shown.

```
x = linspace(0,10);
figure(1); plot(x,sin(x))
set(gca(),'XTick',[0:pi/2:3*pi],...
    'XTickLabel',{'0','\pi/2','\pi','3\pi/2','2\pi','5\pi/2','3\pi'})
set(gca(),'XGrid','on')
set(gca(),'YTick',[-0.5,0,0.4,1])
set(gca(),'YMinorGrid','on');
```

An axis object has many properties to be modified by `set()`. To examine the list of all those use the command `get(gca())`. The list will be rather long!



(a) A plot with tick marks and grid lines



(b) A figure in a figure

Figure 1.16: Tick marks, grid lines and a figure in a figure

A figure in a figure

Octave allows for many more tricks with pictures, e.g. you can generate a figure in a figure, as shown in Figure 1.16(b).

Octave

```
x = linspace(0,10); f1 = sin(x); f2 = cos(x); % generate the data
figure(1); subplot(1,1,1) % assure it is one figure
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]) % this sets the new frame for the graph
set(gca,'xlim',[0,10], '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)')
```

When MATLAB/Octave generate a graphics it has many default options set. You can access those through the command `get()`. Find more information on this in section 15.3 *Graphics Data Structure* of the Octave manual

Size of graphics when printing

When printing or generating a PostScript or PDF file the size is specified by the figure's 'papersize' property and the position on the page by 'paperposition'. In the code below we generate a figure that is wider than usual, leading²³ to Figure 1.17. With the command `gca()` we can get a handle to the current axis, and then modify some of the properties. To find out more, generate an arbitrary graphics and then examine the result of `get(gca())`. In the above example we set the markers on the x -axis at specific locations and used the special symbol π .

```
x = linspace(0,10); y1 = sin(x); y2 = cos(x);

h = figure(1); clf;
plot(x,y1,x,y2)
legend('sin(x)', 'cos(x)'); xlabel('x')
set(h, 'paperunits', 'centimeters')
set(h, 'papersize', [15,6])
set(h, 'paperposition', [0,0,16,6])
set(gca(), 'xtick', [0,pi,2*pi, 3*pi], 'xticklabel', {'0','\pi','2 \pi','3 \pi'})

print -dpdfwrite SizeAndTick.pdf
print -depsc SizeAndTick.eps
```

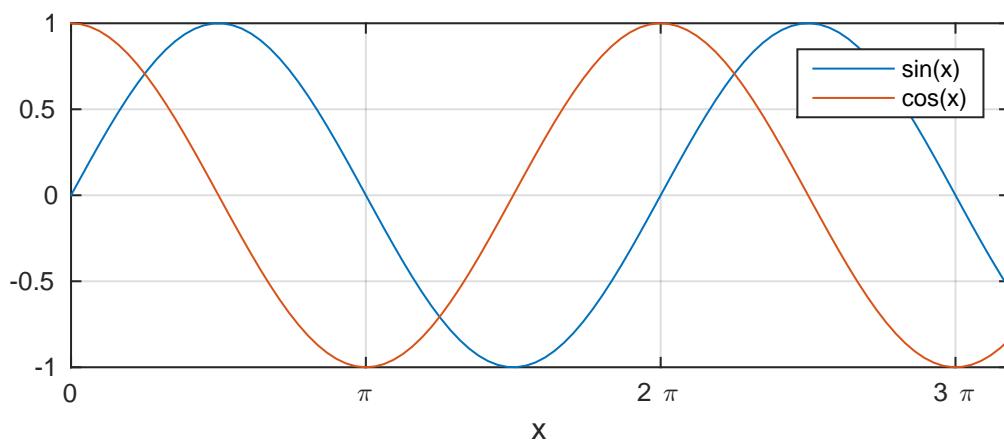


Figure 1.17: A graphics of specific size and with special tick marks

²³Currently the MATLAB version looks nicer than the Octave version.

1.4.2 Printing figures to files

The GUI of *Octave* and *MATLAB* allow you to save a figure in different formats. In many applications it is more convenient to generate the file with the figure by a command. Here you can choose and modify many different aspects of a figure.

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 processing tool or to be used with *L^AT_EX*. 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 with `help print` or `doc print`.

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

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

Octave and *MATLAB* usually choose the file format by looking at the given extension of the given file name. If no device is given explicitly *MATLAB* will send the file to the printer, while *Octave* writes to the given file.

```
print MyFigure.png % Matlab sends to printer, Octave to file or printer
print -dpng MyFigure.png % Matlab and Octave write to the file
```

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 *L^AT_EX* 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 photographs the created files might be unnecessarily 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 image will have a resolution of 600 columns and 400 lines. 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.
- The codes in MATLAB are slightly different. To generate a picture of dimension 6×4 cm with a resolution of 100 dpi use

Matlab

```
set(gcf,'PaperUnits','centimeters','PaperPosition',[0 0 6 4])
print -dpng graph3.png -r100
```

- L^AT_EX and LibreOffice/OpenOffice/Word can handle PNG files.

PDF : Portable Document Format can be used in L^AT_EX or 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, Matlab/Octave
print('graph.pdf',' -dpdfwrite') % for a figure with bounding box, Octave
```

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. Use system tools like `pdfcrop`.

- For photographs the created files might be unnecessarily 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 Unix program `xfig` to modify your picture, e.g. change fonts, colors, thickness of lines, and many more. With `xfig` you can then save the figure in the desired format for the final usage. To generate a colored figure use the option `-color`, e.g.

Octave

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

Converting an image to different formats

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

ImageMagick is a 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 operations to images: resize, rescale, rotate, ... To convert a file `graph.gif` to the PNG format you may type `convert graph.gif graph.png` on a Unix command line. If you want to achieve 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. This can be done within *Octave* by using the `system()` command, as shown above.

Since the command often has to be applied to all `*.eps` files in a sub-directory I created a shell command to convert all images at once. This shell script only works on Unix systems!

doEPStoPDF.sh

```
#!/bin/bash
for file in *.eps
do
    epstopdf $file
done
```

Using `printFigureToPdf.m` to generate nice PDF files

The script file `printFigureToPdf.m` uses features of MATLAB and *Octave* to generate a PDF with a desired size. Observe that the size of the fonts are adapted accordingly²⁴. If you have to fiddle with the exact form of an output, have a closer look at the source of this command. It uses a few `set()` commands to generate the desired size and then calls to standard commands. It might just give you the necessary hints.

Octave

```
% script file to test the PDF output of printFigureToPdf()
x = linspace(0,10);
plot(x, sin(x),x,cos(x))
legend('sin(x)', 'cos(x)')
xlabel('x')
% size given in inches, with a 10% border
printFigureToPdf('Sin_Cos.pdf',[6,4], 'inches',[0.1,0.1,0.1,0.1])
% size given in inches again (problems with cm),
% with a 10% border, except at the top only 5%
printFigureToPdf('Sin_Cos_cm.pdf',[4,3], 'inches',[0.1,0.1,0.1,0.05])
```

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 1.18 illustrate that the values around ± 1 are more likely to show up as results of the `sin`-function on $-5\pi \leq x \leq 5\pi$. 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 of the 20 subintervals and displays the result as height of the column. This leads to Figure 1.18(a). The histogram in Figure 1.18(b) is normalized, such that the sum of all heights equals 1. Thus we can read 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.

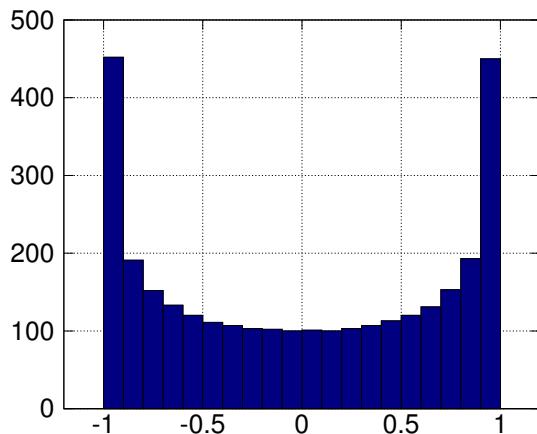
²⁴With versions 3.8.2 and 4.0.* of *Octave* the legends are not handled correctly. With the first release candidate for *Octave* 4.2 the situation is better, but not perfect. One might use `text()` as a fix. On occasion I had to call the command twice to obtain the desired result!

```

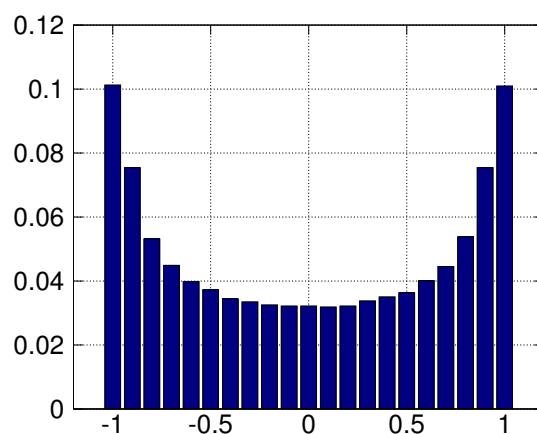
x = -5*pi:0.01:5*pi;    y = sin(x);
figure(1);
hist(y,20)
axis([-1.3 1.3]);        % Matlab can not choose the x-scaling only
%axis([-1.3 1.3 0 500]); % for Matlab use this line

figure(2);
[height,center] = hist(y,-1:0.1:1,1)
height = height/sum(height);
bar(center,height);
axis([-1.2 1.2]);        % Matlab can not choose the x-scaling only
%axis([-1.1 1.1 0 0.12]) % for Matlab use this line

```



(a) counting histogram



(b) normalized histogram

Figure 1.18: 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);

```

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 .

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 of a surface
contourf()	graph the contour lines with colored patches
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

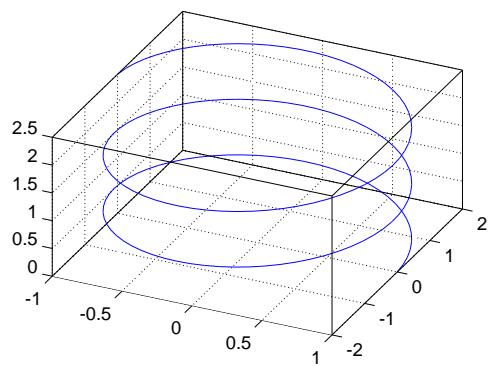


Figure 1.19: A spiral curve in space

- 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)
```

\rightarrow

```
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

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

use the codes below to create Figure 1.20.

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');
```

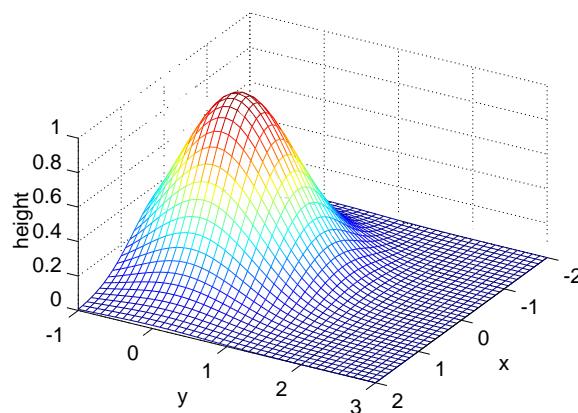


Figure 1.20: The surface $z = \exp(-x^2 - y^2)$

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)
```

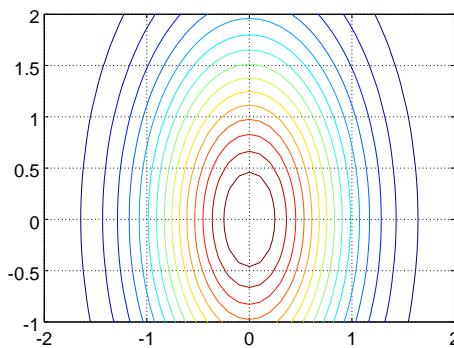


Figure 1.21: The contour lines of the function $z = \exp(-x^2 - 0.3 y^2)$

Instead of a mesh, as shown in Figure 1.20 we can create fully colored patches with the command `surf()`. Find the result in Figure 1.22(a). For the graph we can also insist that the levels shown are between 0 and 1, with steps of 0.1 and we want the levels labeled, as shown in Figure 1.22(b). We can modify the above code.

Octave

```
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
clabel(C,h,cc,'FontSize',10); % display the level curves
xlabel('x'); ylabel('y');
axis equal
```

- 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.

With `contourf()` not only the lines are drawn, but also colored paths. With an option you can not display the contour lines at all. In addition a colorbar is displayed and the shading is based on an interpolation.

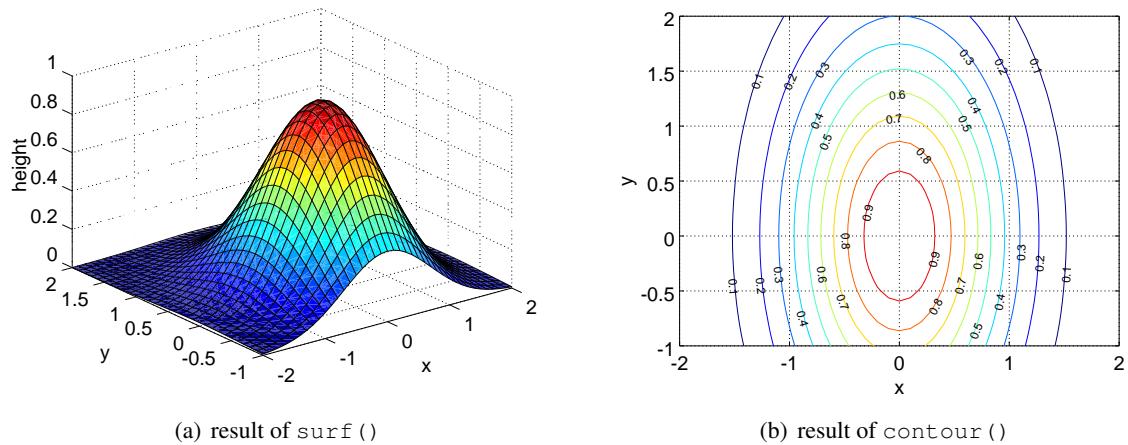


Figure 1.22: Two modifications of the above surface and contour plot

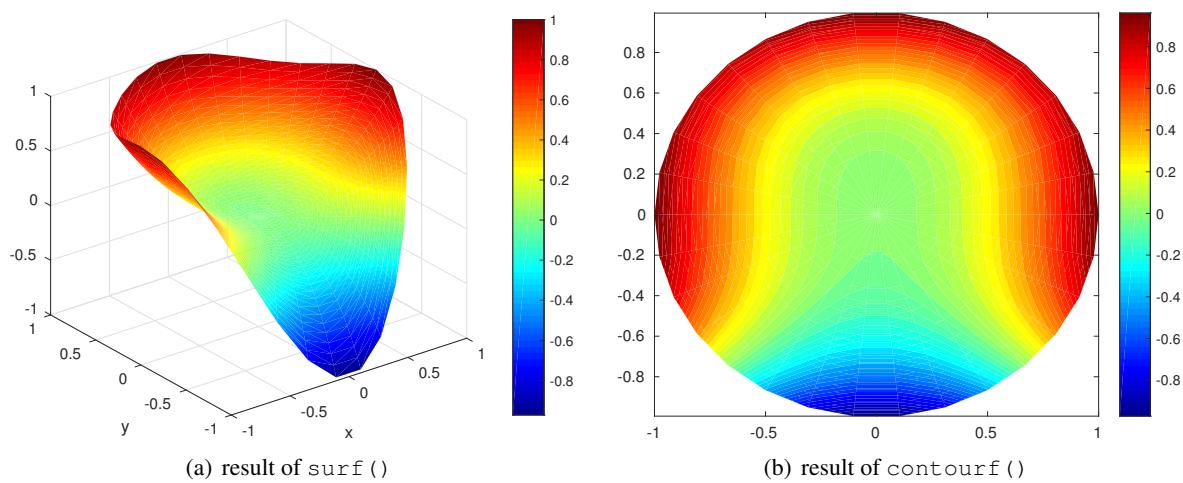


Figure 1.23: Surface and contour plots, without visible lines

```

alpha = linspace(0,2*pi,31)'; radius = linspace(0,1,31);
x = cos(alpha)*radius; y = sin(alpha)*radius;
z = x.^2 + y.^3;
figure(1); H1 = surf(x,y,z); xlabel('x'); ylabel('y')
colormap(jet());
shading interp
set(H1, 'EdgeColor', 'none');
colorbar

figure(2); colormap(jet());
[C,H2] = contourf(x,y,z,50);
colorbar
shading interp
set(H2, 'LineStyle', 'none');

```

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 1.24. The torus is parametrized by 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)

```

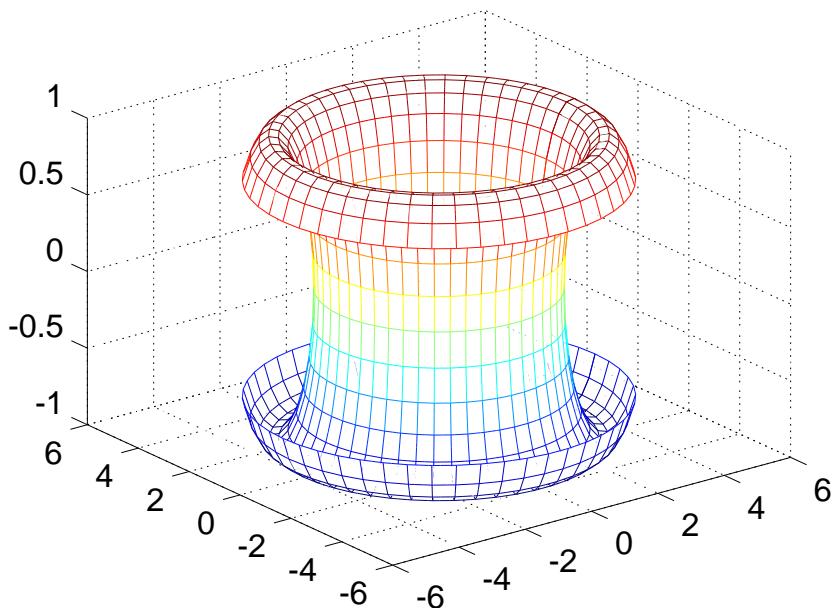


Figure 1.24: A general 3D surface

1.4.5 Generating vector fields

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

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

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. In this example the horizontal component of the vector field is given by $+y$ and the vertical component by $-x$. To obtain a good result the length of the vectors have to be scaled. The effect of the scaling factor might depend on the version of Octave/MATLAB used! Then the vector field is generated, find the result in Figure 1.25.

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.
Vx = y; Vy = -x; % define the vector field
scale = 2; % scaling
quiver(x,y,Vx,Vy,scale) % display the vector field
```

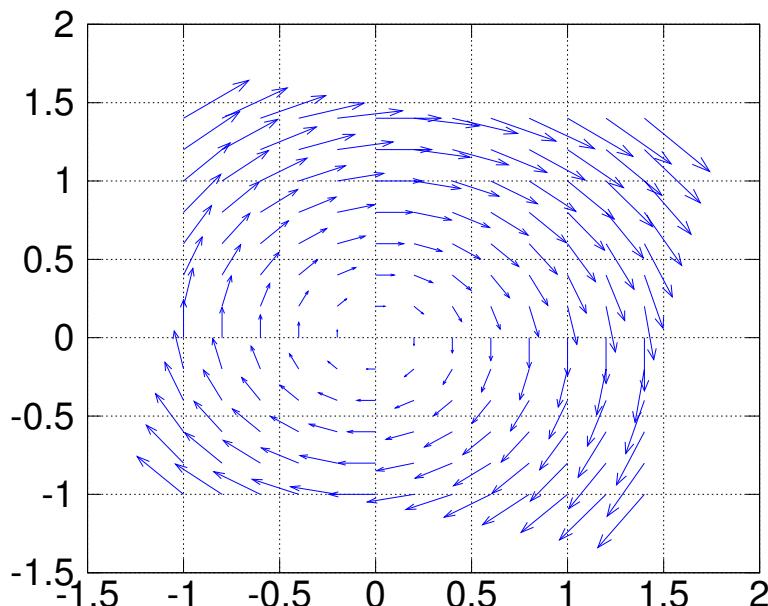


Figure 1.25: A vector field

23 Example : Octave provides the command `peaks` to generate a nice, reasonably complicated surface. If you want to find out about the function used in `peaks.m`, examine its source code. 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)
```



24 Example : As a second example we consider visualizing the magnetic field generated by two vertical conductors. According to Ampère's law the field strength is given by $B = \frac{\mu_0 I}{2\pi r}$ where I is the current and r the horizontal distance from the conductor. The direction of the vector is tangential to a circle with the center at the wire and follows the right hand rule. This can be written in the form

$$\vec{B}(x, y) = \frac{\mu_0 I}{2\pi} \frac{1}{x^2 + y^2} \begin{pmatrix} -y \\ x \end{pmatrix}$$

With this information we can now write code to generate the vector field.

- First set the desired parameters. We put the value of $\frac{\mu_0 I}{2\pi}$ into a constant `cI1`, resp. `cI2`.
- Generate the points where the vector field is to be computed by `linspace()` and `meshgrid()`.
- Compute the distance from the wires with a vectorized call. Then use `find()` to set the values of the distance to `NaN` for points too close to the wire.
- Compute the two components of the vector field and use `quiver()` to generate Figure 1.26.
- Since most of the vectors are very short it is difficult to detect the direction in Figure 1.26(a). Thus we modify the vectors such that they all have length 1 and then generate Figure 1.26(b). In addition one can remove the heads of the vectors by `set(h, 'maxheadsize', 0)`.

MagneticField.m

```
Lx = 2; Ly = +1.5 ; % domain to be examined
cI1 = 1; cI2 = +1 ; % the two currents
D = 1; % half the distance of the two conductors
Nx = 35; Ny = 25; % number of grid points
Dmin = 0.1; % minimal distance from conductor to be examined

x = linspace(-Lx,Lx,Nx); y = linspace(-Ly,+Ly,Ny); % generate the grid
[xx,yy] = meshgrid(x,y);

Dist1 = sqrt((xx-D).^2+ yy.^2); % distance of (x,y) from the first conductor
remove1 = find(Dist1<Dmin); % remove points too close to conductor
Dist1(remove1) = NaN;

Dist2 = sqrt((xx+D).^2+ yy.^2); % distance of (x,y) from the second conductor
remove2 = find(Dist2<Dmin); % remove points too close to conductor
Dist2(remove2) = NaN;

Vy = +cI1*(xx-D)./Dist1.^2 + cI2*(xx+D)./Dist2.^2; % compute the vector field
Vx = -cI1*(yy)./Dist1.^2 - cI2*(yy)./Dist2.^2;

figure(1); h = quiver(xx,yy,Vx,Vy,2);
xlabel('x'); ylabel('y'); axis([-Lx,Lx,-Ly,Ly]); axis equal

norms = sqrt(Vx.^2 + Vy.^2);
Vxn = Vx./norms; Vyn = Vy./norms;
figure(2); h = quiver(xx,yy,Vxn,Vyn);
set(h, 'maxheadsize', 0)
xlabel('x'); ylabel('y'); axis([-Lx,Lx,-Ly,Ly]); axis equal
```

In Figures 1.26(a) and 1.26(b) both currents are positive. In Figures 1.26(c) and 1.26(d) find the similar results with currents of opposite sign. Observe that between the two conductors the behavior of the magnetic field is drastically different²⁵. ◇

²⁵With MATLAB once can use the commands `stream2()` or `streamline()` to generate stream lines. In Octave this is not available yet.

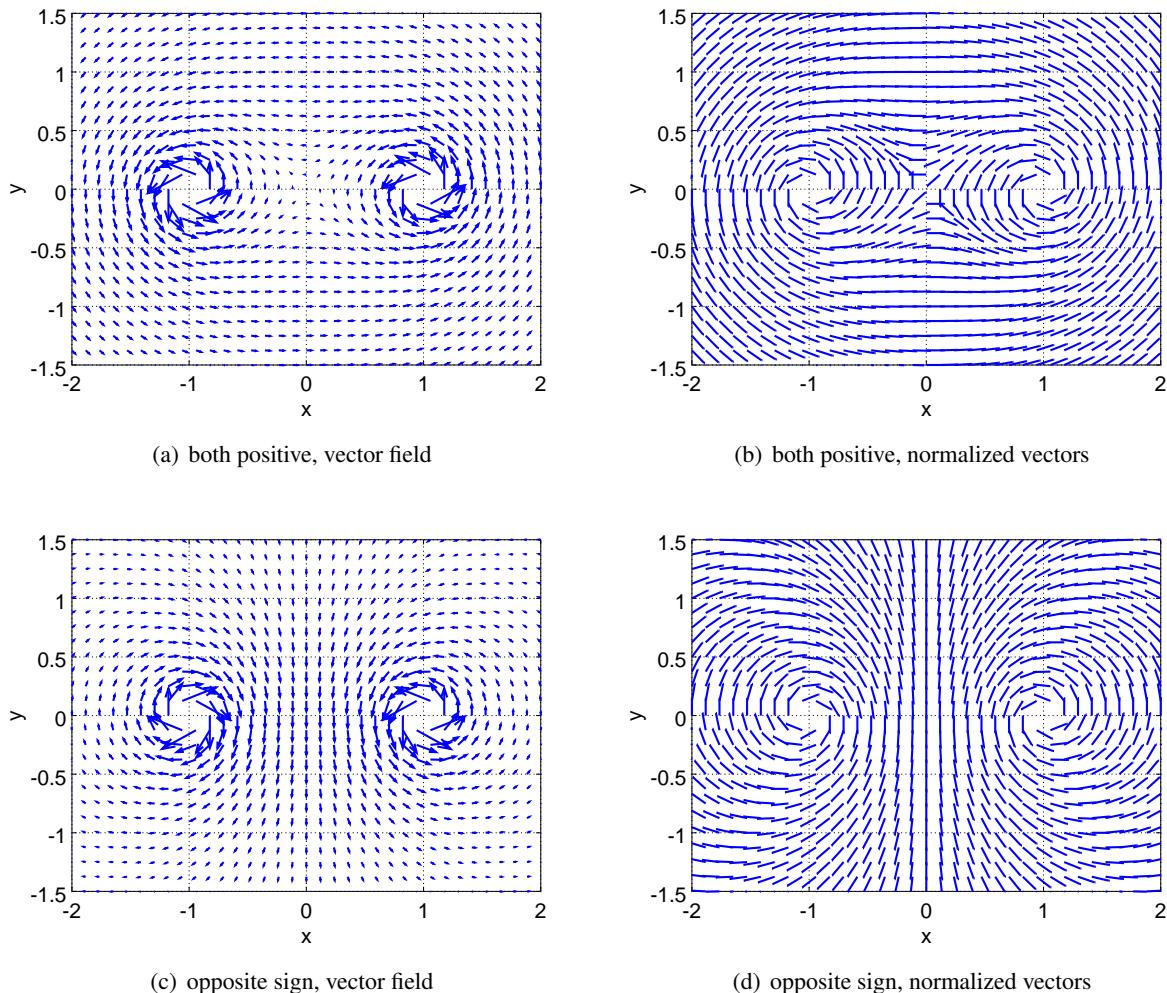


Figure 1.26: Magnetic fields with either both currents positive or opposite sign

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 numbers, 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()`, `gpmmap40()`). 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.
- With the command `imformats()` generate a list of all the image formats available on your platform.

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.

- <http://www.peterkovesi.com/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
imformats()	list all the image formats available
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

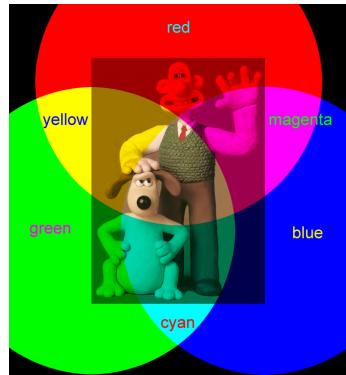
Table 1.10: Image commands

25 Example : RGB, grayscale

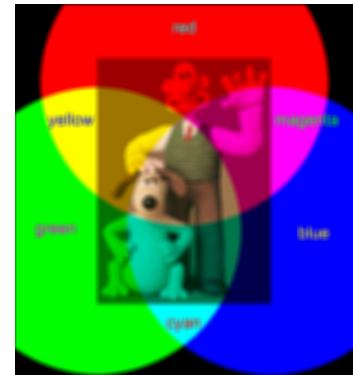
A picture `WallaceGromit.png` in the PNG format (portable network graphics) is loaded into Octave and `imfinfo()` displays all available information on the image. It is an image of size 724×666 and each pixel (picture element) consists of three colors (RGB), encoded by an integer between 0 and 255. Thus the "matrix" `im` in the code below is of size $724 \times 622 \times 3$ and the image is shown in Figure 1.27(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
```



(a) original image



(b) after an averaging filter

Figure 1.27: Wallace and Gromit, original and with an averaging filter applied

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 color. Find the results in Figure 1.28.

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)
```

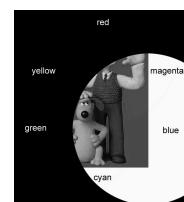
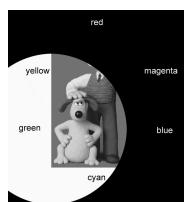
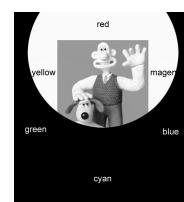
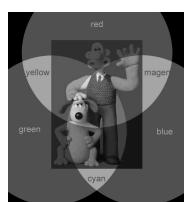


Figure 1.28: Wallace and Gromit, as grayscale and R, G and B images

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

Currently (2016) you can not use different colormaps in Figure 1.28 to see the red, green and blue parts. You need an separate figure for each color.

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 1.27(b) is a smeared out version of the original image 1.27(a).

Octave

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



26 Example : Edge Detection

This is a first example of edge detection, using the command provided by the Octave Forge package. More information is given in a later 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 1.29.

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
```

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 1.29. 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 = bwmorph(imbw,'remove') % run one of the possible edge detections
figure(4)
imshow(1-edgeimbw) % display the picture with edges only
```

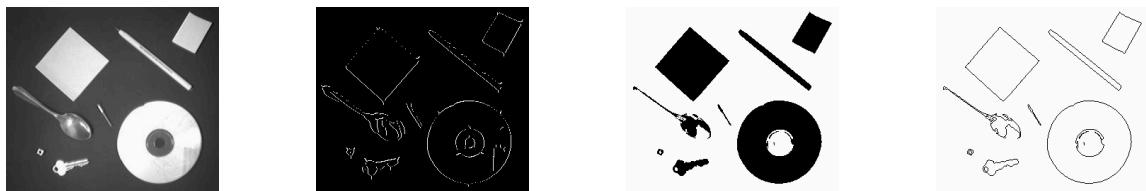


Figure 1.29: A grayscale and BW picture and edge detection



27 Example : Filtering with FFT

The idea presented in this example is also used for the JPEG compression. Find a very readable description in [Stew13, §9].

Using FFT we can write an image as sum of periodic signals with different frequencies. Then we can filter high or low frequencies. As an example we examine the image in Figure 1.31. 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 1.30. Observe that the code below uses block operations instead of multiple loops. This is for speed reasons.

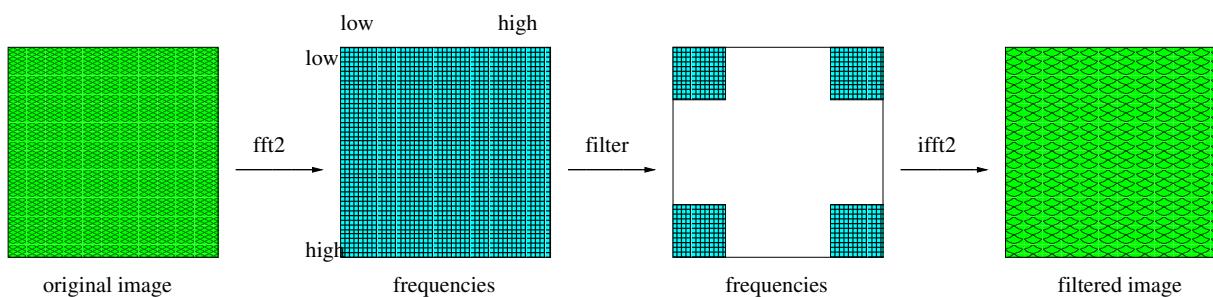


Figure 1.30: Apply a low pass filter to an image, based on FFT

```
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 1.31(b).

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



(a) original image



(b) with low pass filter

Figure 1.31: Original image of Lenna, and with a lowpass filter by FFT



1.5.2 Image processing and vectorization, edge detection

28 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 1.31(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
<pre>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(lin,col) = newIm(lin,col) + NoiseAmp*randn(1);% add noise to the pixel end%for end%for</pre>

```
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(NLines, Ncols)`) and add it to the original matrix.

Octave

```
t0 = cputime();
newIm2 = imG + NoiseAmp*randn(Nlines , Ncols);
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. ◇

29 Example : Edge detection

In many application the first step of image processing is edge detection, e.g. to identify objects. As example consider Figure 1.32 and the goal is to mark the edges of the different objects.



Figure 1.32: 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 shadow below the carabiner, through the Pritt stick and the pocket knife. The darker sections correspond to lower values in Figure 1.33(a).

The basic idea of an edge detection is to look for steep slopes in the graph 1.33(a). Based on the definition of the derivative we examine

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

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

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

or with Octave

Octave

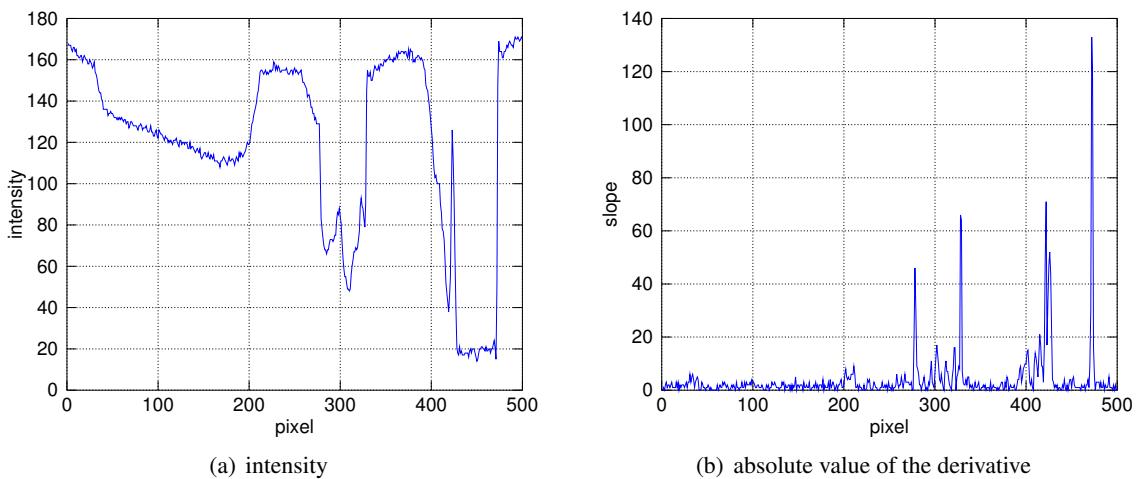


Figure 1.33: Intensity along a horizontal line through the objects

```

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);
edgeLine = test_line(3:n)-test_line(1:n-2);

figure(3)
plot(abs(edgeLine))
xlabel('pixel'); ylabel('slope')

```

This leads to Figure 1.33(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 1.32, which is visually confirmed by scanning along the thin horizontal line in that figure.

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

Octave

The above can also be considered as a convolution²⁶ of the vector of the intensity values along the line to be examined with the vector

-1	0	1
----	---	---

- Detecting horizontal edges, with the Sobel filter

²⁶Check your math lecture notes for the definition of convolution, either in the chapter on Laplace or Fourier transforms.

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

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

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

This indicates an edge with positive slope, i.e. an increasing intensity.

- In the second row and fourth column we obtain

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

This indicates an edge with negative slope, i.e. an decreasing intensity.

- In the second row and fifth column we obtain

$$b_{2,5} = \left\{ \begin{array}{l} +(-1) \cdot 1 + (0) \cdot 1 + (1) \cdot 1 \\ +(-2) \cdot 2 + (0) \cdot 2 + (2) \cdot 2 \\ +(-1) \cdot 3 + (0) \cdot 3 + (1) \cdot 3 \end{array} \right\} = 0$$

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.

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))
```

Find the result on in Figure 1.34(a). Observe that we only marked horizontal edges. The obvious vertical edges in the original image are not detected.

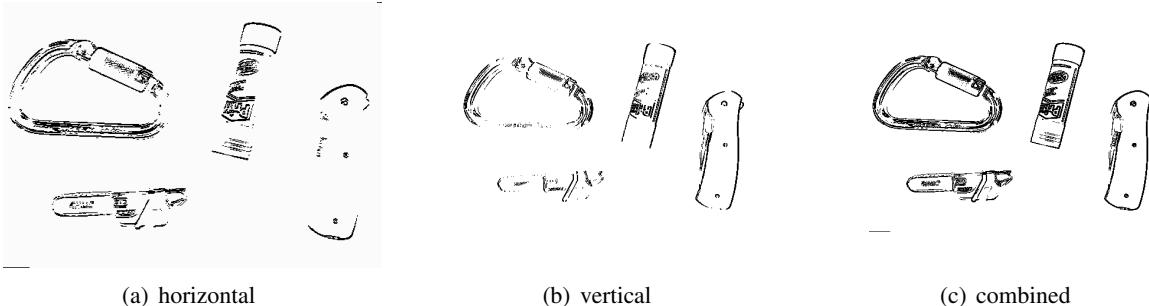


Figure 1.34: Sobel edge detection

- **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 1.34(b).

- **Combining horizontal and vertical edges**

Now we combine the two basic detection algorithms, leading to Figure 1.34(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 1.35. The function `edge()` allows to use a few other filters

for edge detection, e.g. Sobel, Prewitt²⁷, 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)
```

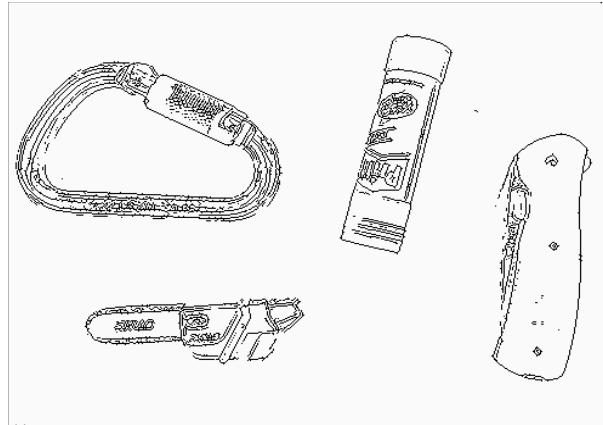


Figure 1.35: Result of a Sobel edge detection



30 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 1.36(a) as result.

Octave

```
imRaw = rgb2gray(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 ]);
```

²⁷For the Prewitt filter use the matrices

$$\begin{bmatrix} +1 & 0 & -1 \\ +1 & 0 & -1 \\ +1 & 0 & -1 \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} +1 & +1 & +1 \\ 0 & 0 & 0 \\ -1 & -1 & -1 \end{bmatrix} .$$

```
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 1.36(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))
```

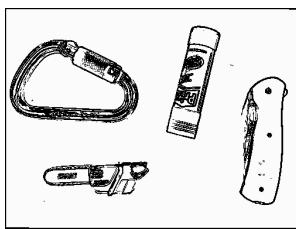
- The effect of noise can sometimes be controlled by an averaging filter. The value at one pixel is replaced by a weighted average of points close to this pixel. To average over a 5×5 section we can (many other options are possible) use the matrix

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

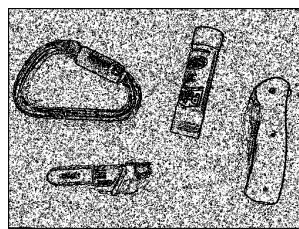
where m is chosen such that the sum of all values in \mathbf{A} equals 1. This assures that the average intensity of the image is not modified. Use a convolution of the noisy image matrix with this averaging matrix to generate a new picture. Now we can detect the edges in a noisy image, as seen in Figure 1.36(c).

Octave

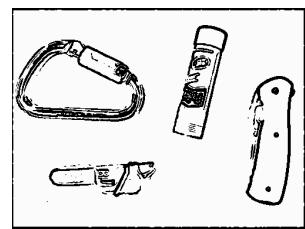
```
AvgMat = [1 3 6 3 1; 3 8 10 8 3; 6 10 12 10 6; 3 8 10 8 3; 1 3 6 3 1];
AvgMat = AvgMat/sum(AvgMat(:));
imNoiseAvg = conv2(imNoiseEdge,AvgMat,'same'); % apply the averaging filter
% now run the two edge detection filters and add
imNoiseAvgEdge = sqrt(conv2(imNoiseAvg,Sx).^2 + conv2(imNoiseAvg,Sy).^2);
figure(5);
imshow(1-(imNoiseAvgEdge>250)) % invert the intensity and display
```



(a) without noise



(b) with noise



(c) with noise and averaging filter

Figure 1.36: Edge detection, using a different filter



31 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. Examine and explain the result!

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);
```



1.5.3 SVD

With a **Singular Value Decomposition (SVD)** of a matrix one can apply good compression algorithms to images.

- Use my file `imageSVD.m`
- Use the good presentation [[HuntLipsRose14](#), p.172ff]

1.6 Ordinary Differential Equations

From your class on Engineering Mathematics or Ordinary Differential Equations you should have some basic 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_0 and initial values x_0 the initial value problem

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

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 options provided by `lsode()`.
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 author's 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 120. MATLAB does not provide the command `lsode()`, you are restricted to `ode45()` and its friends. The most recent version of *Octave* 4.2 has a full set of MATLAB compatible commands, e.g. `ode45()`, `ode23()`, `odeset()` and `odeget()`. Consequently you should use those commands if you want to assure compatibility of your code with *Octave* and MATLAB.

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.

32 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 ;
end%function

% 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 1.37.

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

```

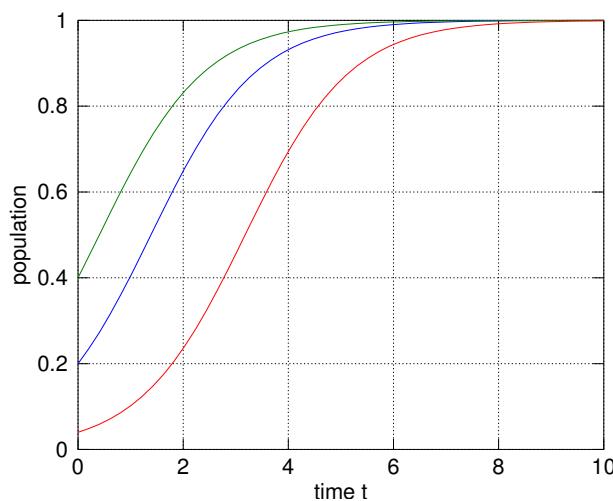


Figure 1.37: Some solutions of the logistic differential equation



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

33 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.

$$\begin{aligned}x(t) & \text{ population size of pray at time } t \\y(t) & \text{ population size of predator at time } t\end{aligned}$$

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 implemented 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 create a vector field plot for this system of two differential equations. Find the result as vector field in Figure 1.38.

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 1.38. 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 1.38, 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

```

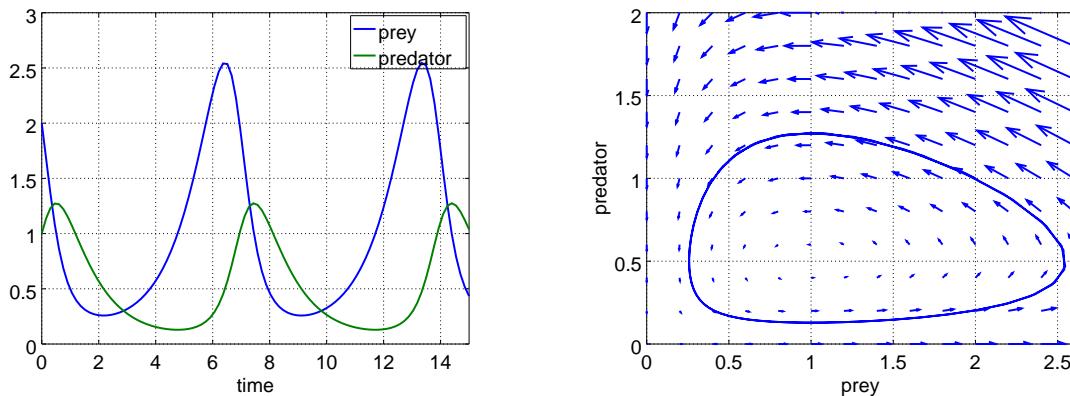


Figure 1.38: One solution and the vector field for the Volterra-Lotka problem



34 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

$$\frac{d}{dt} y_2(t) = \frac{d}{dt} \dot{x}(t) = \ddot{x}(t) = f(t) - \alpha \dot{x}(t) - k x(t) = f(t) - \alpha y_2(t) - k y_1(t)$$

This can be written as a system of first order equations

$$\frac{d}{dt} \begin{pmatrix} y_1(t) \\ y_2(t) \end{pmatrix} = \begin{pmatrix} \dot{y}_1(t) \\ \dot{y}_2(t) \end{pmatrix} = \begin{pmatrix} y_2(t) \\ f(t) - k y_1(t) - \alpha y_2(t) \end{pmatrix}$$

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 1.39 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 1.39 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 1.39 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:

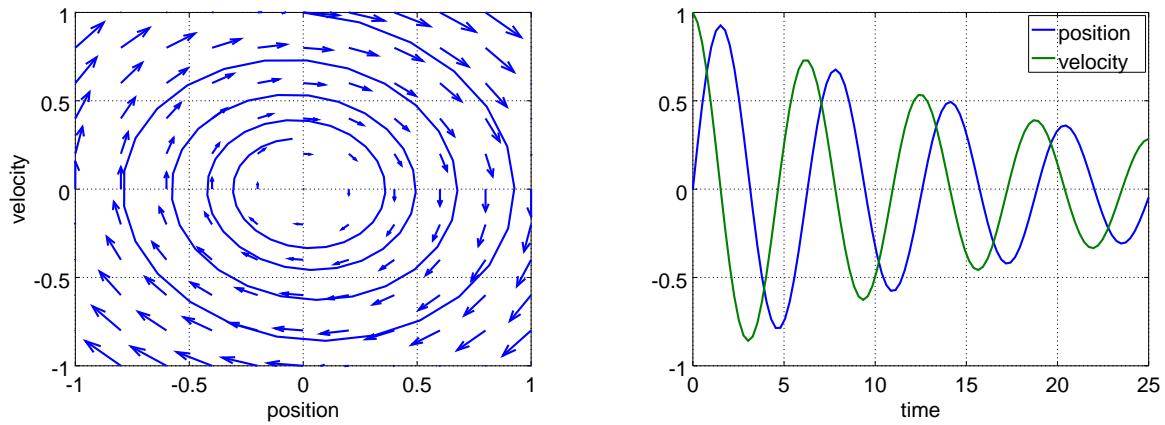


Figure 1.39: Vector field and a solution for a spring-mass problem

- integration method (Adams, stiff, bdf)
- absolute tolerance
- relative tolerance
- initial step size
- minimal and maximal step size

This is done by the command `lsode_options()`. If called without arguments the current values will be returned, e.g.

Octave

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 a smaller absolute 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

There are two reasons to use C/C++ code within Octave or MATLAB:

- Speed: if your code can not be vectorized you might gain a lot of speed by incorporating C/C++ code.
- Hardware: you might want to access special hardware through a library provided by the hardware producer.

There are two ways to incorporate C or C++ code into *Octave* or *MATLAB*:

- Use OCT files with *Octave* only. This approach has better performance, since all structures are based on *Octave*.
- Use MEX files with *Octave* or *MATLAB*. This approach allows to share code between *MATLAB* and *Octave*, but has lower performance. To quote the *Octave* manual: “In particular, to support the manner in which variables are passed to mex functions there are a significant number of additional copies of memory blocks when calling or returning from a mex-file function.”

C++ code in *Octave*, using OCT files

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],0), VolterraLotkaC([2.22,1.12],0)]
→
-2.7528 -2.7528
1.3664 1.3664
```

The main advantage of C++ code is speed. With the code below one can compare the performance 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(@(t,x)VolterraLotka(t,x),[2,1],t);
XY = lsode(@VolterraLotka,[2,1],t);
TimeScript = cputime() - t0

t0 = cputime();
XY = lsode(@VolterraLotkaC,[2,1],t);
TimeCPP = cputime() - t0

ratio = TimeScript/TimeCPP
```

On my current (2019) test system the C++ ran 8.5 times faster than the function file. The difference for more complicated examples can be considerably larger. Calling with `@(x,t) VolterraLotka(x,t)` slows it down considerably,

Other examples are provided with the *Octave* distribution, e.g. `oregonator`.

C++ code in Octave or MATLAB, using MEX files

As an example, given by the *Octave* documentation, examine a function to compute the square of each entry in a matrix.

mypow2.c

```
#include "mex.h"
void
mexFunction ( int nlhs , mxArray *plhs [] ,
              int nrhs , const mxArray *prhs [])
{
    mwSize n;
    mwIndex i;
    double *vri , *vro;
    if (nrhs != 1 || ! mxIsDouble (prhs [0]))
        mexErrMsgTxt ("ARG1 must be a double matrix");

    n = mxGetNumberOfElements (prhs [0]);
    plhs [0] = mxCreateNumericArray (mxGetNumberOfDimensions (prhs [0]),
                                    mxGetDimensions (prhs [0]),
                                    mxGetClassID (prhs [0]),
                                    mxIsComplex (prhs [0]));

    vri = mxGetPr (prhs [0]);
    vro = mxGetPr (plhs [0]);

    for (i = 0; i < n; i++)
        vro [i] = vri [i] * vri [i];
}
```

This code is compiled within *Octave* or *MATLAB* by calling `mex mypow2.c`, leading to a file `mypow2.mex`. Then you can call this function within *Octave/MATLAB* by

```
a = rand(3)
mypow2(a)
```

The above Volterra–Lotka computation can be performed using a mex file.

VolterraLotkaMex.c

```
#include "mex.h"
void mexFunction ( int nlhs, mxArray *plhs [],
                   int nrhs, const mxArray *prhs [])
{
    double *x, *y;
    /* Create matrix for the return argument. */
    plhs[0] = mxCreateDoubleMatrix((mwSize)2, (mwSize)1, mxREAL);

    /* Assign pointers to each input and output. */
    x = mxGetPr(prhs[0]);
    y = mxGetPr(plhs[0]);
    /* compute the expression */
    double c1 = 1.0, c2 = 2.0, c3 = 1.0, c4 = 1.0;
    y[0] = (c1-c2*x[1])*x[0];
    y[1] = (c3*x[0]-c4)*x[1];
}
```

This code is compiled by `mex VolterraLotkaMex.c` and the resulting code, using the function call `XY = lsode(@VolterraLotkaMex, [2,1], t);`, is 6.5 times faster than the script version.

1.6.4 Determine the period of a Volterra–Lotka solution

Using Figure 1.38 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 initial time 0 and generate values of the solution at 1000 times between 6.5 and 7.0. We require an absolute and 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((x,t)VolterraLotkaC(t,x),[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 given 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, then compute the value at T
XYt = lsode (@VolterraLotkaC ,XY(pos,:),[T-dt,T]);
XYt(2,:)-[x0,y0] % difference to 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 commands `ode23()` and `ode45()`

The standard command in *Octave* to solve ordinary differential equations is `lsode()`, as used in the previous section. Starting with version 4.0 *Octave* includes the MATLAB compatible commands `ode45()` and `ode23()`. For earlier versions of *Octave* you can use the package `odepkg` on *Octave Forge* at the site <http://octave.sourceforge.net/>.

- If working with a version of *Octave* earlier than 4.0, you have to install the package `odepkg`. Use the instructions in section 1.1.2 starting on page 12 to assure that the package `odepkg` is installed and loaded.
- With this package many commands from MATLAB are now available in *Octave*, as well as some additional commands. Table 1.11 shows some of the commands in the package.
- Observe a minor, but annoying difference to the command `lsode()`: the arguments in the function describing the differential equation have to be swapped.

$$\begin{aligned} \text{lsode}() &\longleftrightarrow dx = f(x, t) \\ \text{ode??}() &\longleftrightarrow dx = f(t, x) \end{aligned}$$

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 sub-directory with the package. Observe that the implementations of `ode23()` and `ode45()` for *Octave* 4.2.0 are slightly different and the syntax identical to the command in MATLAB.

As a typical example we consider `ode45()`, but the options for other ODE commands are very similar. The command `ode45()` takes three arguments, e.g. `[t, x] = ode45(@ (t, x) t-x, [1, 5], [7])`.

- The first argument is the function handle, e.g. `@ (t, x) t-x` describes the differential equation to be solved, in this example $\frac{dx}{dt} = t - x(t)$.

Solver	Description
<code>lsode ()</code>	efficient, adaptive solver based on Hindmarsh's work ([Hind93])
<code>ode23 ()</code>	adaptive, explicit solver, based on Heun's method
<code>ode45 ()</code>	adaptive, explicit solver, based on Runge-Kutta method of order 4, resp. 5
<code>ode54 ()</code>	Runge Kutta solver
<code>ode78 ()</code>	adaptive, explicit solver, based on Runge-Kutta method of order 7, resp. 8
<code>ode23s ()</code>	solver for stiff problems, based on Hairer and Wanner's code
<code>ode5s ()</code>	solver for stiff problems, based on Hairer and Wanner's code

Table 1.11: Octave commands in `odepkg` to solve ordinary differential equations

Command	Description
<code>odeexamples ()</code>	launch demos for ordinary differential equations
<code>ode23d ()</code>	solver for delay differential equations
<code>ode45d ()</code>	solver for delay differential equations
<code>ode78d ()</code>	solver for delay differential equations

Table 1.12: Additional commands in the ODE package

- The second argument $[1, 5]$ describes the time span, i.e. the times t for which the differential equation will be solved. If more than two values are specified, then the solution will be returned at those values.
- The third argument gives the initial value, while the initial time is specified at the first data point of the time span. In the above example we require $x(1) = 7$.
- In the optional fourth argument you can specify options for the solver, to be examined in the next section.
- The solution can then be plotted by `plot (t, x)`.

The implementation of `ode45 ()` will determine the number and values of the times t_i at which values of the solution are returned based on the requested accuracy. In the above example only 14 time values are returned. If you want the values of the solution at specified times you can provide a vector of time values. With $[t, x] = \text{ode45}(@(\text{t}, \text{x}) \text{t}-\text{x}, \text{linspace}(1, 5, 41), [7])$ the solution is returned at 41 equally spaced time values, only $\Delta t = 0.1$ apart. Internally `ode45 ()` will first determine the solution at the same time values, as if the time span were $[1, 5]$, then an interpolation is used to find the values at the requested time spots. Find details on algorithms of this type in [HairNorsWann08].

35 Example : As a first example we solve the logistic equation from the example on page 111 again, now using the command `ode45 ()`. The differential equation to be solved is given by

$$\frac{d}{dt} x(t) = x(t) - x^2(t) \quad \text{with} \quad x(0) = x_0$$

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

```

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

% generate vector with the times at which solution is desired
T = t0 + linspace(0,Tend,n);
% solve the differential equation with three different initial values
[T1,X1] = ode45(logF,T,x0);
[T2,X2] = ode45(logF,T,2*x0);
[T3,X3] = ode45(logF,T,0.2*x0);

plot(T1,X1,T2,X2,T3,X3)
xlabel('time t'); ylabel('population'); grid on

```



Options for `ode23()` and `ode45()`

For these ODE solvers many options can and should be set. The command `odeset()` will generate a list of the available options and their default values. With `help odeset` you obtain more information on these options. The available options differ slightly for Octave and MATLAB.

The most frequently used options are `AbsTol` (default value 10^{-6}) and `RelTol` (default value 10^{-3}), used to specify the absolute and relative tolerances for the solution.

With the command `odeget()` one can read out specific options for the ode solvers.

Octave `odeset()`

```

odeset()
→
List of the most common ODE solver options.
Default values are in square brackets.
  AbsTol: scalar or vector, >0, [1e-6]
  BDF: binary, {[“off”], “on”}
  Events: function_handle, []
  InitialSlope: vector, []
  InitialStep: scalar, >0, []
  Jacobian: matrix or function_handle, []
  JConstant: binary, {[“off”], “on”}
  JPatten: sparse matrix, []
  Mass: matrix or function_handle, []
  MassSingular: switch, {[“maybe”], “no”, “yes”}
  MaxOrder: switch, {[5], 1, 2, 3, 4, }
  MaxStep: scalar, >0, []
  MStateDependence: switch, {[“weak”], “none”, “strong”}
  MvPattern: sparse matrix, []
  NonNegative: vector of integers, []
  NormControl: binary, {[“off”], “on”}
  OutputFcn: function_handle, []
  OutputSel: scalar or vector, []
  Refine: scalar, integer, >0, []
  RelTol: scalar, >0, [1e-3]
  Stats: binary, {[“off”], “on”}
  Vectorized: binary, {[“off”], “on”}

```

Matlab `odeset()`

```

AbsTol: [ positive scalar or vector {1e-6} ]
RelTol: [ positive scalar {1e-3} ]
NormControl: [ on | {off} ]

```

```

NonNegative: [ vector of integers ]
OutputFcn: [ function_handle ]
OutputSel: [ vector of integers ]
Refine: [ positive integer ]
Stats: [ on | {off} ]
InitialStep: [ positive scalar ]
MaxStep: [ positive scalar ]
BDF: [ on | {off} ]
MaxOrder: [ 1 | 2 | 3 | 4 | {5} ]
Jacobian: [ matrix | function_handle ]
JPATTERN: [ sparse matrix ]
Vectorized: [ on | {off} ]
Mass: [ matrix | function_handle ]
MStateDependence: [ none | {weak} | strong ]
MvPattern: [ sparse matrix ]
MassSingular: [ yes | no | {maybe} ]
InitialSlope: [ vector ]
Events: [ function_handle ]

```

Examples for `ode23()`, `ode45()` and `ode78()`

As an example we consider again the pendulum equation

$$\frac{d}{dt} \begin{pmatrix} y(t) \\ v(t) \end{pmatrix} = \begin{pmatrix} v(t) \\ -y(t) - 0.1v(t) \end{pmatrix} \quad \text{with} \quad \begin{pmatrix} y(0) \\ v(0) \end{pmatrix} = \begin{pmatrix} 0 \\ 0.9 \end{pmatrix}$$

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)];
end%function

```

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 (written by this author) presented in the regular class²⁸ on differential equations we use the example of a diode circuit examined in the corresponding lecture notes. The behavior of the diode is given by a function

$$i = D(u) = \begin{cases} 0 & \text{for } u \geq -u_s \\ R_D(u + u_s) & \text{for } u < -u_s \end{cases}$$

Based on Kirchhoff's law we find the differential equations

$$\begin{aligned}\dot{u}_h(t) &= \frac{1}{C_1} (-D(u_h(t) - u_{in}(t)) + D(u_{out}(t) - u_h(t))) \\ \dot{u}_{out}(t) &= \dot{u}_{in}(t) - \frac{1}{C_2} D(u_{out}(t) - u_h(t))\end{aligned}$$

We define the initial conditions and the two functions in a script file. We examine an input voltage of $u_{in}(t) = 10 \sin(t)$.

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 adaptive

We can use the adaptive Runge-Kutta algorithm with relative and absolute tolerance of 10^{-5} and generate the plot by

Octave

²⁸web.sha1.bfh.science/Math1.pdf

```
t0 = cputime();
[t,u] = rk45('circuit',0,Tend,u0,1e-5,1e-5); % Runge-Kutta adaptive
timer = cputime() - t0
figure(1);
plot(t,u(:,2),'.')
grid on; xlabel('time'); ylabel('tension');
```

The result in Figure 1.40 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 1.40.

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','location','northwest')
```

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 occasions where a fixed size algorithm outperforms an adaptive algorithm.

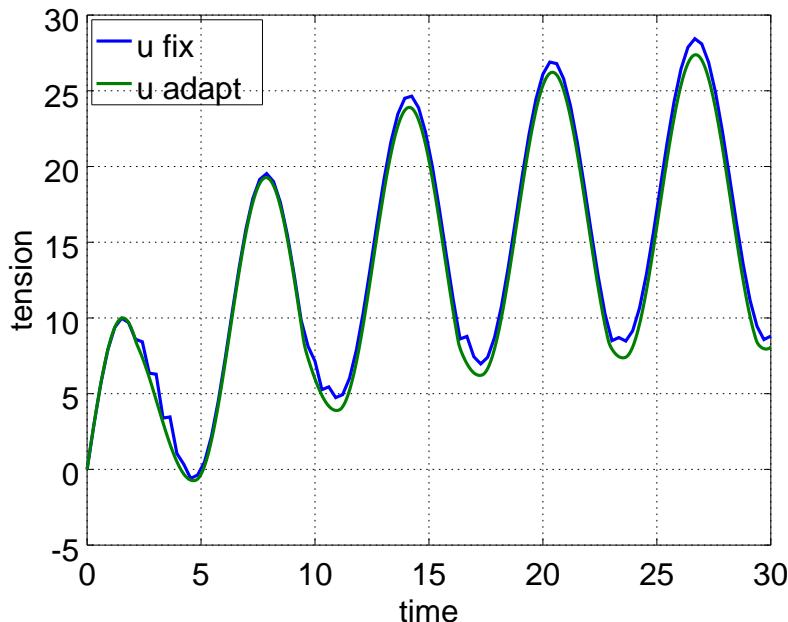


Figure 1.40: Solution for the diode circuit with Runge-Kutta, fixed step and adaptive

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 seconds we find a good solution. This illustrates the quality of the algorithm in `lsode.m`.

DoubleTensionLSODE.m

```

1; % assure script file
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 from 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
<code>logistic.m</code>	script file to solve the logistic equation
<code>VolterraLotka.m</code>	function file for the Volterra-Lotka model
<code>VolterraLotkaField.m</code>	script file to solve the Volterra-Lotka model
<code>VolterraLotkaC.cc</code>	C++ code file for the Volterra-Lotka model
<code>VolterraLotkaPeriod.m</code>	script file to determine the period of solutions
<code>SpringODE.m</code>	script file to solve the damped spring model
<code>ode_Euler.m</code>	algorithm of Euler, fixed step size
<code>ode_Heun.m</code>	algorithm of Heun, fixed step size
<code>ode_Runge.m</code>	algorithm of Runge-Kutta, fixed step size
<code>rk45.m</code>	adaptive Runge Kutta algorithm
<code>DoubleTension.m</code>	sample code for the diode circuit
<code>DoubleTensionLSODE.m</code>	using <code>lsode()</code>

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 are based on works by students . For each section find the *Octave* skills to be used to solve the problems.

- **2.1: Numerical Integration and Magnetic Fields**

Based on the law of Biot–Savart the magnetic field of a wire carrying a current is computed. The Helmholtz configuration of two coils is examined carefully.

- Numerical integration
- Generate a vector field

- **2.2: Linear and Nonlinear Regression**

The basic notations for linear and nonlinear regression are explained and possibles sources of errors discussed. This is followed by a few real world applications.

- Linear regression, using `LinearRegression()`
- Nonlinear regression, using `leasqr()` and `fsolve()`

- **2.3: Regression with Constraints**

Using a linear regression with a constraint fitting of a straight line to data points is performed, using the true geometric distance. Then a plane is fitted to data points and one possible algorithm to fit an ellipse to data points is presented.

- **2.4: Computing Angles on an Embedded Device**

Using integer arithmetic only arbitrary functions are approximated. This is then used to computed angles on an embedded device.

- Integer arithmetic with data type `int16` and similar
- Simulation of operations on a micro controller
- Visualization and analysis of approximation errors

- **2.5: Analysis of Stock Performance, Value of a Stock Option**

A probabilistic analysis of stock performance as presented, leading to the Black–Scholes–Merton approach to put a price tag on a stock option.

- Formatted reading from a file

- Probabilistic analysis of data
- Monte Carlo simulation

- **2.6: Motion Analysis of a Circular Disk**

The motion and deformation of a watch caliber falling on the ground is analyzed and visualized.

- Reading data from a file
- Generating an animation on screen
- Generating a movie, to be played by any movie player

- **2.7: Analysis of a Vibrating Cord**

The performance of a vibrating string based force sensor is examined. The motion of a damped vibrating cord is analyzed and the quality factor determined.

- Fitting of an exponentially decaying vibration to measured data
- Calling external programs within *Octave*
- Construction of *Octave* commands by combining strings and then evaluating the command.

- **2.8: An Example for Fourier Series**

The motion of a beam struck by a hammer is measured by acceleration sensors on beam and hammer. The resulting frequency spectrum is computed, as function of time.

- Reading and displaying data
- Use FFT to determine the frequency spectrum on different time slices

- **2.9: Reading Information from the Screen and Spline Interpolation**

At first mouse clicks on the display are converted to data, then regularly spaced data is generated by interpolation.

- Reading data from screen, either in an MATLAB/*Octave* window (`ginput`) or even anywhere on the screen (`xinput`).
- Interpolation of data.

- **2.10: Intersection of Circles and Spheres, GPS**

An algorithm to determine intersection points of circles and spheres is presented. Then the over-determined system of the intersection of many circles and spheres is examined and reduced to a least square problem. This is then the basis for a short presentation of some Mathematics for the GPS (Global Positioning System).

- **2.11: Scanning a 3-D Object with a Laser**

A solid is scanned by a laser from two different angles. Based on this data the shape of the solid is reconstructed.

- Evaluation irregularly spaced data on a uniform grid.
- Merging two function into one picture.

2.1 Numerical Integration and Magnetic Fields

2.1.1 Basic integration methods

Trapezoidal integration using `trapz()`

The simplest integration in Octave is based on the trapezoidal rule and implemented in the command `trapz()`. Examine the online help. The code below computes

$$\int_0^\pi \sin(x) dx$$

with 100 subintervals 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 $n = 10, 20, 40, \dots, 10 \cdot 2^9$ 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)));
end%for

loglog(n,err);
```

Using the linear regression commands

Octave

```
F = [ones(size(n))', log(n')];
LinearRegression(F, log(err'))
```

we find

$$\ln(\text{err}(n)) \approx 0.5 - 2 \ln(n) \quad \text{and} \quad \text{err}(n) \approx \frac{1.6}{n^2}$$

and this confirms the error estimate for the trapezoidal integration method.

With the command `cumtrapz()` (cumulative trapezoidal) 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 from 0 to π . The result is shown in Figure 2.1.

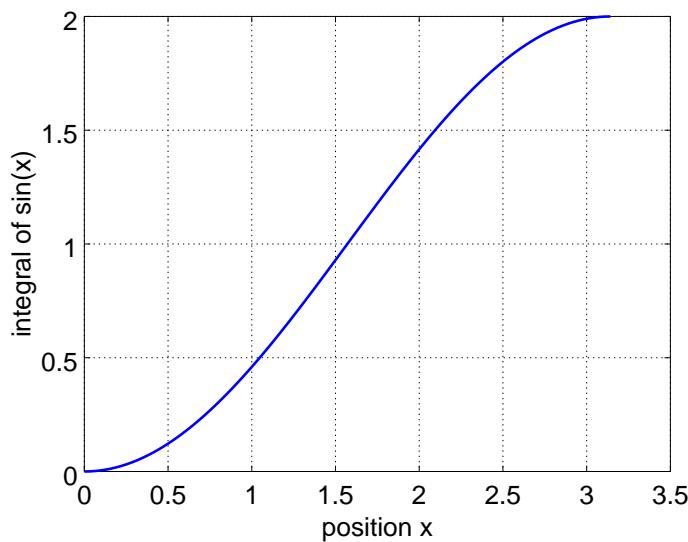


Figure 2.1: Cumulative trapezoidal integration of $\sin(x)$

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 handle, e.g. @sin or a vector of values

if isa(f,'function_handle')
    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%for
else
    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(:)';
    end%if
end%if

w = 2*[ones(1,n/2); 2*ones(1,n/2)]; w = w(:); % construct the simpson weights
w = [w;1]; w(1)=1;
res = (b-a)/(3*n)*f_x*w;

```

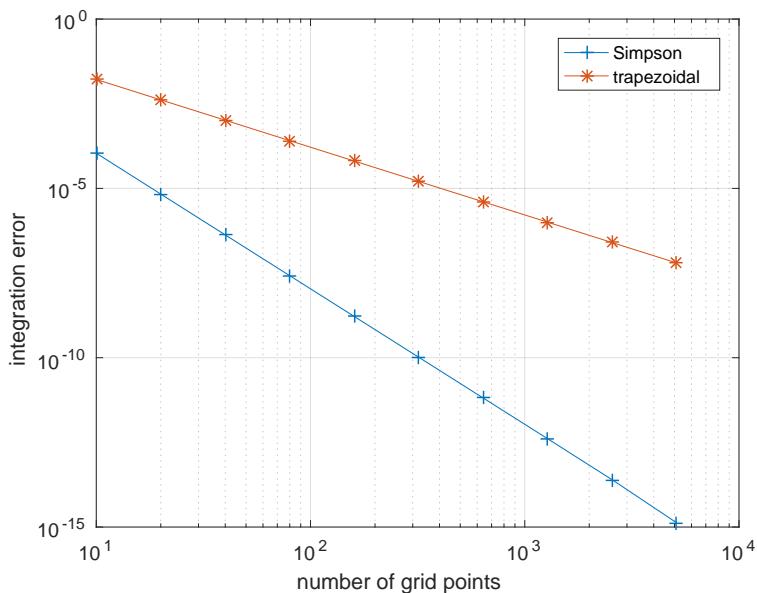


Figure 2.2: Error of trapezoidal and Simpsons integration method

This Simpson integration can now be tested similarly to the above tests. The convergence rate of the trapezoidal and Simpson integration is visualized 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)));
end%for
loglog(n,err,'-+',n,errTrap,'-*');
xlabel('number of grid points'); ylabel('integration error'); grid on
legend('Simpson','trapezoidal')

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()`, using anonymous functions

The built-in MATLAB/Octave command `quad()`¹ (short for quadrature) is based on the **Quadrpack** software to compute integrals numerically. This is a well tested, reliable package. Its usage in Octave is rather simple, as shown by a simple example.

Octave

```
f = @(x)4/(1+x^2);
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 of 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

$$I(p) = \int_0^1 \sin(px2\pi) dx$$

The result will depend on the parameter p . the function $f(x, p) = \sin(px2\pi)$ 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
f = @(x,p) sin(p*x*2*pi);
quad(@(x)f(x,p),0,1) % if 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.

<code>trapz()</code> , <code>cumtrapz()</code>	uses trapezoidal rule to be used for discretized values only uneven spacing is possible
<code>simpson()</code>	uses Simpson's method for discretized values of an anonymous function or by an even number of subintervals of equal length
<code>quad()</code>	uses Quadrpack , adaptive algorithm function name has to be given

Table 2.1: Integration commands in Octave

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.

¹There are other functions available for numerical integration, with different features. E.g the function `quadgk()` can work with discontinuous first derivatives by "WayPoints".

	<code>trapz()</code>	<code>simpson()</code>	<code>quad()</code>
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

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

$$d\vec{H} = \frac{I}{4\pi r^3} \vec{ds} \times \vec{r}$$

where \vec{r} is the vector connecting the point on the conductor to the points at which the field is to be computed.

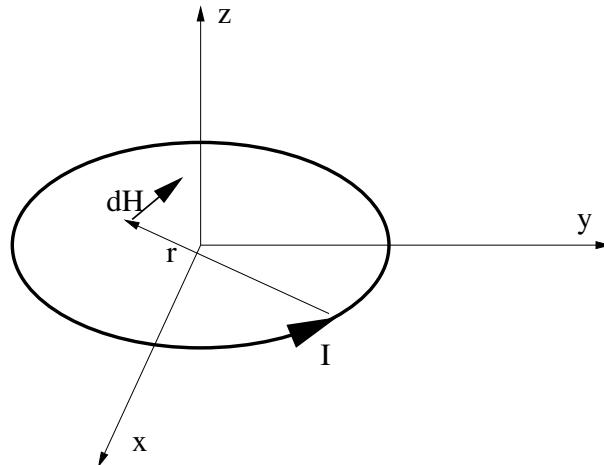


Figure 2.3: Circular conductor for which the magnetic field has to be computed

A parametrization of the circle is given by

$$\begin{pmatrix} R \cos \phi \\ R \sin \phi \\ 0 \end{pmatrix} \quad \text{where } 0 \leq \phi \leq 2\pi$$

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

$$\begin{aligned} r^2 &= (R \cos \phi - x)^2 + R^2 \sin^2 \phi + z^2 \\ &= R^2 - 2xR \cos \phi + x^2 + z^2 \end{aligned}$$

To apply Biot–Savart we need the expression

$$\vec{ds} \times \vec{r} = \begin{pmatrix} -R \sin \phi \\ R \cos \phi \\ 0 \end{pmatrix} \times \begin{pmatrix} x - R \cos \phi \\ -R \sin \phi \\ z \end{pmatrix} d\phi = \begin{pmatrix} zR \cos \phi \\ zR \sin \phi \\ R^2 - xR \cos \phi \end{pmatrix} d\phi$$

and thus obtain an integral for the 3 components of the field \vec{H} at the point $(x, 0, z)$

$$\vec{H}(x, 0, z) = \frac{I}{4\pi} \int_0^{2\pi} \frac{1}{(R^2 - 2xR \cos \phi + x^2 + z^2)^{3/2}} \begin{pmatrix} zR \cos \phi \\ zR \sin \phi \\ R^2 - xR \cos \phi \end{pmatrix} d\phi \quad (2.1)$$

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

$$\vec{H} = \frac{I}{4\pi} \int_0^{2\pi} \frac{1}{(R^2 + z^2)^{3/2}} \begin{pmatrix} zR \cos \phi \\ zR \sin \phi \\ R^2 \end{pmatrix} d\phi$$

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 it 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

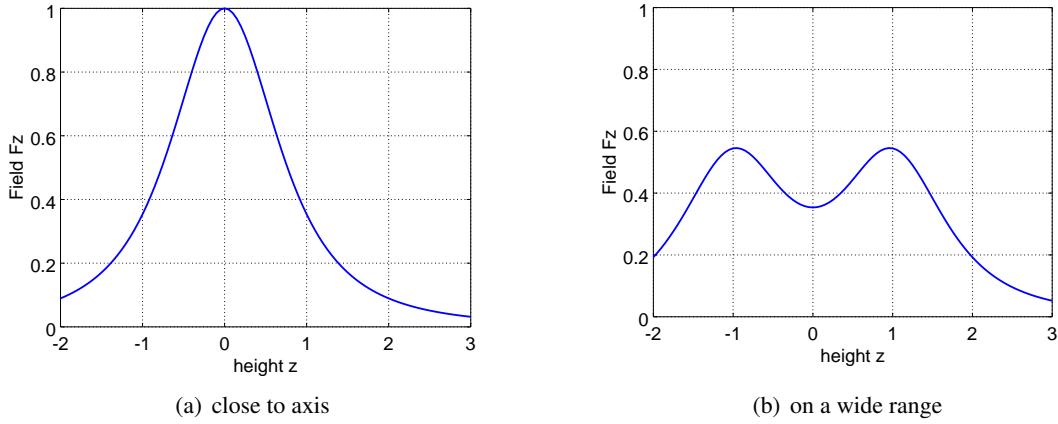


Figure 2.4: Magnetic field along the central axis

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.

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.

$$G(z) \approx G(0) + \frac{dG(0)}{dz} z + \frac{1}{2} \frac{d^2 G(0)}{dz^2} z^2 + \frac{1}{6} \frac{d^3 G(0)}{dz^3} z^3 + \dots$$

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

$$\frac{dG(0)}{dz} = \frac{d}{dz} H(h) + \frac{d}{dz} H(-h) = 0$$

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 $H_z(z)$.

$$\frac{d^2}{dz^2} H_z(z) = \frac{IR^2}{2} \frac{d^2}{dz^2} \left(\frac{1}{(R^2 + z^2)^{3/2}} \right) = 0$$

We find

$$\begin{aligned} \frac{d}{dz} \frac{1}{(R^2 + z^2)^{3/2}} &= \frac{-3 \cdot 2 z}{2(R^2 + z^2)^{5/2}} = \frac{-3 z}{(R^2 + z^2)^{5/2}} \\ \frac{d^2}{dz^2} \frac{1}{(R^2 + z^2)^{3/2}} &= \frac{-3(R^2 + z^2)^{5/2} + 3z\frac{5}{2}(R^2 + z^2)^{3/2}2z}{(R^2 + z^2)^5} \\ &= \frac{-3(R^2 + z^2) + 3z5z}{(R^2 + z^2)^{7/2}} = 3 \frac{4z^2 - R^2}{(R^2 + z^2)^{7/2}} \end{aligned}$$

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. Figures 2.4 and 2.5 are generated by Octave/MATLAB with the help of an anonymous function `HzAxis()` to compute the field along the axis with the commands

Octave

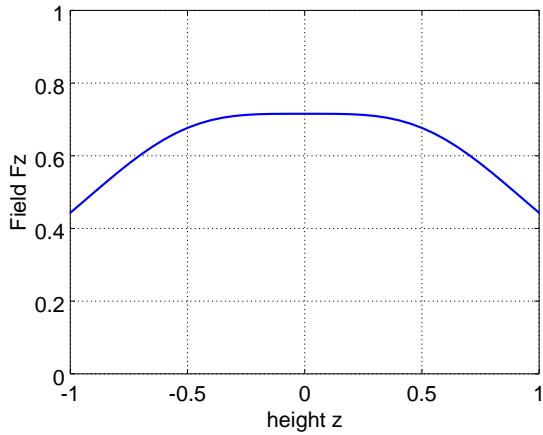


Figure 2.5: Magnetic field along the central axis, Helmholtz configuration

```
HzAxis = @(z)R^2/2*(R^2+z.^2).^(−3/2);
z = linspace(−2,3,101); R = 1;
```

```
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.

$$\vec{H}(x, 0, z) = \frac{I}{4\pi} \int_0^{2\pi} \frac{1}{(R^2 - 2xR \cos \phi + x^2 + z^2)^{3/2}} \begin{pmatrix} zR \cos \phi \\ zR \sin \phi \\ R^2 - xR \cos \phi \end{pmatrix} d\phi$$

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 anonymous function `dHz()`.

Currently we are only interested in z along the x -axis, i.e. $y = z = 0$ and we want to compute

$$H_z(x, 0, 0) = \frac{I}{4\pi} \int_0^{2\pi} \frac{R^2 - xR \cos \phi}{(R^2 - 2xR \cos \phi + x^2)^{3/2}} d\phi$$

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 $-0.5 \leq x \leq 0.8$ and then for $1.2 \leq x \leq 3$. The results are shown in Figure 2.6. Observe that the magnetic 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.

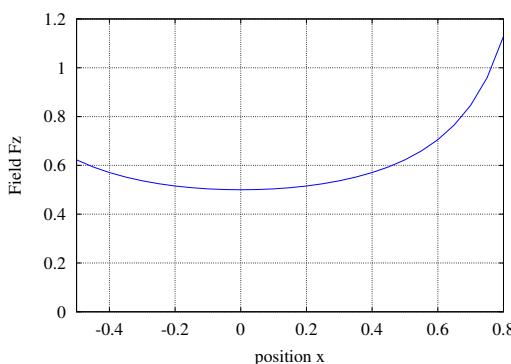
Octave

```
dHz = @(al,R,x,z)R*(R-x.*cos(al))./sqrt(R^2-2*x.*R.*cos(al)+x.^2+z.^2).^3;
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
end%for

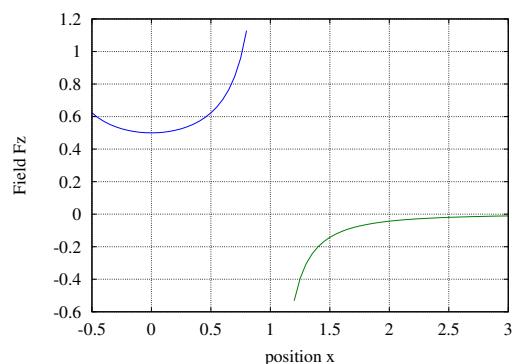
figure(1)
plot(x,Fz)
grid on
axis([-0.5 0.8 0 1.2]);
xlabel('position x'); ylabel('Field Fz');

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
end%for

figure(2)
plot(x,Fz,x2,Fz2)
grid on
axis([-0.5 3 -0.6 1.2]);
xlabel('position x'); ylabel('Field Fz');
```



(a) close to axis



(b) on a wide range

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

$$H_x(x, 0, z) = \frac{I}{4\pi} \int_0^{2\pi} \frac{z R \cos \phi}{(R^2 - 2xR \cos \phi + x^2 + z^2)^{3/2}} d\phi$$

We write an anonymous function `dHx()` for the expression to be integrated. Then 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

```

dHz = @(al,R,x,z)R*(R-x.*cos(al))./sqrt(R^2-2*x.*R.*cos(al)+x.^2+z.^2).^3;
dHx = @(phi,R,x,z)R*z.*cos(phi) ./ sqrt(R^2-2*x.*R.*cos(phi)+x.^2+z.^2).^3;

z = -1:0.2:2; x = -0.4:0.1:0.7;
[xx,zz] = meshgrid(x,z); x = xx(:); z = zz(:); % convert matrix to vector
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
end%for

```

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. Depending on which version of Octave/MATLAB you are using, you might have to adapt the scaling factors in the `quiver()` command.

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,1.5)
grid on; axis([-0.4 0.8 -1 2])

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,0.6)
grid on; axis([-0.4 0.8 -1 2])

```

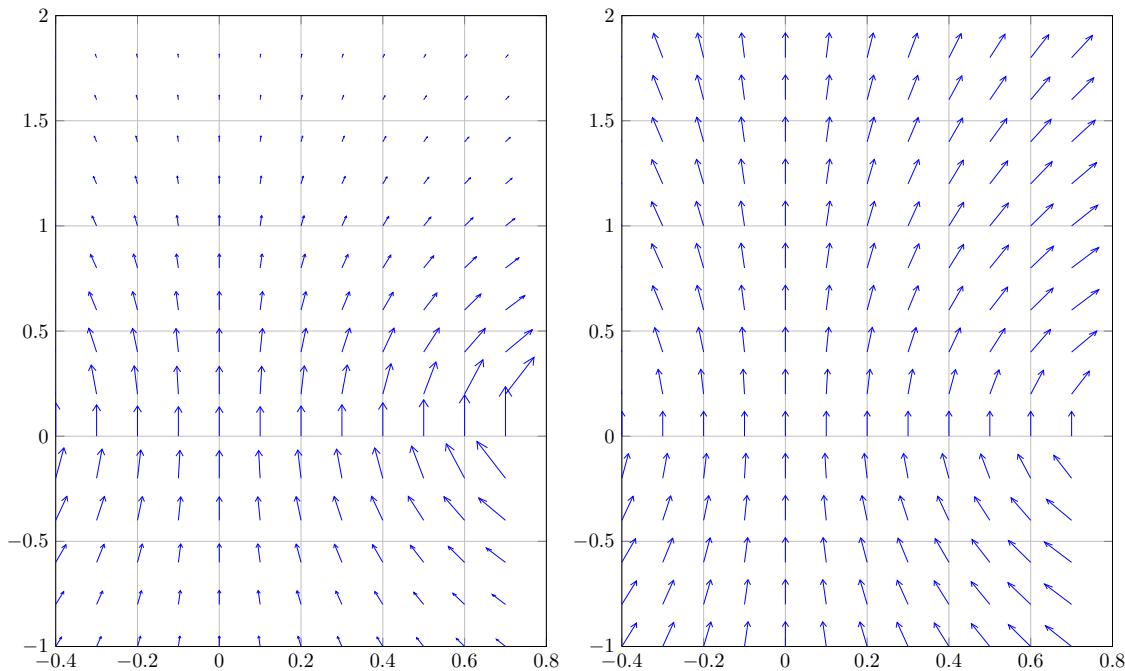


Figure 2.7: Magnetic vector field in a plane, actual length and normalized

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

[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);
end%for

quiver(x,z,Hx,Hz,0.6) % new scaling
grid on; xlabel('x'); ylabel('z')
axis([-0.3 0.3 -0.3 0.3])

```

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 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:

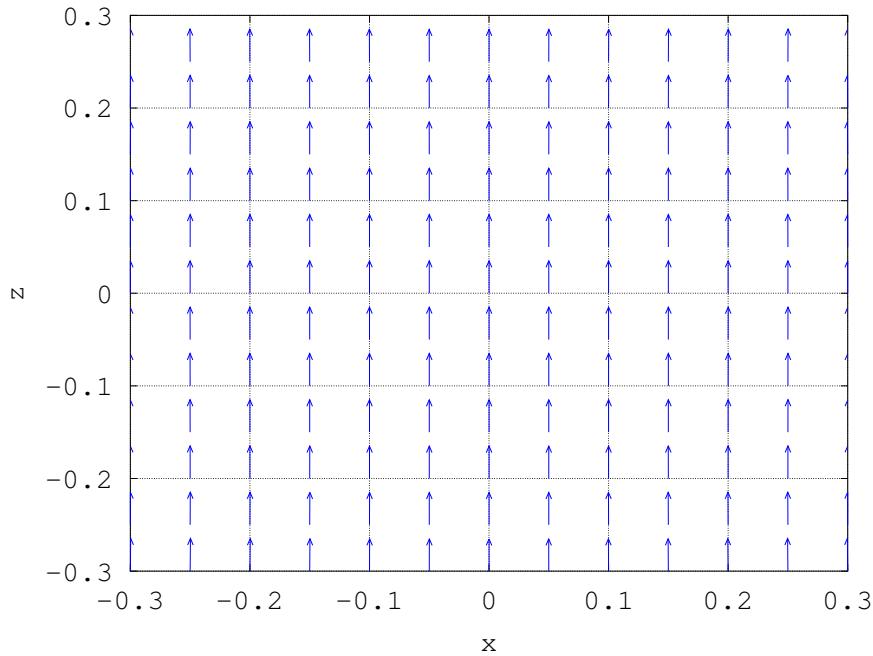


Figure 2.8: Magnetic field for two coils in the Helmholtz configuration

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

$$\text{relative deviation in } H_z = \left| \frac{H_z(x, y, z) - H_z(0, 0, 0)}{H_z(0, 0, 0)} \right|$$

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

$$\text{relative deviation in } \vec{H} = \frac{\|\vec{H}(x, y, z) - \vec{H}(0, 0, 0)\|}{H_z(0, 0, 0)}$$

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

$$\text{relative deviation in strength } \|\vec{H}\| = \left| \frac{\|\vec{H}(x, y, z)\| - H_z(0, 0, 0)}{H_z(0, 0, 0)} \right|$$

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 sharply at the corners of the examined domain of $-0.3 \leq x \leq 0.3$ and $-0.3 \leq z \leq 0.3$.

```

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)

```

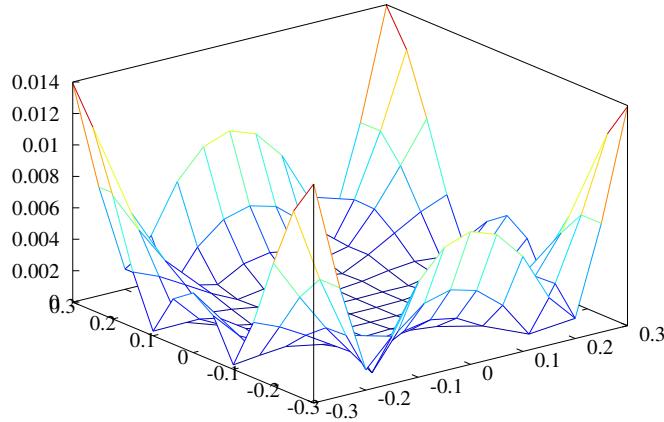


Figure 2.9: Relative changes of H_z in the plane $y = 0$

Level curves for relative deviations

To estimate the domain for which the relative deviation is small we can use the tool of level curves. In Figure 2.10(a) we find the level curves for relative deviation in H_z at levels 0.001, 0.002, 0.005 and 0.01. Observe that the deviation remains small along a few lines, even if we move away from the center. This is confirmed by Figure 2.9. We use a rather fine mesh² to obtain smoother curves. One might have to pay attention to the computation time. If a grid on $n \times n$ points is examined, then $2n^2$ integrals have to be computed. For the sample code below this translates to $2 \cdot 51^2 = 5202$ integrals.

Octave

```

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');

```

²The price to pay is some CPU time. For a quick check one may work at a lower resolution.

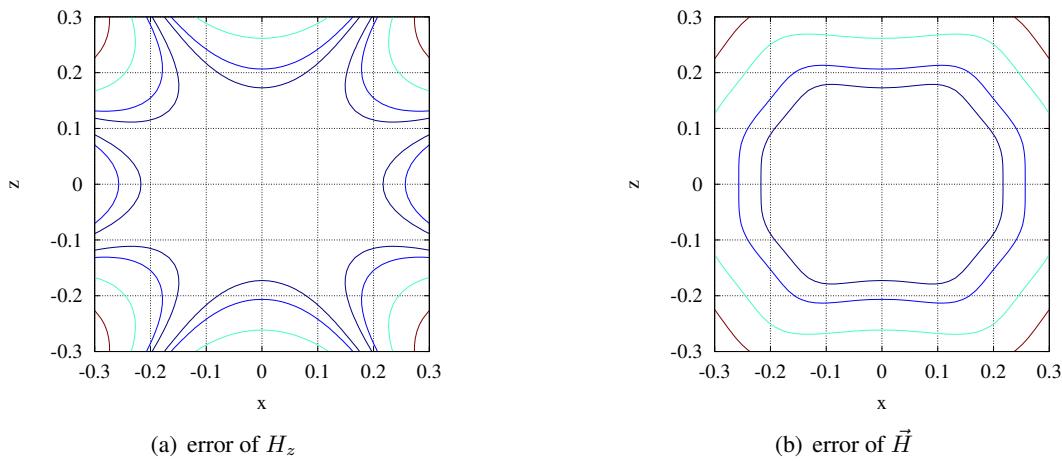


Figure 2.10: Level curves for the relative changes of H_z at levels 0.001, 0.002, 0.005 and 0.01

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 resulting Figure 2.10(b). Observe 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. This is the main advantage of the Helmholtz configuration.

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');
```

2.1.8 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 <code>trapz()</code>
simpson.m	function file, implementing Simpson's algorithm
testsimpson.m	script file for test of <code>simpson()</code>
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

2.2 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 vast literature (e.g. [Stah99],[MontPeckVini12],[Hock05],[Bevi69]) and many pieces of code are available. Obviously Octave and MATLAB 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:

- First we show the example of a straight line regression, the most common case. Only basic *Octave* commands are used. See Section 2.2.1.
- Then a generally applicable matrix notation is introduced to examine all types of linear regression problems. See Section 2.2.2.
- Then we examine the variance (accuracy) of the parameters to be determined. This aspect is often not given the deserved attention by engineers. See Section 2.2.3.
- Using a real example we illustrate how the basis ideas might lead to serious problems (and wrong results), as is the case for many real world problems. We point out how to avoid or eliminate those problems. Some of the mathematical background (QR factorization) is given. See Sections 2.2.5 and 2.2.6.
- Then we present some information on weighted regression problems and the resulting algorithm. See Section 2.2.7.
- All of the above will lead to the code in `LinearRegression.m`. This code is part of the optimization package of *Octave*. You can use the same code with MATLAB. See Section 2.2.9.
- Then all part of the above puzzle will be used to examine four real world, non obvious applications of linear regression.
 1. The performance of a magnetic motor is examined as function of two parameters. In this example we use a linear regression with two independent variables, i.e. we seek a function of two variables. See Section 2.2.10
 2. Using two acceleration sensors one can design an orientation sensor. To calibrate this sensor we use linear regression. See Section 2.2.11.
 3. With an AFM microscope the surface of ball bearing can be examined. With linear regression we determine the exact shape of the bills. See Section 2.2.12.
 4. Using linear regression with a piecewise linear function we examine a system consisting of two springs. In this example the regression is combined with a nonlinear optimization problem. See Section 2.2.13.
- In Section 2.2.14 the commands `leasqr()` and `fsolve()` are used to solve nonlinear regression problems, illustrated by simple examples. This is applied to a real problem in Sections 2.2.15 and 2.2.16. In Section 2.2.18 a real world problem is examined. The importance of obtaining good starting values is illustrated.

For most of the sample code you need the optimization package loaded in *Octave*. Use the command `pkg list` to display the installed packages, the one marked by a star * are currently loaded. To load the optimization package use the command `pkg load optim`.

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 notation 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} .

$$\mathbf{X} \cdot \vec{p} = (\mathbf{F}^T \cdot \mathbf{F}) \cdot \vec{p} = \mathbf{F}^T \cdot \vec{y}$$

This can easily be implemented in Octave, leading to the result in Figure 2.11 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);
xlabel('independent variable x'); ylabel('dependent variable y')
```

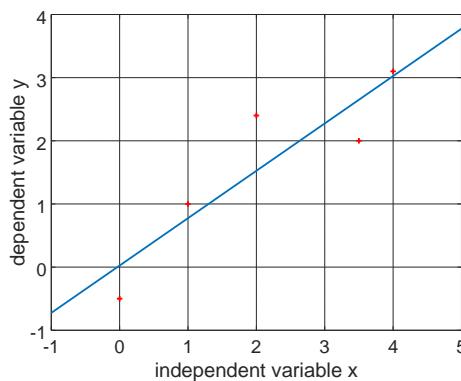


Figure 2.11: Regression of a straight line

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 $\vec{x} = (x_1, x_2, \dots, x_k)^T$ 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 $\vec{p} = (p_1, p_2, \dots, p_m)^T$ 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 a vector and matrix notation this can be written in the form

$$\vec{p} = \begin{pmatrix} p_1 \\ p_2 \\ \vdots \\ p_m \end{pmatrix}, \quad \vec{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}, \quad \mathbf{F} = \begin{bmatrix} f_1(x_1) & f_2(x_1) & \dots & f_m(x_1) \\ f_1(x_2) & f_2(x_2) & \dots & f_m(x_2) \\ \vdots & \vdots & \ddots & \vdots \\ f_1(x_n) & f_2(x_n) & \dots & f_m(x_n) \end{bmatrix}$$

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

$$\mathbf{X} \cdot \vec{p} = (\mathbf{F}^T \cdot \mathbf{F}) \cdot \vec{p} = \mathbf{F}^T \cdot \vec{y}$$

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.

$$(\mathbf{F} \cdot \vec{p})_i = \sum_{j=1}^m p_j \cdot f_j(x_i)$$

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 2.12 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)
xlabel('independent variable x'); ylabel('dependent variable y')

```

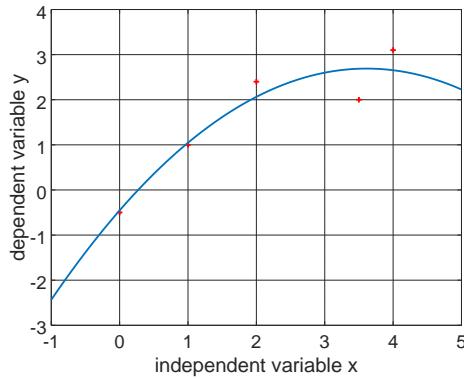


Figure 2.12: Regression of a parabola

2.2.3 Estimation of the variance of parameters, confidence intervals

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

```

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 to 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 p_j . To this end consider the normal equation

$$(\mathbf{F}^T \cdot \mathbf{F}) \cdot \vec{p} = \mathbf{F}^T \cdot \vec{y}$$

and thus the explicit expression for \vec{p}

$$\vec{p} = (\mathbf{F}^T \cdot \mathbf{F})^{-1} \cdot \mathbf{F}^T \cdot \vec{y} = \mathbf{M} \cdot \vec{y} \quad (2.2)$$

or

$$p_j = \sum_{i=1}^n m_{j,i} y_i \quad \text{for } 1 \leq j \leq m$$

where

$$\mathbf{M} = [m_{j,i}]_{1 \leq j \leq m, 1 \leq i \leq n} = (\mathbf{F}^T \cdot \mathbf{F})^{-1} \cdot \mathbf{F}^T$$

is a $m \times n$ -matrix, where $m < n$ (more columns than rows).

This explicit representation of p_j allows³ to compute the variance $\text{var}(p_j)$ of the parameters p_j , using the estimated variance σ^2 of the y -values. The result is given by

$$\text{var}(p_j) = \sum_{i=1}^n m_{j,i}^2 \sigma^2 \quad \text{where } \sigma^2 = \frac{1}{n-m} \sum_{i=1}^n r_i^2$$

Once we know the standard deviation and assume a normal distribution one can readily⁴ determine the 95% **confidence interval** for the parameters, i.e. the probability that the actual value of the parameter is between $p_i - 1.96 \sqrt{\text{var}_i}$ and $p_i + 1.96 \sqrt{\text{var}_i}$ is 95%.

All the above computations can be packed in a function file `LinearRegression.m`⁵ to compute the optimal values of the parameters and the estimated variances.

Octave

```
function [p, e_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
e_var = sum(residual.^2)/(rF-cF); % 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)*e_var; % variance of the parameters
```

The function `LinearRegression()` now allows to solve the straight line problem leading to Figure 2.11 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)
sigma = sqrt(p_v)
alpha = 0.05; scale =
p95 = p + norminv(1-alpha/2)*[-sigma +sigma]
```

³ If z_k are **independent** random variables given by a normal distribution with variances $\text{var}(z_k)$, then a linear combination of the z_i also leads to a normal distribution. The variances are given by the following rules:

$$\begin{aligned} \text{var}(z_1 + z_2) &= \text{var}(z_1) + \text{var}(z_2) \\ \text{var}(\alpha_1 z_1) &= \alpha_1^2 \text{var}(z_1) \\ \text{var}\left(\sum_i \alpha_i z_i\right) &= \sum_i \alpha_i^2 \text{var}(z_i) \end{aligned}$$

⁴Use

$$\int_{-1.96\sigma}^{+1.96\sigma} \frac{1}{\sqrt{2\pi}} \exp(-x^2/(2\sigma^2)) dx \approx 0.95$$

Using the statistics package of Octave this value can be computed by `fsolve (@(x) normcdf(x)-normcdf(-x)-0.95, 2)`.

⁵A better implementation is shown in Figure 2.18 on page 161, thus we use a temporary function name.

The result implies 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 0.55 and the standard deviation of the slope (0.75) is given by 0.21. Thus with a probability of 95% we find for the parameters in $y(x) = \alpha + \beta x$

$$\begin{aligned} -1.05 &= 0.025 - 1.96 \cdot 0.55 < \alpha < 0.025 + 1.96 \cdot 0.55 = +1.10 \\ +0.33 &= 0.75 - 1.96 \cdot 0.21 < \beta < 0.75 + 1.96 \cdot 0.21 = +1.17 \end{aligned}$$

Thus the tolerance for the parameters α and β in this example is huge. This information should prevent you from showing too many digits when analyzing measured data.

The above assumes that the distribution of the parameters are normal distributions. Actually the distribution to use is a Student's t-distribution with $n - 2$ degrees of freedom and the code should be modified to

```
p95 = p + tinv(1-alpha/2, length(x)-2)*[-sigma + sigma]
```

leading to

$$\begin{aligned} -1.720517 &< \alpha < 1.770517 \\ 0.073118 &< \beta < 1.426882 \end{aligned}$$

If we have many data points (only 5 in the above example) the normal distribution and the Student's t-distribution differ very little. Then the estimated confidence intervals will differ very little.

To fit a parabola through the same points replace one line of code by

Octave

```
F = [ones(length(x),1) x x.^2];
```

2.2.4 Estimation of variance of the dependent variable

For the regression of a straight line $y(x) = \alpha + \beta x$ we can also estimate the expected variance of the y -values. We assume that all measured values y_i of y share a common standard deviation of σ . We use the notations $S_x = \sum_i x_i$, $S_{xx} = \sum_i x_i^2$ and $S_{xy} = \sum_i x_i y_i$ and the explicit formulas

$$\Delta = n \cdot S_{xx} - S_x^2 \quad , \quad \alpha = \frac{1}{\Delta} (S_{xx} S_y - S_x S_{xy}) \quad , \quad \beta = \frac{1}{\Delta} (n S_{xy} S_y - S_x S_y)$$

Thus we find⁶

$$\begin{aligned} y &= \alpha + \beta x = \frac{1}{\Delta} (S_{xx} S_y - S_x S_{xy}) + \frac{1}{\Delta} (n \cdot S_{xy} - S_x S_y) x \\ &= \frac{1}{\Delta} \sum_i (S_{xx} - S_x x_i + n x x_i - x S_x) y_i \end{aligned}$$

Then the computational rules for variances lead⁷ to

$$\begin{aligned} V(y) &= \frac{1}{\Delta^2} \sum_i (S_{xx} - S_x x_i + n x x_i - x S_x)^2 \sigma^2 = \text{elementary, tedious algebra} = \\ &= \frac{\sigma^2}{\Delta} \left(n \left(x - \frac{S_x}{n} \right)^2 + \frac{1}{n} (n S_{xx} - S_x^2) \right) = \sigma^2 \left(\frac{1}{n} + \frac{n}{\Delta} (x - \bar{x})^2 \right) \end{aligned}$$

⁶Observe that the simple formula $y = \alpha + \beta x$ does **not** lead to $V(y) = V(\alpha) + V(\beta) x^2$ since the two parameters α and β are not statistically independent.

⁷Ask this author for a printout with all the glorious details shown.

This is the variance of the computed y values on the straight line. Since a new measurement adds another contribution to the variance we obtain a width of the confidence band by

$$\left(1 + \frac{1}{n} + \frac{n}{\Delta} (x - \bar{x})^2\right)^{1/2} \sigma$$

The above formula is correct when fitting a straight line through given data points. For general linear regressions we have to use the general formulas. Let \vec{y}_m denote the set of measured y values and \vec{y}_p the vector of predicted y values, using the result of a linear regression. Based on equation (2.2) and $\vec{y}_p = \mathbf{F} \cdot \vec{p}$ we find

$$\vec{y}_p = \mathbf{F} \cdot (\mathbf{F}^T \cdot \mathbf{F})^{-1} \cdot \mathbf{F}^T \vec{y}_m = \mathbf{B} \vec{y}_m \quad (2.3)$$

Estimate the variance of the straight line

Based on this explicit formula (2.3) for the values of y_i we can estimate the variances of the components of the computed values of y_i .

$$V(y_i) = \sum_{k=1}^n b_{i,k}^2 \sigma^2$$

This is implemented in the function `LinearRegression()` and the values are returned in the variable `fit_var`. With this expression one can determine the confidence band for the straight line.

Estimate the variance of a future measurement

If we want to predict the variance of a new data point at x_i there are two contributions to the variance: the independent variance of the measurement and the variance from the straight line. Since the events are assumed to be independent, we have to add the variances, leading to

$$\sigma^2 + V(y_i) = \sigma^2 + \sum_{k=1}^n b_{i,k}^2 \sigma^2$$

With `LinearRegression()` this can be computed by `e_var+fit_var` and used in the code below, leading to Figure 2.13(a). There find the raw data, the best fitting straight line and the 95% confidence band for straight line and possible new values. The confidence band can be displayed by multiplying the square root of the estimated variance by 1.96 and adding/subtracting this from the fitted value. Observe that the confidence band for the straight line is considerably narrower than the one for the expected new values of y .

```
n = 100; x = sort(rand(n,1)*5-1); y = 1+0.05*x + 0.1*randn(size(x));
F = [ones(n,1),x(:)]; % straight line regression
[p,e_var,r,p_var,y_var] = LinearRegression(F,y);
yFit = F*p;
figure(1)
fac = fsolve(@(x)normcdf(x)-normcdf(-x)-0.95,2); % 95% level , fac = 1.96
plot(x,y,'+b',x,yFit,'-g',...
    x,yFit+fac*sqrt(y_var),'--r',x,yFit+fac*sqrt(e_var+y_var),'--k',...
    x,yFit-fac*sqrt(y_var),'--r',x,yFit-fac*sqrt(e_var+y_var),'--k')
title('straight line by linear regression')
legend('data','fit','+-95% line','+-95% data','location','northwest'); grid on
```

The above result is not restricted to straight line regressions, e.g. we may fit a curve $y(x) = p_1 + p_2 \sin(x)$ through a set of data points and display similar results in Figure 2.13(b).

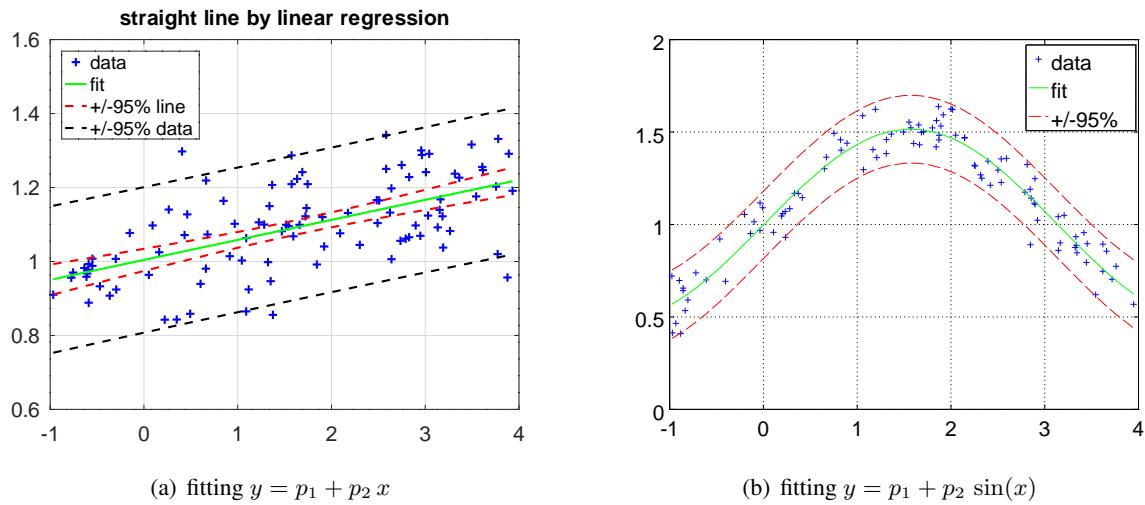


Figure 2.13: Regressions with the fitted data and the 95% confidence bands

```
n = 100; x = sort(rand(n,1)*5-1); y = 1+0.5*sin(x) + 0.1*randn(size(x));
F = [ones(n,1), sin(x(:))];
[p,e_var,r,p_var,y_var] = LinearRegression(F,y);
yFit = F*p;
figure(2)
plot(x,y,'+b',x,yFit,'-g',...
      x,yFit+1.96*sqrt(e_var+y_var),'--r',x,yFit-1.96*sqrt(e_var+y_var),'--r')
legend('data','fit','+/-95%'); grid on
```

2.2.5 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 2.9.3 you find the information on how to import the data from the data sheet into *Octave*. Then Figure 2.14(b) is generated by simple code.

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 5 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

```
LEDdata; % load the data
n = 6; % try with a polynomial of degree 5
F = ones(length(angle),n);
for k = 1:n
    F(:,k) = angle.^(k-1);
end
```

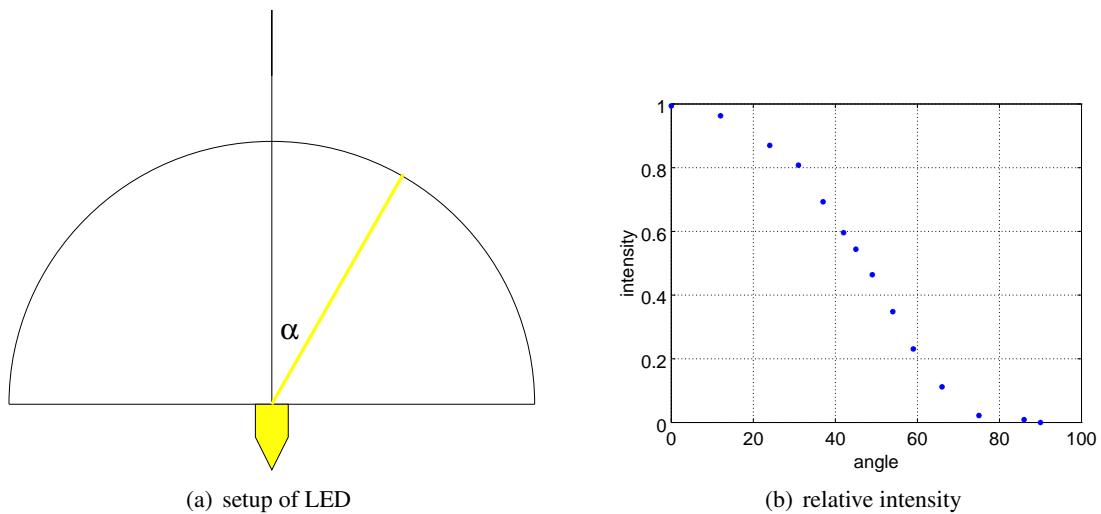


Figure 2.14: Intensity of light as function of the angle

```
[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 ')

```

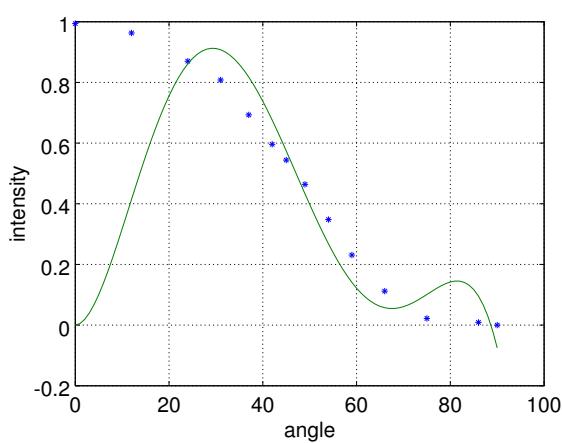


Figure 2.15: Intensity of light as function of the angle and a first regression curve

The result in Figure 2.15 is obviously useless. The estimated variances of the parameters are of the same order of magnitude as the values of the parameters, or even larger. We need to find the reason for the failure and how to avoid the problem.

The above 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						
$\mathbf{F}' \cdot \mathbf{F}$						
→	1.4000e+01	6.7000e+02	4.1114e+04	2.8161e+06	2.0767e+08	1.6113e+10
	6.7000e+02	4.1114e+04	2.8161e+06	2.0767e+08	1.6113e+10	1.2949e+12
	4.1114e+04	2.8161e+06	2.0767e+08	1.6113e+10	1.2949e+12	1.0666e+14
	2.8161e+06	2.0767e+08	1.6113e+10	1.2949e+12	1.0666e+14	8.9414e+15
	2.0767e+08	1.6113e+10	1.2949e+12	1.0666e+14	8.9414e+15	7.5911e+17
	1.6113e+10	1.2949e+12	1.0666e+14	8.9414e+15	7.5911e+17	6.5056e+19

we see that the matrix contains numbers of the order 1 and of the order 10^{19} and one should not be surprised by trouble when solving such a system of equations. Mathematically speaking we have a very large **condition number** of 10^{16} and thus we will lose 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, reliable solution they **should all be used**.

1. Rescaling

For a polynomial of degree 6 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 $90^8 \approx 100^8 = 10^{20}$. If we switch to radians instead of degrees this will be reduced to $(\frac{\pi}{2})^8 \approx 100$ and thus this problem should be taken care of. The code below will generate a good solution.

Octave	
LEDdata;	
scalefactor = 180/pi;	angle = angle/scalefactor;
n = 6;	
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	
a1 = ((0:1:90)')/scalefactor; % consider angles from 0 to 90 degree	
Fnew = ones(length(a1),n);	
for k = 1:n	
Fnew(:,k) = a1.^^(k-1);	
end	
Inew = Fnew*p;	
plot(angle*scalefactor,intensity,'*',a1*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 functions for linear regression very carefully,
based on information about the system to be examined.

There are many software packages (*Mathematica*, MATLAB, *Octave*, Excel, ...) 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**⁸ principle.

3. QR factorization instead of the matrix $\mathbf{F}' \cdot \mathbf{F}$

Idea and consequences of this change in algorithm are based on QR factorization and are given in the next 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, based on the QR factorization.

⁸Garbage In, Garbage Out

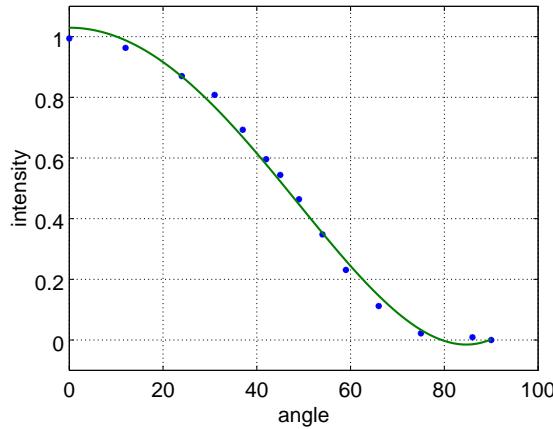


Figure 2.16: Intensity of light as function of the angle and regression with an even function

2.2.6 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. No consider the block matrix notation

$$\mathbf{Q} = \begin{bmatrix} \mathbf{Q}_l & \mathbf{Q}_r \end{bmatrix} \quad \text{and} \quad \mathbf{R} = \begin{bmatrix} \mathbf{R}_u \\ \mathbf{0} \end{bmatrix}$$

The $m \times m$ matrix \mathbf{R}_u is square and upper triangular. The left part \mathbf{Q}_l of the square matrix \mathbf{Q} is of size $n \times m$ and satisfies $\mathbf{Q}_l^T \mathbf{Q}_l = \mathbb{I}_n$. Use the zeros in the lower part of \mathbf{R} to verify that

$$\mathbf{F} = \mathbf{Q} \cdot \mathbf{R} = \mathbf{Q}_l \cdot \mathbf{R}_u$$

Octave can compute the QR factorization by $[\mathbf{Q}, \mathbf{R}] = \text{qr}(\mathbf{F})$ and the reduced form by $[\mathbf{Q}_l, \mathbf{R}_u] = \text{qr}(\mathbf{F}, 0)$. This factorization is very useful to implement linear regression.

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.

$$\begin{aligned} \mathbf{F} \cdot \vec{p} - \vec{y} &= \vec{r} \quad \text{length to be minimized} \\ \mathbf{Q} \cdot \mathbf{R} \cdot \vec{p} - \vec{y} &= \vec{r} \quad \text{length to be minimized} \\ \mathbf{R} \cdot \vec{p} - \mathbf{Q}^T \cdot \vec{y} &= \mathbf{Q}^T \cdot \vec{r} \\ \begin{bmatrix} \mathbf{R}_u \cdot \vec{p} \\ \mathbf{0} \end{bmatrix} - \begin{bmatrix} \mathbf{Q}_l^T \cdot \vec{y} \\ \mathbf{Q}_r^T \cdot \vec{y} \end{bmatrix} &= \begin{bmatrix} \mathbf{Q}_l^T \cdot \vec{r} \\ \mathbf{Q}_r^T \cdot \vec{r} \end{bmatrix} \end{aligned}$$

Since the vector \vec{p} does not change the lower part of the above system, the problem can be replaced by a smaller system of m equations for m unknowns, namely the upper part only of the above system.

$$\mathbf{R}_u \cdot \vec{p} - \mathbf{Q}_l^T \cdot \vec{y} = \mathbf{Q}_l^T \cdot \vec{r} \quad \text{length to be minimized}$$

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} .

$$\begin{aligned} \mathbf{R}_u \cdot \vec{p} &= \mathbf{Q}_l^T \cdot \vec{y} \\ \vec{p} &= \mathbf{R}_u^{-1} \cdot \mathbf{Q}_l^T \cdot \vec{y} \end{aligned}$$

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 QR algorithm is much smaller than 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 reliability⁹.

2.2.7 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 $\|\vec{r}\|^2 = \sum_{i=1}^n r_i^2$. There are situations where not all errors have equal weight and thus we try to minimize a weighted length

$$\|\vec{r}\|_W^2 = \sum_{i=1}^n w_i^2 r_i^2 = \langle \mathbf{W} \cdot \vec{r}, \mathbf{W} \cdot \vec{r} \rangle$$

If the estimated standard deviation for each measurement y_i is given by σ_i , use $w_i = 1/\sigma_i$. Thus points measured with a high accuracy obtain a larger weight. The weight matrix \mathbf{W} is given by

$$\mathbf{W} = \text{diag}(\vec{w}) = \begin{bmatrix} w_1 & & & \\ & w_2 & & \\ & & \ddots & \\ & & & w_n \end{bmatrix}$$

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 2.18 (see page 161).

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

$$\sigma_j^2 \approx \frac{1}{w_j^2} \frac{1}{n-m} \sum_{i=1}^n r_i^2 w_i^2$$

⁹A careful computation shows that using the QR factorization $\mathbf{F} = \mathbf{Q} \mathbf{R}$ in $\mathbf{F}^T \mathbf{F} \vec{p} = \mathbf{F}^T \vec{y}$ also leads to $\mathbf{R}_u \vec{p} = \mathbf{Q}_l^T \vec{y}$.

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

$$\begin{aligned} p_j &= \sum_{i=1}^n m_{j,i} y_i \quad \text{for } 1 \leq j \leq m \\ V(p_j) &= \sum_{i=1}^n m_{j,i}^2 \sigma_i^2 \quad \text{for } 1 \leq j \leq m \end{aligned}$$

Observe that this calculation is only correct if the σ_i^2 are not correlated.

Uniformly distributed errors

If we set all weights to $w_i = 1$ this leads back to the results in Section 2.2.3. The expression to be minimized is

$$\chi^2 = \sum_{i=1}^n (y_i - f(x_i))^2 \quad \text{with } f(x) = \sum_{j=1}^m p_j f_j(x)$$

Uniformly distributed relative errors

In this case we expect the standard deviations to be proportional to the absolute value of y_i and thus we choose the weights $w_1 = 1/|y_i|$. The expression to be minimized is

$$\chi^2 = \sum_{i=1}^n \frac{(y_i - f(x_i))^2}{y_i^2}$$

A priori known error distributions

If we have good estimates σ_i for the standard deviations of the values y_i we choose the weights $w_i = 1/\sigma_i$ and the expression to be minimized is

$$\chi^2 = \sum_{i=1}^n \frac{(y_i - f(x_i))^2}{\sigma_i^2}$$

In this case the standard deviation of $w_i y_i$ is expected to be constant 1. The estimation of the standard deviations has to respect this fact and this leads to the estimates based on the data points and the given weights.

$$\sigma_j^2 w_j^2 \approx \frac{1}{n} \sum_{i=1}^n w_i^2 r_i^2 \quad \Rightarrow \quad \sigma_j^2 \approx \frac{\sum_{i=1}^n w_i^2 r_i^2}{n w_j^2}$$

This leads to the estimate for σ_j in the previous section. The method is implemented in the code of `LinearRegression()` in Figure 2.18.

2.2.8 More commands for regression with Octave or MATLAB

In these notes I mainly use the command `LinearRegression()`, but MATLAB/Octave provide many more commands, some shown in Table 2.4. Consult the manuals for more information.

For nonlinear regression there are special commands too, see Table 2.5. Observe that the syntax and algorithm of these commands might differ between MATLAB and Octave. You definitely have to consult the manuals and examine example applications.

Command	Properties
<code>LinearRegression()</code>	standard and weighted linear regression returns standard deviations for parameters
<code>regress()</code>	standard linear regression returns confidence intervals for parameters
<code>ols()</code>	ordinary least square estimation
<code>gls()</code>	generalized least square estimation
<code>lscov()</code>	generalized least square estimation, with weights
<code>polyfit()</code>	regression with for polynomials only
<code>lsqnonneg()</code>	regression with positivity constraint

Table 2.4: Commands for linear regression

Command	Properties
<code>leasqr()</code>	standard non linear regression, Levenberg-Marquardt see section 2.2.14
<code>fsolve()</code>	can be used for nonlinear regression too
<code>nlinfit()</code>	nonlinear regression
<code>lsqcurvefit()</code> <code>nonlin_curvefit()</code>	nonlinear curve fitting frontend, Octave only
<code>lsqnonlin()</code> <code>nonlin_residmin()</code>	nonlinear minimization of residue frontend, Octave only
<code>nlpaci()</code>	determine confidence intervals of parameters, MATLAB only
<code>expfit()</code>	regression with exponential functions

Table 2.5: Commands for nonlinear regression

2.2.9 Code for the function `LinearRegression()`

The structure of the function file has the typical structure of a Octave function file.

- The first few lines contain the copyright.
- The first section in the file `LinearRegression.m` is the documentation. This text will be displayed by the command `help LinearRegression`. A description of the parameters and the return values is given. Find the result in Figure 2.17.

```
help LinearRegression
→
Function File LinearRegression (F, y, w)
[p, e_var, r, p_var, fit_var] = LinearRegression (...)

general linear regression

determine the parameters p_j (j=1,2,...,m) such that the function
f(x) = sum_(j=1,...,m) p_j*f_j(x) is the best fit to the given values
y_i by f(x_i) for i=1,...,n, i.e. minimize
sum_(i=1,...,n)(y_i-sum_(j=1,...,m) p_j*f_j(x_i))^2 with respect to p_j

parameters:
F is an 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 is a column vector of length n with the given values
w is an optional column vector of length n with the weights of
the data points. 1/w_i is expected to be proportional to the
estimated uncertainty in the y values. Then the weighted expression
sum_(i=1,...,n)(w_i^2*(y_i-f(x_i))^2) is minimized.

return values:
p      is the vector of length m with the estimated values of the parameters
e_var is the vector of estimated variances of the residuals, i.e. the
difference between the provided y values and the fitted function.
If weights are provided, then the product e_var_i * w^2_i is assumed to
be constant.
r      is the weighted norm of the residual
p_var is the vector of estimated variances of the parameters p_j
fit_var is the vector of estimated variances of the fitted function values f(x_i)

To estimate the variance of the difference between future y values
and fitted y values use the sum of e_var and fit_var

Caution: do NOT request fit_var for large data sets, as a n*n matrix is generated
see also: ols, gls, regress, leasqr, nonlin_curvefit, polyfit, wpolyfit, expfit

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```

Figure 2.17: Documentation of the command `LinearRegression()`

- Then the function is defined, showing all possible parameters and return values.
- 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 and the predicted values of y are only computed if the output is requested. This is implemented by counting the return arguments of the call of the function (`nargout`).

The resulting function can be called with 1 to 5 return arguments. The function will return only the requested values.

- `p = LinearRegression(F, y)` will return the estimated value of the parameters \vec{p} only .
- `[p, e_var] = LinearRegression(F, y)` will also return the variance of the y -error.
- `[p, e_var, r, p_var, fit_var] = LinearRegression(F, y)` will return all 5 results.

Find the documentation in Figure 2.17 and the code in Figure 2.18.

LinearRegression.m

```

function [p, e_var, r, p_var, fit_var] = LinearRegression (F, y, weight)

if (nargin < 2 || nargin >= 4)
    print_usage ();
end%if

[rF, cF] = size (F);
[ry, cy] = size (y);

if (rF ~= ry || cy > 1)
    error ('LinearRegression: incorrect matrix dimensions');
end%if

if (nargin == 2) % set uniform weights if not provided
    weight = ones (size (y));
else
    weight = weight (:);
end%if

wF = diag (weight) * F; % this efficient with the diagonal matrix

[Q, R] = qr (wF, 0); % estimate the values of the parameters
p = R \ (Q' * (weight .* y));

%% Compute the residual vector and its weighted norm
residual = F * p - y;
r = norm (weight .* residual);

weight2 = weight.^2;
%% If the variance of data y is sigma^2 * weight.^2, var is an
%% unbiased estimator of sigma^2
var = residual.^2' * weight2 / (rF - cF);
%% Estimated variance of residuals
e_var = var ./ weight2;

%% Compute variance of parameters, only if requested
if (nargout > 3)

    M = R \ (Q' * diag (weight));

    %% compute variance of the fitted values, only if requested
    if (nargout > 4)
        %% WARNING the nonsparse matrix M2 is of size rF by rF,
        %% where rF = number of data points
        M2 = (F * M).^2;
        fit_var = M2 * e_var; % variance of the function values
    end%if

    p_var = M.^2 * e_var; % variance of the parameters
end%if

end%function

```

Figure 2.18: Code for the command `LinearRegression()`

2.2.10 Example 2: Performance of a linear motor

In his diploma thesis in 2005 Alois 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 2.19. With a lengthy computation (approximately 4 hours per configuration) he computed the forces for 25 different configurations. The result is shown in Figure 2.20.

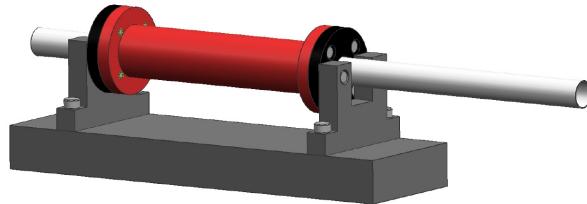


Figure 2.19: A magnetic linear motor

Octave

```
PfennigerData;
figure(1)
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');

figure(2)
mesh(diam, long, force)
xlabel('diameter'); ylabel('length'); zlabel('force');
view(-30,30);
```

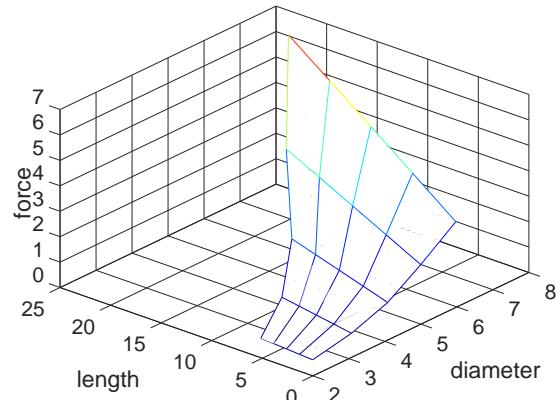
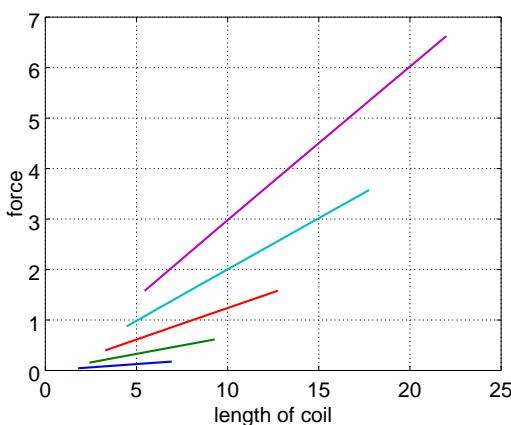


Figure 2.20: Force as function of length of coils, for 5 different diameters

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 2.21 is generated by the code below. The level-curves 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);
```

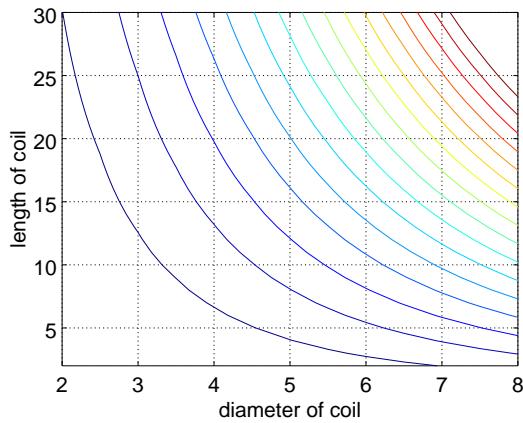


Figure 2.21: Level curves for force as function of length and diameter of coil

```

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');

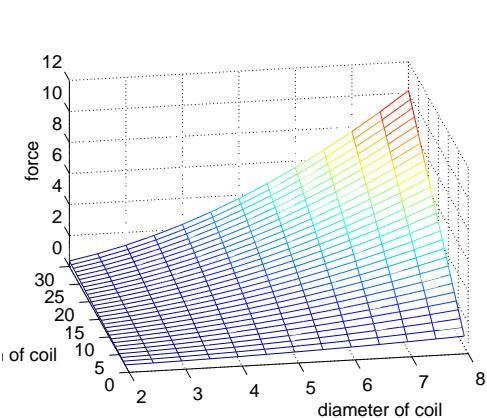
forceB2 = long.* (coef(1)+coef(2)*diam.^2);
maxrelerror = max(max(abs(forceB2-force)./force))
maxerror = max(max(abs(forceB2-force)))

```

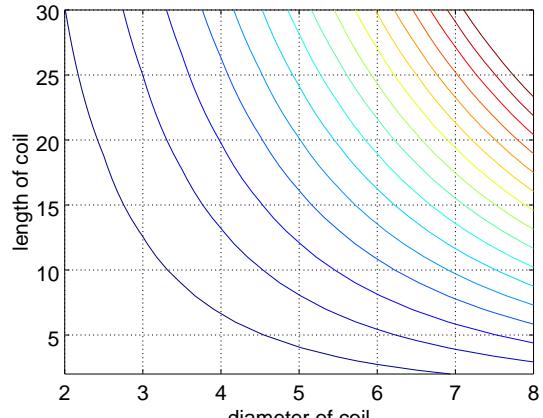
The graphical result can be seen in Figure 2.22 and the numerical results indicates a solution

$$f(l, d) = -0.00990 l + 0.00543975 l d^2$$

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.



(a) the surface



(b) the level curves

Figure 2.22: Computations with simplified function

2.2.11 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

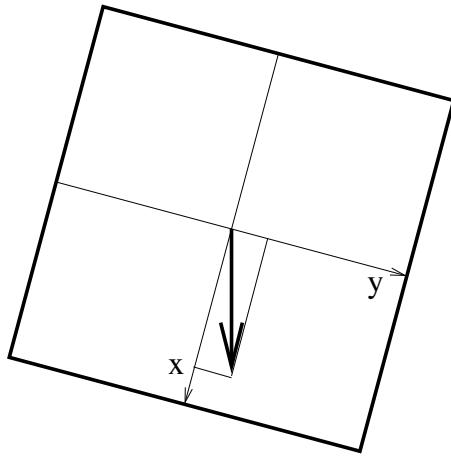


Figure 2.23: A slightly rotated direction sensor

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 $x_0, y_0, r_x, r_y, \phi_x$ and ϕ_y might be different for each 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

$$\begin{bmatrix} g_{x,1} & g_{y,1} & 1 \\ g_{x,2} & g_{y,2} & 1 \\ g_{x,3} & g_{y,3} & 1 \\ \vdots & & \\ g_{x,n} & g_{y,n} & 1 \end{bmatrix} \cdot \begin{pmatrix} m_{x,1} \\ m_{x,2} \\ \vdots \\ c_x \end{pmatrix} - \begin{pmatrix} s_1 \\ s_2 \\ s_3 \\ \vdots \\ s_n \end{pmatrix} = \begin{pmatrix} r_1 \\ r_2 \\ r_3 \\ \vdots \\ r_n \end{pmatrix}$$

A linear regression will give the optimal values of \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
plot(x,y); axis('equal')
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]

xn = F*px; yn = F*py;
hold on
plot(xn,yn,'b')
```

This computation leads to Figure 2.24 and the numerical results below.

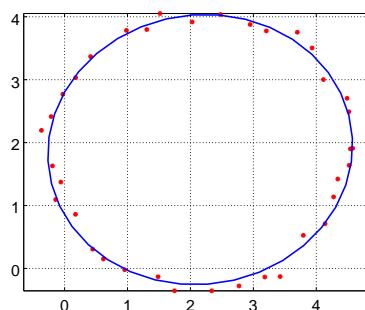


Figure 2.24: Measured data and the fitted circle

$$\vec{s} = \begin{pmatrix} s_x \\ s_y \end{pmatrix} = \begin{bmatrix} 2.40299 & -0.19664 \\ 0.30382 & 2.13793 \end{bmatrix} \cdot \begin{pmatrix} g_1 \\ g_2 \end{pmatrix} + \begin{pmatrix} 2.1549 \\ 1.8899 \end{pmatrix} = \mathbf{M} \cdot \vec{g} + \vec{c}$$

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 $r_x = \sqrt{m_{x,1}^2 + m_{x,2}^2} \approx 2.4221$. 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 similarly 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 $\phi_x \approx 7.21^\circ$ and $\phi_y \approx 5.26^\circ$. 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 of 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

$$\begin{aligned}\phi_x &= \arctan \frac{p_3}{p_2} \\ \frac{\partial}{\partial p_2} \phi_x &= \frac{1}{1+(p_3/p_2)^2} \frac{-p_3}{p_2^2} = \frac{-p_3}{p_2^2 + p_3^2} = \frac{-p_3}{r_x^2} \\ \frac{\partial}{\partial p_3} \phi_x &= \frac{1}{1+(p_3/p_2)^2} \frac{1}{p_2} = \frac{p_2}{p_2^2 + p_3^2} = \frac{p_2}{r_x^2} \\ V(\phi_x) &\approx \frac{1}{r_x^4} (p_3^2 V(p_2) + p_2^2 V(p_3)) \\ \sigma(\phi_x) &= \sqrt{V(\phi_x)} \approx \frac{1}{r_x^2} \sqrt{p_3^2 V(p_2) + p_2^2 V(p_3)}\end{aligned}$$

and similarly¹⁰ 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

$$x_0 = 0.5 , \quad y_0 = 0 , \quad r_x = 1 , \quad r_y = 1.1 , \quad \phi_x = 0^\circ , \quad \phi_y = 5^\circ$$

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

$$x_0 \approx 0.5 , \quad y_0 \approx 0 , \quad r_x \approx 1 , \quad r_y \approx 1.1 , \quad \phi_x \approx 0.01^\circ , \quad \phi_y \approx 4.99^\circ$$

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.

2.2.12 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.

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

¹⁰

$$\begin{aligned}\tan \phi_y = \frac{-p_2}{p_3} \quad \Rightarrow \quad \frac{\partial}{\partial p_2} \phi_y &= \frac{1}{1+(p_2/p_3)^2} \frac{-1}{p_3} = \frac{-p_3}{r_x^2} \quad \Rightarrow \quad V(\phi_x) \approx \frac{1}{r_x^4} (p_3^2 V(p_2) + p_2^2 V(p_3)) \\ \frac{\partial}{\partial p_3} \phi_y &= \frac{1}{1+(p_2/p_3)^2} \frac{+p_2}{p_3^2} = \frac{p_2}{r_x^2}\end{aligned}$$

$(x^2 + y^2)$.

$$\begin{aligned}
 h(x, y) &= h_0 + \sqrt{R^2 - (x - x_0)^2 - (y - y_0)^2} \\
 &= h_0 + R \sqrt{1 - \frac{1}{R^2} ((x - x_0)^2 + (y - y_0)^2)} \\
 &\approx h_0 + R - \frac{(x - x_0)^2}{2R} - \frac{(y - y_0)^2}{2R} \\
 &= h_0 + R - \frac{x_0^2 + y_0^2}{2R} + \frac{x_0}{R} x + \frac{y_0}{R} y - \frac{1}{2R} (x^2 + y^2) \\
 &= p_1 + p_2 x + p_3 y + p_4 (x^2 + y^2)
 \end{aligned}$$

where

$$\begin{aligned}
 p_1 &= h_0 + R - \frac{x_0^2 + y_0^2}{2R} \\
 p_2 &= \frac{x_0}{R} \\
 p_3 &= \frac{y_0}{R} \\
 p_4 &= -\frac{1}{2R}
 \end{aligned}$$

If all values of p_i are known we can solve for the parameters of the sphere.

$$\begin{aligned}
 R &= -\frac{1}{2p_4} \\
 x_0 &= Rp_2 \\
 y_0 &= Rp_3 \\
 h_0 &= p_1 - R + \frac{x_0^2 + y_0^2}{2R}
 \end{aligned}$$

In particular we can read off 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
6.040e-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 = ttt(:,1); y = ttt(:,2); z = ttt(:,3);
N = length(x);
```

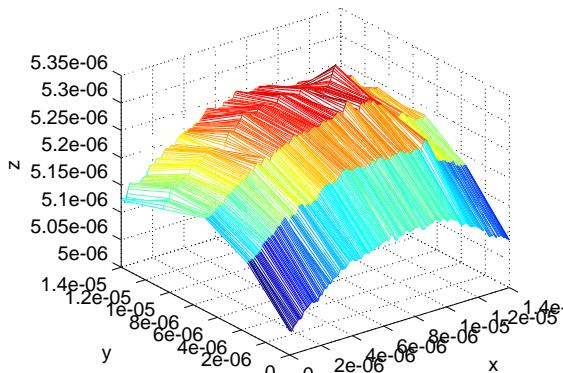
As a next step we generate the plots with the surface and another plot with the level curves. Find the results in Figure 2.25.

Octave

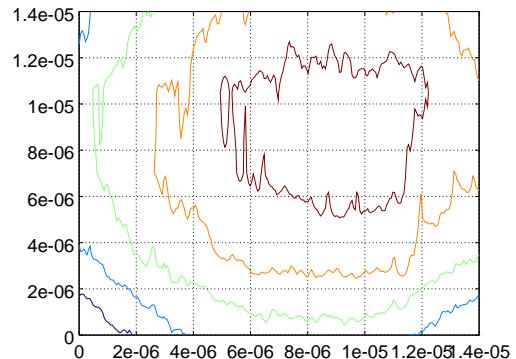
```
steps = 5;
xx = reshape(x,N/steps ,steps );
yy = reshape(y,N/steps ,steps );
zz = reshape(z,N/steps ,steps );

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 2.25: The surface of a ball and the level curves

A quick look at Figure 2.25 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 $300 \mu m$ 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

$$z = \frac{1}{R^2} ((x - x_0)^2 + (y - y_0)^2) \leq 0.0044$$

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 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

$$\mathbf{F} = \begin{bmatrix} 1 & x_1 & y_1 & x_1^2 + y_1^2 \\ 1 & x_2 & y_2 & x_2^2 + y_2^2 \\ 1 & x_3 & y_3 & x_3^2 + y_3^2 \\ \vdots & & & \\ 1 & x_n & y_n & x_n^2 + y_n^2 \end{bmatrix}$$

Then 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,e_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:

$$\begin{aligned} R &= \frac{-1}{2p_4} \\ \Delta R &\approx \left| \frac{\partial R}{\partial p_4} \right| \Delta p_4 = \frac{1}{2p_4^2} \Delta p_4 = 2R^2 \Delta p_4 \\ x_0 &= R p_2 \\ \Delta x_0^2 &\approx \left(\frac{\partial x_0}{\partial p_2} \Delta p_2 \right)^2 + \left(\frac{\partial x_0}{\partial R} \Delta R \right)^2 = (R \Delta p_2)^2 + (p_2 \Delta R)^2 \\ \Delta x_0 &\approx \sqrt{(R \Delta p_2)^2 + (p_2 \Delta R)^2} \\ \Delta y_0 &\approx \sqrt{(R \Delta p_3)^2 + (p_3 \Delta R)^2} \end{aligned}$$

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

$$f(x, y) = p_4 x^2 + p_5 y^2 + p_6 x y = \left\langle \begin{pmatrix} x \\ y \end{pmatrix}, \begin{bmatrix} p_4 & p_6/2 \\ p_6/2 & p_5 \end{bmatrix} \cdot \begin{pmatrix} x \\ y \end{pmatrix} \right\rangle$$

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 $t \vec{e}_1 + s \vec{e}_2$ 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,e_var,r,p_var] = LinearRegression(F2,z);
RadiusNew = -0.5./eig([p(4), p(6)/2;p(6)/2,p(5)])
```

and the results

$$R_1 \approx 267 \mu\text{m} \quad \text{and} \quad R_2 \approx 316 \mu\text{m}$$

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 microscope.

2.2.13 Example 5: A force sensor with two springs

In 2013 Remo Pfaff examined a mechanical spring system consisting of two springs with spring constants k_1 and k_2 . The second spring will only effect the force if a critical x_c position is exceeded. Thus we have the following form of a force (f) distance (x) relation:

$$f(x) = \begin{cases} a + k_1 x & \text{for } x \leq x_c \\ a + (k_1 + k_2) x & \text{for } x \geq x_c \end{cases}$$

Using the offset $p_1 = a$ and the spring constants $p_2 = k_1$, $p_3 = k_2$ this can be written in the form

$$f(x) = p_1 + p_2 x + p_3 \max\{0, x - x_c\} \quad (2.4)$$

For a given data set we can try to find the optimal values for \vec{p} , such that measured data and (2.4) fit together. Find an example in Figure 2.26. There find the measured data, a poorly fitting model and the best possible fit for the value of $x_c = 5$.

For a fixed value of x_c we use the three basis functions

$$f_1(x) = 1, \quad f_2(x) = x \quad \text{and} \quad f_3(x) = \max\{0, x - x_c\}$$

and finding the optimal parameters p_i in equation (2.4) is a linear regression problem. The code below generated Figure 2.26 with the raw data, a poorly fitting model $f(x) = 10 + 2 \cdot x + 3 \cdot \max\{0, x - 5\}$ and the best fitting model with for the fixed value of $x_c = 5$.

Octave

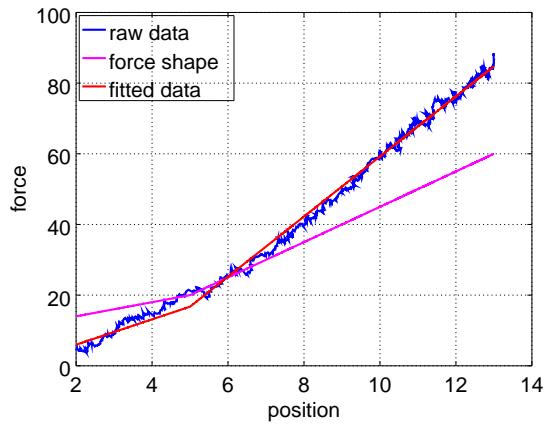


Figure 2.26: A data set for a two spring force distance system and two models

```

force = load('kraftmessung1.dat'); % read the data
dist = load('wegmessung1.dat');

xMin = 2; xMax = 13; % select the useful domain
ind = find ((dist>=xMin).* (dist<=xMax));
dist = dist(ind); force = force(ind);

x_c = 5; % choose a horizontal position for the break point
M = ones(length(dist),3);
M(:,2) = dist(:);
M(:,3) = max(0,dist(:)-x_c);
[p,e_var,r,p_var] = LinearRegression(M,force);
[p sqrt(p_var)]
force_fit = M*p;
force_off = 10 + 2*dist + 3*max(0,dist-x_c);

figure(1)
plot(dist, force, 'b', dist, force_off, 'm', dist, force_fit, 'r')
legend('raw data', 'force shape', 'fitted data', 'location', 'northwest')
xlabel('position'); ylabel('force')

```

In the above algorithm we can compute σ , the standard deviation of the residuals, i.e. the difference between the measurements and the two straight line segments. The smaller the value of σ , the better the fit. Thus we may consider the position x_c of the break as a variable and plot σ as a function of x_c , as shown in Figure 2.27(a).

Octave

```

x_list = 2:0.5:12;
sigma_list = zeros(size(x_list));

function sigma = EvaluateBreak(x_c,dist,force)
M = ones(length(dist),3);
M(:,2) = dist(:);
M(:,3) = max(0,dist(:)-x_c);
[p,sigma] = LinearRegression(M,force);
sigma = mean(sigma);
endfunction

for k = 1:length(x_list)

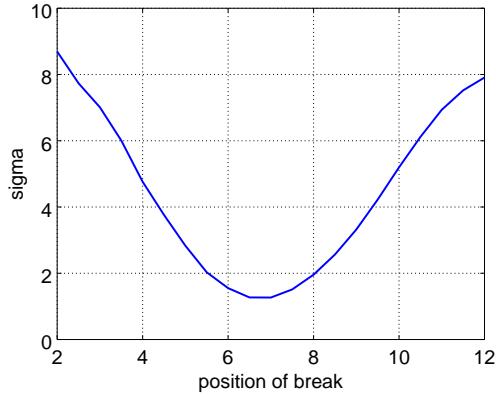
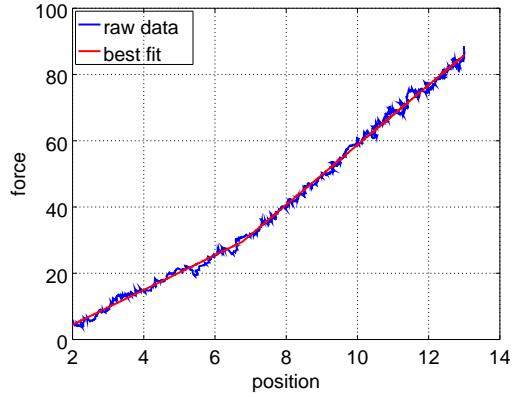
```

```

sigma_list(k) = EvaluateBreak(x_list(k),dist,force);
endfor

figure(2)
plot(x_list,sigma_list)
xlabel('position of break'); ylabel('sigma')

```

(a) σ as function of x_c 

(b) optimal regression

Figure 2.27: Optimal values for the two spring system

In Figure 2.27(a) it is clearly visible that there is an optimal value of x_c , such that σ is minimized. We use the command `fminunc()` to solve the unconstrained minimization problem.

Octave

```

[x_opt,sigma_opt,Info] = fminunc (@(x_c)EvaluateBreak(x_c,dist,force),5)
M = ones(length(dist),3); % redo the linear regression
M(:,2) = dist(:); % with the optimal value for x_c
M(:,3) = max(0,dist(:)-x_opt);
[p,e_var,r,p_var] = LinearRegression(M,force);
param = [p sqrt(p_var)]
force_fit = M*p;

figure(3)
plot(dist, force, 'b', dist, force_fit, 'r')
legend('raw data','best fit')
xlabel('position'); ylabel('force')
->
x_opt = 6.7645
sigma_opt = 1.2391
Info = 3
param = -6.048381 0.138453
      5.252886 0.026087
      3.789025 0.038254

```

Thus the best position of the break point is at $x_c \approx 6.76$ and the resulting minimal value is $\sigma \approx 1.24$. This is confirmed by Figure 2.27(a). Find the optimal result in Figure 2.27(b). The numerical results

$$\begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix} = \begin{pmatrix} -6.05 \\ 5.253 \\ 3.789 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_s \end{pmatrix} = \begin{pmatrix} 0.14 \\ 0.026 \\ 0.038 \end{pmatrix}$$

point towards a best fitting function in equation (2.4)

$$f(x) = p_1 + p_2 x + p_3 \max\{0, x - x_c\} = -6.05 + 5.253x + 3.789 \max\{0, x - 6.76\}$$

2.2.14 Nonlinear Regression, Introduction and a First Example

The commands in the above section are well suited for linear regression problems, but there are many important **nonlinear** regression problems. Examine Table 2.6 to distinguish linear and nonlinear regression problems. 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. This is often not a good idea, as they have special properties that one can and has to take advantage of.

function	parameters	
$y = a + mx$	a, m	linear
$y = ax^2 + bx + c$	a, b, c	linear
$y = ae^{cx}$	a, c	nonlinear
$y = d + ae^{cx}$	a, c, d	nonlinear
$y = ae^{cx}$	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 2.6: Examples for linear and nonlinear regression

Find a list of commands for nonlinear regression in Table 2.5 on page 158. In the next section `leasqr()` is used to illustrate the typical process when solving a nonlinear regression problem. Observe that this may be considerably more difficult than using linear regression.

Nonlinear least square fit with `leasqr()`

The optimization package of Octave provides the command `leasqr()`¹¹. 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 first example we try to fit a function of the type

$$f(t) = A e^{-\alpha t} \cos(\omega t + \phi)$$

through a number of measured points (t_i, y_i) . We search 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 normally distributed random numbers as perturbation of the "exact" result.

¹¹MATLAB users may use the code provided with the samples codes for the class. Use `leasqr.m` and `dfdp.m`.

3. Define the appropriate function and generate the data.

Find the code below and the generated data points are shown in Figure 2.28, together with the best possible approximation by a function of the above type.

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 2.28 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 2π , 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; a10 = 0; omega0 = 1; phi0 = pi/2;
[fr ,p] = leasqr(t ,y ,[A0, a10 ,omega0 ,phi0 ],'f ',1e-10);
p'

yFit = f(t ,p);
plot(t,y ,'+', t ,yFit)
legend('data ','fit ')
-->
p = 1.523957 0.098949 0.891675 1.545294
```

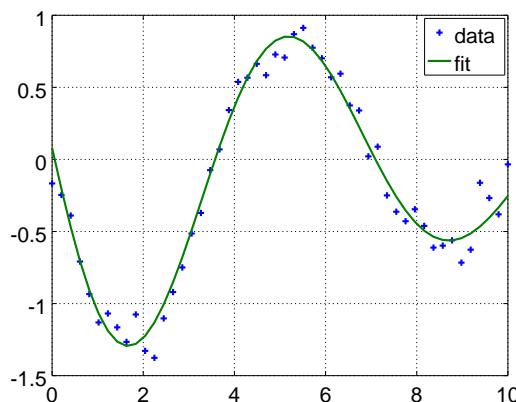


Figure 2.28: Least square approximation of a damped oscillation

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

```
pkg load optim % load the optimization package in Octave
[fr,p,kvg,iter,corp,covp,covr,stdresid,Z,r2] =...
    leasqr(t,y,[A0,a10,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 2.7. 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 2.7: Estimated and exact values of the 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 Regression 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. 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 **over determined** 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

$$\|f(\vec{p}, \vec{x}) - \vec{y}_d\| \text{ is minimized with respect to } \vec{p} \in \mathbb{R}^m$$

It is also possible¹² to estimate the variances of the optimal parameters, using the techniques from Section 2.2.3.

In the example below some data $y = \exp(-0.2x) + 3$ is generated and then some noise added. As initial parameter we use the naive guess $y(x) = \exp(0 \cdot x) + 0$. The best possible fit is determined and displayed in Figure 2.29.

Octave

¹²Ask this author for the sample code `NLRegTest.m`.

```
b0 = 3; a0 = 0.2; % chose the data
x = 0:.5:5;
noise = 0.1 * sin (100*x);
y = exp (-a0*x) + b0 + noise;

[p, fval, info, output] = fsolve (@(p) (exp(-p(1)*x) + p(2) - y), [0, 0]);
plot(x,y,'+', x,exp(-p(1)*x)+p(2))
```

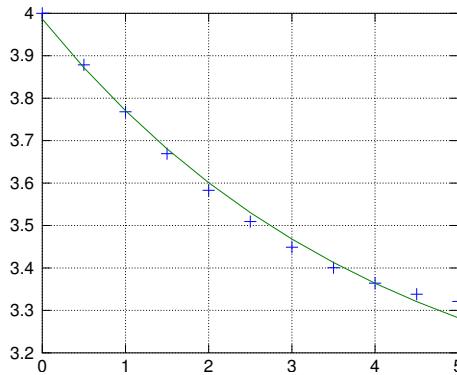


Figure 2.29: Nonlinear least square approximation with `fsolve()`

2.2.15 Nonlinear Regression with a Logistic Function

Many growth phenomena can be described by rescaling and shifting the basic logistic¹³ growth function $\frac{\exp(x)}{1+\exp(x)} = \frac{1}{1+\exp(-x)}$. Thus examine the logistic function

$$f(x) = p_1 + p_2 \frac{\exp(p_3(x - p_4))}{1 + \exp(p_3(x - p_4))} \quad (2.5)$$

with the four parameters p_i , $i = 1, 2, 3, 4$. An example is shown in Figure 2.30. For the given data points (in red) the optimal values for the parameters p_i have to be determined. This is a nonlinear regression problem.

An essential point for a nonlinear regression problems is to find good estimates for the values of the parameters. Thus we examine the graph of the logistic function (2.5) carefully:

- At the midpoint $x = p_4$ find $f(p_4) = p_1 + p_2 \frac{1}{2}$.
- For the extreme values observe $\lim_{x \rightarrow -\infty} f(x) = p_1$ and $\lim_{x \rightarrow +\infty} f(x) = p_1 + p_2$.
- The maximal slope is at the midpoint and given by¹⁴ $f'(p_4) = \frac{p_2 p_3}{4}$.

Assuming $p_2, p_3 > 0$ we can now find good estimates for the parameter values.

- p_1 offset: minimal height of the data points
- p_2 amplitude: difference of maximal and minimal value
- p_3 slope: the maximal slope is $m = \frac{p_2 p_3}{4}$ and thus $p_3 = \frac{4m}{p_2}$
- p_4 midpoint: average of x values

Based on this use the code below to determine the estimated values.

¹³Also called sigmoid function

¹⁴For $g(x) = \frac{\exp(x)}{1+\exp(x)}$ use $g'(0) = \frac{1}{4}$ and then some rescaling to determine $f'(p_4)$.

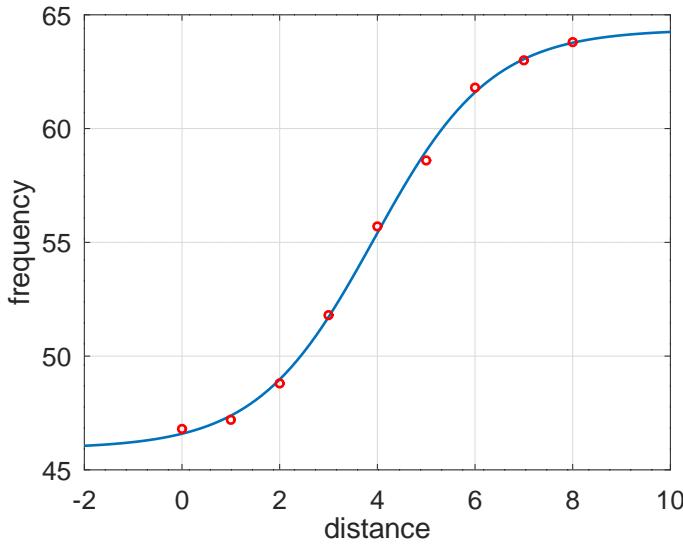


Figure 2.30: Data points and the optimal fit by a logistic function

```
x_data = [0 1 2 3 4 5 6 7 8]';
y_data = [46.8 47.2 48.8 51.8 55.7 58.6 61.8 63 63.8]';

p1 = min(y_data);
p2 = max(y_data)-min(y_data);
p3 = 4*max(diff(y_data)./diff(x_data))/p2;
p4 = mean(x_data);
```

This result can now be used to apply a nonlinear regression, using the functions `leasqr()`, `fsolve()` or `lsqcurvefit()`.

Solution by `leasqr()`

To determine the optimal values of the parameters:

- Define the logistic function, with the parameters p_i .
- Call `leasqr()`, returning the values and the covariance matrix. On the diagonal of the covariance matrix find the estimated variances of the parameters p_i .

Find the result in Figure 2.30. As numerical result the optimal values of p_i and their standard deviations are shown. In addition the number of required iterations and the resulting residual ($\sum_{i=1}^n (f(x_i) - y_i)^2)^{1/2}$ is displayed.

```
f = @(x,p) p(1) + p(2)*exp(p(3)*(x-p(4)))./(1+exp(p(3)*(x-p(4))));
[fr, p,~, iter,~, covp] = leasqr(x_data,y_data,[p1,p2,p3,p4],f);
optimal_values = [p';sqrt(diag(covp))'];
iter_residual = [iter,norm(fr-y_data)]
```

```
figure(1)
plot(x,f(x,p),x_data,y_data,'or')
xlabel('distance'); ylabel('frequency')
-->
optimal_values =
    45.931829    18.428664    0.838742    3.932786
    0.380858    0.645210    0.062353    0.080993
```

```
iter_residual = 4 0.64832
```

Solution by fsolve()

The command `fsolve()` is used to solve systems of nonlinear equations. If more data points than parameters are given (more equations than unknowns), then a nonlinear least square solution is determined. Thus we can solve the above problem using this command.

```
f2 = @(p) p(1) + p(2)*exp(p(3)*(x_data-p(4)))./(1+exp(p(3)*(x_data-p(4)))) - y_data;
[p, fval] = fsolve(f2,[p1,p2,p3,p4]);
optimal_values = p
residual = norm(fval)
→
optimal_values = 45.93183 18.42866 0.83874 3.93279
residual = 0.64832
```

It is no surprise that the same result is found. `fsolve()` does not estimate standard deviations for the parameters. One might use `nlpaci()` to determine confidence intervals.

Solution by lsqcurvefit()

With the command `lsqcurvefit()` the method of nonlinear least squares can be used to fit a function to data points. A solution for the above problem is given by

```
f3 = @(p, x_data) p(1) + p(2)*exp(p(3)*(x_data-p(4)))./(1+exp(p(3)*(x_data-p(4))));
[p, residual] = lsqcurvefit(f3,[p1,p2,p3,p4],x_data,y_data)
optimal_values = p
residual = sqrt(residual)
→
optimal_values = 45.93183 18.42866 0.83874 3.93279
residual = 0.64832
```

It is no surprise that the same result is found. `lsqcurvefit()` does not estimate standard deviations for the parameters.

2.2.16 Nonlinear Regression with an arctan Function

Similar to the previous section on can use a rescaled and shifted arctan function to describe a similar curve. The function for the regression is thus given by

$$f(x) = p_1 + p_2 \arctan(p_3(x - p_4)) \quad (2.6)$$

Examine for this function we observe:

- At the midpoint $x = p_4$ find $f(p_4) = 0$.
- For the extreme values $\lim_{x \rightarrow -\infty} f(x) = -\frac{\pi}{2}$ and $\lim_{x \rightarrow +\infty} f(x) = +\frac{\pi}{2}$ and
- The maximal slope is at the the midpoint and given by $f'(p_4) = p_2 p_3$.

Assuming $p_2, p_3 > 0$ we can now find good estimates for the parameter values.

- p_1 offset: average height of the data points
- p_2 amplitude: difference of maximal and minimal value, divided by π .

- p_3 slope: the maximal slope is $m = p_2 p_3$ and thus $p_3 = \frac{m}{p_2}$
- p_4 midpoint: average of x values

Based on this use the code below to determine the estimated values.

```
p1 = mean(y_data)
p2 = (max(y_data)-min(y_data))/pi
p3 = max(diff(y_data)./diff(x_data))/p2
p4 = mean(x_data)
```

This result can now be used to apply a nonlinear regression, using the functions `leasqr()`, `fsolve()` or `lsqcurvefit()`.

Solution by `leasqr()`

With the code below the optimal values for the parameters p_i and the estimated standard deviations are computed. In addition the number of required iterations and the resulting residual are shown. Find the result in Figure 2.31.

```
f = @(x,p) p(1) + p(2)*atan(p(3)*(x-p(4)));
[fr , p,~, iter,~, covp] = leasqr(x_data,y_data,[p1,p2,p3,p4],f);
optimal_values = [p';sqrt(diag(covp))']
iter_residum = [iter,norm(fr'-y_data)]
```



```
x = linspace(-2,10);
figure(1)
plot(x,f(x,p),x_data,y_data,'or')
xlabel('distance'); ylabel('frequency')
-->
optimal_values =
55.112684    7.731968    0.521908    3.917840
0.244363    0.481495    0.065494    0.106043
```



```
iter_residum = 4 0.79932
```

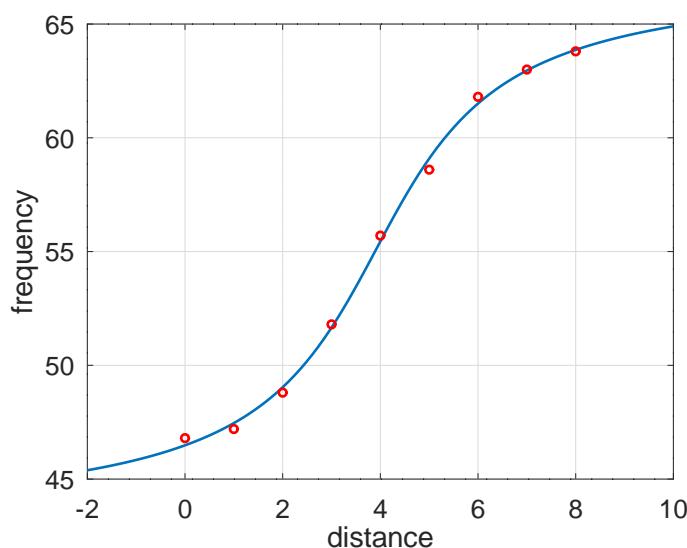


Figure 2.31: Data points and the optimal fit by an arctan function

The residual norm of 0.799 for the arctan function is larger than the residual norm of 0.648 for the approximation by a logistic function. Thus the approximation by an arctan function is slightly worse than the logistic approach.

Solution by `fsolve()`

We may again of `fsolve()` for an over determined system to apply the nonlinear regression algorithm.

```
f2 = @(p) p(1) + p(2)*atan(p(3)*(x_data-p(4)))-y_data;
[p,fval] = fsolve(f2,[p1,p2,p3,p4]);
optimal_values = p
residual = norm(fval)
->
optimal_values = 55.11278    7.73150    0.52198    3.91788
residual        = 0.79932
```

It is no surprise that the same result is found. `fsolve()` does not estimate standard deviations for the parameters.

Solution by `lsqcurvefit()`

With the command `lsqcurvefit()` the method of nonlinear least squares can be used to fit a function to data points. A solution for the above problem is given by

```
f3 = @(p,x_data) p(1) + p(2)*atan(p(3)*(x_data-p(4)));
[p,residual] = lsqcurvefit(f3,[p1,p2,p3,p4],x_data,y_data)
optimal_values = p
residual = sqrt(residual)
->
optimal_values = 55.11268    7.73197    0.52191    3.91784
residual        = 0.79932
```

It is no surprise that the same result is found. `lsqcurvefit()` does not estimate standard deviations for the parameters.

2.2.17 Approximation by a Tikhonov Regularization

A different approach to generate a function fitting the given data points (x_i, y_i) is given by a Tikhonov regularization. For given parameters $\lambda_1 \geq 0$ and $\lambda_2 \geq 0$ find the function $u(x)$ minimizing the functional

$$F(\lambda_1, \lambda_2) = \sum_{i=1}^n (u(x_i) - y_i)^2 + \lambda_1 \int_{-2}^{10} (u'(x))^2 dx + \lambda_2 \int_{-2}^{10} (u''(x))^2 dx$$

Your author¹⁵ has an Octave command solving this problem and the code below leads to Figure 2.32. The shape of the solution can be modified by changing the values of $\lambda_1 = 0.1$ and $\lambda_2 = 0.03$. The residual of 0.413 is smaller than the residuals by the nonlinear regression approaches. An additional advantage of the regularization approach is that one does not have to choose the type of function, i.e. arctan or logistic.

¹⁵Additional documentation is available on request.

```

x_data = [0 1 2 3 4 5 6 7 8];
y_data = [46.8 47.2 48.8 51.8 55.7 58.6 61.8 63 63.8];

F1.lambda = 1e-1;
F2.lambda = 3e-2;
[x,y] = regularization([x_data ',y_data '],[-2,10],100,F1,F2);

figure(1)
plot(x,y,x_data ,y_data , 'or')
xlabel('distance'); ylabel('frequency')

y_fit = interp1(x,y,x_data );
residual = norm(y_fit-y_data )
→
residual = 0.41310

```

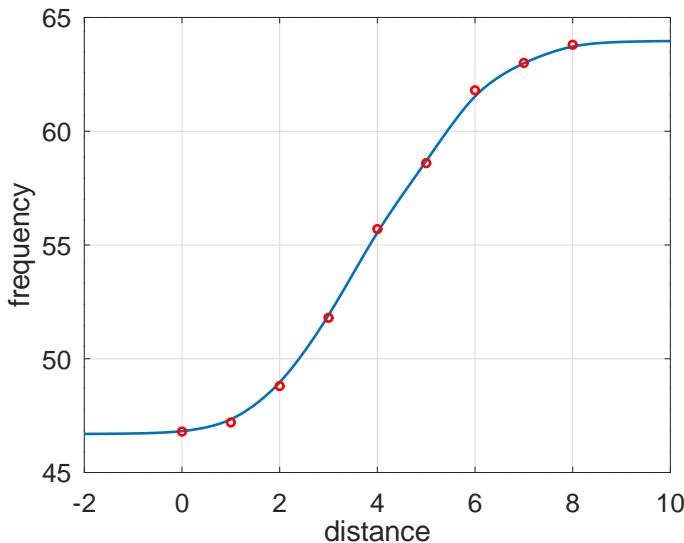


Figure 2.32: Data points and the optimal fit by a Tikhonov regularization

2.2.18 A Real World Nonlinear Regression Problem

For her Bachelor project Linda Welter had to solve a nontrivial nonlinear regression problem. The dependent variable was assumed to be the sum of a linear function and a trigonometric function with exponentially decaying amplitude. For a given set of points examine 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 forward application for the function `leasqr()`, presented in the previous section. Thus we run the code below¹⁶.

Octave

```

ReadData % 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;

```

¹⁶The presented code works with Octave, for MATLAB minor adaptations are required.

```

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

```

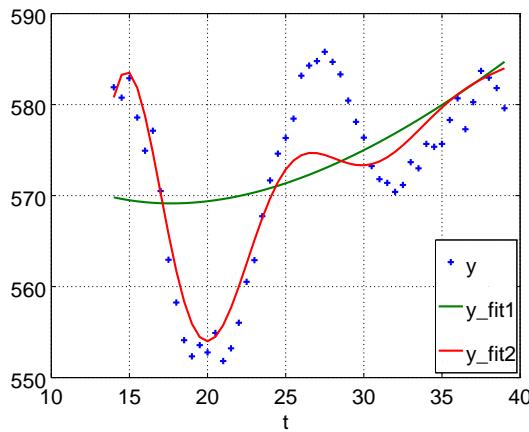


Figure 2.33: Raw data and two failed attempts of nonlinear regression

This first result (green curve in Figure 2.33) 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 (red) in Figure 2.33.

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 determine 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 a 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.

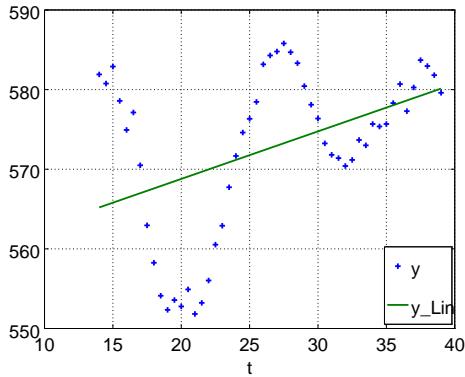
1. Using `LinearRegression()` we fit a straight line through the given data points.

Octave

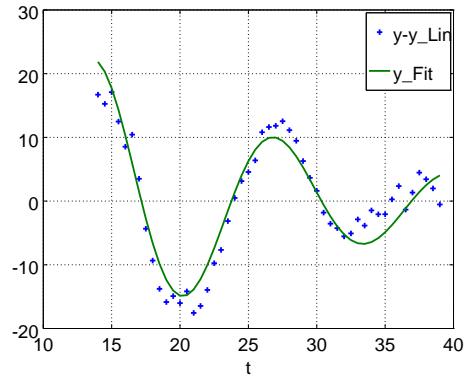
```
%%% fitting a straight line
F = ones(length(t),2); F(:,2) = t;
pLin = LinearRegression(F,y)
yLin = F*pLin;

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 2.34(a).



(a) the straight line fit



(b) exponential regression to difference

Figure 2.34: Regression by a straight line and an exponentially decaying trigonometric function

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 fitting function. The initial parameters are estimated by using Figure 2.34(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

$$y(t) - y_{lin}(t) \approx 51 \exp(-0.06t) \cdot \cos(0.477t - 13)$$

The estimated standard deviations of the parameters are rather large, e.g. for the initial amplitude 51.1 ± 8.6 . Now we can generate Figure 2.34(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 2.35 is obviously superior to the naive attempt shown in Figure 2.33 .

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.

2.2.19 New Functions `lsqcurvefit` and `lsqnonlin`

The above nonlinear problems can probably be solved by the MATLAB/Octave functions `lsqcurvefit()` and/or `lsqnonlin()` too. For a project I used `nlpaci()` to determine the confidence interval, this function is not available yet in Octave.

In Octave those two functions use the more general functions `nonlin_curvefit` and `nonlin_residmin`.

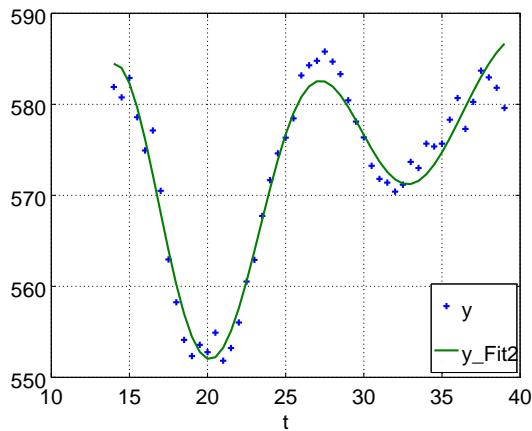


Figure 2.35: The optimal fit, using nonlinear regression

2.2.20 List of codes and data files

In the previous section the codes and data files in Table 2.8 were used.

2.2.21 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

file name	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 analyze 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
Pfaff.m	code for the two spring system
wegmessung1.dat	data the two spring system
kraftmessung1.dat	data the two spring system
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 2.8: Codes and data files for section 2.2

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 2.2.14 with the help of `fsolve()`, i.e. use Section 2.2.14.

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) $\text{cities}(t) = -14.5 + 11.6 t$ where $t = \text{year} - 1994$
- (b) a graphic
- (c) at $t = 251$, i.e. in the year 2245

Exercise 2.2–6 Nova Energy, quadratic

- (a) $\text{cities}(t) = 0.136 + 0.577 t + 1.22 t^2$ where $t = \text{year} - 1994$
- (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 $\text{cities}(t) = 1.85 + e^{0.502 t}$.
- (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; a10 = 0; omega0 = 1; phi0 = pi/2;
% [fr,p]=leasqr(t,y,[A0,a10,omega0,phi0],'f',1e-10); p'
[p, fval, info, output] = fsolve(@(p)(f(t,p)- y), [A0,a10,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 up with the problem to minimize the length of the vector \vec{r} . This leads to the formulation in Figure 2.36.

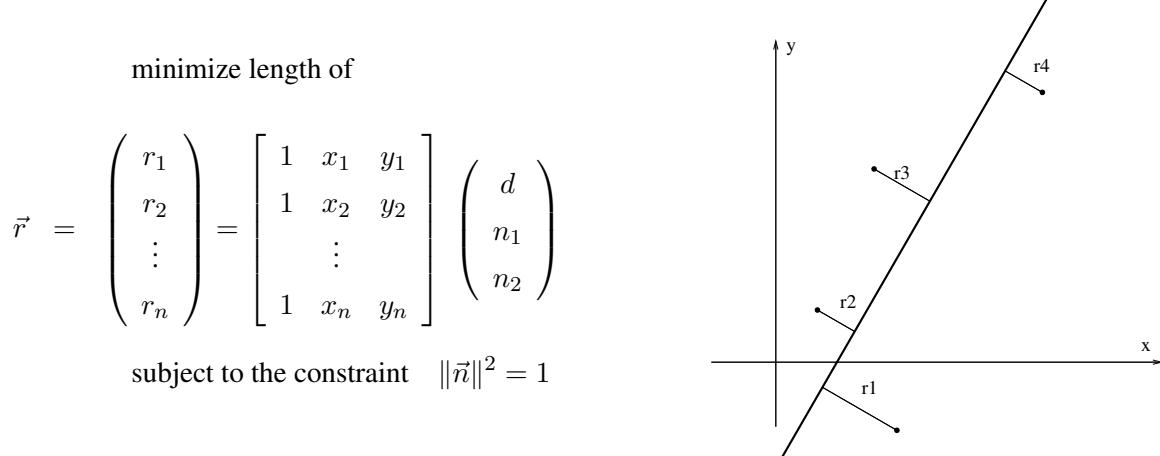


Figure 2.36: A straight line with minimal distance from a set of given points

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

$$\mathbf{F} \cdot \vec{p} = \vec{r} \quad \text{subject to} \quad \|\vec{n}\| = 1 \quad \text{where} \quad \vec{p} = \begin{pmatrix} \vec{d} \\ \vec{n} \end{pmatrix} \in \mathbb{R}^{m_1+m_2} \quad (2.7)$$

The algorithm is based on a QR factorization and one might consult Section 2.2.6.

$$\mathbf{F} \cdot \vec{p} = \mathbf{Q} \cdot \mathbf{R} \cdot \vec{p}$$

The matrix \mathbf{R} may be written in 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

$$\mathbf{R}_{2,2} = \mathbf{U} \cdot \begin{bmatrix} \sigma_1 & & & \\ & \sigma_2 & & \\ & & \ddots & \\ & & & \sigma_k \end{bmatrix} \cdot \mathbf{V}^T \quad \text{where } \sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_k > 0$$

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 (2.7).

Weighted regression with constraint

The result in the previous section can be modified to take weights of the different points into account. Instead 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 be 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 2.37.

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,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
y_var = sum((residual.^2).*(weight.^4))/(n-m+nn);

```

Figure 2.37: 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 2.38 with the slightly smaller slope minimizes the vertical distances to the given set of points.

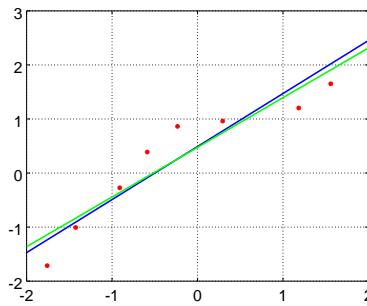


Figure 2.38: Some points with optimal vertical and orthogonal distance fit

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

$$\vec{r} = \begin{pmatrix} r_1 \\ r_2 \\ \vdots \\ r_n \end{pmatrix} = \begin{bmatrix} 1 & x_1 & y_1 & z_1 \\ 1 & x_2 & y_2 & z_2 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & x_n & y_n & z_n \end{bmatrix} \begin{pmatrix} d \\ n_1 \\ n_2 \\ n_3 \end{pmatrix}$$

subject to the constraint $\|\vec{n}\|^2 = 1$. This situation is similar to Figure 2.36 and thus we can use the command `RegressionConstraint()`. As a demo we first generate a cloud of points almost on a plane and display the points in space in Figure 2.39.

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');
```

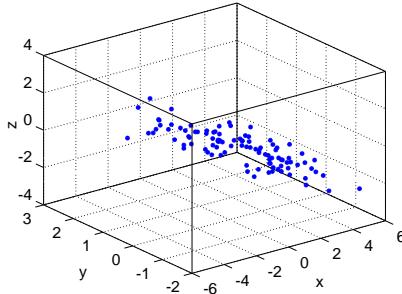


Figure 2.39: A cloud of points, almost on a plane

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

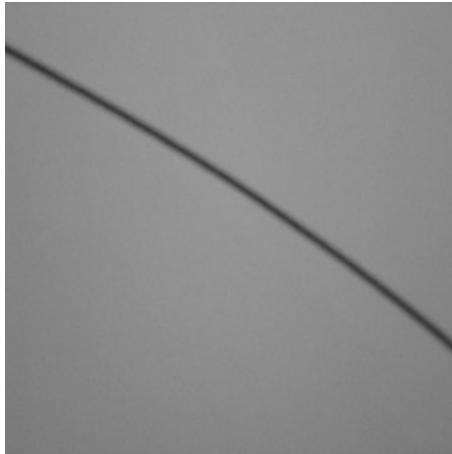
$$\vec{n} \approx \begin{pmatrix} -0.468 \\ -0.555 \\ -0.688 \end{pmatrix} \quad \text{and} \quad d \approx 0.0073$$

2.3.5 Identification of a straight line in a digital image

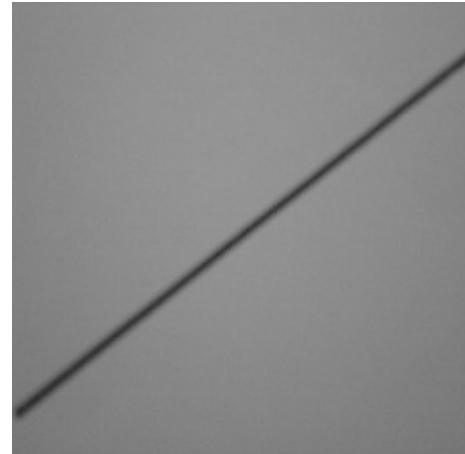
The above method of regression with constraint and weights can be used to identify the parameters of a straight line in a digital image. The basic idea is to use a weighted linear regression where dark points have a large weight and white spots will have no weight.

In Figure 2.40 find photographs of two lines, a freehand version (2.40(a)) and one generated with a ruler (2.40(b)). 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
```



(a) freehand line



(b) straight line by ruler

Figure 2.40: Two photographs of (almost) straight 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 2.40 is of the form

$$\begin{aligned}0 &= 17.02256 + 0.55381x - 0.83264y \\y &= 20.44404 + 0.66513x\end{aligned}$$

- 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 $\sqrt{6.26 \cdot 10^{-7}} \approx 0.0008 \approx 0.05^\circ$.

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 rerun with the image in Figure 2.40(b). The only change is to replace the file name `Line1.bmp` by `Line2.bmp`.

2.3.6 Example 2: Fit an ellipse through some given points in the plane

Ellipse, axes parallel to coordinate axes

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.

$$\begin{aligned} \frac{(x - x_0)^2}{a^2} + \frac{(y - y_0)^2}{b^2} &= 1 \\ \left\langle \begin{bmatrix} 1/a & 0 \\ 0 & 1/b \end{bmatrix} \begin{pmatrix} x - x_0 \\ y - y_0 \end{pmatrix}, \begin{bmatrix} 1/a & 0 \\ 0 & 1/b \end{bmatrix} \begin{pmatrix} x - x_0 \\ y - y_0 \end{pmatrix} \right\rangle &= 1 \\ \frac{1}{a^2} x^2 - \frac{2x_0}{a^2} x + \frac{1}{b^2} y^2 - \frac{2y_0}{b^2} y + \frac{x_0^2}{a^2} + \frac{y_0^2}{b^2} &= 1 \end{aligned}$$

From the last form we could conclude that the search for an ellipse passing through a set of given points might be formulated as a regression problem¹⁷. Multiply the equation by a^2 and set $\gamma = \frac{a}{b}$ to find the equivalent equation

$$\begin{aligned} x^2 - 2x_0 x + \frac{a^2}{b^2} y^2 - \frac{2a^2 y_0}{b^2} y + x_0^2 + \frac{a^2 y_0^2}{b^2} &= a^2 \\ x^2 - 2x_0 x + \gamma^2 y^2 - 2y_0 \gamma^2 y + x_0^2 + \gamma^2 y_0^2 - a^2 &= 0 \end{aligned}$$

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.

$$\begin{aligned} -2x_0 &= p_1 \\ \frac{a^2}{b^2} = \gamma^2 &= p_2 \\ -2y_0 \gamma^2 &= p_3 \\ x_0^2 + \gamma^2 y_0^2 - a^2 &= p_4 \end{aligned}$$

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))
```

¹⁷A straight linear regression in the above form will fail, since there is a constant contribution $\frac{x_0^2}{a^2} + \frac{y_0^2}{b^2}$ on the left hand side. If we would know that $x_0 = y_0 = 0$ then a linear regression of the form $p_1 x^2 + p_2 y^2 = 1$ would work just fine. If a general orientation is asked for use $p_1 x^2 + p_2 y^2 + p_3 x y = 1$

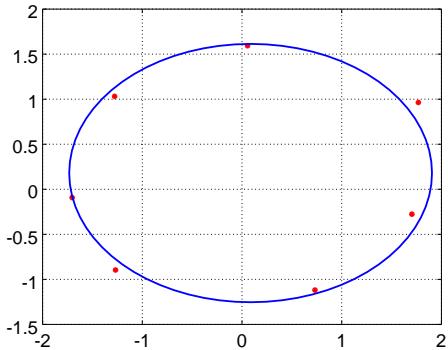
With the computed parameters

$$x_0 = 0.15032, \quad y_0 = -0.17548, \quad a = 1.7109 \quad \text{and} \quad b = 0.79109$$

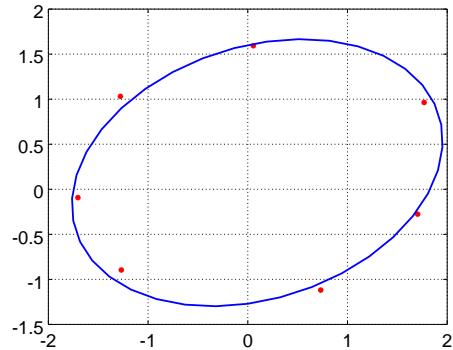
we can draw the ellipse, leading to the left half of Figure 2.41.

Octave

```
phi = (0:5:360)'*pi/180;
x = x0+a*cos(phi);
y = y0+b*sin(phi);
plot(xi,yi,'*r',x,y,'b');
```



(a) parallel axis



(b) general orientation

Figure 2.41: Some points and best fit ellipses, parallel to axes and general orientation

Ellipse with general orientation

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

$$\left\langle \begin{bmatrix} 1/a & 0 \\ 0 & 1/b \end{bmatrix} \begin{pmatrix} x - x_0 \\ y - y_0 \end{pmatrix}, \begin{bmatrix} 1/a & 0 \\ 0 & 1/b \end{bmatrix} \begin{pmatrix} x - x_0 \\ y - y_0 \end{pmatrix} \right\rangle = 1$$

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

$$\begin{aligned}
 1 &= \langle \mathbf{M} \cdot \begin{pmatrix} x - x_0 \\ y - y_0 \end{pmatrix}, \mathbf{M} \cdot \begin{pmatrix} x - x_0 \\ y - y_0 \end{pmatrix} \rangle \\
 &= \left\langle \begin{pmatrix} x - x_0 \\ y - y_0 \end{pmatrix}, \begin{bmatrix} \frac{n_1^2}{a^2} + \frac{n_2^2}{b^2} & \frac{-n_1 n_2}{a^2} + \frac{n_1 n_2}{b^2} \\ \frac{-n_1 n_2}{a^2} + \frac{n_1 n_2}{b^2} & \frac{n_2^2}{a^2} + \frac{n_1^2}{b^2} \end{bmatrix} \begin{pmatrix} x - x_0 \\ y - y_0 \end{pmatrix} \right\rangle \\
 &= \left\langle \begin{pmatrix} x - x_0 \\ y - y_0 \end{pmatrix}, \mathbf{A} \cdot \begin{pmatrix} x - x_0 \\ y - y_0 \end{pmatrix} \right\rangle \\
 &= \left\langle \begin{pmatrix} x \\ y \end{pmatrix}, \mathbf{A} \cdot \begin{pmatrix} x \\ y \end{pmatrix} \right\rangle - 2 \left\langle \begin{pmatrix} x_0 \\ y_0 \end{pmatrix}, \mathbf{A} \cdot \begin{pmatrix} x \\ y \end{pmatrix} \right\rangle + \left\langle \begin{pmatrix} x_0 \\ y_0 \end{pmatrix}, \mathbf{A} \cdot \begin{pmatrix} x_0 \\ y_0 \end{pmatrix} \right\rangle
 \end{aligned}$$

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 2.41.

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 \mathbf{x}_i and \mathbf{y}_i .

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 2.42.

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

```

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:

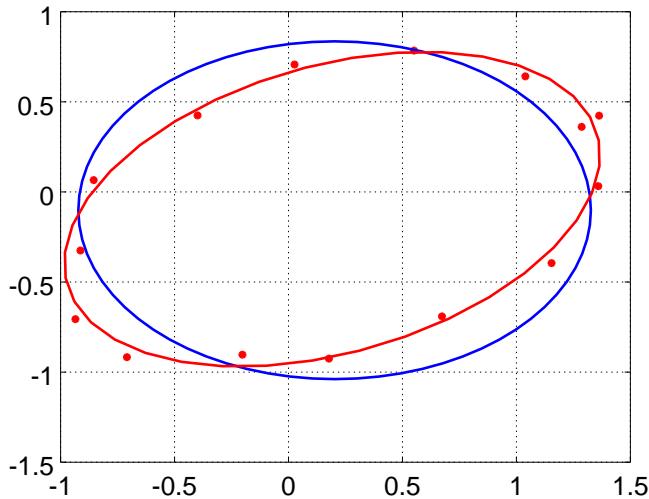


Figure 2.42: Some random points and a best fit ellipses, parallel to axes and general

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 2.9 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 compare the two methods
EllipseClick.m	script file to read points with mouse and fit ellipses

Table 2.9: 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 2.40. 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_i) where $1 \leq i \leq n$.

Exercise 2.3–3 Circle, arbitrary 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_i) 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.

$$\begin{aligned} \text{minimize } \|\vec{r}\|^2 &= \sum_{k=1}^n ((x_k^2 + y_k^2) p - 1)^2 = \sum_{k=1}^n ((x_k^2 + y_k^2)^2 p^2 - 2(x_k^2 + y_k^2)p + 1) \\ \frac{\partial}{\partial p} \|\vec{r}\|^2 = 0 &= \sum_{k=1}^n (2(x_k^2 + y_k^2)^2 p - 2(x_k^2 + y_k^2)) \\ p &= \frac{\sum_{k=1}^n (x_k^2 + y_k^2)}{\sum_{k=1}^n (x_k^2 + y_k^2)^2} \\ R^2 &= \frac{\sum_{k=1}^n (x_k^2 + y_k^2)^2}{\sum_{k=1}^n (x_k^2 + y_k^2)} \end{aligned}$$

Exercise 2.3–3 Circle, arbitrary center

The equation of a circle with radius R is given by

$$\begin{aligned} (x - x_0)^2 + (y - y_0)^2 - R^2 &= 0 \\ x^2 + y^2 - 2x_0 x - 2y_0 y + x_0^2 + y_0^2 - R^2 &= 0 \end{aligned}$$

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

$$p_1 = -2x_0, \quad p_2 = -2y_0 \quad \text{and} \quad p_3 = +x_0^2 + y_0^2 - R^2$$

Thus we try to minimize the length of

$$\left[\begin{array}{ccc} x_1 & y_1 & 1 \\ x_2 & y_2 & 1 \\ \vdots & & \\ x_n & y_n & 1 \end{array} \right] \cdot \begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix} + \begin{pmatrix} x_1^2 + y_1^2 \\ x_2^2 + y_2^2 \\ \vdots \\ x_n^2 + y_n^2 \end{pmatrix} = \begin{pmatrix} r_1 \\ r_2 \\ \vdots \\ r_n \end{pmatrix}$$

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 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 in 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 subtractions 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.
 - 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 $y = f(x) = 1 - 0.8x^2$ for $0 \leq x \leq 2$ on an 16-bit processor, assuming that for x and y we need an 8-bit resolution. The code is developed with MATLAB/Octave and we first generate a graph of the function.

```

x = linspace(0,2,1001);
%function y = f(x) % test function
% y = 1 - 0.8*x.^2;
%endfunction
f = @(x)1-0.8*x.^2;
y = f(x);

figure(1)
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 $-3 \leq y \leq 1$ 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 $0 \leq x \leq 2$. To use an 8-bit resolution we pass the values $x8 = x \cdot 2^6 = x \cdot 64$. We know $0 \leq x8 \leq 127$ and thus we use it as an `int8` data type.

```
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.

```
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 2^16 (uint16)
→
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.

```
% 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 $2^5 = 32$.

```
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.

```
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.

```
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 2.43, but for a good implementation in an actual device some further aspect have to be taken into account.

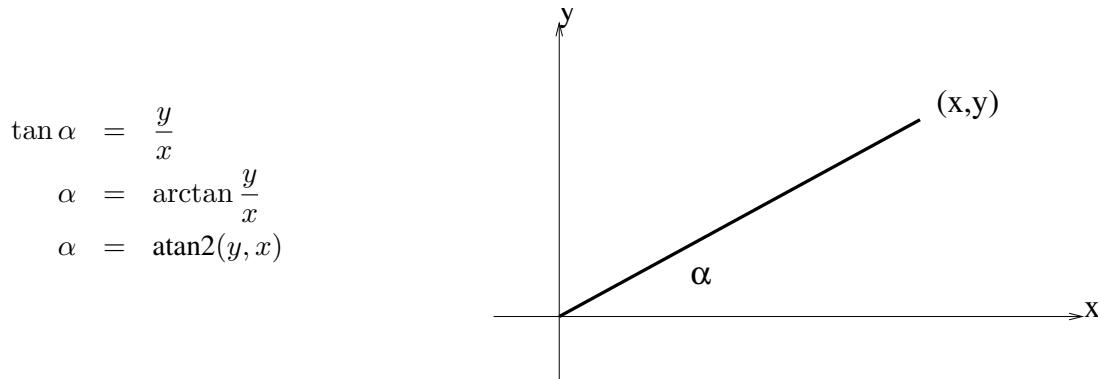


Figure 2.43: The angle α as function of x and y

- 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

$$\begin{aligned}
 V(\alpha) &= \frac{1}{r^4} (y^2 V(x) + x^2 V(y)) \\
 \sigma_\alpha &= \frac{1}{r^2} \sqrt{y^2 \sigma_x^2 + x^2 \sigma_y^2}
 \end{aligned}$$

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 influenced by the hardware (e.g. resolution of AD converters) and might be determined by statistical methods, see also Section 2.2.11.

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 2.44.

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	$x \leq 0$	$y > 0$	$ x \leq y$	$\alpha = \frac{\pi}{2} + \arctan \frac{-x}{y}$
4	$x < 0$	$y \geq 0$	$y \leq x $	$\alpha = \pi - \arctan \frac{y}{-x}$
5	$x < 0$	$y \leq 0$	$ y \leq x $	$\alpha = -\pi + \arctan \frac{-y}{-x}$
6	$x \leq 0$	$y < 0$	$ x \leq y $	$\alpha = -\frac{\pi}{2} - \arctan \frac{-x}{-y}$
7	$x \geq 0$	$y < 0$	$ x \leq y $	$\alpha = -\frac{\pi}{2} + \arctan \frac{x}{-y}$
8	$x > 0$	$y \leq 0$	$ y \leq x $	$\alpha = -\arctan \frac{-y}{x}$

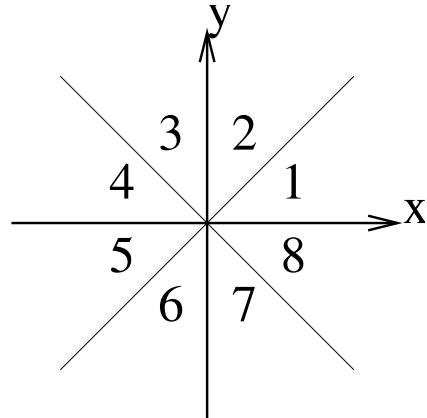


Figure 2.44: The eight sectors used to compute $\tan \alpha = \frac{y}{x}$

Using the table in Figure 2.44 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/MATLAB.

```
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

$$\arctan z = \sum_{k=0}^n \frac{(-1)^k}{2k+1} z^{2k+1} + R_n$$

where the approximation error is $|R_n| \approx \frac{1}{2k+3} z^{2k+3}$. Since we examine $0 \leq z \leq 1$ we would need $2k+3 \approx 500$, 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

$$\begin{aligned}\arctan z &\approx -0.003113205848 + 1.073115615 z - 0.283642707 z^2 \\ &= -0.003113205848 + z(1.073115615 - z \cdot 0.283642707)\end{aligned}$$

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

$$\arctan z \approx -0.0031 + z(1.0731 - z \cdot 0.2836) \quad \text{for } 0 \leq z \leq 1$$

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.

```
a0 = 0.283642707;      i0 = uint16(a0*2^8)
a1 = 1.073115615;      i1 = uint16(a1*2^15)
a2 = 0.003113205848;   i2 = uint16(a2*2^16)

myatan = @(z)-0.003113205848 + z.*(
    1.073115615 - z*0.283642707);
```

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.

```
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}

```
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}

```
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}

```
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}

```
r4 = uint16(r3-i2);
limits4 = [min(r4) max(r4)]
```

This result is converted back to floats and then Figure 2.45 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 2.45 shows that the contributions from the Chebyshev approximation and the integer arithmetic are both of the same size.

```
res = single(r4)/2**16;
plot(z,res-atan(z), 'r', z, myatan(z)-atan(z), 'b')
legend('int16', 'float')
xlabel('z'); ylabel('difference')
grid on; legend('show')
```

This can all be crammed into one lengthy formula

$$\arctan z \approx 2^{-16} (-0.0031 \cdot 2^{16} + (z \cdot 2^8) \cdot (2^{-7}(1.0731 \cdot 2^{15} - 2^{-1}(z \cdot 2^8) \cdot (0.2836 \cdot 2^8))))$$

but for an implementation it is wise to use the above description.

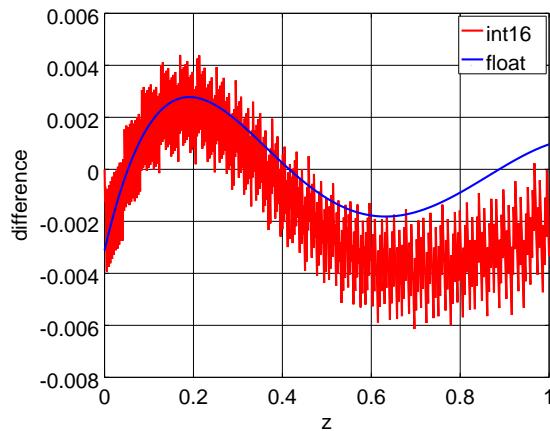


Figure 2.45: Comparison of errors for a Chebyshev approximation and its integer implementation

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.

```
zc = linspace(0,1,256);
atantab = round(atan(zc)*255*4/pi);
```

For a given value of $0 \leq z \leq 1$ 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.

```
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;
end%for

figure(1);
plot(z,res-atan(z), 'r')
grid on; legend('difference')
```

The resulting Figure 2.46 shows a maximal error of approximately 0.003, which corresponds to 0.17° .

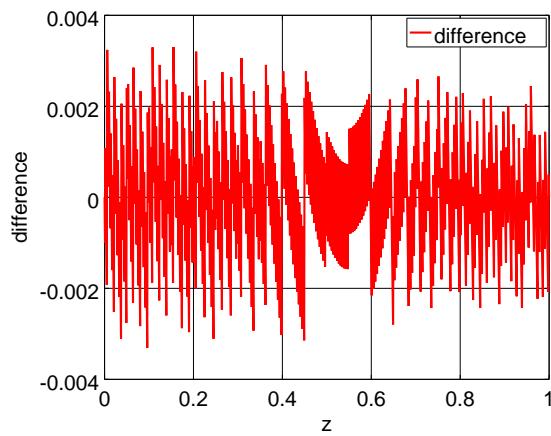


Figure 2.46: The difference for a tabulated approximation of the arctan–function

Piecewise linear interpolation

Lets us divide the interval $0 \leq z \leq 1$ 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 $i = 0, 1, 2, \dots, n$. 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 2.47 the interpolated value is given by

$$f(z_i + \Delta z) \approx f(z_i) + \frac{f(z_{i+1}) - f(z_i)}{z_{i+1} - z_i} \Delta z = f(z_i) + m_i \cdot \Delta z \quad (2.8)$$

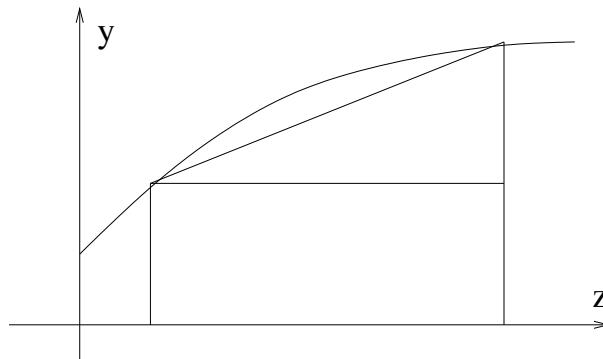


Figure 2.47: Linear interpolation of a function

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

$$|\text{error}| \leq \frac{1}{8} M_2 h^2$$

where M_2 is the maximal absolute value of the second derivative of the function. For our function $f(z) =$

$\arctan z$ with $0 \leq z \leq 1$ we have to determine M_2 by the calculations below.

$$\begin{aligned} f''(z) &= \frac{-2z}{(1+z^2)^2} \\ f'''(z) &= \frac{-2(1+z^2)^2 + 8z^2(1+z^2)}{(1+z^2)^2} = 2 \frac{-1-z^2+4z^2}{(1+z^2)} = 0 \\ z_m &= \frac{1}{\sqrt{3}} \\ M_2 &= |f''(1/\sqrt{3})| = \frac{2/\sqrt{3}}{(1+1/3)^2} = \frac{3\sqrt{3}}{8} \approx 0.64 < 1 \end{aligned}$$

If we divide the interval $0 \leq z \leq 1$ into $2^5 = 32$ subintervals of equal length we find $h = \frac{1}{32}$ and thus

$$|\text{error}| \leq \frac{1}{8} M_2 h^2 \leq \frac{1}{8 \cdot 32^2} \approx 1.3 \cdot 10^{-4}$$

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 (2.8) 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 $i = 0, 1, \dots, 31$ 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 $i = 0, 1, \dots, 31$ 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 addition¹⁸. The code below is one possible implementation and leads to Figure 2.48. The maximal error of $1.2 \cdot 10^{-4}$ leads to a value of $\text{bitaccuracy} \approx -12.9$ and thus we find at least 12-bit resolution of this implementation.

LinearInterpol.m

```

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));
end%for

res = res/2^(31);

figure(1);
plot(z,res-atan(z), 'r')
legend('difference')
grid on
accuracybits = log(max(abs(res-atan(z))*4/pi))/log(2)

```

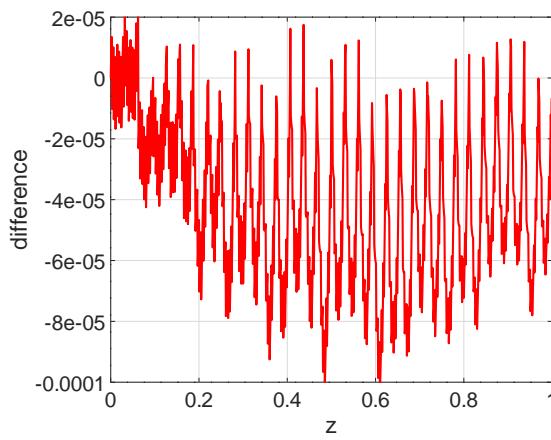


Figure 2.48: The errors for a piecewise linear approximation of the arctan–function

Figure 2.47 and the graph of $\arctan z$ explain why the piecewise linear interpolation is below the actual function. Thus the error in Figure 2.48 is everywhere negative. Since we have an estimate for the maximal

¹⁸This 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 ($0 \leq z \leq 2^{16} - 1 = 65535$), return an integer value y ($0 \leq y \leq 2^{15} - 1 = 32767$), 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 fractional 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 2.10 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 two other options in Table 2.10 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 2.10 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 2.10: Comparison of 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.

$$\begin{aligned} \cos(+\alpha + n\alpha) &= \cos(\alpha) \cos(n\alpha) - \sin(\alpha) \sin(n\alpha) = x T_n(x) - \sin(\alpha) \sin(n\alpha) \\ \cos(-\alpha + n\alpha) &= \cos(-\alpha) \cos(n\alpha) + \sin(\alpha) \sin(n\alpha) = x T_n(x) + \sin(\alpha) \sin(n\alpha) \\ T_{n+1}(x) + T_{n-1}(x) &= 2x T_n(x) \\ T_{n+1}(x) &= 2x T_n(x) - T_{n-1}(x) \end{aligned}$$

This leads to

$$\begin{aligned} T_0(x) &= \cos(0) = 1 \\ T_1(x) &= \cos(\arccos(x)) = x \\ T_2(x) &= 2x(x) - 1 = 2x^2 - 1 \\ T_3(x) &= 2x(2x^2 - 1) + x = 4x^3 - 3x \\ T_4(x) &= 2x(4x^3 - 3x) - 2x^2 + 1 = 8x^4 - 8x^2 + 1 \\ &\vdots \end{aligned}$$

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;
    end%for
end%if

```

The code below will generate the graphs of the first few Chebyshev polynomials in Figure 2.49.

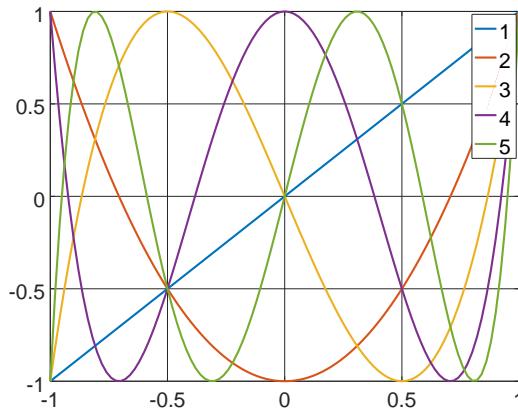


Figure 2.49: Graphs of the first 5 Chebyshev polynomials

```

nn = 5; x = -1:0.02:1; y = zeros(nn,length(x));
for n = 1:nn
    y(n,:) = polyval(Chebyshev(n),x);
end%for
plot(x,y)
legend('1','2','3','4','5')

```

Orthogonality of the Chebyshev polynomials

These polynomials are orthogonal on the interval $[-1, 1]$ with respect to the integration weight $1/\sqrt{1-x^2}$.

$$\begin{aligned}
 \langle T_n(x), T_m(x) \rangle &= \int_{-1}^1 T_n(x) T_m(x) \frac{1}{\sqrt{1-x^2}} dx \\
 &= \int_{-1}^1 \cos(n \cdot \arccos(x)) \cos(m \cdot \arccos(x)) \frac{1}{\sqrt{1-x^2}} dx \\
 \text{substitution} \quad \cos \phi &= x \quad , \quad -\sin(\phi) \frac{d\phi}{dx} = 1 \quad , \quad \sqrt{1-x^2} = \sqrt{1-\cos^2(\phi)} = \sin(\phi) \\
 &= \int_{\pi}^0 \cos(n \phi) \cos(m \phi) \frac{-\sin(\phi)}{\sin(\phi)} d\phi \\
 &= \int_0^{\pi} \cos(n \phi) \cos(m \phi) d\phi = 0 \quad \text{if } n \neq m \\
 \langle T_n(x), T_n(x) \rangle &= \int_0^{\pi} \cos(n \phi) \cos(n \phi) d\phi = \frac{\pi}{2} \quad \text{if } n \geq 1
 \end{aligned}$$

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

$$\begin{aligned}
 \frac{\pi}{2} c_n &= \int_{-1}^1 f(x) T_n(x) \frac{1}{\sqrt{1-x^2}} dx \\
 &= \int_{-1}^1 f(x) \cos(n \cdot \arccos(x)) \frac{1}{\sqrt{1-x^2}} dx \\
 \text{substitution} \quad \cos \phi &= x \quad , \quad -\sin(\phi) \frac{d\phi}{dx} = 1 \quad , \quad \sqrt{1-x^2} = \sqrt{1-\cos^2(\phi)} = \sin(\phi) \\
 &= \int_{\pi}^0 f(\cos(\phi)) \cos(n \phi) \frac{-\sin(\phi)}{\sin(\phi)} d\phi \\
 &= \int_0^{\pi} f(\cos(\phi)) \cos(n \phi) d\phi
 \end{aligned}$$

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

$$\begin{aligned}
 z &= -1 + 2 \frac{x-a}{b-a} \quad a \leq x \leq b \\
 x &= a + \frac{1}{2} (z+1)(b-a) = \frac{a+b}{2} + z \frac{b-a}{2} \\
 g(z) &= f\left(\frac{a+b}{2} + z \frac{b-a}{2}\right) \quad -1 \leq z \leq 1
 \end{aligned}$$

and then the coefficients for this new function $g(z)$ have to be computed. We find

$$f(x) = g(z) = \frac{c_0}{2} + \sum_{n=1}^N c_n T_n(z) = \frac{c_0}{2} + \sum_{n=1}^N c_n T_n\left(-1 + 2 \frac{x-a}{b-a}\right) \quad (2.9)$$

Octave code

The above results are readily implemented in Octave for the exemplary function $f(x) = \arctan(x)$ on the interval $A = 0 \leq x \leq 1 = B$.

```
%>> %% compute the Chebyshev approximation of order n of the function fun
n = 2;
accuracy = 1e-8; % accuracy for the numerical integration
A = 0; % left endpoint
B = 1; % right endpoint
fun = @(x) atan(x); % function to be approximated
```

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.

```
%>> % redefine function on standard interval [-1,1]
newFun = @(x,A,B)fun(A+0.5*(x+1)*(B-A));

% function to be integrated
intFun = @(p,A,B,k)newFun(cos(p),A,B).*cos(k*p)

c = zeros(n+1,1);
c(1) = quad(@(p)intFun(p,A,B,0),0,pi,accuracy)*1/pi;
for k = 1:n
    c(k+1) = quad(@(p)intFun(p,A,B,k),0,pi,accuracy)*2/pi;
end%for

coeff = zeros(n+1,n+1);
for i = 1:n+1;
    coeff(i,n-i+2:n+1) = Chebyshev(i-1);
end%for

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 (2.9) and seek the coefficients p_k such that

$$y_i = g\left(-1 + i \frac{2}{n}\right) = p(x_i) = p\left(A + i \frac{B - A}{n}\right) = \sum_{k=0}^n p_k x_i^k \quad \text{for } i = 0, 1, 2, 3, \dots, n$$

This can be regarded as a system of $n + 1$ linear equations with a Vandermonde matrix.

$$\begin{bmatrix} x_0^n & x_0^{n-1} & x_0^{n-2} & \dots & 1 \\ x_1^n & x_1^{n-1} & x_1^{n-2} & \dots & 1 \\ x_2^n & x_2^{n-1} & x_2^{n-2} & \dots & 1 \\ \vdots & & \ddots & \vdots & \\ x_n^n & x_n^{n-1} & x_n^{n-2} & \dots & 1 \end{bmatrix} \cdot \begin{pmatrix} p_n \\ p_{n-1} \\ p_{n-2} \\ \vdots \\ p_0 \end{pmatrix} = \begin{pmatrix} y_0 \\ y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}$$

This is easily implemented in *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 2.45.

```
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 2.11 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 to 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 2.11: Codes and data files 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 2.10 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 $0 \leq z \leq 1$. 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

$$\begin{aligned}\arctan z \approx & -0.00007717176023065795 + 1.0031357062620350346 z - 0.015262708673125458 z^2 \\ & - 0.34245381909783135 z^3 + 0.14017184670506358 z^4\end{aligned}$$

shows a maximal error of 0.0001 for $0 \leq z \leq 1$. Since $\log_2\left(\frac{0.0001^4}{\pi}\right) \approx -13$ this approximation might allow 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 2.10 with the information on this algorithm.

Exercise 2.4–4 Piecewise quadratic interpolation

Use a piecewise quadratic interpolation for the function $f(z) = \arctan z$ on the intervall $0 \leq z \leq 1$ with 32 subintervals of equal length. The interpolation error ist estimated by

$$|\text{error}| \leq \frac{1}{6} M_3 h^3$$

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.

- Determine the coefficients of the approximating polynomial.
- 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

```
Chebyshev3.m
```

```

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)

myatan = @(z)-0.0011722644 +z.* (1.038178669 + z.* (-0.1904775175-z*0.06211012633));

z = 0:0.001:1;
zi = int32(z*2^15);

r1 = int32(zi.*i0); %% 15+16
limits1 = [min(r1) max(r1)]

r2 = 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 = 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)]

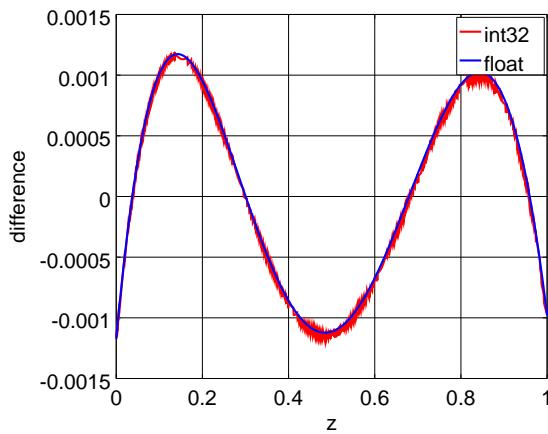
r6 = int16(bitshift(r5,-15))+i3; %% 29-15
limits6 = [min(r4) max(r4)]

res = single(r6)*2^-14;

plot(z,res-atan(z), 'r', z, myatan(z)-atan(z), 'b')
legend('int32', '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

```
// 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

Chebyshev4.m	
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)
myatan = @(x)-0.00007717176023065795 + 1.0031357062620350346*x ...	
- 0.015262708673125458*x.^2 - 0.34245381909783135*x.^3 ...	
+ 0.14017184670506358*x.^4;	
z = 0:0.001:1;	
zi = int32(z*2^15);	
r1 = int32(zi.*i0); %% 15+16=30	
limits1 = [min(r1) max(r1)]	
r2 = 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(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(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)]	

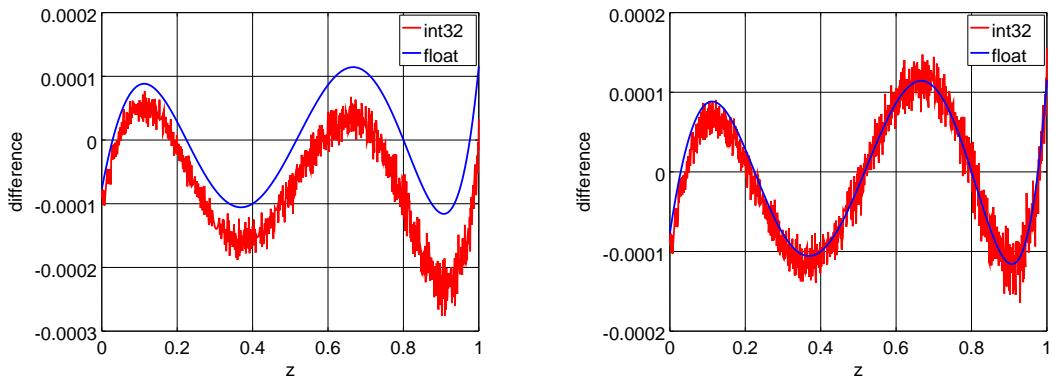
```
r8 = int16(bitshift(r7,-14))+i4; %% 29-14=15
limits6 = [min(r8) max(r8)]

res = double(r8)*2^15;

plot(z,res-atan(z), 'r', z, myatan(z)-atan(z), 'b')
legend('int32', 'float')
xlabel('z'); ylabel('errors')
grid on; legend('show')

bitaccuracy = log2(1.4e-4/pi*4)
```

leading to the result on the left in the figure below. The value of `bitaccuracy` ≈ -11.8 shows that we achieved the desired 12-bit resolution is not fully preserved. The graph also shows that the maximal error of approximately 0.00027 is dominated by the Chebyshev approximation, but has a slightly negative slope.



By modifying the coefficient for the linear contribution we may correct the slope, leading to the right part of the figure. Now the `bitaccuracy` ≈ -12.5 is good enough and the difference are clearly 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

$$\log_2\left(\frac{4}{\pi} 10^{-5}\right) = \frac{\ln(\frac{4}{\pi} 10^{-5})}{\ln 2} \approx -16.2$$

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

$$\sin(x) \approx 2.8566 \cdot 10^{-2} x^4 - 2.0312 \cdot 10^{-1} x^3 + 1.9516 \cdot 10^{-2} x^2 + 9.9629 \cdot 10^{-1} x + 1.1389 \cdot 10^{-4}$$

- (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 1999¹⁹.

2.5.1 Reading the data from the file, using `dlmread()`

The data retrieved from the internet is stored in a file, whose first few lines are shown below in a file `IBM.csv`.

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, showing the value of the stock at the opening of each trading day. Find the result in Figure 2.50.

IBMsriptDLM.m

```
% read all the data, starting at column 2 and row 2
data = dlmread('IBM.csv', ',', ',1,1');

indata = data(:,1)'; % use second column only
k = length(data) ;
indata = fliplr(indata);
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

¹⁹The results were found at <http://finance.yahoo.com> trough <http://finance.yahoo.com/stock-center/>. The package financial of Octave has functions to read this type of data from the web site, but lately yahoo does not accept the commands. You obtain the data by selecting your stock, the dates, then use APPLY and download the data. Values of Swiss stock is available on Yahoo too. Similar information is available at <https://www.macrotrends.net/>

- 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
 - 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 2.50.

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 ischar(inline)              % test for end of input file
  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                                % close the file

fclose(infile);

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

```

Another option would be to use the command `textread()` and then can line by line with a well constructed format string.

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 2.51.

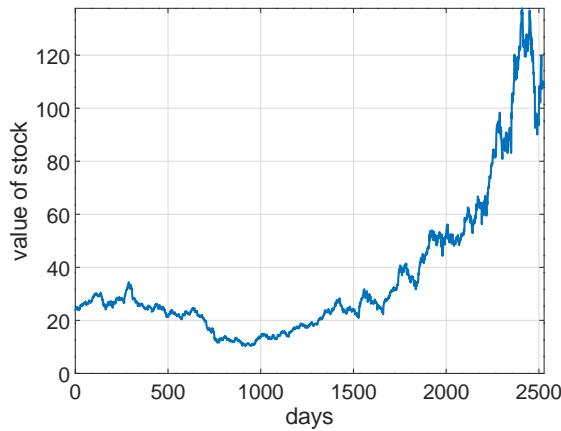


Figure 2.50: The price of IBM stock from 1990 to 1999

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 ii = 1:k
    avgdata(ii) = mean(indata(max(1,ii-avg):ii));
end%for
% 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')
legend('data','moving average')
```

Daily change rates

Using the above data we can compute a daily (per trading day) change rate r by

$$S(n) = S(0) e^{nr}$$

where r is the change rate per day and $S(n)$ the value of the investment after n days. If one year has N trading days then the annual change rate can be computed by

$$e^{Nr} - 1 \approx Nr \quad \text{if } Nr \ll 1.$$

Based of this we can compute the change rate rate by using the starting and final value of the stock

$$S(n) = S(0) e^{nr} \implies e^{nr} = \frac{S(n)}{S(0)} \implies r = \frac{1}{n} \ln \frac{S(n)}{S(0)}.$$

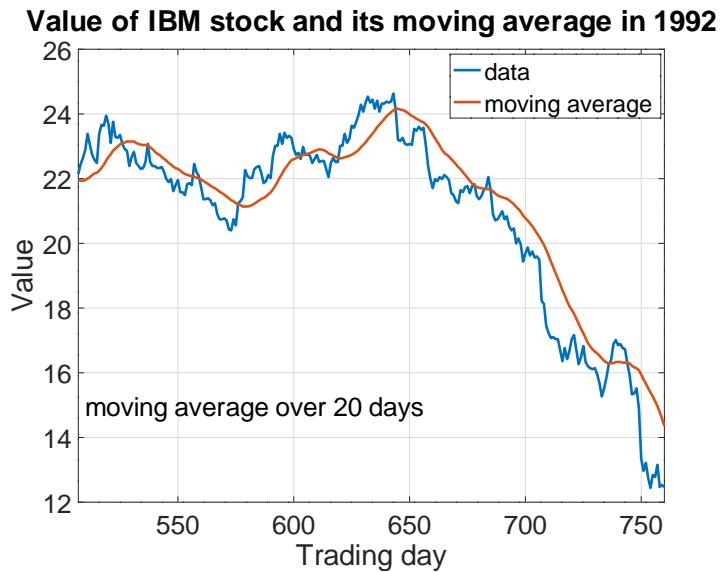


Figure 2.51: The price of IBM stock from 1992 and its average value over 20 days

The code below implements this formula.

Octave

```
n = length(indata);
rcomp = log(indata(n)/indata(1))/(n-1)
→
rcomp = 6.0481e-04
```

This change rate can be compared to the average of the daily change 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 change rates and we may consider their statistical distribution of the values, i.e. determine mean and standard deviation.

Octave

```
% mean value and standard deviation of daily change rate
rates = log(indata(2:n)./indata(1:n-1));
rmean = mean(rates)
rstd = std(rates)
→
rmean = 6.0481e-04
rstd = 0.019396
```

As one would expect the average of the daily change rates (computed day by day) coincides with the average daily change rate (computed by using initial and final value only).

To illustrate the distribution of the daily rates rates a histogram can be used, as shown in Figure 2.52(a).

Octave

```
dr = 0.005; edges = [-inf,-0.1:dr:0.1,inf]; nn = length(edges);
histdata = hist(rates,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')
```

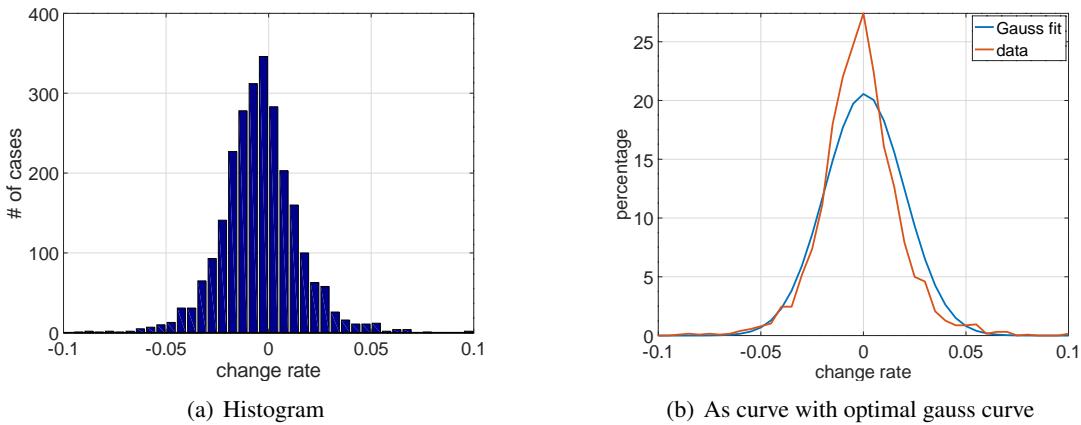


Figure 2.52: Histogram of daily interest rate of IBM stock

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

$$\text{gauss}(x) = \frac{1}{\sigma \sqrt{2\pi}} e^{-\frac{(x-\bar{x})^2}{2\sigma^2}}$$

can be defined²⁰ by (the code has to be stored in a file 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 Figure 2.52(b).

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('change rate'); ylabel('percentage')
legend('Gauss fit','data')

```

One might use the correlation coefficient of two vectors to obtain a numerical criterion on how similar the shape of the functions are. 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

²⁰On newer versions of Octave one may use `normpdf()`. In MATLAB this function is unfortunately part of the statistics toolbox, i.e. extra \$\$. .

two functions (resp. vectors) in Figure 2.52 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 change rates is quite close to a normal distribution.

2.5.4 A Monte Carlo Simulation

Since we found an average daily change rate and its standard deviation we can use random numbers to simulate the behavior of stock values. We generate random numbers for the daily change rates with the known average value and standard deviation. Then we use these change rates to compute the behavior of the value of the stock when those change 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 change 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 Figure 2.53(a). Observe that at the $(k + 1)$ -th day the value is given by

$$S(k + 1) = S(1) \cdot e^{r(1)} \cdot e^{r(2)} \cdot e^{r(3)} \cdots e^{r(k)} = S(1) \exp(r(1) + r(2) + r(3) + \cdots + r(k))$$

and thus we can use the command `cumsum()` (cumulative summation) to determine the values at all days, without using a loop.

IBMsimulation.m

```
days = 250; % number of trading days to be simulated
rates = randn(1, days-1)*rstd + rmean; % daily change rates

%% solution with a loop, slow
% values = ones(1, days); % value of stock
% for k = 2:days
%   values(k) = values(k-1)*exp(rates(k-1));
% end

%% solution without a loop, thus fast
values = [1, exp(cumsum(rates))];

plot(values)
xlabel('trading day'); ylabel('relative value'); grid on
```

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 2.53. Observe that most final results are rather close together, but individual runs may show a large deviation. Thus it is a good idea to examine the statistical behavior of the final value of the stock.

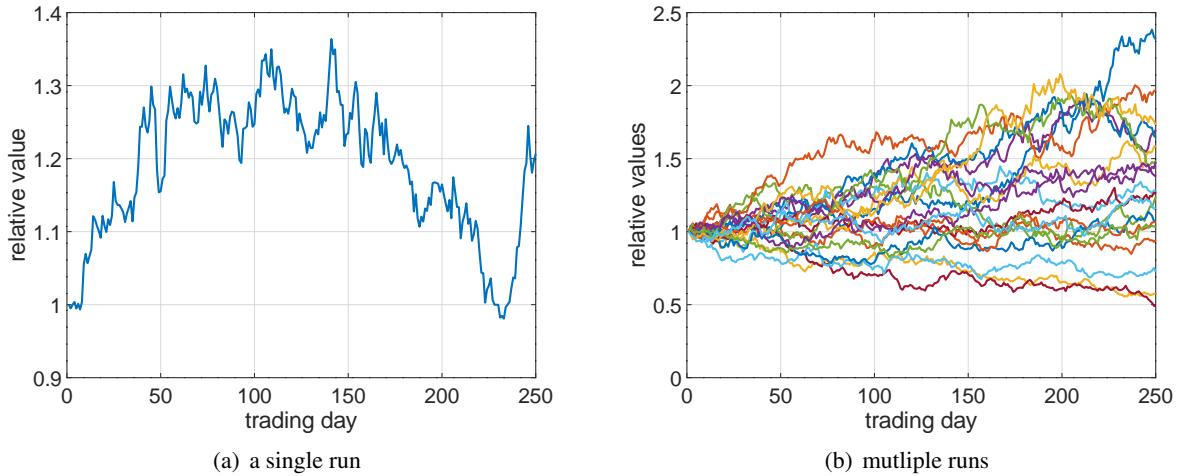


Figure 2.53: Simulation of annual performance of IBM stock

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 Figure 2.53(b). 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. Observe that we removed another loop from the previous code by applying the command `cumsum()` directly to the matrix of all daily change rates. Since we only need the final values we can even use `sum()` instead of `cumsum()`. This will lead to a large speed gain, compared to the original code with two nested loops.

Octave

```
days = 250;           % number of trading days to be simulated
runs = 1000;           % number of trial runs

rates = randn(runs, days-1)*rstd + rmean;    % daily change rates
finalvalues = exp(sum(rates, 2));

MeanValue = mean(finalvalues)
StandardDeviation = std(finalvalues)
LogMeanValue = mean(log(finalvalues))
LogStandardDeviation = std(log(finalvalues))
```

One specific run of the above code leads to the numerical values shown below. Be aware that the numbers change from one run to the next, as they depend on the random simulation.

Octave

- Create the histogram of the final values, as function of the value of the stock. Find the result in Figure 2.54(a).

- 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 values, as function of the logarithm of value of the stock. Find the result in Figure 2.54(b).

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 for one simulation are shown above and the graphs are given in Figure 2.54 . 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. Observe that the shape of this figure changes slightly from run to run, since the result is based on a Monte Carlo simulation.

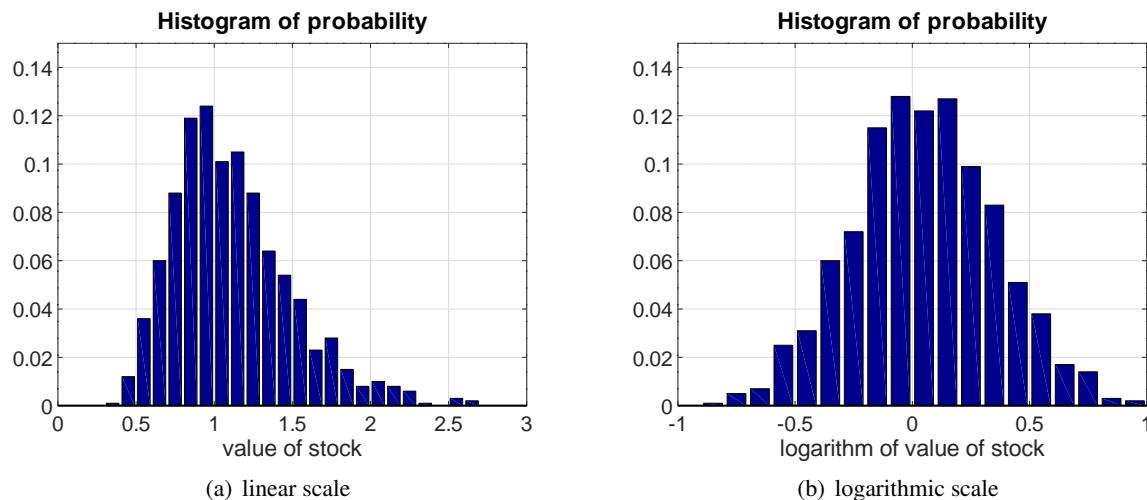


Figure 2.54: Histograms of the final values of IBM stock after one year

If the daily change 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

$$\text{PDF}(z) = \frac{1}{\sigma \sqrt{N} \sqrt{2\pi}} \exp \left(-\frac{(z - N r)^2}{2 \sigma^2 N} \right).$$

Thus the probability that $\ln S(N)$ is between z and $z + \Delta z$ is given by $\text{PDF}(z) \Delta z$, as long as Δz is small.

$$P(z \leq \ln S(N) \leq z + \Delta z) \approx \text{PDF}(z) \cdot \Delta z$$

With the above numbers $r = 6.0481 \cdot 10^{-4}$, $\sigma = 0.0194$ and $N = 250$ we obtain

$$r N = 0.1512 \quad \text{and} \quad \sigma \sqrt{N} = 0.3067$$

The predicted values are very close to the simulation results $\text{LogMeanValue} = 0.1490$ and $\text{LogStandardDeviation} = 0.3096$ 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 at the end of the year.

- 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 lose on the option, but you might win, if the actual value after one year is larger than the strike 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

$$\text{PDF}(z) \cdot \Delta z = \frac{1}{\sigma \sqrt{N} \sqrt{2\pi}} \exp\left(-\frac{(z - N r)^2}{2 \sigma^2 N}\right) \cdot \Delta z$$

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 value of the option.

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

$$\text{PDF}(z) \cdot \Delta z = \frac{1}{\sigma \sqrt{N} \sqrt{2\pi}} \exp\left(-\frac{(z - N r)^2}{2 \sigma^2 N}\right) \cdot \Delta z.$$

The graph of this function is shown in Figure 2.55. This figure has to be compared with the left part in Figure 2.54.

With the help of this probability density 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

$$\int_{\ln 2}^{\infty} \text{PDF}(z) dz = \frac{1}{\sigma \sqrt{N} \sqrt{2\pi}} \int_{\ln 2}^{\infty} \exp\left(-\frac{(z - N r)^2}{2 \sigma^2 N}\right) dz \approx 0.039.$$

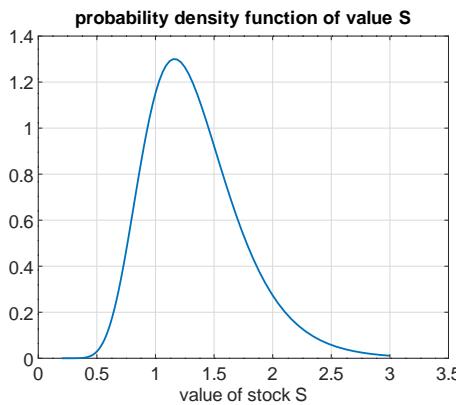


Figure 2.55: Probability density function of final values

Thus there is only a 4% chance to double the value within one year. The integral

$$\int_{\ln 1}^{\infty} \text{PDF}(z) dz = \frac{1}{\sigma \sqrt{N} \sqrt{2\pi}} \int_{\ln 1}^{\infty} \exp\left(-\frac{(z - N r)^2}{2 \sigma^2 N}\right) dz \approx 0.69$$

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 $\max\{0, S_1 - C\}$.

- 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 $\text{PDF}(z) \cdot \Delta z$ we find

$$\text{payoff of } e^z - C \quad \text{with probability} \quad \text{PDF}(z) \cdot \Delta z = \frac{1}{\sigma \sqrt{N} \sqrt{2\pi}} \exp\left(-\frac{(z - N r)^2}{2 \sigma^2 N}\right) \cdot \Delta z.$$

To examine the expected payoff we plot the product of the payoff with the probability density function. The result is shown in Figure 2.56 . 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 .

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

$$\begin{aligned} p &= \lim_{\Delta z_i \rightarrow 0} \left(\sum_{z_i=\ln C}^{\infty} (e^{z_i} - C) \text{PDF}(z_i) \Delta z_i \right) \\ &= \int_{\ln C}^{\infty} (e^z - C) \text{PDF}(z) dz = \frac{1}{\sigma \sqrt{N} \sqrt{2\pi}} \int_{\ln C}^{\infty} (e^z - C) \exp\left(-\frac{(z - N r)^2}{2 \sigma^2 N}\right) dz \approx 0.23887. \end{aligned}$$

Thus the fair value of the option is $p \approx 0.24$ for a strike of $C = 1.05$.

The above computations can be repeated for multiple values of the strike price C , leading to Figure 2.57 .

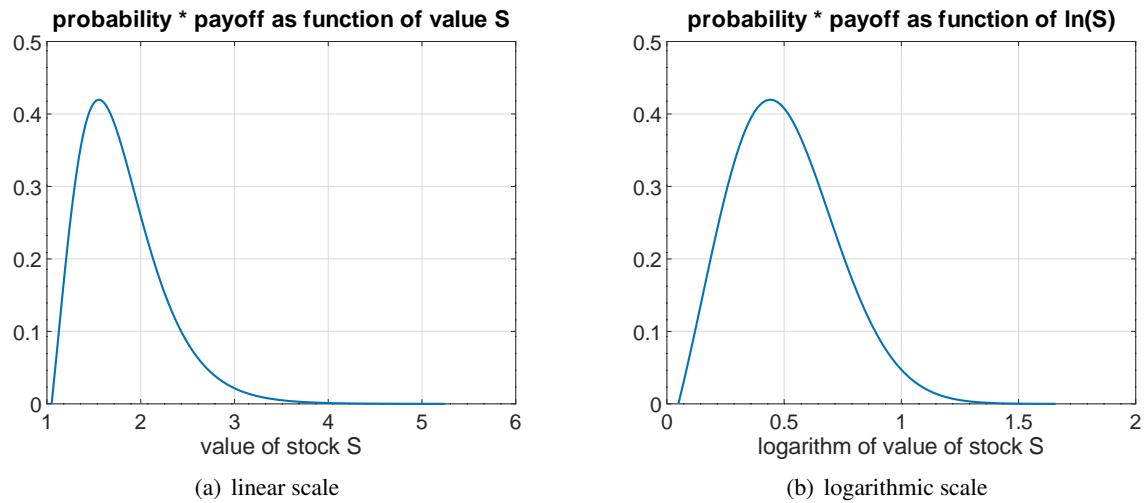
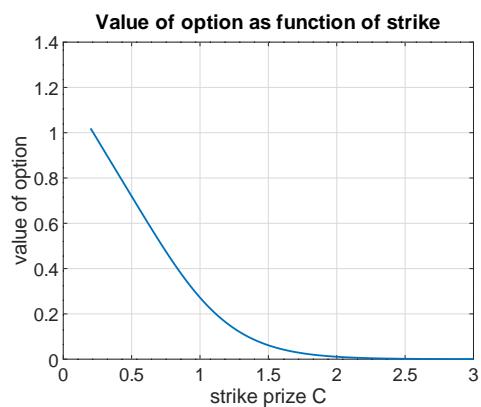


Figure 2.56: Product of payoff with probability density function

Figure 2.57: Value 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-codes.

- Give the basic data and plot the probability density function. Find the result in Figure 2.55.

Octave

```
rmean = 6.0481e-4      % mean of the daily change rate
rstd  = 0.0194          % standard deviation of the daily change 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 density 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)
->
prob1 = 0.68892
prob2 = 0.038648
```

The result show that with a probability of 69% the value of the stock will increase and with a probability of 3.8% the value will at least double.

- 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)
xlabel('logarithm of value of stock S')
title('probability * payoff as function of ln(S)'); grid on

figure(3);
plot(exp(zval),payoffProb)
xlabel('value of stock S')
title('probability * payoff as function of value S'); grid on
OptionValue = trapz(zval,payoffProb) % use built-in trapezoidal rule
->
OptionValue = 0.23884
```

The result states that the option with a strike prize of $C = 1.05$ has a value of 0.24.

- Now examine different values for the strike price C and plot the resulting values of the option. Find the result in Figure 2.57.

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('Value of option as function of strike')
xlabel('strike prize C'); ylabel('value of option'); grid on

```

Nobel Price in Economics in 1997

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. changing rates and other types of options. The theory was developed by Fischer Black, Myron Scholes and Robert Merton in 1973. Since then their methods are used extensively by the financial “industry”. The 1997 Nobel Prize in Economics was awarded to Merton and Scholes. Fisher Black died in 1995 and thus did not obtain the Nobel prize. Further information on the Black–Scholes–Merton method and its applications in finance can be found in many books, e.g. [Seyd00] or [Wilm98].

2.5.6 List of codes and data files

In the previous sections the codes and data files in Table 2.12 were used.

Script file	task to perform
IBMscripDLM.m	read the data and create basic plot
IBMscrip.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
IBMBlaScholes.m	find the value of a stock option

Table 2.12: Codes and data files for section 2.5

2.6 Motion 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 2.58.

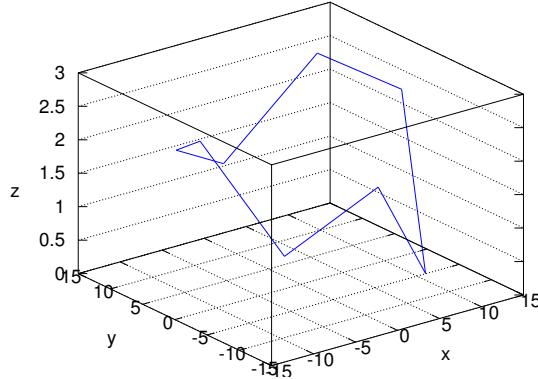


Figure 2.58: Deformed circle for a given time

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 9th, 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 row²¹, 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 scanning (`sscanf()`) to extract the two numbers.

ReadData.m

²¹With very recent versions of MATLAB this works too.

```

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 circle.

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 2.58.

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 2.58 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 sub-directory `pngmovie` in a bitmap format (png)²². Then an external command (`mencoder`) is used to generate a movie file `Circle.avi` to be used without Octave or MATLAB. The command is composed of two strings, for them to fit on one display line. Subsequently the directory is cleaned up.

²²With the current version of Octave (4.0.0) the graphics toolkit `qt` seems to have a problem generating the PNG files. Thus one should first switch to another graphics toolkit by `graphics_toolkit('fltk')`

MovieAVI.m

```

graphics_toolkit('fltk') % due to a bug in the QT toolkit with
                         % Octave, not required for Matlab
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')
    end%if
end%for

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 movie 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

```

- Instead of the command `mencoder` one might use the FFmpeg suite of codes, to be found at the site <http://www.ffmpeg.org/>. A possible call to create a movie with 5 frames per second is given by

```

ffmpeg -r 5 -i movie%03d.png -c:v libx264 -r 30 -pix_fmt yuv420p out.mp4

```

- Similarly the command `ffmpeg` might be used (www.libav.org)

```

ffmpeg -i /* movie%03d.png out.mp4

```

or

```
ffmpeg -r 10 -i ./movie%03d.png -c:v libx264 -r 10 -pix_fmt yuv420p out.mp4
```

To play the movie you may use any movie player, e.g. vlc or xine.

2.6.4 Decompose the motion into displacement and deformation

The movement of the circle can be decomposed into four different actions:

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 . The value of p_1 corresponds to the height of the center and p_2 , p_3 show the slopes in x and y direction.

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 2.59. In Figure 2.59(a) find the height as function of time. The down an up movement of the circle is clearly recognizable. In Figure 2.59(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%for

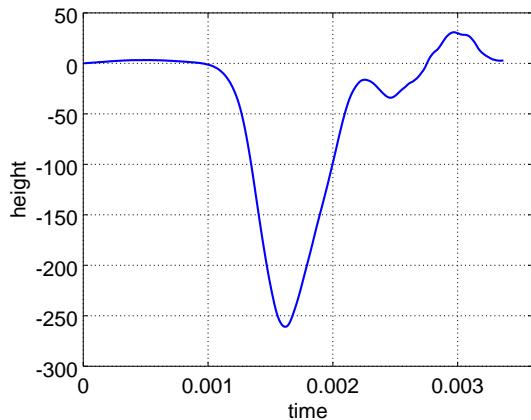
figure(3);
```

```

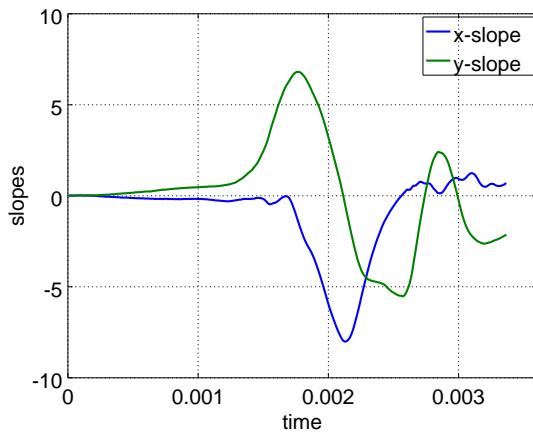
plot(t(1,:),par(1,:));
grid on; axis([0 0.0036, -300, 50])
xlabel('time'); ylabel('height'); grid on

figure(4);
plot(t(1,:),par(2:3,:));
grid on; axis([t(1,1), max(t(1,:)), -10, 10])
xlabel('time'); ylabel('slopes');
legend('x-slope','y-slope')
axis([0, 0.0036 -10 10])

```



(a) height as function of time



(b) the two slopes as function of time

Figure 2.59: Height and slopes of the moving circle

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
    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
end%for

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')
    end%if
end%for

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 2.13 were used.

Script file	task to perform
cg*a.txt	data files
ReadDataDLM.m	read all data files, using <code>dlmread()</code>
ReadData.m	read all data files, using <code>sscanf()</code>
MovieAVI.m	display movie and create <code>Circle.avi</code>
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 2.13: 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 2.60. 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.

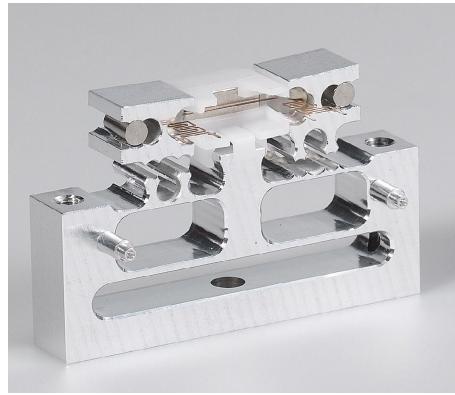


Figure 2.60: A vibrating cord sensor produced by DIGI SENS AG

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 2.61. At first the cord is vibrating with a constant amplitude and then the amplitude seems to converge to zero, exponentially. Thus we find functions of the form

$$\text{first: } y(t) = A \cos(\omega t) \quad \text{then: } y(t) = A e^{-\alpha(t-t_0)} \cos(\omega t)$$

To characterize the behavior of the sensor the initial amplitude A and the decay exponent α have to be determined reliably.

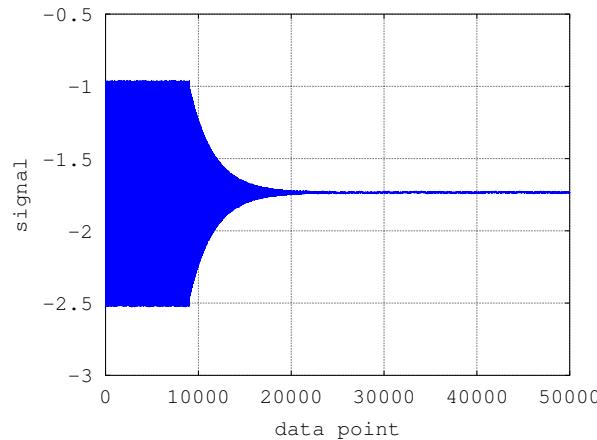


Figure 2.61: The signal of a vibrating cord sensor

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 an *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
end%function
```

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.mat`) is generated. On subsequent calls of this function the binary file will be read, leading to sizable time savings²³.

- 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()` .
- 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.

²³On this authors PC the time was cut from 12 seconds to 1 second.

Readm4.m

```

%% script file to read one data set
filename = 'm4';
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 ,'.mat'], 'file') ==2)
    eval(['load ',filename ,'.mat'])
else
    inFile = fopen(filename , 'rt' ) ; %% read the information from the file
    for k = 1:5
        inLine = fgetl(inFile);
    end%for
    k = 1;
    for j = 1:Nmax
        inLine = fgetl(inFile);
        counter = find(inLine=='E');
        y(j) = sscanf(inLine(counter-9:length(inLine)) ,'%f');
    end%for
    fclose(inFile) ;
    eval([' save -mat ',filename ,'.mat y'])
end%if

figure(1);
plot(y) %% plot the raw data
xlabel('dada point'); ylabel('signal'); grid on

```

Determine the amplitude as function of time

The result of the above code is shown in Figure 2.61. 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 $y = \text{abs}(\sin(\omega t))$ at equidistant times, as shown in Figure 2.62. 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
    y3(k) = mean(y2(k:k+FilterLength));
end%for
tt = cputime-t0

```

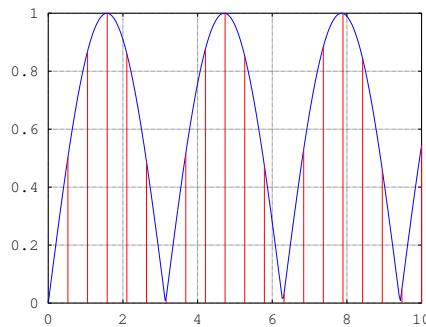


Figure 2.62: A function $y = \text{abs}(\sin(\omega t))$ and a sampling

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 2.63(a), generated by

Octave

```
figure(2);
t = linspace(0,(N-1)*dt,N)';
plot(t,log(y3)); grid on
xlabel('time t'); ylabel('log of amplitude')
```

In Figure 2.63(a) we clearly recognize the constant amplitude in the first sector and then a straight line segment. This is caused by

$$A = A_0 e^{-\alpha t} \implies \ln A = \ln A_0 - \alpha t$$

The wild variations on the right part in Figure 2.63(a) 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

```

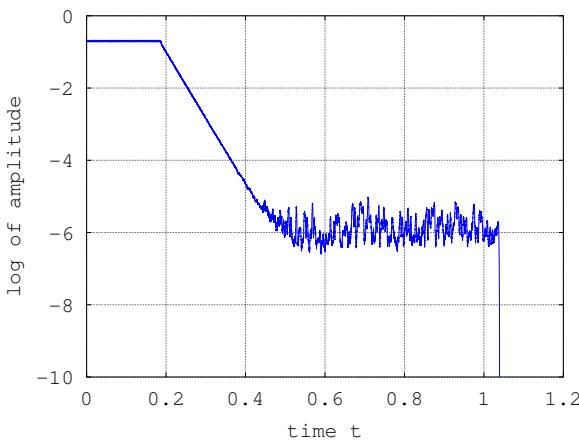
%% run the linear regression
F = ones(N,2); F(:,2) = t;
[p,y_var,r,p_var] = LinearRegression(F,y4');
yFit = F*p;

figure(3);
plot(t,y4,t,yFit) % display the real data and the regression line
xlabel('time t'); ylabel('log of amplitude'); grid on

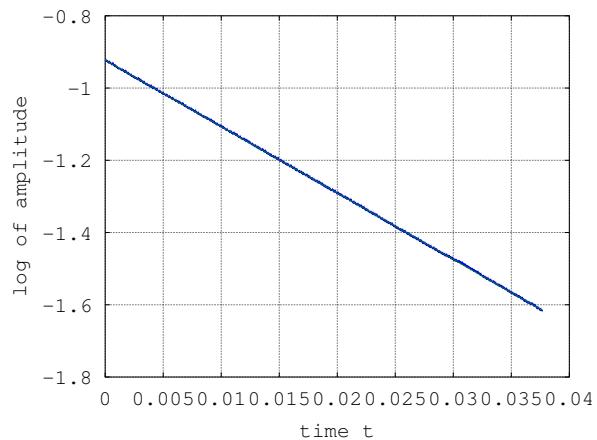
fprintf('Slope: %g, Variance of slope: %g, relative error:%g\n',...
        p(2), sqrt(p_var(2)), -sqrt(p_var(2))/p(2));
factor = 1/p(2);

```

The numerical result and Figure 2.63(b) clearly indicate that we have **one exponential function** on the decaying section of the signal.



(a) log of the amplitude



(b) result of linear regression

Figure 2.63: The logarithm of the amplitude and the regression result for the straight line section

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 analyze one data set for a single measurement. For each frequency multiple measurements should be made and analyzed, to estimate the variance of the results. These measurements have to be repeated for many different frequencies and a useful graph has to be generated, to be

included in reports on the development of new sensors. A possible result is given in Figure 2.64. Graphs of this type could not be generated directly by Octave²⁴.

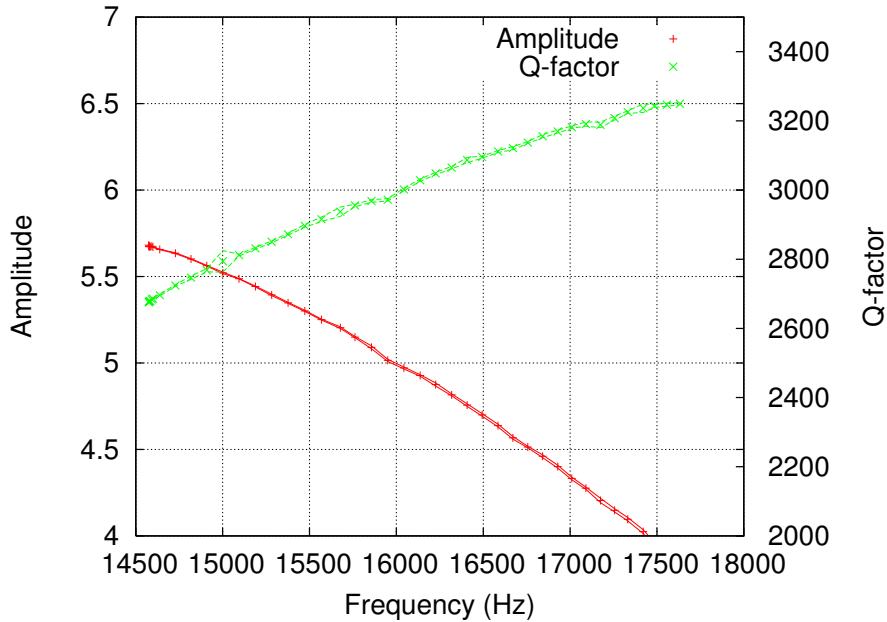


Figure 2.64: Amplitude and Q-factor as function of frequency, including error

We expect the following features for the final graphics:

- For each frequency the average value of all the measurements is shown and error lines at a distance of one standard deviation are drawn.
- 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 too.
- 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.

²⁴Up to date versions of Octave have the command `plotyy()` and can now not generate graphs with two different vertical axis. Thus one of the reasons to use an external program disappeared.

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 open a data file `gnu.dat` for writing the data to be used by *Gnuplot*, a powerful program to generate graphs.
- 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 2.64 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, or consult the web page <http://www.gnuplot.info/>.

- 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` fulfills the above requirements²⁵. 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
% 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))
    error('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');

```

²⁵On Win* system the last line might have to be replaced by `system('pgnuplot AmpQ.gnu');`

```

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);
end%for

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);
    end%for
    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));
end%for
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(
'minimal 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\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));
end%for
fclose(outfile);

system('gnuplot AmpQ.gnu');
end%function

```

With very similar tools the results in Figure 2.65 are generated. The file AmpQ.gnu will create all three graphs in this section.

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 Figures 2.66 and 2.67. They are created by

Octave

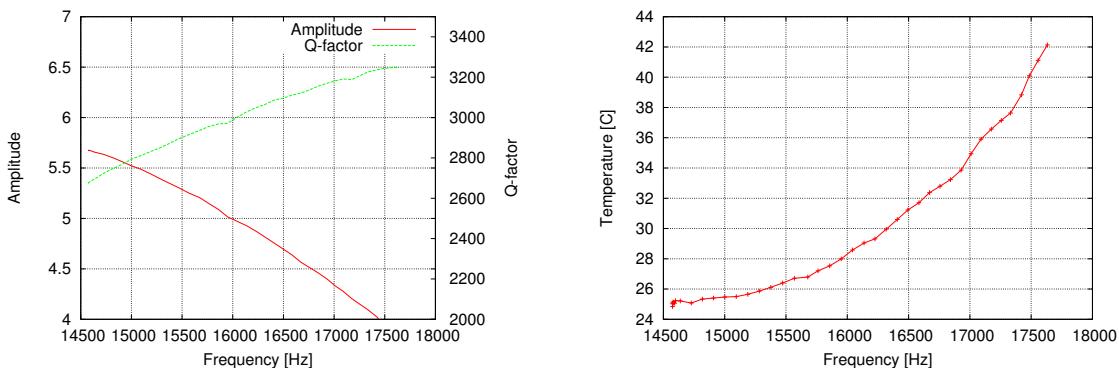


Figure 2.65: Amplitude, Q-factor and temperature as function of frequency

```
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')
```

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

```
if ((nargin ~=3))
    error('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; cmdLegend = 'legend(';
for sensor = 1:length(numbers)
    filename = [basename, num2str(numbers(sensor)), ext];
    infile = fopen(filename, 'rt');
```

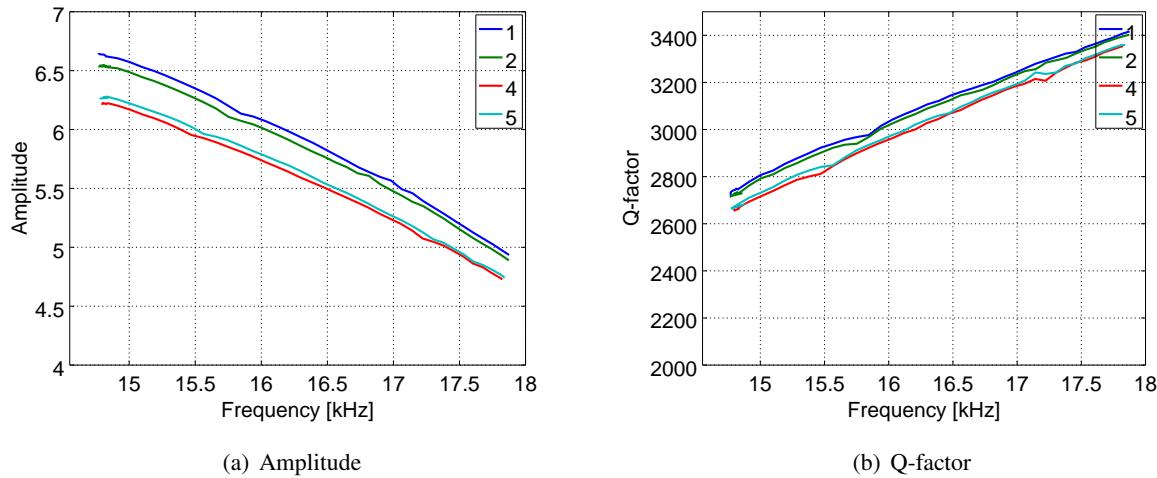


Figure 2.66: Results for multiple measurements

```
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);
end%for

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);
    end%for % 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));
end%for % meas
freqA = [freqA; freq]; ampA = [ampA; amp];
qualiA = [qualiA; quali]; tempA = [tempA; temp];
fclose(infile);

key = num2str(numbers(sensor));
freqn = ['freq ',key,'=freq/1000;']; eval(freqn);
```

```

ampn = [ 'amp', key, '=amp; ']; eval(ampn);
qualin = [ 'quali', key, '=quali; ']; eval(qualin);
cmd1 = [cmd1, ' freq ', key, ', amp', ' key, ', '];
cmd2 = [cmd2, ' freq ', key, ', quali', key, ', '];
cmdLegend = [cmdLegend, char(39), key, char(39), ', '];
end%for % loop over all files

cmdLegend = [cmdLegend(1:end-1), ')'];
cmd1 = [cmd1(1:end-1), ')'];
cmd2 = [cmd2(1:end-1), ')'];

figure(1); clf;
eval(cmd1)
grid('on')
axis([14500 18000 4 7]);
xlabel('Frequency [kHz]'); ylabel('Amplitude')
eval(cmdLegend)
print('AmpAll.png',' -dpng');

figure(2); clf;
eval(cmd2);
grid('on')
axis([14500 18000 2000 3500]);
xlabel('Frequency [kHz]'); ylabel('Q-factor')
eval(cmdLegend)
print('QAll.png',' -dpng');

NN = length(freqA);
F = ones(NN,3);
F(:,1) = freqA; F(:,2)=tempA;
[p,y_var,r,p_var] = LinearRegression(F,ampA);
display(sprintf('estimated temperature dependence of amplitude: %g um/C\n',p(2)))
[p,y_var,r,p_var] = LinearRegression(F,qualiA);
display(sprintf('estimated temperature dependence of Q-factor: %g /C\n',p(2)))

figure(3); clf; axis();
plot3(freqA/1000,tempA,ampA,'+')
xlabel('frequency [kHz]'); ylabel('Temperature'); zlabel('Amplitude')

```

- 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/1000; ']; eval(freqn);
```

will generate the string '`freq3=freq/1000;`' and then evaluate this command. The variable `freq3` contains the frequencies from the data file `Elektro3.data`.

- The plot command to generate Figure 2.66(a) is constructed step by step. Examine the patches of code.

Octave

```
cmd1 = [ ' plot( '];
for sensor = 1:length(numbers) % loop over all data files
    key = num2str(numbers(sensor));
    cmd1 = [cmd1, ' freq ',key,' ,amp', ' key , ',' ];
    cmdLegend = [cmdLegend, char(39),key,char(39),',',''];
end%for
cmd1 = [cmd1(1:end - 1),');'];
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,freq3,amp3,freq5,amp5);
```

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 graphics 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 2.67, generated by

Octave

```
figure(3); clf; axis()
plot3(freqA/1000,tempA,ampA, '+')
xlabel(' frequency [kHz]'); ylabel('Temperature'); zlabel('Amplitude')
```

- By rotating Figure 2.67 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);
fprintf('estimated temperature dependence of amplitude: %g um/C\n',p(2))
```

As a result we find that the amplitude A decreases by $0.047 \mu\text{m}$ per degree of temperature increase.

- A similar computation shows that the Q-factor is diminished by 10 units per degree of temperature increase.

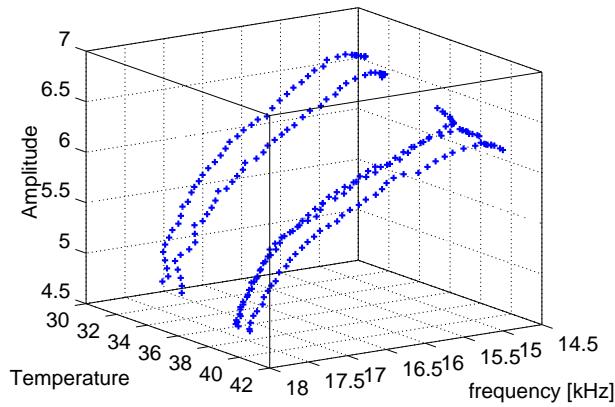


Figure 2.67: Amplitude as function of frequency and temperature

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 2.14 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 <i>Gnuplot</i>
WriteDataAll.m	function file to analyse multiple data sets
Elektro*.data	sample data files

Table 2.14: 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 2.68.

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
```

- If you want to avoid `dlmread()` one may 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 ischar(inline) % test for end of input file
    A = sscanf(inline,'%f,%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 2.68.
- 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
xlabel('time'); ylabel('amplitude')

figure(2)
dom = 1070:1170;
plot(timedataIn(dom),ampdataIn(dom))
title('Amplitude of input'); grid on
xlabel('time'); ylabel('amplitude')

```

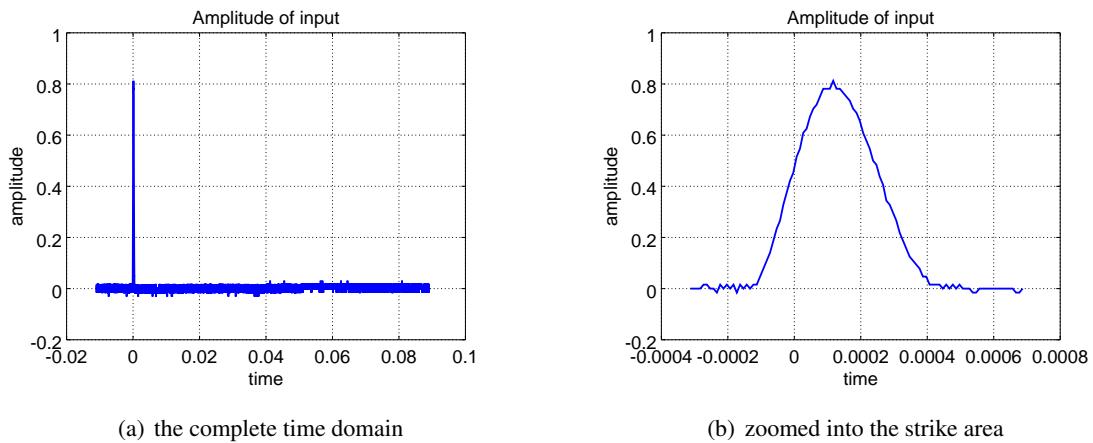


Figure 2.68: Acceleration of the hammer

2.8.2 Further information

- Time of contact

The result in Figure 2.68(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 threshold
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 2.68(b).

- Octave

```

speed1 = trapz(timedataIn ,ampdataIn.* contact)
speed2 = trapz(timedataIn(dom),ampdataIn(dom)) % dom is defined in ReadDataDLM
→
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 Using FFT, Fast Fourier Transform

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 (aliasing) 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 2.69 .

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 2.69 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.

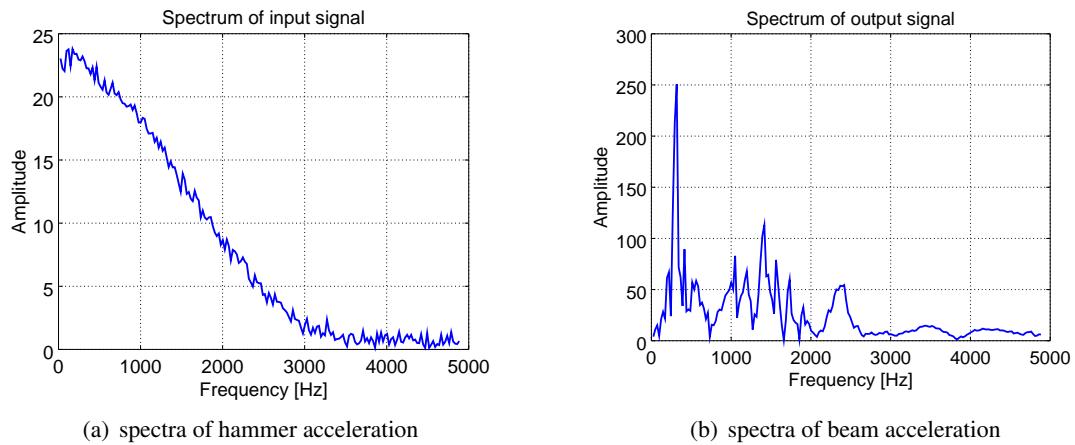


Figure 2.69: Spectra of the accelerations of hammer and bar

- The graphs of the above 6 computations are shown in Figure 2.70 . 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
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)
xlabel('frequency'); ylabel('amplitude')
```

Another option would be to consider even more starting times and generate a 3D-graph. The code below²⁶ does just this. The result in Figure 2.71 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 = 1:250:5000;
levels = 1:200:8000;

spectrum = zeros(length(levels),Ndisp);
PeriodIn = timedataIn(2^N2)-timedataIn(1);
frequencies = linspace(1,Ndisp,Ndisp)/PeriodIn;
```

²⁶Recently your author learned about the command `specgram()` which applies a similar procedure.

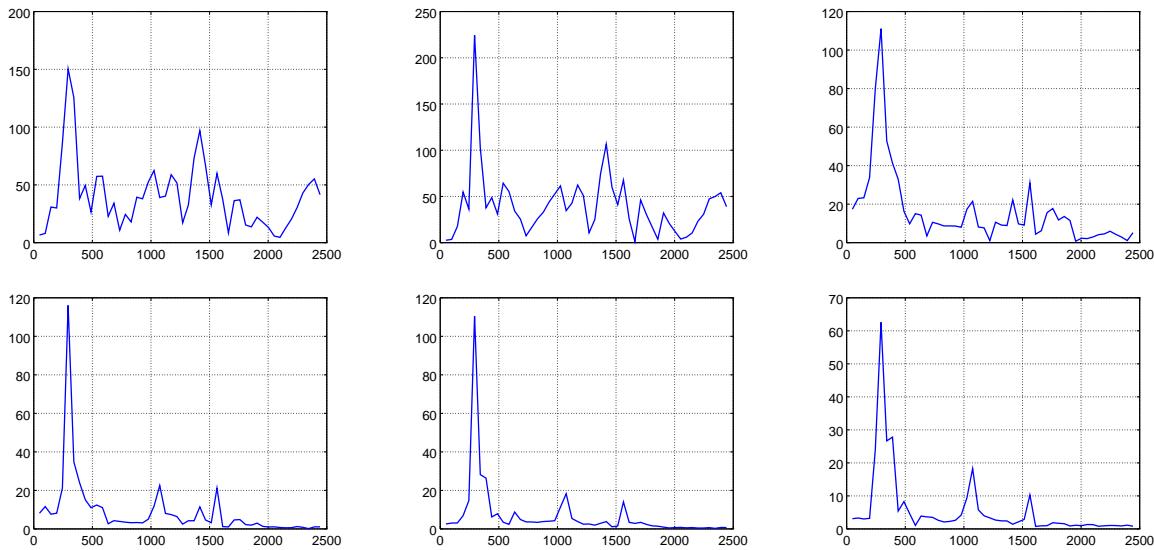


Figure 2.70: Spectra at different times

```

for kl = 1:length(levels)
    adata = ampdataOut(levels(kl):levels(kl)+2^N2-1);
    fftOut = fft(adata);
    spectrum(kl,:) = abs(fftOut(2:Ndisp+1));
end%for
figure(3);
mesh(frequencies , levels/FreqIn*1000,spectrum)
xlabel('frequency [Hz]'); ylabel('time [ms]'); zlabel('amplitude')
title('spectrum as function of starting time');
view(35,25)

```

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 2.72 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

```

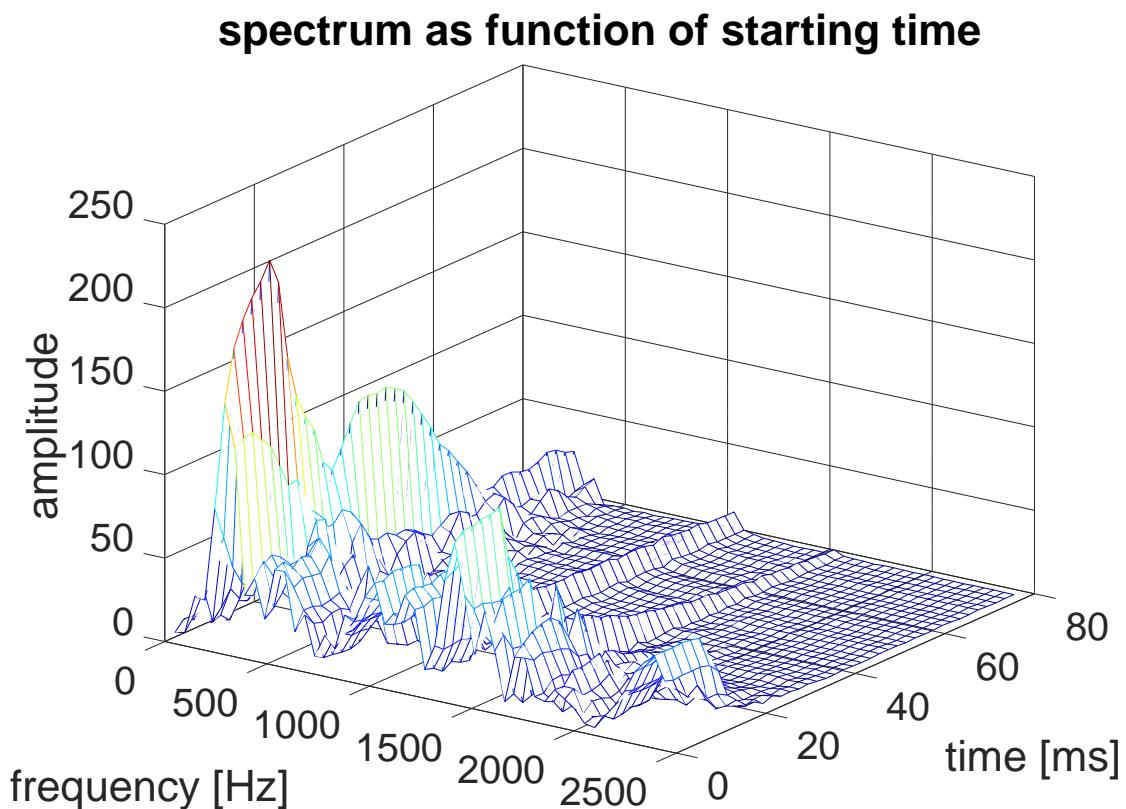


Figure 2.71: Spectra at different times as 3D graph

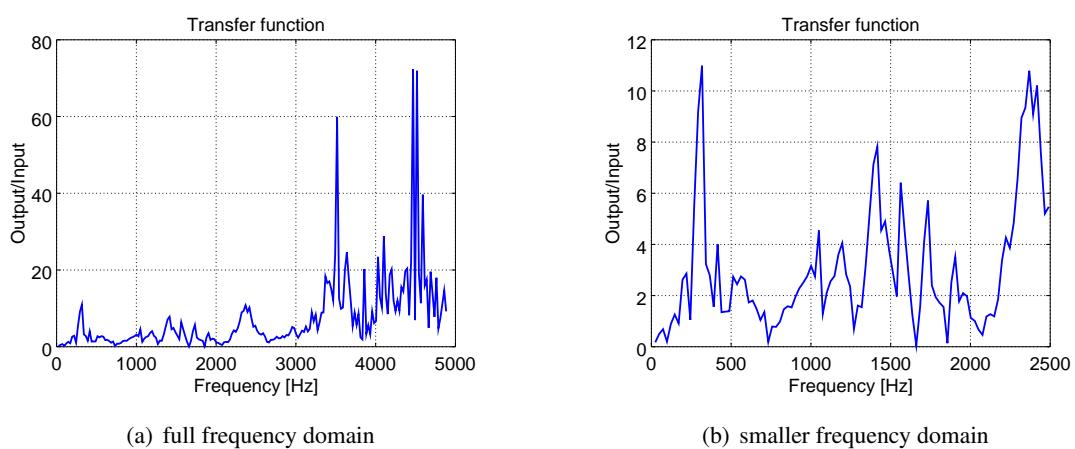


Figure 2.72: Transfer function for the acceleration of hammer and bar

2.8.6 List of codes and data files

In the previous section the codes and data files in Table 2.15 were used.

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 2.15: Codes and data files for section 2.8

2.9 Reading Information from the Screen and Spline Interpolation

In this section we:

- First examine how to read coordinate information from a MATLAB/*Octave* graphics window.
- Then we show how to read data from 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 Reading form an *Octave/MATLAB* graphics window by `ginput()`

With the command `ginput()` you can read information from an *Octave* or MATLAB graphics window. With the code below we

- open a graphics window and fix the axis.
- display some information for the user
- use the left mouse button to collect positions and display the corresponding points.
- exit the loop with the last point, marked by the right mouse button.

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.')
button = 1; % boolean variable to indicate the last point
while button == 1 % while loop, picking up the points.
    [xi,yi,button] = ginput(1); % get coordinates of one point
    x = [x,xi]; y = [y,yi];
    plot(x,y,'ro') % plot all points
    axis(axislimits); % fix the axis
end
plot(x,y,'ro-')
xlabel('x'); ylabel('y')
```

The command `ginput()` should work with *Octave* and MATLAB on any platform.

2.9.2 Create `xinput()` to replace `ginput()`

With recent versions 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 no longer read 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 instructions 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


```
mkostfile -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()`. With newer versions of *Octave* calling `mkostfile` `grab.cc` does the same job. 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 `~/.octaverc` 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. It does not directly read from the screen, can work with many formats for graphics.

2.9.3 Reading an LED data sheet with Octave

In Figure 2.73 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*²⁷. 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. `evince`) on a command line or through the GUI of the operating system to display the file `NSHUS550ALEDwide.pdf`. Locate the page shown in Figure 2.73. 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 2.74(a).

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');
```

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 2.74(b).

Octave

²⁷With MATLAB this is unfortunately not possible, and *Octave* on Win?? systems seems to be problematic too.

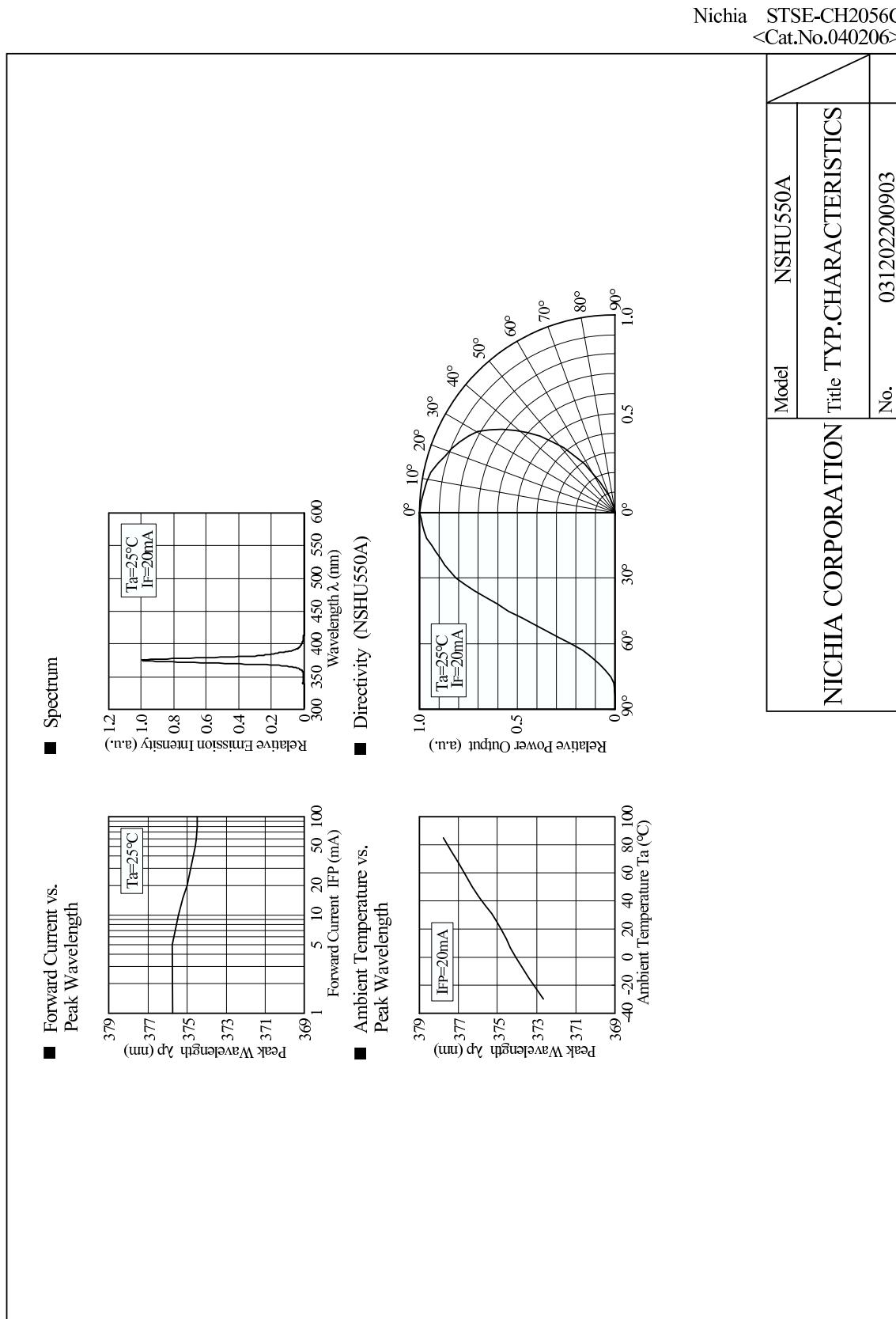


Figure 2.73: Data sheet for an LED

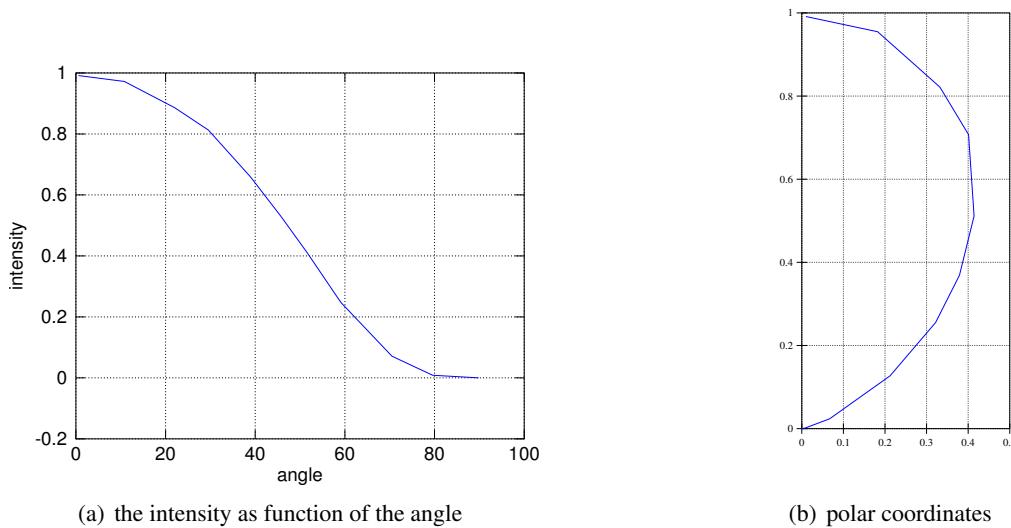


Figure 2.74: Light intensity data for an LED

```
figure(2);
polar(pi/2-xi/180*pi ,yi)
axis([0 0.5 0 1], 'equal')
```

In section 2.2.5 (page 151) 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 2.73.

- 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 2.74(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);

a1 = pi/2-atan2(yi,xi);
Intensity = sqrt(xi.^2 + yi.^2);
```

```
figure(2);
plot(al*180/pi , Intensity ),
grid on
axis('normal');
```

2.9.4 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 is shown on page 275 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.

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); % integers from 1 to n
t = 1:n;          % from 1 to n, stepsize 0.2
ts = 1: .2: n;    % do the spline interpolation
xys = spline(t,[x;y],ts);
xs = xys(1,:);   ys = xys(2,:);
ys = ys';         % 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 2.75 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.

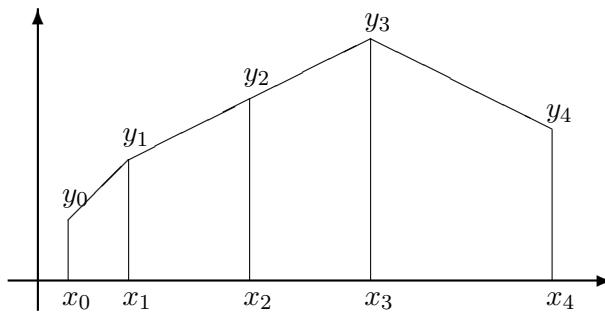


Figure 2.75: Trapezoidal integration

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;
endfor
figure(3);
axis(axislimits)
plot(xs,ys,"function",xs,integral,"integral")
```

The identical result can be obtained by the command `cumtrapz()`, short for cumulative 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 an 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 2.76. With the sorted values we then call the function `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

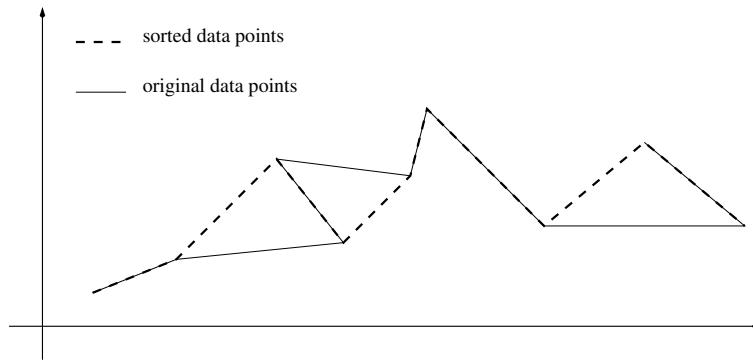


Figure 2.76: Data points in original order and sorted

```
% 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.

2.9.5 List of codes and data files

In the previous section the codes and data files in Table 2.16 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, (<i>Octave only</i>)
grab.cc	C++ source for the command grab(), (<i>Octave only</i>)

Table 2.16: Codes and data files for section 2.9

2.10 Intersection of Circles and Spheres, GPS

In this section we build up some of the Mathematics used for the Global Positioning System (GPS). It turns out the problem of finding intersection points of spheres is one of the essential tools used for the GPS, see [Thomp98].

- We start with the geometric problem of finding the two intersection points of two circles in the plane. This can be used to determine the position of a robot in a plane, if the distance to two fixed points is known.
- A MATLAB/Octave function is written to determine the two intersection points.
- Similar ideas are used to determine the intersection points of three spheres in space and an application in robotics is mentioned.
- Then the problem of approximating the common intersection point of many circles in the plane is examined. The system of over-determined quadratic equations is replaced by a linear least square problem.
- The identical algorithm can be used to search for the intersection point of many spheres in space.
- By adding the additional dimension time one can use the same idea to determine the position if information of a few GPS satellites is available.

The following examples will show you how to implement the mathematical operations with MATLAB or Octave. We start with a geometric problem, solved by algebraic methods.

2.10.1 Intersection of two circles

As can be seen in Figure 2.77 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.

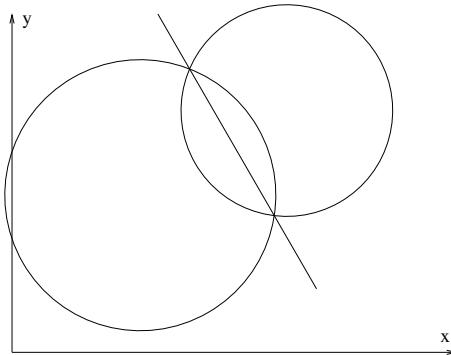


Figure 2.77: Intersection of two circles

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

$$\begin{pmatrix} x(t) \\ y(t) \end{pmatrix} = \begin{pmatrix} x_1 \\ y_1 \end{pmatrix} + r_1 \begin{pmatrix} \cos(t) \\ \sin(t) \end{pmatrix} \quad \text{for } 0 \leq t \leq 2\pi$$

First choose the parameters for the first circle

```
x1m = 2; y1m = 3; % coordinates of the center
r1 = 1.5; % radius
```

then create the graph.

```
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
plot(x1,y1); % create the plot
axis([0,5,0,5],"equal") % choose a domain
```

A second circle is plotted using similar code.

```
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

$$\begin{aligned} x^2 - 2x x_1 + x_1^2 + y^2 - 2y y_1 + y_1^2 &= r_1^2 \\ x^2 - 2x x_2 + x_2^2 + y^2 - 2y y_2 + y_2^2 &= r_2^2 \end{aligned}$$

Subtracting the two equations we find the equation for a straight line on which both points of intersection have to be.

$$-2x(x_1 - x_2) + x_1^2 - x_2^2 - 2y(y_1 - y_2) + y_1^2 - y_2^2 = r_1^2 - r_2^2$$

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

$$\vec{x}(t) = \vec{x}_p + t \vec{v} \quad \text{with } t \in \mathbb{R}$$

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

$$t_{1,2} = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a} = \frac{-2\langle \vec{v}, \vec{x}_p - \vec{x}_m \rangle \pm \sqrt{D}}{2\|\vec{v}\|^2}$$

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 to determine the intersection points of two circles

All the above computation can be put in one function file `IntersectCircles.m`

IntersectCircles.m

```
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
axis equal

% 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

```
IntersectionPoints = 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 2.78 are moving 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 Sébastien Perroud in 2004, to be used as a pick and place robot. At the CSEM Sébastien did develop the concept and the results are PoketDelta and MicroDelta robots.

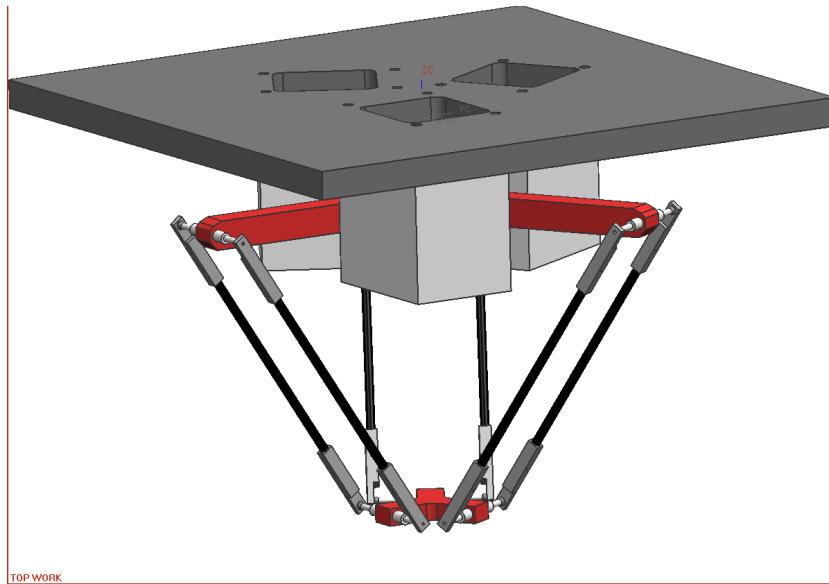


Figure 2.78: A Delta Robot

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.

$$\begin{aligned} -2(x_1 - x_2)x - 2(y_1 - y_2)y - 2(z_1 - z_2)z &= r_1^2 - x_1^2 - y_1^2 - z_1^2 - r_2^2 + x_2^2 + y_2^2 + z_2^2 \\ -2(x_2 - x_3)x - 2(y_2 - y_3)y - 2(z_2 - z_3)z &= r_2^2 - x_2^2 - y_2^2 - z_2^2 - r_3^2 + x_3^2 + y_3^2 + z_3^2 \end{aligned}$$

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 \vec{v} of the homogeneous problem $\mathbf{A} \vec{v} = \vec{0}$.

$$\vec{x}_p = \mathbf{A} \setminus \vec{b} \quad \text{and} \quad \vec{v} = \ker(\mathbf{A})$$

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 Intersection of multiple circles

In Section 2.10.1 we observed that the intersection points of two circles are characterized by a system of quadratic equations

$$\begin{aligned} x^2 - 2x x_1 + x_1^2 + y^2 - 2y y_1 + y_1^2 &= r_1^2 \\ x^2 - 2x x_2 + x_2^2 + y^2 - 2y y_2 + y_2^2 &= r_2^2 \end{aligned}$$

Subtraction these two leads to one linear equation

$$2x(x_2 - x_1) + (x_1^2 - x_2^2) + 2y(y_2 - y_1) + (y_1^2 - y_2^2) = r_1^2 - r_2^2$$

or

$$2(x_2 - x_1)x + 2(y_2 - y_1)y = (r_1^2 - r_2^2) - (x_1^2 - x_2^2) - (y_1^2 - y_2^2)$$

If the intersection points of more than two circles are examined, then we have multiple of these equations. For N circles with centers at (x_i, y_i) and radii r_i for $i = 1, 2, 3, \dots, N$ we have

$$2(x_j - x_i)x + 2(y_j - y_i)y = (r_i^2 - r_j^2) - (x_i^2 - x_j^2) - (y_i^2 - y_j^2) \quad \text{for } 1 \leq i \neq j \leq N \quad (2.10)$$

It is obvious that for $N > 3$ we have too many equations to determine the two unknown coordinates (x, y) of the point of intersection. This is mirrored by the fact that in general N circles do not have a unique point of intersection.

number of circles	2	3	4	5	N
number of equations	1	3	6	10	$\frac{1}{2}N(N - 1)$

Thus it seems that we have $\frac{1}{2}N(N - 1)$ equations, but this is not the full truth. Many equations are linearly dependent. The difference generated by the intersections of the pair $(1, i)$ of circles and by the pair $(1, j)$ is identical to the equation generated by the pair (i, j) . Consequently we have only $N - 1$ independent equations. This confirms that three circles with a unique point of intersection lead to two equations for the two unknowns of the position of the point of intersection. The implementation below uses the pairs $(1, 2), (2, 3), (3, 4), \dots, (N - 1, N)$

Thus we have usually an over-determined system of $N - 1$ linear equations of the type (2.10) and this can be written using a matrix $\mathbf{M} \in \mathbb{R}^{(N-1) \times 2}$

$$\mathbf{M} \begin{pmatrix} x \\ y \end{pmatrix} = \vec{b} \in \mathbb{R}^{N-1}$$

When solving this over-determined system with the backslash operator \backslash Octave/MATLAB will determine the least square solution, i.e. the norm of the residual vector \vec{r}

$$\vec{r} = \mathbf{M} \begin{pmatrix} x \\ y \end{pmatrix} - \vec{b}$$

will be minimized.

- If the given circles happen to have a unique point of intersection, it will be determined by MATLAB/Octave.
- If there is not exact point of intersection, an approximation is generated.
- Even if there is no intersection point at all, the algorithm will return a result. It is the best possible result in the above least square sense.
- A major advantage of the above algorithm is that a linear regression problem is used, instead of a nonlinear system of equations.

As a first example examine the three circles with center at the origin, radius 2.3, center at $(3, 3)$, radius 2.2 and center at $(0, 3)$, radius 1.7. The approximate intersection point is at $(1.175, 1.900)$. Find the resulting graphics in Figure 2.79. Since the three straight lines have an exact point of intersection, the norm of the residual vector \vec{r} is zero, but this does not imply the we have an exact point of intersection for the tree circles.

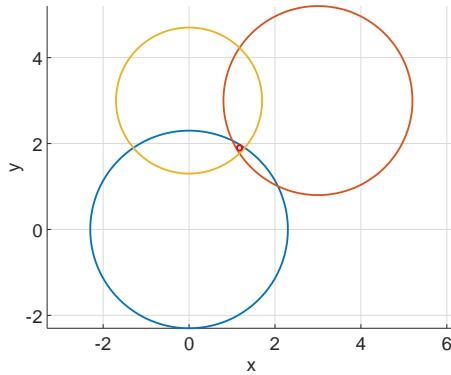


Figure 2.79: Approximate intersection point of three circles

```
% intersect three circles
centers = [0,0; 3,3; 0 3];
radii = [ 2.3;2.2;1.7];

% generate the plots
angle = linspace(0,2*pi,200); xr = cos(angle); yr = sin(angle);
figure(1); clf
hold on
for ii = 1:length(radii)
    plot(centers(ii,1)+radii(ii)*xr,centers(ii,2)+radii(ii)*yr)
end%for
hold off

% construct the overdetermined linear system
N = length(radii);
M = zeros(N-1,2); b = zeros(N-1,1);

for ii = 1:N-1
    M(ii,:) = 2*(centers(ii,:)-centers(ii+1,:));
    b(ii) = radii(ii+1)^2-radii(ii)^2-sum(centers(ii+1,:).^2)+sum(centers(ii,:).^2);
end%for
xy = M\b
residum = norm(M*xy-b)

hold on
plot(xy(1),xy(2),'or') % mark the point of intersection in red
hold off
axis equal
xlabel('x'); ylabel('y')
```

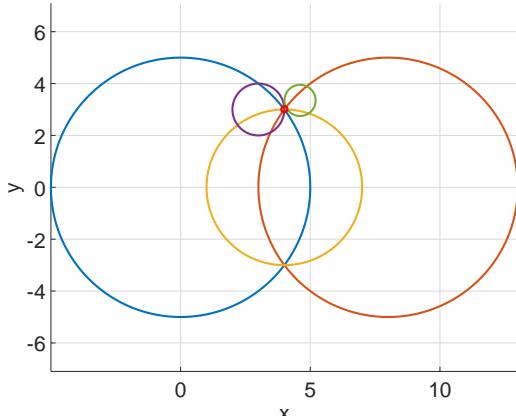
The above code can be reused to examine possible points of intersection of more circles.

circle	center	radius
1	(0, 0)	5
2	(8, 0)	5
3	(4, 0)	3
4	(3, 3)	1
5	(4.6062, 3.35)	0.6

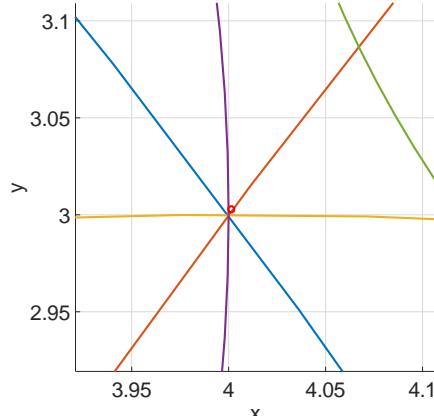
Replace the first section in the code above by the data of these five circles.

```
% a set of four circles
centers = [0,0;8,0;4,0;3,3];
radii = [5;5;3;1];
% add a fifth circle
c5 = [4,3] + 0.7*[cos(pi/6), sin(pi/6)];
centers = [centers;c5]; radii = [radii;0.6];
```

The approximation for the point of intersection is $(x, y) \approx (4.0013, 3.0028)$ and clearly visible in Figure 2.80(a). But these five circles have no common point of intersection, illustrated by the zoom into the critical area in Figure 2.80(b). The length of the residual vector is $\|\vec{r}\| \approx 0.18$. If the fifth circle is dropped from the list of circles, then the exact point of intersection (4, 3) is computed.



(a) global situation



(b) zoomed into critical area

Figure 2.80: Intersection of five circles

2.10.5 Intersection of multiple spheres

The problem of intersecting multiple spheres is very similar to the above question. The only additional aspect is the third coordinate z . For two spheres we have the quadratic equations

$$\begin{aligned} x^2 - 2x x_1 + x_1^2 + y^2 - 2y y_1 + y_1^2 + z^2 - 2z z_1 + z_1^2 &= r_1^2 \\ x^2 - 2x x_2 + x_2^2 + y^2 - 2y y_2 + y_2^2 + z^2 - 2z z_2 + z_2^2 &= r_2^2 \end{aligned}$$

Subtraction these two leads to one linear equation

$$2x(x_2 - x_1) + (x_1^2 - x_2^2) + 2y(y_2 - y_1) + (y_1^2 - y_2^2) + 2z(z_2 - z_1) + (z_1^2 - z_2^2) = r_1^2 - r_2^2$$

or

$$2(x_2 - x_1)x + 2(y_2 - y_1)y + 2(z_2 - z_1)z = (r_1^2 - r_2^2) - (x_1^2 - x_2^2) - (y_1^2 - y_2^2) - (z_1^2 - z_2^2)$$

If the intersection points of more than two spheres are examined we have multiple of these equations. For spheres with centers at (x_i, y_i, z_i) and radii r_i for $i = 1, 2, 3, \dots, N$ we have for $1 \leq i \neq j \leq N$

$$2(x_j - x_i)x + 2(y_j - y_i)y + 2(z_j - z_i)z = (r_i^2 - r_j^2) - (x_i^2 - x_j^2) - (y_i^2 - y_j^2) - (z_i^2 - z_j^2) \quad (2.11)$$

Thus the problem of intersection spheres in space is very similar to the problem of intersecting circles in the plane. To have a unique point of intersection we need at least 4 spheres, but we can use information of more and examine the corresponding least square problem.

The implementation of the algorithm is very similar to the code shown in the previous Section 2.10.4.

2.10.6 GPS

The context and some of the Mathematics of the global positioning system (GPS) is explained in the very nice article [Thomp98]. The basic facts are:

- Each satellite sends accurate information on its own position and the time at which the signal was sent.
- The GPS receiver has information from N satellites and uses its own clock to determine the current distance r_i to the satellite by multiplying the measured travel time by the speed of light c .
- The clock of the GPS receiver might be off by ΔT , leading to a fixed error of $D = c\Delta T$ for the distance to each satellite.

With the above each satellite leads to a quadratic equation

$$\begin{aligned} (x - x_i)^2 + (y - y_i)^2 + (z - z_i)^2 &= (r_i - D)^2 \\ x^2 - 2x x_i + x_i^2 + y^2 - 2y y_i + y_i^2 + z^2 - 2z z_i + z_i^2 &= r_i^2 - 2r_i D + D^2 \end{aligned}$$

Subtracting two of these equations leads to

$$2(x_j - x_i)x + 2(y_j - y_i)y + 2(z_j - z_i)z - 2(r_j - r_i)D = (r_i^2 - r_j^2) - (x_i^2 - x_j^2) - (y_i^2 - y_j^2) - (z_i^2 - z_j^2) \quad (2.12)$$

This is one linear equation for the four unknowns x, y, z and D . With the information of at least 5 satellites we can determine the current position and the offset $\Delta T = \frac{D}{c}$ of the clock of the GPS receiver.

The implementation of the algorithm is again very similar to the code shown in Section 2.10.4.

2.10.7 List of codes and data files

In the previous section the codes in Table 2.17 were used.

filename	function
twocircles.m	script file to determine intersection points
IntersectCircles.m	function file to compute intersection points

Table 2.17: Codes and data files for section 2.10

2.10.8 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

IntersectSpheres.m

```

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 given angle. A CCD camera is placed straight above the object and is recording the laser spot on the solid. With this information one can determine the height of the solid at these 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.

Since some sections of the solid is shaded, i.e. not visible by the laser, the object is then rotated by 90° and rescanned. The two scans have to be combined.

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 describe the goal for each line of code.

ReadData.m

```
% 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 2.81, generated by the code below.

Octave

```
kk = 175; plot(x(:,kk),z(:,kk))
xlabel('x'); ylabel('z');
```

In Figure 2.82 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 2.83. 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 2.82.

The command `mesh (x,y,z)` will create Figure 2.84, 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 from a different angle and then try to merge the two pictures.

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

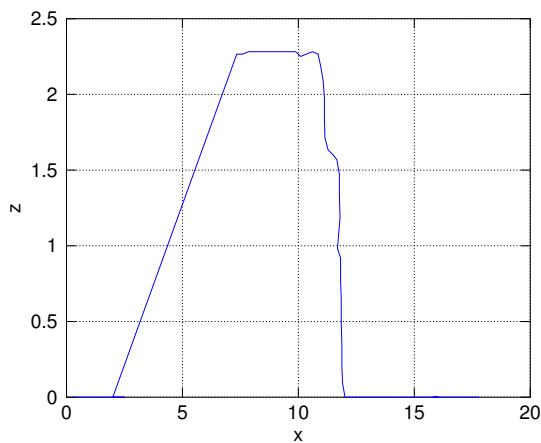
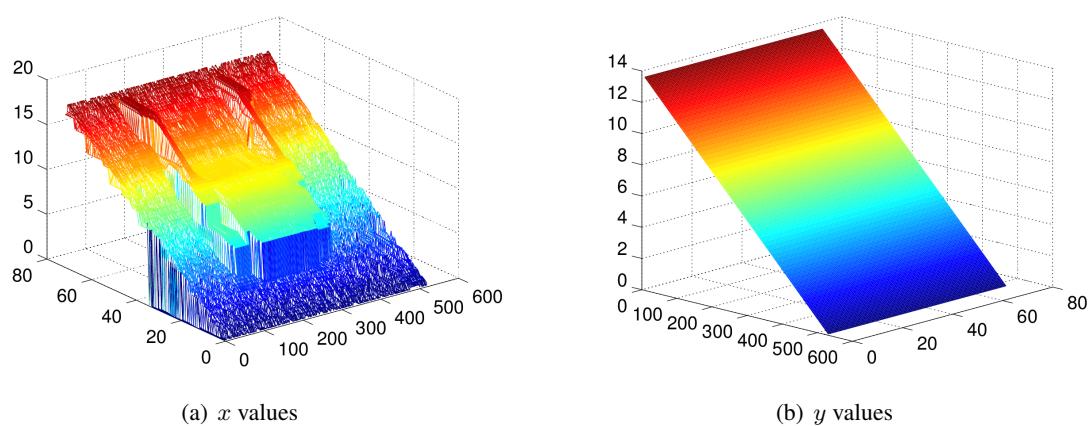
Figure 2.81: Cross section in x directionFigure 2.82: Location of laser spot, varied in x direction

Figure 2.83: Values of the measured coordinates

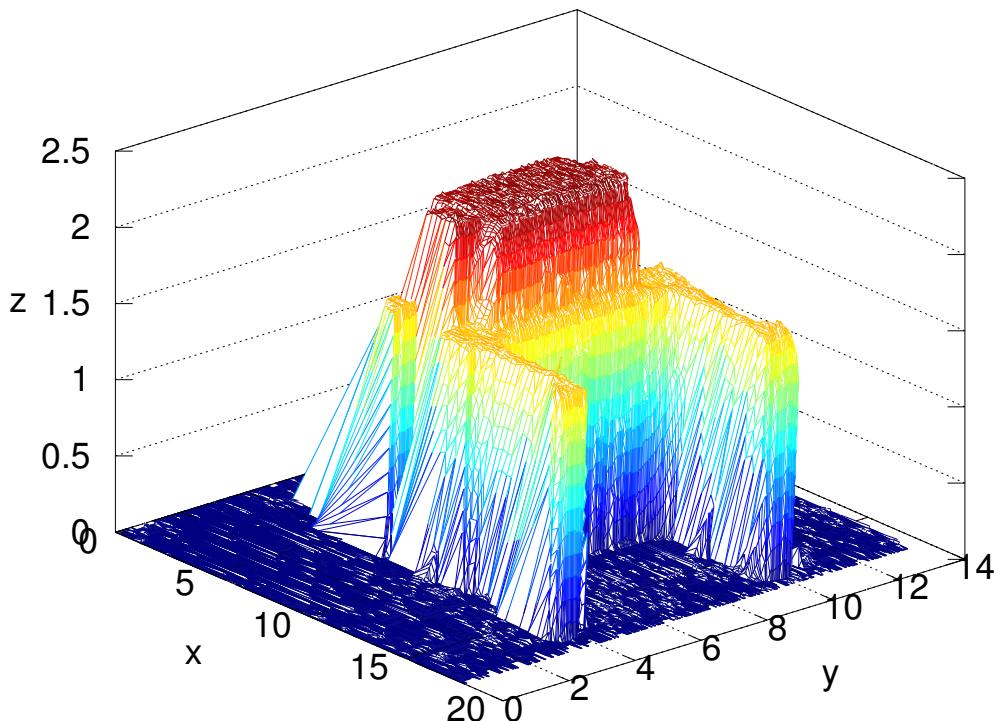


Figure 2.84: 3-D scan of solid from one direction

1. choose the number of grid points in either direction.
2. along each line in x direction (see Figure 2.81) 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; % add 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%for

xlin = xlin'*ones(1,npix); % create the uniformly spaced x and y values
ylin = ones(1,npix)*y(1,:);

% plot the interpolated data
figure(2);
mesh(xlin,ylin,zlin)

```

```
xlabel('x'); ylabel('y'); zlabel('z');
```

As the 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 $\alpha = 30^\circ = \pi/6$ and 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

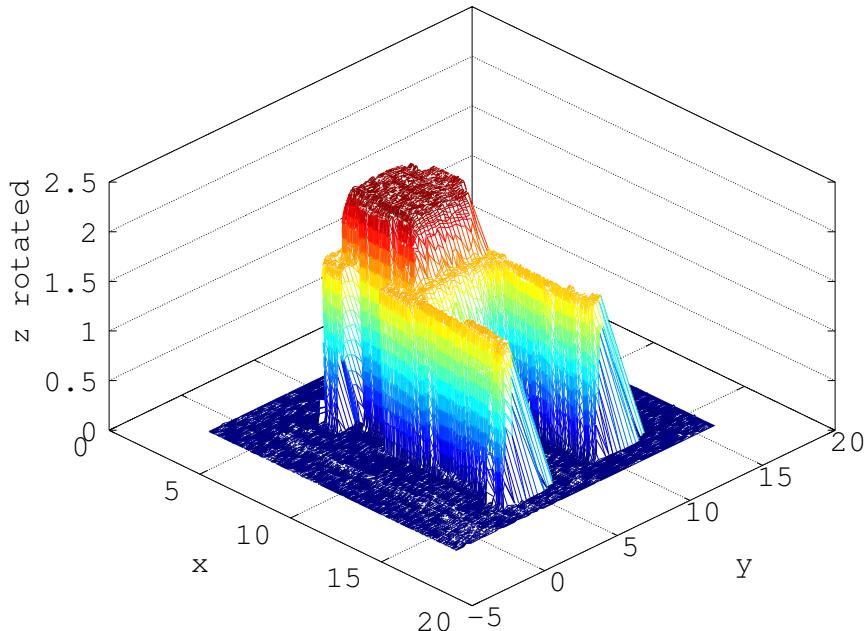


Figure 2.85: 3-D scan of solid from a second direction

Now the solid is rotated by 90° on the mounting plate and a second scan generates independent results, shown in Figure 2.85. The result has to be compared with Figure 2.84. 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 2.84 is in a shadowed area, replace the height by the result from Figure 2.85.
3. Plot the new, combined picture.

With 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 2.86.

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 2.18 were used. The following sequence of commands in Octave or MATLAB should reproduce the results in this section. Use `ReadData.m` to read all data files and generate a first plot. Then use `UniformMesh.m` to examine the solid on a uniform mesh and determine the shadow areas. Finally the two scans are combined with the help of `RotateShape.m`.

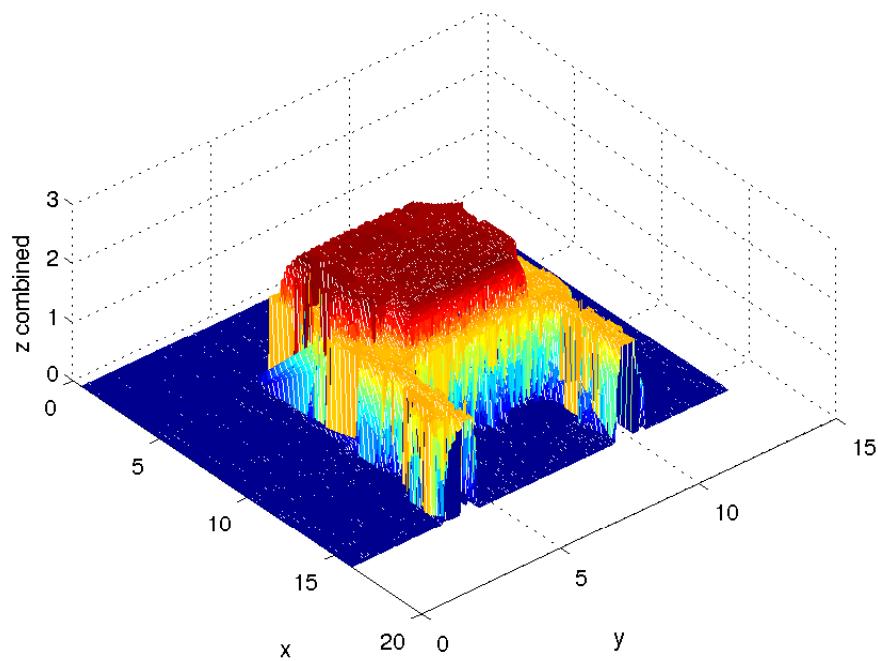


Figure 2.86: Combination of the two scans

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 2.18: 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

$$G(s) = \frac{4 + 4.8s}{5.5 + 17.5s + 14.5s^2 + 3.5s^3 + s^4}$$

By writing 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 2.87.

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 2.88 . 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 2.89. 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

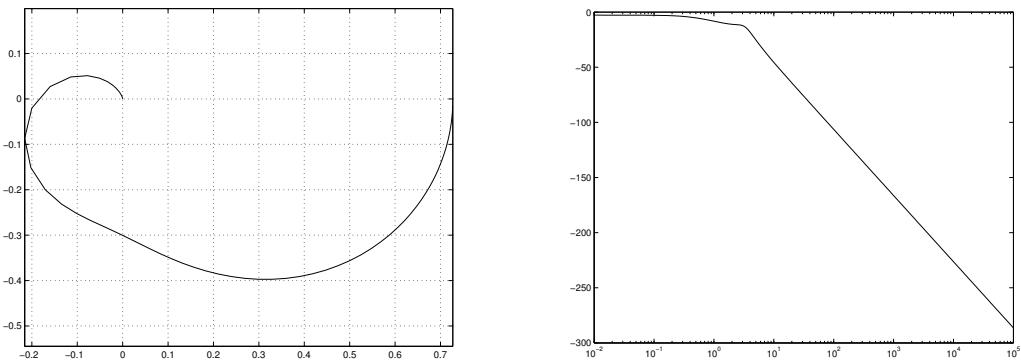


Figure 2.87: Nyquist and Bode plots of the system, programmed with MATLAB

```
num = [4.8 4];
denum = [1 3.5 14.5 17.5 5.5];
nyquist(num,denum);
bode(num,denum);
```

Nyquist Diagram

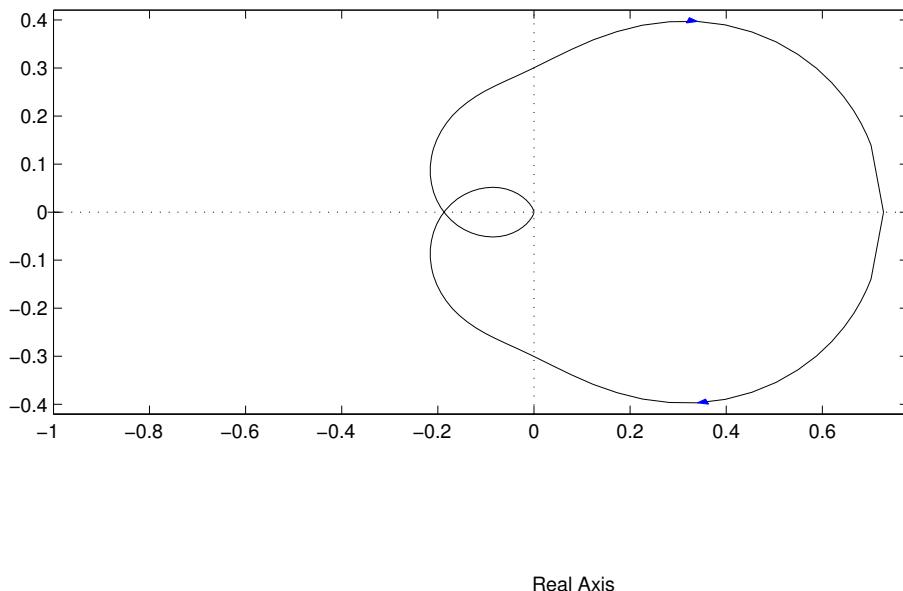


Figure 2.88: Nyquist plot of the system, with control toolbox of MATLAB

2.12.3 Create the Bode and Nyquist plots of a system with Octave commands

The Octave Forge package `control` of Octave provides a set of commands for control theory, including Bode and Nyquist plots. The code below leads to the Figures 2.90 and 2.91. You may want to consult the online help on the commands `tf()`, `bode()` and `nyquist()`.

Octave

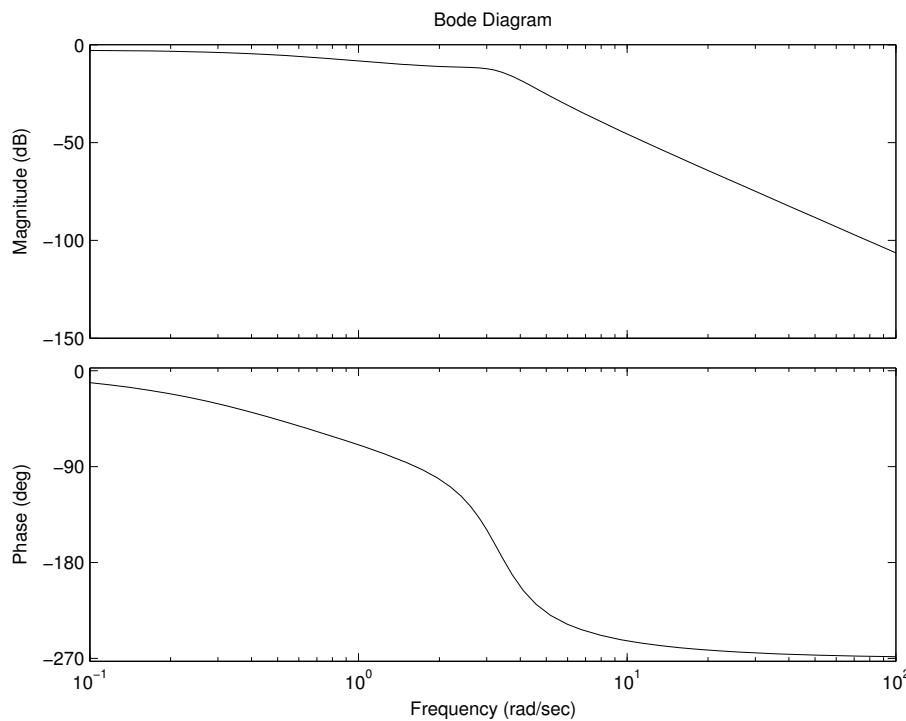


Figure 2.89: Bode plots of the system, with control toolbox of MATLAB

```
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 2.91 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 and 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 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;
```

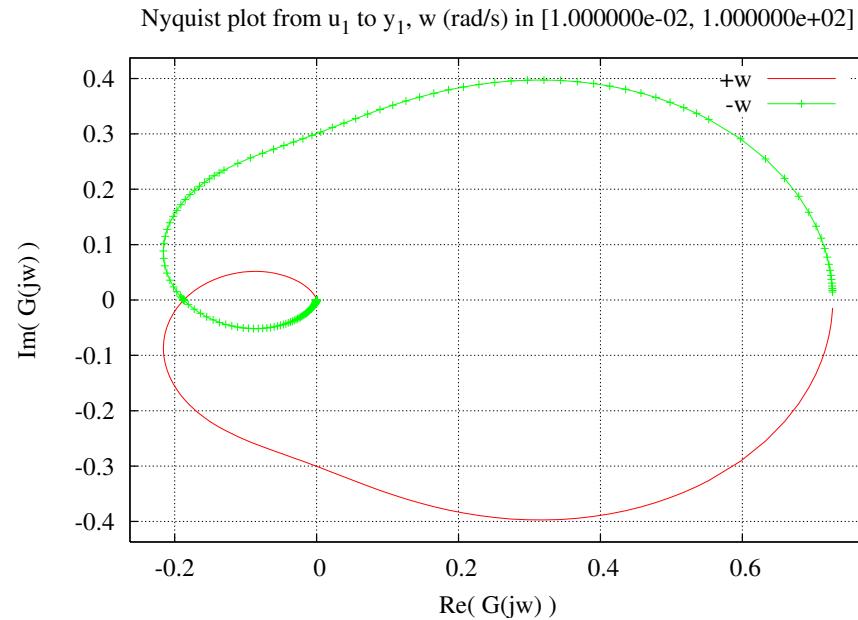


Figure 2.90: Nyquist plot of the system, created by Octave

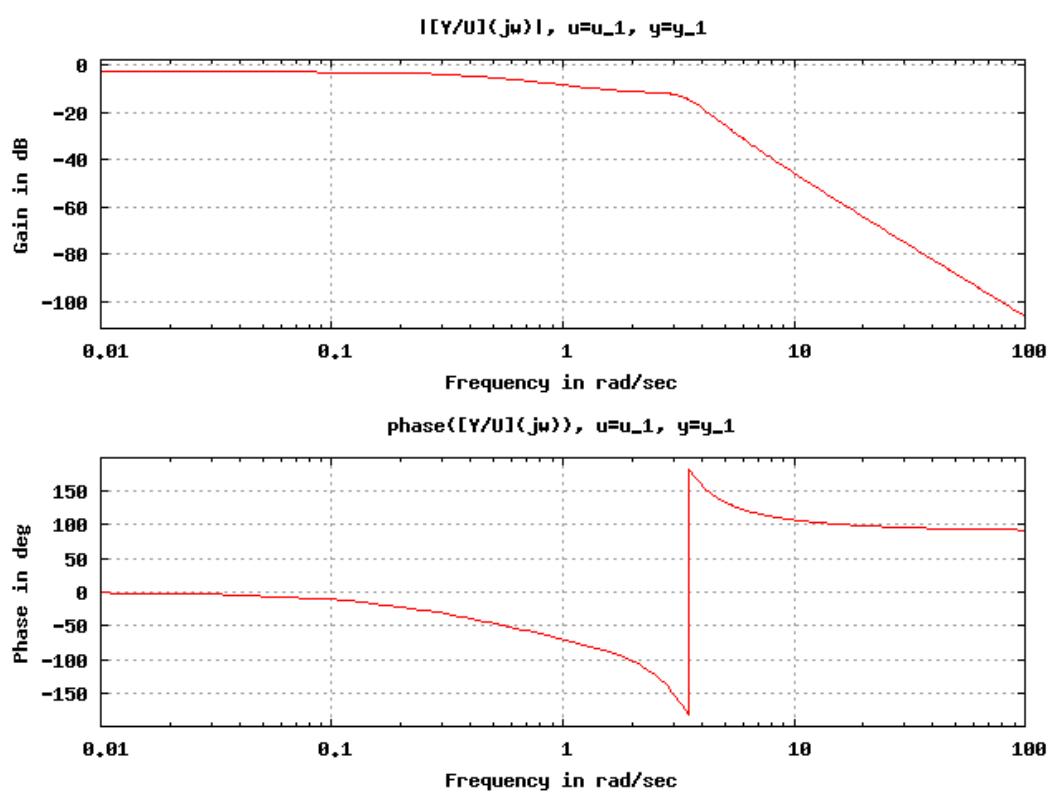


Figure 2.91: Bode plots of the system, created by Octave

```

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 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)

```

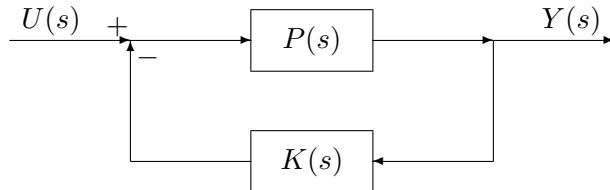
The result shows that the system is in fact stable, since all poles (zeros of the denominator) have negative real part.

There are some demos of the specialized commands, all documented in the section `OCST demos` of the Octave Forge 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

36 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

$$T(s) = \frac{P(s)}{1 + K(s)G(s)} = \frac{\frac{1}{s+2}}{1 + \frac{s+1}{s} \cdot \frac{1}{s+2}} = \frac{s}{s^2 + 3s + 1}$$

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

```

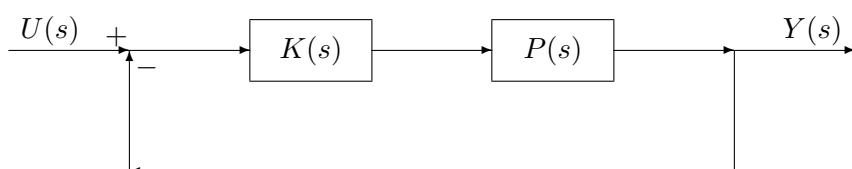
num = 1 0
den = 1 3 1

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 $p_2 \approx -0.38$. \diamond

37 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

$$\begin{aligned}
 Y(s) &= K(s)P(s) (U(s) - Y(s)) \\
 (1 + K(s)P(s)) Y(s) &= K(s)P(s) U(s) \\
 Y(s) &= \frac{K(s)P(s)}{1 + K(s)P(s)} U(s) \\
 &= \frac{\frac{s+1}{s^2+2s}}{1 + \frac{s+1}{s^2+2s}} U(s) = \frac{s+1}{s^2+3s+1} U(s)
 \end{aligned}$$

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 your 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 object 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 2.88 and the poles are given by

Octave

```

-1.0000 + 3.1623 i
-1.0000 - 3.1623 i
-1.0000
-0.5000

```

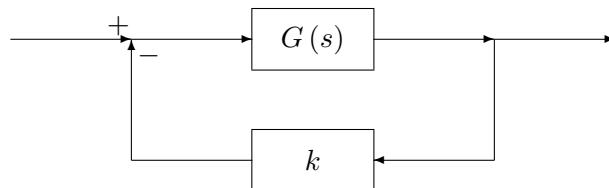
With Octave the command `sys2zp()` determines zeros and poles of the transfer function. Since all real parts of the poles are negative we conclude that the open loop system is stable.

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 2.88 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 `backsyst=tf(kvalues(j),1)`; the feedback part of the system is created. The amplification factor given by `kvalues(j)`. Then with `FeedbackSys=feedback(mysys, backsyst)`; 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 2.92 shows that all poles are 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,'bo');
title('All poles'); xlabel('Real'); ylabel('Imaginary')

```

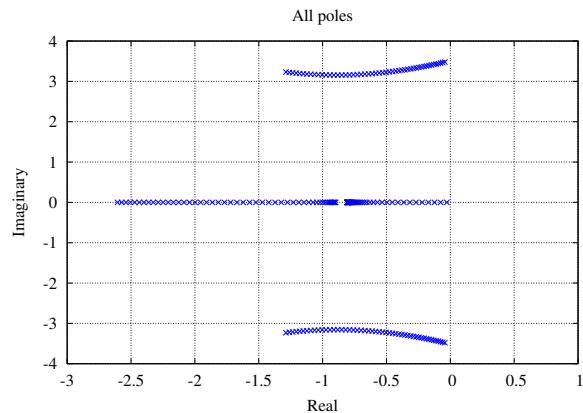


Figure 2.92: Pole location of the closed loop system

2.12.7 List of codes and data files

In the previous section the codes in Table 2.19 were used.

filename	function
fixangles.m	function file to eliminate artificial phase jumps
mybode.m	a modified version of the command <code>bode()</code>
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 2.19: 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 playrec 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. Use the command `toeplitz()` to generate matrices for periodic boundary conditions.
- Sparse matrix operations, use `LinearSystems.tex` and the test provided in that directory.
- Present my solution of KdV, using the conservation law
- Add an index with the keywords. DONE
- Terminal interaction by `input()`, `menu()`, `yes_or_no()`, `kbhit()`
- GUI using `inputdlg()`, `uicontrol()`, `demo_uicontrol.m`
- `dlmread()` might be extremely slow on large data files, see
`/Projects/Miracor/CSP_LDAP/Dec13/OCCLUDED`. Use awk to write better file with the numerical data only.

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