Scientific Computing with **MATLAB**

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About the author

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http://www.gribblelab.org

This document

This document was typeset using LaTeX version 3.14159265-2.6-1.40.16 (TeX Live 2015). These notes in their entirety, including the LaTeX source, are available on GitHub[8] here:

https://github.com/paulgribble/SciComp

License

Links

[1] http://www.uwo.ca

[2] http://psychology.uwo.ca

[3] http://www.schulich.uwo.ca/physpharm/

[4] http://www.schulich.uwo.ca

[5] http://www.uwo.ca/bmi

[6] http://www.schulich.uwo.ca/neuroscience/

[7] http://www.mcgill.ca

[8] https://github.com

[9] http://creativecommons.org/licenses/by/4.0/

Preface

These are the course notes associated with my graduate-level course called Scientific Computing (Psychology 9040a), given in the Department of Psychology[10] at the University of Western Ontario[11]. The goal of the course is to provide you with skills in scientific computing: tools and techniques that you can use in your own scientific research. We will focus on learning to think about experiments and data in a computational framework, and we will learn to implement specific algorithms using a high-level programming language (MATLAB). Learning how to program will significantly enhance your ability to conduct scientific research today and in the future. Programming skills will provide you with the ability to go beyond what is available in pre-packaged analysis tools, and code your own custom data processing, analysis and visualization pipelines.

The course (and these notes) are organized around using MATLAB[12] (MathWorks[13]), a high-level language and interactive environment for scientific computing. MATLAB version R2015b is used throughout.

Chapters 13 and 14 on integrating ordinary differential equations and simulating dynamical systems are based on notes from a previous course that were developed in collaboration with Dr. Dinant Kistemaker (VU Amsterdam).

For a much more detailed, comprehensive book on MATLAB and all of its functionality, I can recommend:

Mastering MATLAB by Duane Hanselman & Bruce Littlefield. Pearson Eduction, Inc., publishing as Prentice Hall, Upper Saddle River, NJ, 2012. ISBN: 978-0-13-601330-3.

They have a website associated with their book here:

http://www.masteringmatlab.com

Conventions in the notes

Web links are given in blue font and are clickable when viewing this document as a .pdf on your computer, for example: Gribble Lab[14]. Code snippets are shown in monospaced font within a box with a gray backround such as this:

```
>> disp('Hello, world!')
Hello, world!
```

Also note that Chapter headings, sections and subsections in the Table of Contents are hyperlinks in this .pdf, so that if you click on them you are taken directly to the appropriate page.

Comments

Do you have ideas about how to improve these notes? Please get in touch, send me an email at paul@gribblelab.org

Links

[10] http://psychology.uwo.ca

[11] http://www.uwo.ca

[12] http://www.mathworks.com/products/matlab/

[13] http://www.mathworks.com

[14] http://www.gribblelab.org

Contents

1 What is computer code?

What is a computer program? What is code? What is a computer language? A computer program is simply a series of instructions that the computer executes, one after the other. An instruction is a single command. A program is a series of instructions. Code is another way of referring to a single instruction or a series of instructions (a program).

1.1 High-level vs low-level languages

The CPU[15] (central processing unit) chip(s) that sit on the motherboard[16] of your computer is the piece of hardware that actually executes instructions. A CPU only understands a relatively low-level language called machine code[17]. Often machine code is generated automatically by translating code written in assembly language[18], which is a low-level programming language[19] that has a relatively direcy relationship to machine code (but is more readable by a human). A utility program called an assembler[20] is what translates assembly language code into machine code.

In this course we will be learning how to program in MATLAB, which is a high-level programming language[21]. The "high-level" refers to the fact that the language has a strong abstraction from the details of the computer (the details of the machine code). A "strong abstraction" means that one can operate using high-level instructions without having to worry about the low-level details of carrying out those instructions.

An analogy is motor skill learning. A high-level language for human action

might be *drive your car to the grocery store and buy apples*. A low-level version of this might be something like: (1) walk to your car; (2) open the door; (3) start the ignition; (4) put the transmission into Drive; (5) step on the gas pedal, and so on. An even lower-level description might involve instructions like: (1) activate your gastrocnemius muscle[22] until you feel 2 kg of pressure on the underside of your right foot, maintain this pressure for 2.7 seconds, then release (stepping on the gas pedal); (2) move your left and right eyeballs 27 degrees to the left (check for oncoming cars); (3) activate your pectoralis muscle on the right side of your chest and simultaneously squeeze the steering wheel with the fingers on your right hand (steer the car to the left); and so on.

For scientific programming, we would like to deal at the highest level we can, so that we can avoid worrying about the low-level details. We might for example want to plot a line in a Figure and colour it blue. We don't want to have to program the low-level details of how each pixel on the screen is set, and how to generate each letter of the font that is used to specify the x-axis label.

As an example, here is a *hello, world* program written in a variety of languages, just to give you a sense of things. You can see the high-level languages like MATLAB, Python and R are extremely readable and understandable, even though you may not know anything about these languages (yet). The C code is less readable, there are lots of details one may not know about... and the assembly language example is a bit of a nightmare, obviously too low-level for our needs here.

MATLAB

```
disp('hello, world')
```

Python

```
print "hello, world"
```

R

```
cat("hello, world\n")
```

Javascript

```
document.write("hello, world");
```

Fortran

```
print *,"hello, world"
```

C

```
#include <stdio.h>
int main (int argc, char *argv[]) {
  printf("hello, world\n");
  return 0;
}
```

8086 Assembly language

```
; this example prints out  "hello world!"
; by writing directly to video memory.
; in vga memory: first byte is ascii character, byte that follows is
    character attribute.
; if you change the second byte, you can change the color of
; the character even after it is printed.
; character attribute is 8 bit value,
; high 4 bits set background color and low 4 bits set foreground color.

; hex    bin        color
;
; 0      0000      black
; 1      0001      blue
; 2      0010      green
; 3      0011      cyan
; 4      0100      red
```

```
; 5      0101      magenta
; 6      0110      brown
; 7      0111      light gray
; 8      1000      dark gray
; 9      1001      light blue
; a      1010      light green
; b      1011      light cyan
; c      1100      light red
; d      1101      light magenta
; e      1110      yellow
; f      1111      white

org 100h

; set video mode
mov ax, 3     ; text mode 80x25, 16 colors, 8 pages (ah=0, al=3)
int 10h       ; do it!

; cancel blinking and enable all 16 colors:
mov ax, 1003h
mov bx, 0
int 10h

; set segment register:
mov     ax, 0b800h
mov     ds, ax

; print "hello world"
; first byte is ascii code, second byte is color code.

mov [02h], 'H'
mov [04h], 'e'
mov [06h], 'l'
mov [08h], 'l'
mov [0ah], 'o'
mov [0ch], ','
mov [0eh], 'W'
mov [10h], 'o'
mov [12h], 'r'
mov [14h], 'l'
```

```
mov [16h], 'd'
mov [18h], '!'

; color all characters:
mov cx, 12  ; number of characters.
mov di, 03h ; start from byte after 'h'

c:  mov [di], 11101100b   ; light red(1100) on yellow(1110)
    add di, 2 ; skip over next ascii code in vga memory.
    loop c

; wait for any key press:
mov ah, 0
int 16h

ret
```

1.2 Interpreted vs compiled languages

Some languages like C and Fortran are compiled languages[23], meaning that we write code in C or Fortran, and then to run the code (to have the computer execute those instructions) we first have to translate the code into machine code, and then run the machine code. The utility function that performs this translation (compilation) is called a compiler[24]. In addition to simply translating a high-level language into machine code, modern compilers will also perform a number of optimizations to ensure that the resulting machine code runs fast, and uses little memory. Typically we write a program in C, then compile it, and if there are no errors, we then run it. We deal with the entire program as a whole. Compiled program tend to be fast since the entire program is compiled and optimized as a whole, into machine code, and then run on the CPU as a whole.

Other languages, like MATLAB, Python and R, are interpreted languages[25], meaning that we write code which is then translated, command by command, into machine language instructions which are run one after another. This is

done using a utility called an interpreter[26]. We don't have to compile the whole program all together in order to run it. Instead we can run it one instruction at a time. Typically we do this in an interactive programming environment where we can type in a command, and observe the result, and then type a next command, etc. This is known as the read-eval-print (REPL) loop[27]. This is advantageous for scientific programming, where we typically spend a lot of time exploring our data in an interactive way. One can of course run a program such as this in a batch mode, all at once, without the interactive REPL environment... but this doesn't change the fact that the translation to machine code still happens one line at a time, each in isolation. Interpreted languages tend to be slow, because every single command is taken in isolation, one after the other, and in real time translated into machine code which is then executed in a piecemeal fashion.

For interactive programming, when we are exploring our data, interpreted languages like MATLAB, Python and R shine. They may be slow but it (typically) doesn't matter, because what's many orders of magnitude slower, is the firing of the neurons in our brain as we consider the output of each command and decide what to do next, how to analyse our data differently, what to plot next, etc. For batch programming (for example fMRI processing pipelines, or electrophysiological recording signal processing, or numerical optimizations, or statistical bootstrapping operations), where we want to run a large set of instructions all at once, without looking at the result of each step along the way, compiled languages really shine. They are much faster than interpreted languages, often several orders of magnitude faster. It's not unusual for even a simple program written in C to run 100x or even 1000x faster than the same program written in MATLAB, Python or R.

A 1000x speedup may not be very important when the program runs in 5 seconds (versus 5 milliseconds) but when a program takes 60 seconds to run in MATLAB, for example, things can start to get problematic.

Imagine you write some MATLAB code to read in data from one subject, process that data, and write the result to a file, and that operation takes 60 seconds. Is

that so bad? Not if you only have to run it once. Now let's imagine you have 15 subjects in your group. Now 60 seconds is 15 minutes. Now let's say you have 4 groups. Now 15 minutes is one hour. You run your program, go have lunch, and come back an hour later and you find there was an error. You fix the error and re-run. Another hour. Even if you get it right, now imagine your supervisor asks you to re-run the analysis 5 different ways, varying some parameter of the analysis (maybe filtering the data at a different frequency, for example). Now you need 5 hours to see the result. It doesn't take a huge amount of data to run into this sort of situation.

Now imagine if you could program this data processing pipeline in C instead, and you could achieve a 500x speedup (not unusual), now those 5 hours turn into 36 seconds (you could run your analysis twice and it would still take less time than listening to Stairway to Heaven a dozen times). All of a sudden it's the difference between an overnight operation and a 30 second operation. That makes a big difference to the kind of work you can do, and the kinds of questions you can pursue.

MATLAB is pretty good about using optimized, compiled subroutines for operations that it knows it can farm out (e.g. many matrix algebra operations), so in many cases the difference between MATLAB and C performance isn't as great as it is for others. MATLAB also has a toolbox (called the MATLAB Coder[28]) that will allow you to generate C code from your MATLAB code, so in principle you can take slow MATLAB code and generate faster, compiled C code. In practice this can be tricky though.

My own approach is to use interpreted languages like Python, R, MATLAB, etc, for prototyping: exploring small amounts of data, for developing an approach, and algorithms, for analysing data, and for generating graphics. When I have a computation, or a simulation, or a series of operations that are time-consuming, I think about implementing them in C. Interpreted languages for *prototyping* and *exploration*, and C for *performance*.

Links

[15] https://en.wikipedia.org/wiki/Central_processing_unit

[16] https://en.wikipedia.org/wiki/Motherboard

[17] https://en.wikipedia.org/wiki/Machine_code

[18] https://en.wikipedia.org/wiki/Assembly_language

[19] https://en.wikipedia.org/wiki/Low-level_programming_language

[20] https://en.wikipedia.org/wiki/Assembly_language#Assembler

[21] https://en.wikipedia.org/wiki/High-level_programming_language

[22] https://en.wikipedia.org/wiki/Gastrocnemius_muscle

[23] https://en.wikipedia.org/wiki/Compiled_language

[24] https://en.wikipedia.org/wiki/Compiler

[25] https://en.wikipedia.org/wiki/Interpreted_language

[26] https://en.wikipedia.org/wiki/Interpreter_(computing)

[27] https://en.wikipedia.org/wiki/Read-eval-print_loop

[28] http://www.mathworks.com/products/matlab-coder/

2 Digital representation of data

Here we review how data are stored in a digital format on computers.

2.1 Binary

At its core, all information on a digital computer is stored in a binary[29] format. Binary format represents information using a series of 0s and 1s. If there are n digits of a binary code, one can represent 2^n bits[30] of information.

So for example the binary number denoted by:

```
0001
```

represents the number 1. The convention here is called little-endian[31] because the least significant value is on the right, and as one reads right to left, the value of each binary digit doubles. So for example the number 2 would be represented as:

```
0010
```

This is a 4-bit code since there are 4 binary digits. The full list of all values that can be represented using a 4-bit code are shown in Table 2.1.

So with a 4-bit binary code one can represent $2^4 = 16$ different values (0-15). Each additional bit doubles the number of values one can represent. So a 5-bit code enables us to represent 32 distinct values, a 6-bit code 64, a 7-bit code 128

Binary	Decimal
0000	0
0001	1
0010	2
0011	3
0100	4
0101	5
0110	6
0111	7
1000	8
1001	9
1010	10
1011	11
1100	12
1101	13
1110	14
1111	15

Table 2.1: Binary and decimal values for a 4-bit code.

and an 8-bit code 256 values (0-255).

Another piece of terminology: a given sequence of binary digits that forms the natural unit of data for a given processor (CPU) is called a word[32].

Have a look at the ASCII table[33]. The standard ASCII table represents 128 different characters and the extended ASCII codes enable another 128 for a total of 256 characters. How many binary bits are used for each?

2.2 Hexadecimal

You will also see in the ASCII table that it gives the decimal representation of each character but also the Hexadecimal and Octal representations. The hexadecimal[34] system is a base-16 code and the octal[35] system is a base-8 code. Hex values for a single hexadecimal digit can range over:

```
0 1 2 3 4 5 6 7 8 9 A B C D E F
```

If we use a 2-digit hex code we can represent $16 * 16 = 256$ distinct values. In computer science, engineering and programming, a common practice is to represent successive 4-bit binary sequences using single-digit hex codes.

Table 2.2 shows 4-bit values of Binary, Decimal and Hexadecimal.

Binary	Decimal	Hexadecimal
0000	0	0
0001	1	1
0010	2	2
0011	3	3
0100	4	4
0101	5	5
0110	6	6
0111	7	7
1000	8	8
1001	9	9
1010	10	A
1011	11	B
1100	12	C
1101	13	D
1110	14	E
1111	15	F

Table 2.2: Binary, Decimal and Hexadecimal values for a 4-bit code.

If we have 8-bit binary codes we would use successive hex digits to represent each 4-bit word of the 8-bit byte[36] (another piece of lingo). Table 2.3 shows how this would look for some 8-bit values in binary, decimal and hexadecimal.

The left chunk of 4-bit binary digits (the left word) is represented in hex as a single hex digit (0-F) and the next chunk of 4-bit binary digits (the right word) is represented as another single hex digit (0-F).

Hex is typically used to represent bytes (8-bits long) because it is a more compact notation than using 8 binary digits (hex uses just 2 hex digits).

Binary	Decimal	Hexadecimal
0000 0000	0	00
0000 0001	1	01
0000 0010	2	02
…	…	…
1111 1101	253	FD
1111 1110	254	FE
1111 1111	255	FF

Table 2.3: Binary, Decimal and Hexadecimal values for an 8-bit (1-byte) code.

2.3 Floating point values

The material above talks about the decimal representation of bytes in terms of integer values (e.g. 0-255). Frequently however in science we want the ability to represent real numbers[37] on a continuous scale, for example 3.14159, or 5.5, or 0.123, etc. For this, the convention is to use floating point[38] representations of numbers.

The idea behind the floating point representation is that it allows us to represent an approximation of a real number in a way that allows for a large number of possible values. Floating point numbers are represented to a fixed number of *significant digits* (called a *significand*) and then this is scaled using a *base* raised to an *exponent*:

$$s \times b^e \tag{2.1}$$

This is related to something you may have come across in high-school science, namely scientific notation[39]. In scientific notation, the base is 10 and so a real number like 123.4 is represented as 1.234×10^2.

In computers there are different conventions for different CPUs but there are standards, like the IEEE 754[40] floating-point standard. As an example, a so-called single-precision floating point format[41] is represented in binary (using a base of 2) using 32 bits (4 bytes) and a /double precision/ floating point number

is represented using 64 bits (8 bytes). In C you can find out how many bytes are used for various types using the `sizeof()` function:

```
#include <stdio.h>
int main(int argc, char *argv[]) {
  printf("a single precision float uses %ld bytes\n", sizeof(float));
  printf("a double precision float uses %ld bytes\n", sizeof(double));
  return 0;
}
```

On my macbook pro laptop this results in this output:

```
a single precision float uses 4 bytes
a double precision float uses 8 bytes
```

According to the IEEE 754 standard, a single precision 32-bit binary floating point representation is composed of a *1-bit sign bit* (signifying whether the number is positive or negative), an *8-bit exponent* and a *23-bit significand*. See the various wikipedia pages for full details.

There is a key phrase in the description of floating point values above, which is that floating point representation allows us to store an *approximation* of a real number. If we attempt to represent a number that has more significant digits than can be store in a 32-bit floating point value, then we have to approximate that real number, typically by rounding off the digits that cannot fit in the 32 bits. This introduces rounding error[42].

Now with 32 bits, or even 64-bits in the case of double precision floating point values, rounding error is likely to be relatively small. However it's not zero, and depending on what your program is doing with these values, the rounding errors can accumulate (for example if you're simulating a dynamical system over thousands of time steps, and at each time step there is a small rounding error).

We don't need a fancy simulation however to see the results of floating point rounding error. Open up your favourite programming language (MATLAB,

Python, R, C, etc) and type the following (adjust the syntax as needed for your language of choice):

```
(0.1 + 0.2) == 0.3
```

What do you get? In MATLAB I get:

```
>> (0.1 + 0.2) == 0.3

ans =

     0
```

In MATLAB, `0` is synonymous with the logical value `FALSE`. What's going on here? What's happening is that these decimal numbers, 0.1, 0.2 and 0.3 are being represented by the computer in a binary floating-point format, that is, using a base 2 representation. The issue is that in base 2, the decimal number 0.1 cannot be represented precisely, no matter how many bits you use. Plug in the decimal number 0.1 into an online binary/decimal/hexadecimal converter (such as here[43]) and you will see that the binary representation of 0.1 is an infinitely repeating sequence:

```
0.0001100110011001100110011001100... (base 2)
```

This shouldn't be an unfamiliar situation, if we remember that there are also real numbers that cannot be represented precisely in decimal format, either, because they involve an infintely repeating sequence. For example the real number $\frac{1}{3}$ when represented in decimal[44] is:

```
0.3333333333... (base 10)
```

If we try to represent $\frac{1}{3}$ using n decimal digits then we have to chop off the digits to the right that we cannot include, thereby rounding the number. We lose some

amount of precision that depends on how many significant digits we retain in our representation.

So the same is true in binary. There are some real numbers that cannot be represented precisely in binary floating-point format.

See here[45] for some examples of significant adverse events (i.e. disasters) cause by numerical errors.

Rounding can be used to your advantage, if you're in the business of stealing from people (see salami slicing[46]). In the awesomely kitchy 1980s movie Superman III[47], Richard Pryor's character plays a "bumbling computer genius" who embezzles a ton of money by stealing a large number of fractions of cents (which in the movie are said to be lost anyway due to rounding) from his company's payroll (YouTube clip here[48]).

There is a comprehensive theoretical summary of these issues here: What Every Computer Scientist Should Know About Floating-Point Arithmetic[49].

Also see these webpages from the MathWorks online documentation about how MATLAB represents floating-point numbers:

Floating-Point Numbers[50]

and this section on avoiding common problems with Floating-Point Arithmetic:

Avoiding Common Problems with Floating-Point Arithmetic[51]

2.4 ASCII

ASCII stands for *American Standard Code for Information Interchange*. ASCII codes delineate how text is represented in digital format for computers (as well as other communications equipment).

ASCII uses a 7-bit binary code to represent 128 specific characters of text. The first 32 codes (decimal 0 through 31) are non-printable codes like TAB, BEL (play a bell sound), CR (carriage return), etc. Decimal codes 32 through 47 are more

typical text symbols like # and &. Decimal codes 48 through 57 are the numbers 0 through 9. Decimal codes 65 through 90 are capital letters A through Z, and codes 97 through 122 are lowercase letters a through z. Table 2.4 shows codes in decimal, hexadecimal and octal (base-8) for the numbers 0 through 9. Table 2.5 shows codes for uppercase and lowercase letters.

Dec	Hex	Oct	Chr
48	30	060	0
49	31	061	1
50	32	062	2
51	33	063	3
52	34	064	4
53	35	065	5
54	36	066	6
55	37	067	7
56	38	070	8
57	39	071	9

Table 2.4: 7-bit ASCII codes for the numbers 0 through 9.

For a full description of the 7-bit ascii codes in their entirety, including the *extended ASCII codes* (where you will find things like ö and é), see this webpage:

http://www.asciitable.com[52] (ASCII Table and Extended ASCII Codes).

In MATLAB, all individual text characters (variable type `char`) are represented, under the hood, as decimal ASCII values. Have a look at this code, in which we ask for the numeric value of individual characters. You can see that the result corresponds to their decimal ASCII values in Table 2.5.

```
>> double('a')

ans =

    97

>> double('b')

ans =
```

```
    98

>> double('z')

ans =

   122
```

You can get the character value of an ASCII code in MATLAB using the `char()` function:

```
>> char(65)

ans =

A
```

You can use your knowledge of ASCII codes to do tricky things in MATLAB, like convert to and from uppercase and lowercase, given your knowledge that the difference (in decimal) between ASCII `A` and ASCII `a` is 32 (see Table 2.5).

```
>> char('A' + 32)

ans =

a

>> char('a' - 32)

ans =

A
```

Exercises

E 2.1 Convert the following decimal integer values into hexadecimal (resist the urge to use an online decimal-to-hex tool, try to do it using your brain):

1. 64206
2. 47806
3. 4013
4. 64222
5. 47802

E 2.2 Convert the following decimal integer values into binary (little-endian format):

1. 2
2. 20
3. 200
4. 17
5. 170

E 2.3 Convert the following (little-endian) binary values into hexadecimal:

1. 0001
2. 1000
3. 1001
4. 1000 0001
5. 1011 1010 1011 1010

Links

[29] http://en.wikipedia.org/wiki/Binary_code

[30] http://en.wikipedia.org/wiki/Bit

[31] http://en.wikipedia.org/wiki/Endianness

[32] http://en.wikipedia.org/wiki/Word_(computer_architecture)

[33] http://www.asciitable.com

[34] http://en.wikipedia.org/wiki/Hexadecimal

[35] http://en.wikipedia.org/wiki/Octal

[36] http://en.wikipedia.org/wiki/Byte

[37] http://en.wikipedia.org/wiki/Real_number

[38] http://en.wikipedia.org/wiki/Floating_point

[39] http://en.wikipedia.org/wiki/Scientific_notation

[40] http://en.wikipedia.org/wiki/IEEE_floating_point

[41] http://en.wikipedia.org/wiki/Binary32

[42] http://en.wikipedia.org/wiki/Round-off_error

[43] http://www.wolframalpha.com/input/?i=0.1+to+binary

[44] http://www.wolframalpha.com/input/?i=1%2F3+in+decimal

[45] http://ta.twi.tudelft.nl/users/vuik/wi211/disasters.html

[46] http://en.wikipedia.org/wiki/Salami_slicing

[47] http://en.wikipedia.org/wiki/Superman_III

[48] http://www.youtube.com/watch?v=iLw9OBV7HYA

[49] http://docs.oracle.com/cd/E19957-01/806-3568/ncg_goldberg.html

[50] http://www.mathworks.com/help/matlab/matlab_prog/floating-point-numbers.html

[51] http://www.mathworks.com/help/matlab/matlab_prog/floating-point-numbers.html#bqxyrhp

[52] http://www.asciitable.com

Dec	Hex	Oct	Chr	Dec	Hex	Oct	Chr
65	41	101	A	97	61	141	a
66	42	102	B	98	62	142	b
67	43	103	C	99	63	143	c
68	44	104	D	100	64	144	d
69	45	105	E	101	65	145	e
70	46	106	F	102	66	146	f
71	47	107	G	103	67	147	g
72	48	110	H	104	68	150	h
73	49	111	I	105	69	151	i
74	4A	112	J	106	6A	152	j
75	4B	113	K	107	6B	153	k
76	4C	114	L	108	6C	154	l
77	4D	115	M	109	6D	155	m
78	4E	116	N	110	6E	156	n
79	4F	117	O	111	6F	157	o
80	50	120	P	112	70	160	p
81	51	121	Q	113	71	161	q
82	52	122	R	114	72	162	r
83	53	123	S	115	73	163	s
84	54	124	T	116	74	164	t
85	55	125	U	117	75	165	u
86	56	126	V	118	76	166	v
87	57	127	W	119	77	167	w
88	58	130	X	120	78	170	x
89	59	131	Y	121	79	171	y
90	5A	132	Z	122	7A	172	z

Table 2.5: 7-bit ASCII codes for uppercase and lowercase letters.

3 Basic data types, operators & expressions

3.1 Expressions

When you start MATLAB you are greeted with a command prompt:

```
>>
```

You are now in the read-eval-print loop[53] and MATLAB is waiting for you to enter an *expression*, so that MATLAB can evaluate that expression and provide you with the result. For example, you might enter something that looks like arithmetic:

```
>> 1+2

ans =

     3
```

MATLAB evaluates that expression `1+2` and prints out the value of that expression, which is `3`, and assigns that output value to a new *variable* called `ans`. We will talk about variables soon.

Try typing in another arithmetic expression, for example:

```
>> 1/3

ans =
```

```
    0.3333
```

So you can see that MATLAB can do division too.

Expressions don't have to be arithmetic. They could be logical expressions, such as:

```
>> 1+2 == 3

ans =

     1
```

In this case the double-equal sign is an *operator* which means "is equal to?". Essentially our expression is asking MATLAB a logical question (a question with a TRUE or FALSE answer): Is `1+2` equal to `3`? MATLAB evaluates that expression and returns the answer: `1`. In MATLAB a logical TRUE is the same as the number `1`, and a logical FALSE is the same as the number `0`. Try another logical expression:

```
>> 1+1 == 0

ans =

     0
```

In this case we are asking MATLAB "Does `1+1` equal `0`?" and MATLAB returns `0`, which is MATLAB's way of saying `FALSE`.

Here's another one in which we combine multiple operators into one expression:

```
>> 5+6-1+20>25

ans =
```

```
    1
```

With the numbers and operators all squished next to each other this is a bit hard to read. I might prefer to write this expression with spaces in between, and round brackets surrounding the left hand side, to make it more readable:

```
>> (5 + 6 - 1 + 20) > 25

ans =

     1
```

It's up to you how to write your code, but I would suggest to you that writing your code in such a way that it is easy to read is a good idea in the long run. It will make it easier for other people to read your code (including yourself in the future).

Here's an example to illustrate this point. Can you figure out what the result of this expression is?

```
>> 2*6*3*4/3/4/2/5>1
```

It's difficult and annoying to try to do this. How about this re-written version:

```
>> (2*6 * 3*4) / (3*4 * 2*5)  >  1

ans =

     1
```

They are both valid code, they both evaluate to the same result, but one version (the second version) is much more readable (in my opinion).

Here's a puzzling result:

```
>> 0.1 + 0.2 == 0.3

ans =

     0
```

This is a rather surprising result, isn't it. I'll leave it as an exercise for you to research why this happens, and what a potential solution to this kind of unexpected result might be. Hint: look at the course notes on digital representation of data[54].

Let's move on and talk about operators.

3.2 Operators

In the example code snippets above we saw a number of operators already. We saw the `+` and `/` mathematical operators, and we saw the logical operator `==`. There are in fact a wide variety of operators in MATLAB. The MathWorks (the company that makes MATLAB) has a web page that lists them all:

Operators and Elementary Operations[55]

There are a variety of arithmetics operators, relational and logical operators, and others that you can read about as well.

One concept that is important to talk about is *operator precedence*. This refers to the order in which MATLAB evaluates expressions and operators when there are multiple operations in a single expression. Take the following expression for example:

```
>> 2 + 3 * 5
```

What does this evaluate to? There are two possibilities. If you proceed left-to-right and evaluate each operator in the order in which it appears, then this

would evaulate to `2+3`, which is `5`, multiplied by `5`, which equals `25`. This is not what happens in MATLAB (nor in most programming languages). Instead the multiply operator `*` takes precedence over the addition operator `+`, and the `3*5` sub-expression is evaluated first, and then the result (which is `15`) is substituted, and then the resulting expression `2+15` is evaulated, which returns `17`.

```
>> 2 + 3 * 5

ans =

    17
```

Here is a page from the MathWorks documentation on MATLAB that describes operator precedence in MATLAB:

Operator Precedence[56]

For arithmetic the easy rule to remember is that multiply and divide take precedence over add and subtract.

You can force particular parts of an expression to be evaluated first by using round brackets, which take the highest precedence in MATLAB. For example we could rewrite the expression above to force the `2+3` to occur first, like this:

```
>> (2 + 3) * 5

ans =

    25
```

3.3 Variables

In the above examples we have been typing in numbers, along with arithmetic and logical or relational operators, and MATLAB evaluates those expressions and returns the result. In fact when you don't provide any output variable to

store the results of your expression, MATLAB automatically stores the result in a variable called `ans` (short for *answer*). So for example:

```
>> 1 + 2

ans =

     3
```

MATLAB has stored the answer in a *variable* called `ans`. You can think of a variable as a human-readable name of some data that is stored in MATLAB's memory. You can refer to data by it's variable name. Under the hood, MATLAB keeps track of how these variable names correspond to the location (and type) of the data stored in memory.

This memory we are referring to is RAM or Random-access memory[57]. This is a form of data storage in your computer which is to be considered temporary. Once MATLAB quits, or your computer is turned off, the data that was stored in RAM is gone. To permanently store data on your computer you need to store it on a more permanent form of memory, such as the hard drive in your computer, or an external drive such as a memory stick.

By naming your data using a variable name, you can easily view and manipulate those data. Here's an example where we store the result of a calculation in a variable that we will name `fred`:

```
>> fred = 1 + 2

fred =

     3
```

We type our expression `1+2` and on the left hand side we type our variable name `fred`, and set it to be equal to (using the equal sign `=`) the expression. MATLAB evaluates this whole expression and in its return statement we can see that now

`fred` is equal to `3`.

Here's another one:

```
>> bob = 4 * 5

bob =

    20
```

Now we have defined a second variable called `bob` which we have set to be equal to the result of the expression `4*5`. We can see in MATLAB's return statement that now bob is equal to `20`.

We can use variable names within expressions and MATLAB will substitute the value of those variables within the expression:

```
>> joe = bob + fred

joe =

    23
```

We have defined a new variable called `joe` and assigned it to be equal to the value of `bob` (which is `20`) added to the value of `fred` (which is `3`). MATLAB returns that now `joe` is equal to `23`.

What happens if we do this?

```
>> mike = joe + bob + fred + danny
Undefined function or variable 'danny'.
```

MATLAB returns an error: `Undefined function or variable 'danny'`. The problem here is that we have never defined a variable called `danny` and so when MATLAB attempts to evaluate `danny`, it can't find anything. When it evaluates `joe` and `bob` and `fred` MATLAB knows the data that those variable names refers to, but we

have not named any data using a variable called `danny` and so MATLAB has no idea what we are referring to.

In fact this is exactly the right way to think about this error: when we type `danny`, MATLAB does not know what we are referring to.

At any time we can get a list of which variables are defined in MATLAB by using a command called `who`:

```
Your variables are:

bob   fred  joe
```

We can see we have three variables defined. You can use a command called `whos` to get a more detailed list:

```
>> whos
  Name      Size            Bytes  Class     Attributes

  bob       1x1                 8  double
  fred      1x1                 8  double
  joe       1x1                 8  double
```

We see our variables in a table now with their name, their size, the number of Bytes that they occupy in MATLAB's memory, their class (what *type* of variable they are, which relates to what kind of digital representation holds those data) and a column called `Attributes`.

Note that if you assign a new value to an existing variable, the old data is wiped out. Here is an example. We first assign the number `3` to the new variable `jane`:

```
>> jane = 3

jane =

     3
```

Now we verify that indeed `jane` is `3`:

```
>> jane

jane =

     3
```

Now we reassign the number `4` to `jane`, and check the value:

```
>> jane = 4

jane =

     4

>> jane

jane =

     4
```

Indeed, `jane` is now `4` and there is no trace of `3`.

There are some rules governing how you can name your variables. Variable names cannot start with a number or a symbol, only with a letter. There can be no spaces or symbols in variable names. Capitalization matters, so `joe` is different than `Joe`.

The other thing to talk about in this context is that MATLAB has some commands and functions that are already defined by MATLAB, and so you should avoid using those as your own variable names. So for example MATLAB has a built-in function called `sort()` that will sort a vector of values:

```
>> sort([4 3 2 6 5 7 9 8 1])

ans =
```

```
    1     2     3     4     5     6     7     8     9
```

When you type `sort` MATLAB executes its built-in sorting algorithm. Nothing stops you however from defining your own variable with the same name:

```
>> sort = 23

sort =

    23
```

Now when you try typing the sorting expression in again you get this:

```
>> sort([4 3 2 6 5 7 9 8 1])
Index exceeds matrix dimensions.
```

MATLAB throws an error. Now when MATLAB sees `sort` it thinks you are referring to your variable called `sort` which equals `23`. Actually it equals a `1x1` matrix (a single value) containing `23`.

Why do we get this particular error message? The round brackets when put next to a variable cause MATLAB to try to index into a vector or matrix, and since our variable sort has only a single value, when MATLAB tries to retrieve the 4th, then 3rd, then 2nd, values, etc, it throws an error. We haven't talked about vectors or matrices or indexing yet, so don't worry about that. The point here is that we have essentially wiped out the reference to the sorting algorithm originally referred to by sort by defining our own variable called `sort`. Oops!

We can remedy this situation by clearing the variable `sort` using the built-in command `clear`:

```
>> clear sort
```

Now we have erased our variable called `sort` and when we type `sort` again, MATLAB will no longer refer to our variable containing `23` (since we just cleared it from memory) and MATLAB will go back to referring to its own built-in function called `sort()`:

```
>> sort([4 3 2 6 5 7 9 8 1])

ans =

     1     2     3     4     5     6     7     8     9
```

Now it's time to talk about variable types.

3.4 Basic Data Types

So far we have been dealing with data in the form of single numbers. The number `1` for example, or the number `0.5`. There are in fact a number of different numeric *types* of data that MATLAB can store in variables. Here is a webpage from the MathWorks that describes the full constellation of data types used in MATLAB:

Data Types[58]

Numeric data can be stored in a number of different Numeric Types[59]. The default type of numeric data in MATLAB is `double`, which stands for double-precision floating-point format[60]. The *floating-point* part of this means essentially that this data type can store a real number[61], i.e. numbers along a continuous line such as `1.0` or `1.33` or `3.14159`. The *double-precision* part of this refers to how many *bytes* are used by MATLAB to represent that number. More bytes means more precision. You can read about this in more detail in Chapter 2, *Digital representation of data*.

When you just type in numbers, or have MATLAB compute the result of an arithmetic expression, you will typically be using, by default, the `double` data type:

```
>> a = 1

a =

     1

>> b = 2

b =

     2

>> c = a/b

c =

    0.5000

>> d = b/a

d =

     2

>> whos
  Name      Size            Bytes  Class     Attributes

  a         1x1                 8  double
  b         1x1                 8  double
  c         1x1                 8  double
  d         1x1                 8  double
```

If you want to convert a variable to another numeric data type, you can do it using one of MATLAB's built-in conversion functions. So for example to convert a `double` variable to a 32-bit integer, use `int32()`:

```
>> x = 1.3
```

```
x =

    1.3000

>> y = int32(x)

y =

           1

>> whos
  Name      Size            Bytes  Class     Attributes

  x         1x1                 8  double
  y         1x1                 4  int32
```

You can see that when the `double` `x` (which equals `1.3`) is converted into an `int32` it is rounded down to `1`.

MATLAB also has data types to deal with individual characters (letters like `'a'` and `'b'`) and strings of characters (like `'joe'`), and a selection of built-in functions to manipulate strings:

Characters and Strings[62]

For example:

```
>> x = 'a'

x =

a

>> y = 'b'

y =

b
```

```
>> z = 'fred'

z =

fred

>> whos
  Name      Size            Bytes  Class    Attributes

  x         1x1                 2  char
  y         1x1                 2  char
  z         1x4                 8  char
```

Above we have defined three variables all of type `char` (which stands for character string). The first two, named `x` and `y` both contain a single character (`'a'` and `'b'`, respectively) and the third, `z`, contains a string of four characters (`'fred'`). You can see that `x` and `y` occupy 2 bytes of memory and `z` uses 8 bytes. Two bytes are required to store a single character in MATLAB.

You can dive deeper here in the documentation for the char function[63], which describes how characters are represented. The first 7 bits (values 0 to 127) code 7-bit ASCII characters. The next 9 bits code values 128 to 65535 and represent characters that depend on your locale (i.e. other languages besides plain english ASCII).

You can quickly see the integer codes for different characters in MATLAB by doing the following:

```
>> int8('a')

ans =

   97

>> int8('b')

ans =
```

```
   98

>> int8('z')

ans =

  122
```

In fact you can get the integer codes for all 26 lower case letters in one go, like this:

```
>> int8('a':'z')

ans =

  Columns 1 through 15

   97   98   99  100  101  102  103  104  105  106  107  108  109  110  111

  Columns 16 through 26

  112  113  114  115  116  117  118  119  120  121  122
```

You can display a string to the screen using the `disp` command:

```
>> disp('hello, world, my name is fred')
hello, world, my name is fred
```

You can concatenate multiple strings using the square brackets `[` and `]` to construct a new string:

```
>> a = 'fred';
>> b = 'joe';
>> c = 'jane';
>> s = ' ';
>> z = [a,s,b,s,c];
```

```
>> disp(z)
fred joe jane
```

I've introduced some new syntax here, the use of the semicolon ; after an expression. This prevents MATLAB from echoing the value of the expression to the screen. The expression is still evaluated but MATLAB doesn't echo the result back to us on the screen. Use this when you want to suppress the output of expressions. If you don't need to see the result of an expression on the screen then this makes for a cleaner MATLAB session.

You can get attributes of a string such as its length:

```
>> disp(['z is ', num2str(l), ' characters long'])
z is 13 characters long
```

I've also introducted the built-in function `num2str()` which will convert a numeric type into a character string.

Another way to generate a character string out of many parts is to use the `sprintf()` function. This mimics the `printf()` function[64] that is famililar to C programmers:

```
>> m = sprintf('z is %d characters long, & pi is approx. %.5f', l, pi);
>> disp(m)
z is 13 characters long, and pi is approximately 3.14159
```

The `%d` notation tells the sprintf function that an integer numeric type will be provided here. The `%.5f` notation says that a floating-point value will be provided, and please show it using 5 decimal places. At the end of the string is where you supply the needed values, in the order in which they appear in the string. Note that `pi` is a built-in value in MATLAB.

In MATLAB you can use the `class()` function to get the type of a variable. For example:

```
>> a = 3.14159

a =

    3.1416

>> class(a)

ans =

double
```

You can use the `isa()` function to ask whether a variable is a certain type. For example:

```
>> isa(a,'char')

ans =

     0

>> isa(a,'double')

ans =

     1
```

Remember in MATLAB `0` is "FALSE" or "NO" and `1` is "TRUE" or "YES".

So far we have seen numeric types and character string types. These are basic data types. MATLAB also allows for complex data types such as vectors, matrices, structures and cell arrays. These you can think of as container types, in other words data types that can store not just one value but many values.

Actually, the character string is already a sort of container type, in that it stores many single characters all strung together. You can think of a character string

as a vector of single characters.

In the next section in the notes we will talk about some of these complex data types and how to use them.

3.5 Special values

The MathWorks online documentation has a page on various special values built-in to MATLAB:

Special Values[65]

There is a special numeric value in MATLAB called `NaN` (not a number). It is often used to denote missing data.

There is also a special value called `Inf` which stands for infinity. Try typing the expression `1/0` and you will get `Inf`.

There are other mathematical special values such as `pi`:

```
>> pi

ans =

    3.1416

>> help pi
 PI     3.1415926535897....
    PI = 4*atan(1) = imag(log(-1)) = 3.1415926535897....

    Reference page in Help browser
       doc pi
```

and imaginary numbers `i` and `j`:

```
>> help i
 I  Imaginary unit.
    As the basic imaginary unit SQRT(-1), i and j are used to enter
    complex numbers.  For example, the expressions 3+2i, 3+2*i, 3+2j,
```

```
    3+2*j and 3+2*sqrt(-1) all have the same value.

    Since both i and j are functions, they can be overridden and used
    as a variable.  This permits you to use i or j as an index in FOR
    loops, etc.

    See also J.

    Reference page in Help browser
       doc i

>> help j
 J  Imaginary unit.
    As the basic imaginary unit SQRT(-1), i and j are used to enter
    complex numbers.  For example, the expressions 3+2i, 3+2*i, 3+2j,
    3+2*j and 3+2*sqrt(-1) all have the same value.

    Since both i and j are functions, they can be overridden and used
    as a variable.  This permits you to use i or j as an index in FOR
    loops, subscripts, etc.

    See also I.

    Reference page in Help browser
       doc j
```

Also of note is the special function `eps()`:

```
>> help eps
 EPS  Spacing of floating point numbers.
    D = EPS(X), is the positive distance from ABS(X) to the next larger in
    magnitude floating point number of the same precision as X.
    X may be either double precision or single precision.
    For all X, EPS(X) is equal to EPS(ABS(X)).

    EPS, with no arguments, is the distance from 1.0 to the next larger
    double
    precision number, that is EPS with no arguments returns 2^(-52).
```

```
...
```

If we type `eps(1.0)` we get:

```
>> eps(1.0)

ans =

   2.2204e-16
```

which is a pretty small number: `0.0000000000000022204`. This is the distance between the floating-point representation of `1.0` and the next largest number that the `double` floating-point representation can represent. You can think of it as the precision of the `double` floating-point representation of numbers, near the number `1.0`.

Try `eps(2^54)` (which equals `18,014,000,000,000,000`):

```
>> eps(2^54)

ans =

     4
```

Huh? So near the number `2^54`, the precision of our `double` floating-point representation of continuous numbers is `4.0`! This is terrible! This is however just a limitation of representing continuous (infinite) numbers using a finite digital representation. See Chapter 2 for more information about this kind of thing.

3.6 Getting help

We can get help about MATLAB built-in commands and functions using the `help` command:

```
>> help who
```

```
WHO    List current variables.
   WHO lists the variables in the current workspace.

   In a nested function, variables are grouped into those in the nested
   function and those in each of the containing functions.  WHO displays
   only the variables names, not the function to which each variable
   belongs.  For this information, use WHOS.  In nested functions and
   in functions containing nested functions, even unassigned variables
   are listed.

   WHOS lists more information about each variable.
   WHO GLOBAL and WHOS GLOBAL list the variables in the global workspace.
   WHO -FILE FILENAME lists the variables in the specified .MAT file.

   WHO ... VAR1 VAR2 restricts the display to the variables specified. The
   wildcard character '*' can be used to display variables that match a
   pattern.  For instance, WHO A* finds all variables in the current
   workspace that start with A.

   WHO -REGEXP PAT1 PAT2 can be used to display all variables matching the
   specified patterns using regular expressions. For more information on
   using regular expressions, type "doc regexp" at the command prompt.

   Use the functional form of WHO, such as WHO('-file',FILE,V1,V2),
   when the filename or variable names are stored in strings.

   S = WHO(...) returns a cell array containing the names of the variables
   in the workspace or file. You must use the functional form of WHO when
   there is an output argument.

   Examples for pattern matching:
       who a*                      % Show variable names starting with "a"
       who -regexp ^b\d{3}$        % Show variable names starting with "b"
                                   %   and followed by 3 digits
       who -file fname -regexp \d  % Show variable names containing any
                                   %   digits that exist in MAT-file fname

   See also WHOS, CLEAR, CLEARVARS, SAVE, LOAD.

   Other functions named who:
```

```
      Simulink.who

   Reference page in Help browser
      doc who
```

We can also get a GUI interface to help using the `doc` command.

There is also a way of searching the help documentation files for keywords, using the `lookfor` command. The `lookfor` command will return the names of all functions or commands for which the associated help documentation contains the given keyword. So for example let's say we need to find the `invkine()` function but we've forgotten what it's called, we just remember it's something to do with a robot. We can search using: `lookfor robot`

```
>> lookfor robot
invkine                        - Inverse kinematics of a robot arm.
invkine_codepad                - Modeling Inverse Kinematics in a Robotic Arm
idnlgreydemo13                 - Modeling an Industrial Robot Arm
idnlgreydemo8                  - Industrial Three-Degrees-of-Freedom Robot: C
     MEX-File Modeling of MIMO System Using Vector/Matrix Parameters
robot_m                        - A simplified Manutec r3 robot with three
    arms.
robotarm_m                     - A physically parameterized robot arm.
refmodel_dataset               - ROBOTARM_DATASET Reference model dataset
robotarm_dataset               - Robot arm dataset
mech_robot_data                - Data defining the manutec robot.
RobotArmExample                - Multi-Loop PID Control of a Robot Arm
```

3.7 Script M-files

Instead of typing in commands into the MATLAB command-line, you can instead save them in a file, called a MATLAB script, and then type the name of the script on the command line to execute all code within that script. Scripts typically have a `.m` filename suffix.

So for example you might have a file called `random8.m` that contains the following code:

```
% script M-file example random8.m
%
rlist = round(rand(1,8)*10);
disp(rlist);
disp(['mean = ',num2str(mean(rlist))]);
disp(['median = ',num2str(median(rlist))]);
disp(['standard deviation = ',num2str(std(rlist))]);
```

The script generates a list of 8 random numbers chosen from a uniform distribution between 0 and 10, and then displays the mean, median and standard deviation of those values.

If the script file called `random8.m` is in your MATLAB path, then typing `random8.m` on the MATLAB command line will execute the script:

```
>> random8
     8     9     1     9     6     1     3     5

mean = 5.25
median = 5.5
standard deviation = 3.3274
```

3.8 MATLAB path

When you first start MATLAB, you will be faced with the command line prompt, and MATLAB will be started up looking at a particular location in your file system. This location is known as the *current working directory*. If you are using the MATLAB GUI (graphical user interface) you will see your current working directory displayed in a toolbar just above the command line. On my computer it shows as `/Users/plg/Desktop`. On your computer it will be something different.

The other way to query MATLAB about the current working directory is to type

`pwd` into the command line:

```
>> pwd

ans =

/Users/plg/Desktop
```

When you type something into the command line, like `random8`, MATLAB will go through a number of steps to find out what you mean:

- is `random8` defined as a variable in memory?
- is `random8` defined as a function or script file or data file in MATLAB's current working directory?
- is `random8` defined as a function or script file or data file somewhere else in MATLAB's path?

The MATLAB *path* is a list of directories on your computer's hard disk where MATLAB knows to look for scripts and functions. You can see what's defined in your MATLAB path by typing `path` at the MATLAB command line:

```
>> path

                MATLABPATH

        /Users/plg/Documents/MATLAB
        /Applications/MATLAB_R2015a.app/toolbox/matlab/addons
        /Applications/MATLAB_R2015a.app/toolbox/matlab/addons/cef
        /Applications/MATLAB_R2015a.app/toolbox/matlab/addons/fallbackmanager
        /Applications/MATLAB_R2015a.app/toolbox/matlab/demos
        /Applications/MATLAB_R2015a.app/toolbox/matlab/graph2d
        /Applications/MATLAB_R2015a.app/toolbox/matlab/graph3d
        /Applications/MATLAB_R2015a.app/toolbox/matlab/graphics
        ...
        ...
```

On my computer I get a list of more than 600 directories—almost all of them sub-

directories of the MATLAB main application directory. This is where all of MATLAB's built-in functions and scripts are located, and where the various MATLAB toolbox code is located.

The other way to see (and alter) your MATLAB path is by using the MATLAB GUI. Type `pathtool` on the MATLAB command line and you get a nice GUI interface where you can scroll through all of the directories that are in your MATLAB path, you can delete some, add some, and change the order.

On the issue of the order: remember that MATLAB goes through its path in the order in which the directories appear in the path list. So if you have a function called `random8()` defined in multiple places in your path, when you type `random8` on the MATLAB command line, MATLAB will use the first one it finds in the path.

My personal approach to the MATLAB path is to basically never mess with it. Instead of adding data directories and script directories associated with my various projects to the MATLAB path, instead I just start MATLAB from the appropriate location when I am working on different projects.

To change the current working directory you can either click on the toolbar in the MATLAB GUI, or use the `cd` command on the MATLAB command line, for example:

```
>> cd /Users/plg/Documents/Research/projects/Heather_fMRI/
>> pwd

ans =

/Users/plg/Documents/Research/projects/Heather_fMRI
```

Exercises

E 3.1 Write a program to convert temperature values from Celsius to Fahrenheit according to the equation:

$$F = \frac{9}{5}C + 32 \tag{3.1}$$

The program should as the user to input the temperature in Celsius, and then print out a sentence giving the temperature in Fahrenheit, like this:

```
enter the temperature in Celsius: 22
22.0 degrees Celsius is 71.6 degrees Fahrenheit
```

E 3.2 Given parabolic flight, the height of a ball y is given by the equation:

$$y = x\tan(\theta) - \left[\frac{1}{2v_0^2}\right]\left[\frac{gx^2}{cos(\theta)^2}\right] + y_0 \tag{3.2}$$

where x is a horizontal coordinate (metres), g is the acceleration of gravity (metres per second per second), v_0 is the size of the initial velocity vector (metres per second) at an angle θ (radians) with the x-axis, and $(0, y_0)$ is the initial position of the ball (metres).

Write a program to compute the vertical height of a ball. The program should ask the user to input values for g, v_0, θ, x, and y_0, and print out a sentence giving the vertical height of the ball.

Test your program with this example:

```
enter a value for g: 9.8
enter a value for v0: 6.789
enter a value for theta: 0.123
enter a value for x: 4.5
enter a value for y0: 5.4
The vertical height of the ball is:  3.77057803072
```

E 3.3 As an egg cooks, the proteins first denature and then coagulate. When the temperature exceeds a critical point, reactions begin and proceed faster as the temperature increases. In the egg white the proteins start to coagulate for temperatures above 63 C, while in the yolk the proteins start to coagulate for temperatures above 70 C. For a soft-boiled egg, the white needs to have been heated long enough to coagulate at a temperature above 63 C, but the yolk should not be heated above 70 C. For a hard-boiled egg, the centre of the yolk should be allowed to reach 70 C.

The following equation gives the time t it takes (in seconds) for the centre of the yolk to reach the temperature T_y (Celsius):

$$t = \frac{M^{2/3} c \rho^{1/3}}{K\pi^2 (4\pi/3)^{2/3}} \ln\left[0.76 \frac{T_o - T_w}{T_y - T_w}\right] \tag{3.3}$$

where M, ρ, c and K are properties of the egg: M is mass, ρ is the density, c is the specific heat capacity, and K is the thermal conductivity. Relevant values are $M = 47$ g for a small egg and $M = 67$ g for a large egg, $\rho = 1.038\,\text{g cm}^{-3}$, $c = 3.7\,\text{J g}^{-1}\,\text{K}^{-1}$, and $K = 0.0054\,\text{W cm}^{-1}\,\text{K}^{-1}$. The parameter T_w is the temperature (in Celsius) of the boiling water, and T_o is the original temperature of the egg before being put in the water.

Implement the equation in a program, set $T_w = 100$ C and $T_y = 70$ C, and compute t for a large egg taken from the fridge ($T_o = 4$ C) and from room temperature ($T_o = 20$ C).

Test your program with this example:

```
Is the egg large (1) or small (0)? 1
enter the initial temperature of the egg
reminder 4.0 for fridge, 20.0 for room: 15.0
time taken to cook the egg is: 342.271 seconds (5 minutes, 42 seconds)
```

Links

[53] https://en.wikipedia.org/wiki/Read–eval–print_loop

[54] file:digital_representation_of_data.html

[55] http://www.mathworks.com/help/matlab/operators-and-elementary-operations.html

[56] http://www.mathworks.com/help/matlab/matlab_prog/operator-precedence.html

[57] https://en.wikipedia.org/wiki/Random-access_memory

[58] http://www.mathworks.com/help/matlab/data-types_data-types.html

[59] http://www.mathworks.com/help/matlab/numeric-types.html

[60] https://en.wikipedia.org/wiki/Double-precision_floating-point_format

[61] https://en.wikipedia.org/wiki/Real_number

[62] http://www.mathworks.com/help/matlab/characters-and-strings.html

[63] http://www.mathworks.com/help/matlab/ref/char.html

[64] https://en.wikipedia.org/wiki/Printf_format_string

[65] http://www.mathworks.com/help/matlab/matlab_prog/special-values.html

4 Complex data types

In Chapter 3 we saw data types such as `double` and `char` which are used to represent individual values such as the number `1.234` or the character `'G'`. Here we will learn about a number of complex data types that MATLAB uses to store multiple values in one data structure. We will start with the *array* and *matrix*—and in fact a matrix is just a two-dimensional array. What's more, a scalar value (like `3.14`) is just an array with one row and one column. We will also cover *cell arrays* and *structures*, which are data types designed to hold different kinds of information together in a single type.

4.1 Arrays

Arrays are simply ordered lists of values, such as the list of five numbers: `1,2,3,4,5`. In MATLAB we can define this array using square brackets:

```
>> a = [1,2,3,4,5]

a =

     1     2     3     4     5

>> whos
  Name      Size            Bytes  Class     Attributes

  a         1x5                40  double
```

We can see that `a` is a `1x5` (1 row, 5 columns) array of `double` values.

We can also get the length of an array using the `length` function:

```
>> length(a)

ans =

     5
```

We can in fact leave out the commas if we want, when we construct the array—we can use spaced instead. It's up to you to decide which is more readable.

```
>> a = [1 2 3 4 5]

a =

     1     2     3     4     5
```

MATLAB has a number of built-in functions and operators for creating arrays and matrices. We can create the above array using a colon (`:`) operator like so:

```
>> a = 1:5

a =

     1     2     3     4     5
```

We can create a list of only odd numbers from `1` to `10` like so, again using the colon operator:

```
>> b = 1:2:10

b =

     1     3     5     7     9
```

4.1.1 Array indexing

We can get the value of a specific item within an array by *indexing* into the array using round brackets `()`. For example to get the third value of the array `b`:

```
>> third_value_of_b = b(3)

third_value_of_b =

     5
```

To get the first three values of `b`:

```
>> b(1:3)

ans =

     1     3     5
```

We can get the 4th value onwards to the end by using the `end` keyword:

```
>> b(4:end)

ans =

     7     9
```

Remember, array indexing in MATLAB starts at 1. In other languages like C and Python, array indexing starts at 0. This can be the source of significant confusion when translating code from one language into another.

Another useful array construction built-in function in MATLAB is the `linspace` function:

```
>> c = linspace(0,1,11)

c =
```

```
  Columns 1 through 8

         0    0.1000    0.2000    0.3000    0.4000    0.5000    0.6000    0.
    7000

  Columns 9 through 11

    0.8000    0.9000    1.0000
```

By default arrays in MATLAB are defined as row arrays, like the array `a` above which is size `1x5`—one row and 5 columns. We can however define arrays as columns instead, if we need to. One way is to simply transpose our row array using the transpose operator `'`:

```
>> a2 = a'

a2 =

     1
     2
     3
     4
     5

>> size(a2)

ans =

     5     1
```

Now we can see `a2` is a `5x1` column array.

We can directly define column arrays using the semicolon `;` notation instead of commas or spaces, like so:

```
>> a2 = [1;2;3;4;5]
```

```
a2 =

     1
     2
     3
     4
     5
```

So in general, commas or spaces denote moving from one column to another, and semicolons denote moving from one row to another. This will become useful when we talk about matrices (otherwise know as two-dimensional arrays).

4.1.2 Array sorting

MATLAB has a built-in function called `sort()` to sort arrays (and other structures). The algorithm used by MATLAB under the hood is the quicksort[66] algorithm. To sort an array of numbers is simple:

```
>> a = [5 3 2 0 8 1 4 8 5 6]

a =

     5     3     2     0     8     1     4     8     5     6

>> a_sorted = sort(a)

a_sorted =

     0     1     2     3     4     5     5     6     8     8
```

If you give the `sort` function two output variables then it also returns the indices corresponding to the sorted values of the input:

```
>> [aSorted, iSorted] = sort(a)

aSorted =
```

```
     0     1     2     3     4     5     5     6     8     8


iSorted =

     4     6     3     2     7     1     9    10     5     8
```

The `iSorted` array contains the indices into the original array `a`, in sorted order. So this tells us that the first value in the sorted array is the 4th value of the original array; the second value of the sorted array is the 6th value of the original array, and so on.

The default sort happens in ascending order. If we want to reverse this we can specify this as an option to the `sort()` function:

```
>> sort(a, 'descend')

ans =

     8     8     6     5     5     4     3     2     1     0
```

4.1.3 Searching arrays

We can use MATLAB's built-in function called `find()` to search arrays (or other structures) for particular values. So for example if we wanted to find all values of the above array `a` which are greater than 5, we could use:

```
>> ix = find(a > 5)

ix =

     5     8    10
```

This tells us that the 5th, 8th and 10th values of `a` are greater than 5. If we want

to see what those values are, we index into `a` using those found indices `idx`:

```
>> a(ix)

ans =

     8     8     6
```

We could combine these two steps into one line of code like this:

```
>> a(find(a>5))

ans =

     8     8     6
```

4.1.4 Array arithmetic

One great feature of MATLAB is that arithmetic (and many other) operations can be carried out on an entire array at once—and what's more, under the hood MATLAB uses optimized, compiled code to carry out these so-called *vectorized* operations. Vectorized code is typically many times faster than the equivalent code organized in a naive way (for example using for-loops). We will talk about vectorized code and other ways to speed up computation in Chapter 8.

We can multiply each element of the array `a2` by a scalar value:

```
>> a2 * 5

ans =

     5
    10
    15
    20
    25
```

We can perform a series of operations all at once:

```
>> a3 = (a2 * 5) + 2.5

a3 =

    7.5000
   12.5000
   17.5000
   22.5000
   27.5000
```

These mathematical operations are performed *elementwise*, meaning element-by-element.

We can also perform arithmetic operations between arrays. For example let's say we wanted to multiply two 1x5 arrays together to get a third:

```
>> a = [1,2,3,4,5];
>> b = [2,4,6,8,10];
>> c = a*b
Error using  *
Inner matrix dimensions must agree.
```

Oops! We get an error message. When you perform arithmetic operations between arrays in MATLAB, the default assumption is that you are doing matrix (or matrix-vector) algebra, not elementwise operations. To force elementwise operations in MATLAB we use *dot-notation*:

```
>> c = a.*b

c =

     2     8    18    32    50
```

Now the multiplication happens elementwise. Needless to say we still need the

dimensions to agree. If we tried multiplying, elementwise, a 1x5 array with a 1x6 array we would get an error message:

```
>> d = [1,2,3,4,5,6];
>> e = c.*d
Error using  .*
Matrix dimensions must agree.

>> size(c)

ans =

     1     5

>> size(d)

ans =

     1     6
```

4.2 Matrices

In mathematics a matrix is generally considered to have two dimensions: a row dimension and a column dimension. We can define a matrix in MATLAB in the following way. Here we define a matrix A that has two rows and 5 columns:

```
>> A = [1,2,3,4,5; 1,4,6,8,10]

A =

     1     2     3     4     5
     1     4     6     8    10

>> size(A)

ans =
```

```
     2     5
```

We use commas (or we could have used spaces) to denote moving from column to column, and we use a semicolon to denote moving from the first row to the second row.

If we want a 5x2 matrix instead we can either just transpose our 2x5 matrix:

```
>> A2 = A'

A2 =

     1     1
     2     4
     3     6
     4     8
     5    10
```

Or we can define it directly:

```
>> A2 = [1,2; 2,4; 3,6; 4,8; 5,10]

A2 =

     1     2
     2     4
     3     6
     4     8
     5    10
```

There are other functions in MATLAB that we can use to generate a matrix. The `repmat` function in particular is useful when we want to repeat certain values and stick them into a matrix:

```
>> G = repmat([1,2,3],3,1)
```

```
G =

     1     2     3
     1     2     3
     1     2     3
```

This means repeat the row vector `[1,2,3]` three times down columns, and one time across rows. Here's another example:

```
>> H = repmat(G,1,3)

H =

     1     2     3     1     2     3     1     2     3
     1     2     3     1     2     3     1     2     3
     1     2     3     1     2     3     1     2     3
```

Now we've repeated the matrix `G` once down rows and three times across columns.

There are also special functions `zeros()` and `ones()` to create arrays or matrices filled with zeros or ones:

```
>> I = ones(4,5)

I =

     1     1     1     1     1
     1     1     1     1     1
     1     1     1     1     1
     1     1     1     1     1

>> J = zeros(7,3)

J =

     0     0     0
     0     0     0
```

```
     0     0     0
     0     0     0
     0     0     0
     0     0     0
     0     0     0
```

Of course we can fill a matrix with any value we want by multiplying a matrix of ones by a scalar:

```
>> P = ones(3,4) * pi

P =

    3.1416    3.1416    3.1416    3.1416
    3.1416    3.1416    3.1416    3.1416
    3.1416    3.1416    3.1416    3.1416
```

If we use `zeros` or `ones` with just a single input argument we end up with a square matrix (same number of rows and columns):

```
>> Q = ones(5)

Q =

     1     1     1     1     1
     1     1     1     1     1
     1     1     1     1     1
     1     1     1     1     1
     1     1     1     1     1
```

There is also a special MATLAB function called `eye` which will generate the identity matrix (a special matrix in linear algebra sort of equivalent to the number `1` in scalar arithmetic):

```
>> eye(3)
```

```
ans =

     1     0     0
     0     1     0
     0     0     1
```

4.2.1 Matrix indexing

We can *index* into a matrix using round brackets, just like with an array. Now however we need to specify both a row and a column index. So for example the entry in the matrix `A2` corresponding to the 3rd row and the second column is:

```
>> A2(3,2)

ans =

     6
```

To get the value in the last row, and the first column:

```
>> A2(end,1)

ans =

     5
```

We can also specify a range in our index values. So to get rows 1 through 3 and columns 1 through 2:

```
>> A2(1:3,1:2)

ans =

     1     2
     2     4
     3     6
```

We can use a shorthand for "all columns" (also works for all rows) using the colon operator:

```
>> A2(1:3,:)

ans =

     1     2
     2     4
     3     6
```

We can use indexing to replace parts of a matrix. For example to replace the first row of `A2` (which is presently `[1 2]` with `[99 99]` we could use this code:

```
>> A2(1,:) = [99 99]

A2 =

    99    99
     2     4
     3     6
     4     8
     5    10
```

To replace the second column of `A2` with 5 random numbers chosen from a gaussian normal distribution with mean zero and standard deviation one, we could use this code:

```
>> A2(:,2) = randn(5,1)

A2 =

   99.0000    0.5377
    2.0000    1.8339
    3.0000   -2.2588
    4.0000    0.8622
    5.0000    0.3188
```

Note the use of the `randn()` function to generate (pseudo)random deviates from a gaussian normal distribution.

4.2.2 Matrix reshaping

MATLAB has a built-in function called `reshape()` which is handy for reshaping matrices into new dimensions. For example let's say we have a `4x3` matrix `M`:

```
>> M = [1,2,3; 4,5,6; 7,8,9; 10,11,12]

M =

     1     2     3
     4     5     6
     7     8     9
    10    11    12
```

We can use `reshape()` to reshape `M` into a `6x2` matrix `Mr`:

```
>> Mr = reshape(M,6,2)

Mr =

     1     8
     4    11
     7     3
    10     6
     2     9
     5    12
```

Note that `reshape()` does its work by taking values *columnwise* from the original input matrix `M`. If we want to perform the reshaping in the other way—row-wise—we can do this by transposing the original matrix:

```
>> Mr2 = reshape(M',6,2)

Mr2 =
```

```
     1     7
     2     8
     3     9
     4    10
     5    11
     6    12
```

To reshape a matrix (or indeed any multi-dimensional array) into a column vector, there is a convenient shorthand in MATLAB, namely the colon operator `(:)`:

```
>> M_col = M(:)

M_col =

     1
     4
     7
    10
     2
     5
     8
    11
     3
     6
     9
    12
```

If we want a row vector instead we can just transpose the result:

```
>> M_row = M(:)'

M_row =

     1     4     7    10     2     5     8    11     3     6     9    12
```

4.2.3 Matrix arithmetic

In MATLAB as with arrays, matrix-scalar operations happen elementwise, whereas matrix-matrix operations are assumed to be based on the rules of matrix algebra. We won't go through matrix algebra in all its glory here, but you can see a reminder of the basic operations on this wikipedia page:

Matrix Basic Operations[67]

I can recommend a great book on Linear Algebra by Gilbert Strang:

Introduction to Linear Algebra, 4th Edition[68] by Gilbert Strang. Wellesley-Cambridge Press, 2009

He also has his course on MIT's open-courseware, complete with videos for all lectures here:

video lectures of Professor Gilbert Strang teaching 18.06 (Fall 1999)[69]

The Mathworks has a web page with a matrix algebra "refresher" that might serve as a useful reminder for those who have had linear algebra in the past:

Matrix Algebra Refresher[70]

Here is an example of a scalar-matrix operation on our matrix `A2` from above:

```
>> A2 * 10

ans =

    10    20
    20    40
    30    60
    40    80
    50   100
```

Let's say we wanted to multiply, elementwise, a `5x2` matrix `A3` by `A2`:

```
>> A3 = rand(5,2)
```

```
A3 =

    0.2785    0.9706
    0.5469    0.9572
    0.9575    0.4854
    0.9649    0.8003
    0.1576    0.1419
```

As with arrays, we can use dot notation to force elementwise multiplication:

```
>> A4 = A2 .* A3

A4 =

    0.2785    1.9412
    1.0938    3.8287
    2.8725    2.9123
    3.8596    6.4022
    0.7881    1.4189
```

Without the dot notation we would get an error message:

```
>> A4 = A2 * A3
Error using  *
Inner matrix dimensions must agree.

>> size(A2)

ans =

     5     2

>> size(A3)

ans =

     5     2
```

To perform matrix multiplication we need a right-hand-side that has legal dimensions, in other words the same number of rows as `A2` has columns. For example, if we have another matrix A5 sized `2x3`:

```
>> A5 = rand(2,3)

A5 =

    0.8147    0.1270    0.6324
    0.9058    0.9134    0.0975
```

then we can perform matrix multiplication:

```
>> A6 = A2 * A5

A6 =

    2.6263    1.9537    0.8274
    5.2526    3.9075    1.6549
    7.8789    5.8612    2.4823
   10.5052    7.8150    3.3098
   13.1315    9.7687    4.1372
```

Again, review your linear algebra if you have forgotten about the rules of matrix multiplication. Just remember that to force elementwise operations, use dot-notation.

Addition and subtraction are always elementwise.

4.2.4 Matrix Algebra

As we saw above, MATLAB assumes that matrix-matrix operations are not elementwise, but conform to the rules of linear algebra and matrix arithmetic. The exception is matrix addition and subtraction, which happen elementwise even in matrix algebra. Multiplication is special however, as we saw above.

What about division (`/`)? In MATLAB the so-called *slash operator* is the gateway

to much complexity.

```
>> help slash
 Matrix division.
  \   Backslash or left division.
      A\B is the matrix division of A into B, which is roughly the
      same as INV(A)*B , except it is computed in a different way.
      If A is an N-by-N matrix and B is a column vector with N
      components, or a matrix with several such columns, then
      X = A\B is the solution to the equation A*X = B. A warning
      message is printed if A is badly scaled or nearly
      singular.  A\EYE(SIZE(A)) produces the inverse of A.

      If A is an M-by-N matrix with M < or > N and B is a column
      vector with M components, or a matrix with several such columns,
      then X = A\B is the solution in the least squares sense to the
      under- or overdetermined system of equations A*X = B. The
      effective rank, K, of A is determined from the QR decomposition
      with pivoting. A solution X is computed which has at most K
      nonzero components per column. If K < N this will usually not
      be the same solution as PINV(A)*B.  A\EYE(SIZE(A)) produces a
      generalized inverse of A.

  /   Slash or right division.
      B/A is the matrix division of A into B, which is roughly the
      same as B*INV(A) , except it is computed in a different way.
      More precisely, B/A = (A'\B')'. See \.

  ./  Array right division.
      B./A denotes element-by-element division.  A and B
      must have the same dimensions unless one is a scalar.
      A scalar can be divided with anything.

  .\  Array left division.
      A.\B. denotes element-by-element division.  A and B
      must have the same dimensions unless one is a scalar.
      A scalar can be divided with anything.
```

The backslash (left division) when used like this: `A\B` performs matrix division

of `B` into `A`. As the documentation says, this is roughly like `INV(A)*B` but it's not computed this way under the hood. The typical way you will use the backslash matrix operator in MATLAB is to solve systems of linear equations. So for example `X = A\B` is the solution to the matrix equation `A*X=B`. For example, if `B` is a column representing measurements of a dependent variable, and `A` is a matrix representing measurements of several independent variables, then `X` is the vector of regression weights that minimize the sum of squared deviations between `B` and `A*X`. More on this later in the course.

MATLAB has many, many built-in (and compiled and optimized) functions for matrix algebra and matrix algorithms of all sorts. After all, the origins of MATLAB[71] are "Matrix Laboratory", and so from the start the emphasis has been on matrix computation.

In their web documentation, the MathWorks has a listing of some linear algebra algorithms implemented in MATLAB:

Linear Algebra[72]

These include algorithms for solving linear equations, for matrix decomposition, for finding eigenvalues and singular values, for matrix analysis and so on.

4.3 Multidimensional arrays

We have seen one-dimensional (row or column) arrays and we have seen (two dimensional) matrices. In MATLAB you can create arrays with more than two dimensions. Here is an example of a three dimensional array:

```
>> A = ones([2,3,4])

A(:,:,1) =

     1     1     1
     1     1     1


A(:,:,2) =
```

```
     1     1     1
     1     1     1


A(:,:,3) =

     1     1     1
     1     1     1


A(:,:,4) =

     1     1     1
     1     1     1
```

We have created a three-dimensional array `A` that is size `2x3x4`:

```
>> size(A)

ans =

     2     3     4
```

You can think of it like this: `A` is a `2x3` matrix that is repeated `4` times (in a third dimension). Perhaps the third dimension is time. Perhaps it is something else (e.g. spatial third dimension).

We can even create 4-dimensional arrays:

```
>> B = rand(256,256,10,50);
>> whos
  Name      Size                Bytes  Class     Attributes

  B         4-D             262144000  double

>> size(B)
```

```
ans =

   256   256    10    50
```

Here is a 4-dimensional array `B`. You can think of it as a `256x256x128` dimensional 3D array repeated 50 times in a fourth dimension. Note how large the array is (262,144,000 bytes, about 250 megabytes). Depending on how much RAM you have in your computer, you can potentially have MATLAB work with very large data structures indeed.

A quick example, we could take the mean across the 4th dimension like so:

```
>> Bm = mean(B,4);
>> whos
  Name        Size                    Bytes  Class     Attributes

  B           4-D                 262144000  double
  Bm        256x256x10              5242880  double
```

Another useful function to know about is the `squeeze()` function in MATLAB. This will remove any singleton dimensions—that is, dimensions that have size 1. So for example consider the following three-dimensional array:

```
>> A = reshape(1:12,[3,1,4])

A(:,:,1) =

     1
     2
     3


A(:,:,2) =

     4
     5
     6
```

```
A(:,:,3) =

     7
     8
     9


A(:,:,4) =

    10
    11
    12

>> size(A)

ans =

     3     1     4
```

The second (middle) dimension is size `1`, so we can use `squeeze` to reshape this three-dimensional array into a two-dimensional array of size `[3x4]`:

```
>> As = squeeze(A)

As =

     1     4     7    10
     2     5     8    11
     3     6     9    12

>> size(As)

ans =

     3     4
```

4.4 Cell arrays

Arrays (single-dimensional vectors as well as two-dimensional matrices and multi-dimensional arrays) must contain values of the same type. MATLAB has another data structure called a *cell array* that allows one to store data of different types in a structed similar to an array—namely it's an indexed data container containing *cells*, and each cell can contain different data types. Cell arrays use curly brackets instead of square brackets.

The MathWorks online documentation has a page devoted to cell arrays here:

Cell Arrays[73]

So for example we can create a cell array called myCell that contains 5 cells:

```
>> myCell = {1, 2, 3, 'hello', rand(1,10)}

myCell =

    [1]    [2]    [3]    'hello'    [1x10 double]
```

Cells 1 through 3 are numeric, cell 4 is a character string, and cell 5 is a `[1x10]` array of `double` values. We can index into a cell array just like a regular array:

```
>> myCell{4}

ans =

hello

>> myCell{5}

ans =

  Columns 1 through 8

    0.7577    0.7431    0.3922    0.6555    0.1712    0.7060    0.0318    0.
    2769
```

```
  Columns 9 through 10

    0.0462    0.0971
```

You can create an empty cell array like this:

```
>> emptyCell = {}

emptyCell =

     {}
```

Or a cell array with a certain structure that is empty, like this:

```
>> emptyCell = cell(3,5)

emptyCell =

    []    []    []    []    []
    []    []    []    []    []
    []    []    []    []    []

>> emptyCell{2,3} = 'hello'

emptyCell =

    []    []          []    []    []
    []    []    'hello'    []    []
    []    []          []    []    []
```

4.5 Structures

MATLAB has another data type called a *structure* that is similar to what you might have seen in other languages like Python, and is called a Dictionary. In

MATLAB a structure is an array with *named fields* that can contain any data type.

The MathWorks online documentation has a page devoted to structures here:

Structures[74]

Let's create a structure called subject1 that contains a character string corresponding to their name, a numeric value corresponding to their age, a numeric value correponding to their height, a value corresponding to the date the experiment was run, and an array corresponding to some recorded empirical data during an experiment:

```
>> subject1.name = 'Mr. T';
>> subject1.age = 63;
>> subject1.height = 1.78;
>> subject1.date = datetime(2015,08,12);
>> subject1.data = rand(100,2);
>> subject1.catchphrase = 'I pity the fool!';
>> subject1

subject1  =

           name: 'Mr. T'
            age: 63
         height: 1.7800
           date: [1x1 datetime]
           data: [100x2 double]
    catchphrase: 'I pity the fool!'
```

As you can see we use dot-notation to denote a *field* of a structure. As soon as you introduce dot notation into a variable, it becomes a structure type. If a field with the given name does not exist, it is created. Note the use of the `datetime()` function which is a built-in function in MATLAB that handles dates and times.

We can access a field of a structure using dot-notation:

```
>> subject1.name
```

```
ans =

Mr. T

>> subject1.date

ans =

   12-Aug-2015
```

4.5.1 Arrays of structures

We can of course form arrays of structures. An array can hold any data type as long as each element is the same.

```
subject1.name = 'Mr. T';
subject1.age = 63;
subject1.height = 1.78;
subject1.date = datetime(2015,08,12);
subject1.data = rand(100,2);
subject1.catchphrase = 'I pity the fool!';

subject2.name = 'Polly Holliday';
subject2.age = 78;
subject2.height = [];
subject2.date = datetime(2015,08,12);
subject2.data = rand(100,2);
subject2.catchphrase = 'Kiss my grits!';

subject3.name = 'Leonard Nimoy';
subject3.age = 83;
subject3.height = [];
subject3.date = datetime(2015,02,26);
subject3.data = rand(100,2);
subject3.catchphrase = 'Live long and prosper';

allSubjects = [subject1, subject2, subject3];
```

```
>> allSubjects

allSubjects =

1x3 struct array with fields:

    name
    age
    height
    date
    data
    catchphrase
```

Now we can do convenient things like look at all of the age fields across the whole array:

```
>> allSubjects.age

ans =

    63


ans =

    78


ans =

    83
```

We can collect these into an array:

```
>> allAges = [allSubjects.age]

all_ages =
```

```
    63    78    83
```

Or we could collect all the `data` fields together into a three-dimensional array, and then average across subjects:

```
>> allData = [allSubjects.data];
>> size(allData);
>> allData = [allSubjects.data];
>> size(allData)

ans =

   100     6

>> allData = reshape(allData,100,2,3);
>> size(allData)

ans =

   100     2     3

>> allDataMean = mean(allData,3);
>> size(allDataMean)

ans =

   100     2
```

Note that if all elements of an array are not the same identical structure (i.e. do not have the same fields defined) then we get an error:

```
>> subject4.name = 'me'

subject4 =

    name: 'me'

>> allSubjects = [subject1, subject2, subject3, subject4];
```

```
Error using horzcat
Number of fields in structure arrays being concatenated do not match.
Concatenation of structure arrays requires that these arrays have the
same set of fields.
```

The solution here would be to use a cell array instead of a plain array—remember, in a cell array the cells do not have to be the same type:

```
>> allSubjects = {subject1, subject2, subject3, subject4}

allSubjects =

    [1x1 struct]    [1x1 struct]    [1x1 struct]    [1x1 struct]
```

Exercises

E 4.1 If we have a vector X containing n values, then the mean $\bar{X}$ is:

$$\bar{X} = \frac{1}{n} \sum_{i=1}^{N} (X_i) \tag{4.1}$$

In MATLAB there is a built-in function for computing the mean of a vector, called `mean()`.

```
x = [2,1,5,4,8,3,4,3];
mean(x)

ans =

    3.7500
```

Write a MATLAB script that computes the mean of a vector. Do it from scratch, in other words don't use the built-in function `mean()`. Ask the user to enter a vector using square brackets, and then compute the mean, and tell the user what it is. For example:

```
enter a vector, e.g. [3,1,4,1,5,9]: [1,2,3,4,5]
the mean of the vector is: 3.00
```

E 4.2 If we have a vector X containing n values, then the unbiased sample variance[75] s^2 is:

$$s^2 = \frac{1}{n-1} \sum_{i=1}^{n} \left(X_i - \bar{X}\right)^2 \tag{4.2}$$

where $\bar{X}$ is the mean of the vector.

In MATLAB there is a built-in function for computing the variance of a vector, called `var()`.

```
x = [2,1,5,4,8,3,4,3];
var(x)

ans =

    4.5000
```

Write a MATLAB script that computes the unbiased variance of a list of numbers. Do it from scratch, in other words don't use the built-in functions `var()` or `mean()`.

```
enter a vector, e.g. [3,1,4,1,5,9]: [1,2,3,4,5]
the variance of the vector is: 2.50
```

Links

[66] https://en.wikipedia.org/wiki/Quicksort

[67] https://en.wikipedia.org/wiki/Matrix_(mathematics)#Basic_operations

[68] http://math.mit.edu/~gs/linearalgebra/

[69] http://ocw.mit.edu/courses/mathematics/18-06-linear-algebra-spring-2010/video-lectures/

[70] http://www.mathworks.com/help/finance/matrix-algebra-refresher.html

[71] http://www.mathworks.com/company/newsletters/articles/the-origins-of-matlab.html

[72] http://www.mathworks.com/help/matlab/linear-algebra.html

[73] http://www.mathworks.com/help/matlab/cell-arrays.html

[74] http://www.mathworks.com/help/matlab/structures.html

[75] http://en.wikipedia.org/wiki/Variance#Sample_variance

5 Control flow

Here we will learn above several ways to specify the flow of information as your code gets executed. We will learn about *loops*, which are constructs that allow you to repeat blocks of code multiple times, typically while changing the values of variables inside the repeating block. We will learn about *conditionals*, which allow you to execute different branches of code depending on the values of variables. We will see how to *pause* your code, and to *break* out of a code block.

5.1 Loops

Loops are used when you have a chunk of code that you need to repeat over and over again, each time changing one (or more) parameters. Here is a simple example for the purposes of demonstration. Let's say you want to load data from 5 files, named `data1.txt`, `data2.txt`, ..., `data5.txt`. Let's say each file contains a one-dimensional array of 10 values. Let's say you want to take the average of each data file and then report the overall mean and overall variance of those 5 values. Here's one way to do it:

```
d1 = load('data1.txt');
d1m = mean(d1);
d2 = load('data2.txt');
d2m = mean(d2);
d3 = load('data3.txt');
d3m = mean(d3);
d4 = load('data4.txt');
d4m = mean(d4);
d5 = load('data5.txt');
```

```
d5m = mean(d5);
%
% report overall mean and overall variance of 5 data file means
alldata = [d1m d2m d3m d4m d5m];
datamean = mean(alldata);
datavar = var(alldata);
disp(sprintf('mean=%.3f and variance=%.3f', datamean, datavar))
```

You can see that there is a lot of repetition in this code. What if we had to load data from 1000 data files? There would be a lot of copying and pasting of code chunks. This is error prone and inefficient. Instead let's use a *for loop*. A for loop allows you to repeat a block of code some predetermined number of times, and includes a counter so that you know which iteration of the loop is currently running. Here is what the code above would look like if we used a for loop:

```
nfiles = 5;
alldata = ones(1,nfiles)*NaN; % pre-allocate array and fill with NaN
for i=1:nfiles
    d = load(['data',num2str(i),'.txt']);
    alldata(i) = mean(d);
end
datamean = mean(alldata);
datavar = var(alldata);
disp(sprintf('mean=%.3f and variance=%.3f', datamean, datavar))
```

Now all we would need to change if we have 1000 data files (or one million) is the value of our variable `nfiles=1000;` or `nfiles=1e6;`—nothing else in the code would have to change. This makes our code much more resilient against programming errors.

You can see a for loop begins with the keyword `for` followed by a name of a variable (your choice) that will keep track of which iteration of the loop is currently running. Then the equal sign `=` followed by a list of values to be iterated through. This list can be a constructed list using the colon operator (as in the example above) or it can be a variable such as an array containing several values as in the

example below. Next is the block of code to be repeated. The end of this code block is denoted by the `end` keyword.

```
x = 1:3:15;
for i=x
    disp(sprintf('i=%d', i))
end
```

which prints out:

```
i=1
i=4
i=7
i=10
i=13
```

For loops are executed in a serial fashion, one repetition after another. When we talk later about parallel programming we will see that one can pretty easily *parallelize* a for loop in MATLAB so that different iterations are distributed over multiple cores of a CPU (or indeed over multiple CPUs in different machines over a network).

There is a second sort of loop called a *while loop*. This kind of loop is typically used when the number of iterations is not known in advance. A while loop keeps repeating until the value of a logical expression changes from TRUE to FALSE (changes from 1 to 0). As a little demo, here is an example of a while loop that prints out successive integers starting from 1, until they exceed a critical value, in this case 10:

```
i=1;
while (i<9)
    disp(sprintf('i=%d', i))
    i=i+1;
end
```

which displays:

```
i=1
i=2
i=3
i=4
i=5
i=6
i=7
i=8
```

The expression that determines whether a while loop will continue repeating can be any valid MATLAB expression that evaluates to 0 (FALSE) or 1 (TRUE). In fact, in MATLAB 0 is FALSE and any other value is considered to be TRUE.

For both for loops and while loops, there are two keywords to know about that can break you out of a loop (`break`) and can move you to the next iteration of the loop (`continue`). I tend not to use these, but you can see the MathWorks online help to read more about them:

break[76]

continue[77]

5.2 Conditionals

So far we have seen how to use loops to repeat sections of code over and over again as needed. The other major control flow mechanism in high-level languages such as MATLAB is the *conditional*, which allows you to specify how code branches in one direction or another depending on some logical condition.

So for example let's say you ask the user to enter a number, and if the number is even you output "The number is even." and if the number is odd you output "The number is odd.":

```
x = input('Enter a number: ');
if (mod(x,2)==0)
```

```
    disp('The number is even.');
elseif (mod(x,2)~=0)
    disp('The number is odd.');
end
```

which produces:

```
Enter a number: 15
The number is odd.
```

and

```
Enter a number: 12
The number is even.
```

In general one can string together any number of `elseif` branches (including none of them). For example:

```
x = input('Enter a number: ');
if (x<10)
    disp('The number is less than 10');
elseif (x<20)
    disp('The number is less than 20');
elseif (x<30)
    disp('The number is less than 30');
else
    disp('I don''t have anything to say');
end
```

You don't need any `else` statements at all if is suits your needs:

```
x = input('Enter a number: ');
if (x<0)
    disp('That is a negative number');
end
```

The MathWorks online documentation has a page on conditional statements here:

Conditional Statements[78]

5.3 Switch statements

The other type of conditional you might come across (though I rarely use them) is called a *switch statement*. Typically these are used when there is some relatively large list of potential cases and for each you have a defined (and different) course of action. Here is an example adapted from the MathWorks help page on conditionals:

```
d = input('Enter a day of the week: ','s');
switch d
    case 'Monday'
        disp('First day of the week')
    case 'Tuesday'
        disp('Day 2')
    case 'Wednesday'
        disp('Day 3')
    case 'Thursday'
        disp('Day 4')
    case 'Friday'
        disp('Last day of the work week')
    otherwise
        disp('Weekend!')
end
```

Side note: can you spot any potential problem(s) with the above code?

5.4 Pause, break, continue, return

There are some keywords in MATLAB that give you finer control over the flow of a program.

The `pause` keyword by itself will simply cause MATLAB to stop at that point in the code, and wait until the user strikes any key—then MATLAB will continue. Try this:

```
for i=1:10
    if (i==5)
        disp('i is 5! hit any key to continue');
        pause
    else
        disp(sprintf('i is not 5, continuing... (i is %d)', i));
    end
end
```

which produces:

```
i is not 5, continuing... (i is 1)
i is not 5, continuing... (i is 2)
i is not 5, continuing... (i is 3)
i is not 5, continuing... (i is 4)
i is 5! hit any key to continue
i is not 5, continuing... (i is 6)
i is not 5, continuing... (i is 7)
i is not 5, continuing... (i is 8)
i is not 5, continuing... (i is 9)
i is not 5, continuing... (i is 10)
```

The `break` keyword in MATLAB will terminate the execution of a loop. Any code appearing after the `break` keyword will not be executed. In nested loops the `break` keyword only exits from the loop in which it appears. Here is an example of how `break` works:

```
for i=1:10
    if (i==5)
        disp('i is 5! stopping...');
        break
    else
        disp(sprintf('i is not 5, continuing... (i is %d)', i));
```

```
    end
end
```

which produces:

```
i is not 5, continuing... (i is 1)
i is not 5, continuing... (i is 2)
i is not 5, continuing... (i is 3)
i is not 5, continuing... (i is 4)
i is 5! stopping...
```

I tend not to use `break` to exit out of loops but rather write code that more gracefully determines what to do. It's a personal preference.

The `continue` keyword passes control to the next iteration of a loop, and skips any code appearing below where it appears. Like the `break` keyword, when `continue` appears in nested loops it only applies to the loop in which it appears. Here is an example of how `continue` works:

```
for i=1:10
    if mod(i,2)==0
        continue
    end
    disp(sprintf('the number %d is odd', i));
end
```

which produces:

```
the number 1 is odd
the number 3 is odd
the number 5 is odd
the number 7 is odd
the number 9 is odd
```

Again, I tend not to use `continue` but this is perhaps a personal preference.

The `return` keyword forces MATLAB to return control to the "invoking function", which means that when used within a function, `return` will exit the function without executing any of the remaining code. See Chapter 6 on Functions for more about how functions work in MATLAB.

Exercises

E 5.1 Write a program that computes the sum of the first 10 positive integers. Print the resulting sum to the screen like this:

```
the sum of the first 10 positive integers is: 55
```

E 5.2 Some people use an approximate formula for quickly converting Fahrenheit (F) to Celsius (C):

$$C \approx \hat{C} = (F - 30)/2 \tag{5.1}$$

Write a program that prints three columns: F, C and the approximate value of $\hat{C}$. The table should print for values of F from 0 to 100, in steps of 10 degrees, each to two decimal places.

Your program output should look like this:

```
Fahrenheit Celsius      C
      0.00  -17.78 -15.00
     10.00  -12.22 -10.00
     20.00   -6.67  -5.00
     30.00   -1.11   0.00
     40.00    4.44   5.00
     50.00   10.00  10.00
     60.00   15.56  15.00
     70.00   21.11  20.00
     80.00   26.67  25.00
     90.00   32.22  30.00
```

E 5.3 Write a program that computes the sum of the first n positive integers, where n is specified by the user. Let's assume for now that $n > 0$ and $n < 500$. Test it on $n = 5$, $n = 50$ and $n = 500$, the output should be:

```
the sum of the first 5 positive integers is: 15
the sum of the first 50 positive integers is: 1275
```

```
the sum of the first 500 positive integers is: 125250
```

E 5.4 Write a program to estimate the square root of 612 using Newton's method[79]. Write it so that the number whose square root is to be taken, and the number of iterations are both parameters (variables) that can be set by the user or the programmer. You can choose the initial guess on your own, use whatever you like. I suggest the number 10.0 as in the wikipedia example.

Find the square root of 612 using 5 iterations. Try it again using 10 iterations.

Links

[76] http://www.mathworks.com/help/matlab/ref/break.html

[77] http://www.mathworks.com/help/matlab/ref/continue.html

[78] http://www.mathworks.com/help/matlab/matlab_prog/conditional-statements.html

[79] http://en.wikipedia.org/wiki/Newton's_method#Square_root_of_a_number

6 Functions

Functions are one of the most useful programming facilities that you will run into because they allow you to make your code more modular.

6.1 Encapsulation

We have seen functions already, for example functions to print stuff to the screen like `disp()` in MATLAB, functions for mathematics like `sqrt()`, and so on. The advantage of putting things like these into functions is that we avoid the need to write everything from scratch each time we want to repeat a common operation. Imagine if every time we wanted to take the square root of a number, we had to write an entire algorithm (like Newton's method) to do so. It would be ridiculous. By encapsulating this operation into a function, all we need to do is write `sqrt()` and the program goes and looks up the definition of that function, and executes that code, without us having to type it in again, and again.

Here we will be going through how to write our own functions to encapsulate our own operations, whatever they may be.

You can even imagine a series of functions that you write to perform the various steps of your data analysis, so that each time you collect more data in your experiment, you simply have to type:

```
>> go_my_analysis();
```

and all of your data analysis will be repeated, including the incorporation of any

new data that may be residing in your data directory. Of course you have to define what happens inside of `go_my_analysis()` for this to be useful. Maybe inside your function you have defined other functions like:

```
>> load_all_data();
>> filter_data();
>> average_across_subjects();
>> perform_statistics();
>> generate_plots();
>> save_processed_data();
```

You get the idea.

The other situation where modularity in your code is useful, is for when you want to share code with other people (or use someone else's code). If you (or someone else) has a specific input/output functionality in mind, then you can swap in and out one of many potential functions that claim to achieve the desired functionality, as long as it preserves the input/output relationship(s) that you specify.

For example, let's say you discover that as part of your data analysis you will need to compute the square root of a number, and let's pretend that you don't have a function to do so built in to your language. (In fact you do of course—but for the purpose of this thought experiment let's imagine you don't.) The input/output requirements for your square root function are that it takes as input a single floating-point number and returns a single floating point number. Now you can go shopping, among your friends, colleagues, or on the internet, for an implementation of the square root function, and you can simply plug it in to your program and use it, as long as it takes a single floating-point number as input, and returns a single floating-point number as output. This specification is sometimes called the *function prototype*. You might find that several functions that you have found work equally well in terms of returning the correct answer, but that one in particular is way faster than the rest (perhaps it was written by a mathematician who knows some clever numerical tricks).

6.2 Function specification

In MATLAB usually sits in its own `.m` file, and starts with the word `function`, such as in this file called `mydeg2rad.m`:

```
function radsOut = mydeg2rad(degIn)

% radsOut = mydeg2rad(degIn)
%
% accepts an angle in degrees and returns
% the equivalent in radians
%

conversion = pi / 180;
radsOut = degIn * conversion;
```

The first line of the file begins with the word `function`, followed by (1) output variable(s), (2) the function name, and (3) input variables. In the above case there is a single output variable which we have named `radsOut`, and a single input variable named `degIn`. A function in MATLAB can have zero, one, or more output variables, and zero, one or more intput variables.

Following the function protype on line 1, is a series of commented lines—lines beginning with the `%` symbol. This tells MATLAB not to execute those lines as MATLAB code but that rather, these are human-readable comments. In addition now when you type `help mydeg2rad` on the MATLAB command line, MATLAB will display those comments as help for your function:

```
>> help mydeg2rad
  radsOut = mydeg2rad(degIn)

  accepts an angle in degrees and returns
  the equivalent in radians
```

The last two lines of the file is where the work happens in the function. In this

case our function has just two lines of code that do the work—but in general your function can have many lines of code. The thing that your function has to have, is a definition of the value of the output variable(s)—the names of which are defined on line 1, in the function prototoype—so in our case this is a variable called `radsOut`. This is how a function in MATLAB sends it output back to the code that called the function.

We can use our function like this:

```
>> mydeg2rad(180)

ans =

    3.1416
```

6.3 Variable scope

In MATLAB, we named the output variable(s) of our function and we also named the input variable(s) of our function. In the `mydeg2rad` function above, the output variable is named `radsOut` and the input variable is named `degIn`. The *scope* of these variable definitions is only within the function itself. Outside of the function, MATLAB does not know about these variables.

Similarly, the `conversion` variable defined on the second-to-last line of the `mydeg2rad` function also has a scope within the function itself, and outside of the function, MATLAB doesn't know about it.

You can think of a function like a black box, and to the outside user, the innards are unknown and inaccessible.

We can show this by trying to access the within-function variables:

```
>> mydeg2rad(180)

ans =
```

```
    3.1416

>> degIn
Undefined function or variable 'degIn'.

>> radsOut
Undefined function or variable 'radsOut'.

>> conversion
Undefined function or variable 'conversion'.
```

If we want to collect the output of the function we have to define a new variable to hold it:

```
>> myValue = mydeg2rad(180)

myValue =

    3.1416
```

Similarly, within a function, MATLAB does not know about variables outside of the function. So if we try to access, from within a function, variables defined outside of the function, we get an error message:

```
function out = newFun(in)

out = (myValue * 2) + 10;
```

```
>> newFun(10)
Undefined function or variable 'myValue'.

Error in newFun (line 3)
out = (myValue * 2) + in;
```

MATLAB functions *do* know about scripts and functions defined elsewhere how-

ever. It's only *variables* that have limited scope in MATLAB.

6.4 Anonymous functions

I have said that usually functions in MATLAB are located in their own `.m` file. However there is a way to define a function that is not stored in a file, but is associated with a variable defined in the MATLAB workspace. The hitch is that functions defined in this way can only contain a single executable statement. Here is an example of an *anonymous function* that returns the square of an input value:

```
>> sqr = @(x) x.^2;
>> a = sqr(5)

a =

    25
```

Line 1 says define an anonymous function, named `sqr()` that is a function of one input variable which we shall call `x` (within the function—remember variable scope), and the output of that function ought to be `x.^2`.

See the MATLAB documentation on anonyous functions for more details and examples:

Anonymous Functions[80]

Exercises

E 6.1 Write a function that determines whether a given number is a prime number. Remember, a prime number[81] is a (natural) number greater than 1 that is only divisible (with zero remainder) by the number 1, and itself. The first few prime numbers are 2,3,5,7,11,13,17,19,23,29, ...

For now you don't have to implement a fancy algorithm for testing primeness (e.g. Sieve of Eratosthenes[82]). For now, it's ok to implement a brute force method.

Hint: you will probably want to use the modulo[83] operator to test whether the remainder is zero after dividing a number n by another number m. In MATLAB, modulo is achieved using a function `mod(n,m)`.

So for example we can test whether the number 5 is prime by testing whether (5 modulo m) equals 0 for m=2,3,4.

E 6.2 Write a function that computes the nth Fibonacci number[84]. Your function should be called `fib()` and should take as input a single integer value n, and should return a single integer value representing the nth Fibonacci number.

Use a loop to accomplish this. Count how many arithmetic operations take place for computing the 10th Fibonacci number, and count also for the 20th.

bonus: write a second version of your function that uses recursion[85] instead of a loop. Note how much more succint the code is. Count how many arithmetic operations take place for computing the 10th Fibonacci number, and for the 20th as well. Now you see the potential downside of recursive algorithms.

bonus 2: incorporate memoization[86] to make your recursive version more efficient. Count again the number of arithmetic operations for the 10th and 20th Fibonacci numbers.

E 6.3 The following equation can be used to estimate an approximate derivative of a mathematical function $f(x)$ if h is sufficiently small:

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h} \tag{6.1}$$

Write a function `numdiff(f,x,h)` that returns an approximate estimate of the derivative of a mathematical function in a single variable x. Apply it to the four mathematical functions given below to estimate derivatives at the given values:

1. $f(x) = (e^x)$ at $x = 0$
2. $f(x) = \left(e^{-2x^2}\right)$ at $x = 1$
3. $f(x) = (\cos x)$ at $x = \pi/2$
4. $f(x) = (\ln x)$ at $x = 1$

Use $h = 0.01$

In each case write out the error, i.e., the difference between the exact derivative and the result of the approximation. Use 10 decimal places of precision.

If you need help finding out what the exact solutions to these derivatives are, (1) try to remember your calculus!, (2) ask a classmate, (3) google it, or (4) ask me (at which point I will direct you to WolframAlpha[87]).

hint: the $\ln()$ function (logarithm, base e) is typically called `log()` in programming languages like MATLAB whereas the logarithm, base 10 (typically referred to in math class as $\log()$, is typically called `log10()`.

Here is some code scaffolding to get you started:

In a file called `numdiff.m`:

```
function out = numdiff(f,x,h)

out = (feval(f,x+h) - feval(f,x-h)) / (2*h);

end
```

In a file called `myfun1.m`:

```
function out = myfun1(x)

out = exp(x);

end
```

In a file called `numerical_differentiation.m` (this is your main script):

```
% exercise on numerical differentiation
%

% estimate derivative of e^x at x=0, h=0.01:
%
est1 = numdiff('myfun1',0,0.01);
% est1 = 1.000016666749992
true1 = 1.00; % from calculus, d(e^x)/dx = e^x
err1 = est1-true1;
disp(sprintf('error for e^x is %.10f', err1))
```

```
error for e^x is 0.0000166667
```

E 6.4 The wikipedia article about pi (here[88]) describes a monte carlo method of estimating pi that involves repeated sampling from a random distribution.

The basic idea is to imagine a circle of radius r inscribed inside a square with side length $2r$. Now imagine placing a dot at some random location within the square. Sometimes the dot will be inside the circle and sometimes it will not. If you count the number of dots that land inside the circle and divide that by the total number of dots, that ratio ought to equal $\frac{\pi}{4}$.

As an exercise, implement this method of estimating pi. Write the program so that you can use any number of random dots n. Start with 1000 dots and then try larger numbers. See how close you can get to the actual value of π. Here are the first 100,000 digits[89] of π.

Note that this algorithm is not a very efficient or fast way of getting the digits of π, but it's a fun programming exercise nevertheless and a way to get you coding.

hint: you will need a function that generates random numbers. In MATLAB the `rand()` function samples from a uniform (pseudo)random distribution over the interval $(0, 1)$. Typing `rand` will return a single random value.

hint: to determine whether each point is inside or outside of the circle you can compute the distance between the point and the centre of the circle. If this distance is greater than the radius of the circle, it must be outside of the circle. Using the Pythagorean theorem[90] you can easily show that the equation for the distance d between two points (x_1, y_1) and (x_2, y_2) is:

$$d = \sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2} \tag{6.2}$$

Links

[80] http://www.mathworks.com/help/matlab/matlab_prog/anonymous-functions.html

[81] http://en.wikipedia.org/wiki/Prime_number

[82] http://en.wikipedia.org/wiki/Sieve_of_Eratosthenes

[83] http://en.wikipedia.org/wiki/Modulo_operation

[84] http://en.wikipedia.org/wiki/Fibonacci_number

[85] http://en.wikipedia.org/wiki/Recursion_(computer_science)

[86] http://en.wikipedia.org/wiki/Memoization

[87] http://www.wolframalpha.com

[88] http://en.wikipedia.org/wiki/Pi#Geometry_and_trigonometry

[89] http://www.geom.uiuc.edu/~huberty/math5337/groupe/digits.html

[90] http://en.wikipedia.org/wiki/Pythagorean_theorem

7 Input & Output

Most of the time you will be writing programs that analyse data—whether those data are collected from experiments, or generated by models and simulations. We will need to be able to read in data from a file. It will also be useful to be able to write data out to a file.

The MathWorks online documentation has a page devoted to importing and exporting data, here:

Data Import and Export[91]

Here we will go over how to read and write to some common types of files including ASCII files (plain text), MATLAB `.mat` files, as well as other binary formats. The MathWorks has a page listing all of the various file formats that MATLAB knows how to import, it is quite lengthy:

Supported File Formats for Import and Export[92]

In general, there are two types of file formats, ASCII files (otherwise known as plain text files) and binary files. In fact, this is a lie and there really is only one file type, namely binary files, since all data are ultimately stored as `0`s and `1`s (binary)—but we have conventions, like the ASCII code, which allow us to make assumptions, to make life easier. So we know that if a (binary) file is coded using a series of bytes, each of which corresponds to an ASCII code, then this file is in fact a "plain text" or ASCII file (and you can read it using any plain text editor like vim, emacs, sublime text, notepad, even MS Turd will open plain text files). Binary files include things like image formats such as `.png`, `.jpeg`, sound files such as `.mp3` and video files such as `.mp4` and `.mov`. Like I said before though,

really, all files are binary. It's just that we can open files containing ASCII code using many programs which know how to interpret the 0s and 1s as ASCII codes.

7.1 Plain text files

If your data are stored in a plan text file (ascii) then you can use the MATLAB function `load` to load in the file. For example let's say we have a plain text file called `mydata.txt` that contains the following:

```
2 3
4 5
6 7
8 9
```

Then we can use the `load` command to load the data:

```
>> d = load('mydata.txt');
>> whos
  Name      Size            Bytes  Class     Attributes

  d         4x2                64  double

>> d

d =

     2     3
     4     5
     6     7
     8     9
```

You can also load the data without giving the `load` function an output variable to store the data—in this case the data will be stored in a new variable with the same name as the filename (but any file suffix, such as `.txt` stripped):

```
>> load mydata.txt
```

```
>> whos
  Name        Size            Bytes  Class     Attributes

  mydata      4x2                64  double

>> mydata

mydata =

     2     3
     4     5
     6     7
     8     9
```

For loading ASCII files, the file must contain a rectangular table of numbers, with an equal number of elements in each row. Delimiters such as spaces, commas, semicolons or tabs can be used—but they have to the same througout the file. If these conditions are not met, MATLAB will complain. For example if our data file `mydata2.txt` looks like this:

```
2 3
4 5
6 7 8
8 9
```

MATLAB will complain about number of columns not being the same:

```
>> load mydata2.txt
Error using load
Number of columns on line 3 of ASCII file mydata2.txt must be the same as
    previous lines.
```

To save data to an ASCII file, you can use the `save` command. For example let's say we have data store in a variable called `data` that looks like this:

```
data =
```

```
    0.6557    0.7577
    0.0357    0.7431
    0.8491    0.3922
    0.9340    0.6555
    0.6787    0.1712
```

Then we can use `save` with the `-ascii` flag to save this into an ASCII file:

```
>> save mynewdata.txt data -ascii
```

The first argument (`mynewdata.txt`) is the filename of the new file to be created. The second argument (`data`) is the name of the variable to be saved to the file, and the third argument (`-ascii`) is a flag to the `save` command that tells MATLAB to save the data in plain text (ASCII) format. Now if we look at the new file (for example by opening it in the MATLAB text editor) that was created, `mynewdata.txt` it looks like this:

```
   6.5574070e-01   7.5774013e-01
   3.5711679e-02   7.4313247e-01
   8.4912931e-01   3.9222702e-01
   9.3399325e-01   6.5547789e-01
   6.7873515e-01   1.7118669e-01
```

Note how it has been saved in scientific notation.

If you want finer control over how things are stored in an ASCII file, you can read (as well as write) using lower-level control using MATLAB's built-in functions `fprintf` and `fscanf`. These mirror the functions with the same name that may be familiar to you if you have programmed in C before. Here is an example of writing to an ASCII file where we want a very specific format:

```
data = [
    0.6557    0.7577
    0.0357    0.7431
```

```
    0.8491    0.3922
    0.9340    0.6555
    0.6787    0.1712
];

fid = fopen('myfile.txt','w');
fprintf(fid, 'myfile.txt contains some data\n');
for i=1:size(data,1)
    fprintf(fid,'item 1.1: %.4f, item 1.2: %.4f\n', data(i,1), data(i,2));
end
fprintf(fid, 'end of data\n');
fclose(fid);
```

This creates a file called `myfile.txt` that looks like this:

```
myfile.txt contains some data
item 1.1: 0.6557, item 1.2: 0.7577
item 1.1: 0.0357, item 1.2: 0.7431
item 1.1: 0.8491, item 1.2: 0.3922
item 1.1: 0.9340, item 1.2: 0.6555
item 1.1: 0.6787, item 1.2: 0.1712
end of data
```

7.2 Binary files

MATLAB has its own binary format for files, denoted using a `.mat` file suffix. The `save` and `load` functions in MATLAB with no other options use this default binary format. The advantage of MATLAB's binary format over an ASCII format is (1) your data files will be smaller in size, and (2) with MATLAB's `.mat` format you can store more than one variable (and variables of different kinds) in a single file. For example here we store a scalar variable called `mynumber`, a vector called `myvector`, a matrix called `mymatrix` and a structure called `mystructure` in a single binary `.mat` file called `myfile.mat`:

```
>> whos
```

```
  Name             Size            Bytes  Class     Attributes

  mymatrix         4x2                64  double
  mynumber         1x1                 8  double
  mystructure      1x1               840  struct
  myvector         1x7                56  double

>> save myfile mynumber myvector mymatrix mystructure
```

Now there is a file in my working directory called `myfile.mat`. I can now load the file (and all the variables contained within it) into MATLAB's memory using the `load` function. First I clear the memory to demonstrate that I'm not cheating:

```
>> clear
>> whos
```

Now I load the file:

```
>> load myfile
>> whos
  Name             Size            Bytes  Class     Attributes

  mymatrix         4x2                64  double
  mynumber         1x1                 8  double
  mystructure      1x1               840  struct
  myvector         1x7                56  double
```

7.3 ASCII or binary?

The question of which file format to use as you go forward and write programs for analysing your data is an interesting one to consider. For long-term archival purposes, I would suggest storing your data in an ASCII format, so that it remains readable by human eyes. There will always be programs to read ASCII files. The risk of storing data in a binary format is that (a) whatever program you used to

save the data will no longer be easily accessible in the future, and/or (b) you may not even remember what the binary format is. The disadvantage of storing data in ASCII format is that the files will be larger than if they were stored in a binary format. The availability and affordability of large amounts of storage is growing so quickly however, so perhaps one does not have to worry too much about this.

Links

[91] http://www.mathworks.com/help/matlab/data-import-and-export.html

[92] http://www.mathworks.com/help/matlab/import_export/supported-file-formats.html

8 Debugging, profiling and speedy code

In this chapter we will look at ways of solving problems with your code using the various debugging tools in MATLAB. We will also look at profiling your code using the built-in *profiler* in MATLAB, which can be used to identify parts of your code that are taking the most time to execute. We will go over a number of ways to make sure your code runs fast. In some cases this amounts to telling you about what *not* to do to make your code run slow. Finally we will look at the MATLAB Coder, which is a toolbox included in MATLAB that can generate standalone C and C++ code from MATLAB code. It can also generate so-called binary MEX functions that allow you to call compiled versions of your MATLAB code, potentially speeding up computations.

8.1 Debugging

There are at least two kinds of errors you will encounter in programming. The first is when you run your code and it aborts because of some kind of error, and you recieve an error message. Sometimes those error messages are useful and you can determine immediately what is wrong. Other times the error message is cryptic and it takes some detective work on your part to figure out what part of the code is failing, and why it is failing.

The second type of error is when your code runs without aborting, and without reporting any problem to you, but you do not get the expected result. This is much more difficult to debug.

In general the approach you should use for debugging is to step through your

code, line by line, and ensure that each step is (a) performing the operation you think it is, and (b) is performing the appropriate operation.

The built-in MATLAB editor that you can use to edit your MATLAB code files has a handy feature called *breakpoints* that allows you to set a breakpoint (or multiple breakpoints) on a specific line (or lines) of your code, such that as you run your code, MATLAB stops at a breakpoint and enters a special mode called the *debugger*. Once in the debugger you can examine values of variables, step to the next line of code, step in or out of functions, and continue executing the rest of the code. It's a very useful way to halt execution at specific places in your code, so that you can examine what is going on. Often this is how will find bugs and errors in your code—when you assumed a variable had a specific value, or an operation resulted in a specific value, and in fact it didn't.

Here is an example of a MATLAB script called `go.m` which computes some values, and executes a for-loop in which is fills a vector `v` with some numbers. By clicking with the mouse on the little dash (–) next to the line number 7 (on the left hand side of the editor window) I have inserted a breakpoint, which appears as a filled red circle. Figure 8.1 shows what this looks like.

Now when we run the program, MATLAB stops the first time it encounters the breakpoint on line 7. You will see this at the MATLAB command prompt:

```
>> go
7       d = c / 12;
K>>
```

It reports the line number (7) and the code appearing on that line, and it puts you in to debugger mode, as indicated by the prompt `K>>`. Now you can enter the names of variables to query their value, for example we can see what the value of `i`, and `c` are:

```
K>> i

i =
```

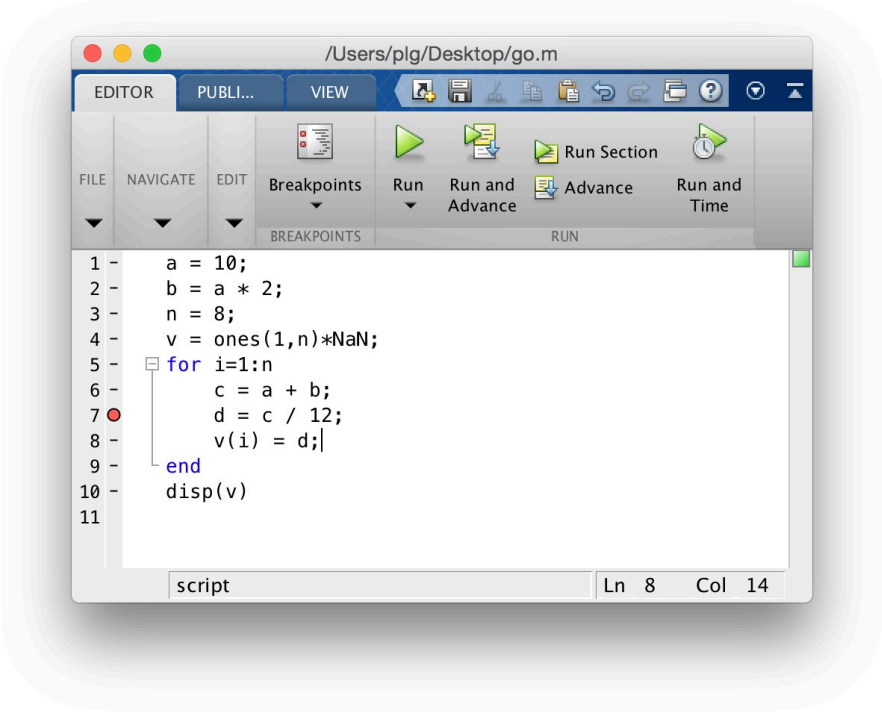


Figure 8.1: Setting a breakpoint at line 7.

```
     1

K>> c

c =

    30
```

We can step to the next line of code by clicking on the "Step" button appearing at the top of the editor window, as shown in Figure 8.2.

You will see that there is now a little green arror pointing to the right, at line 8 in the code. This indicates the line of code where the debugger has stopped, and is waiting for you to tell it what to do next. We can click on the "Continue"

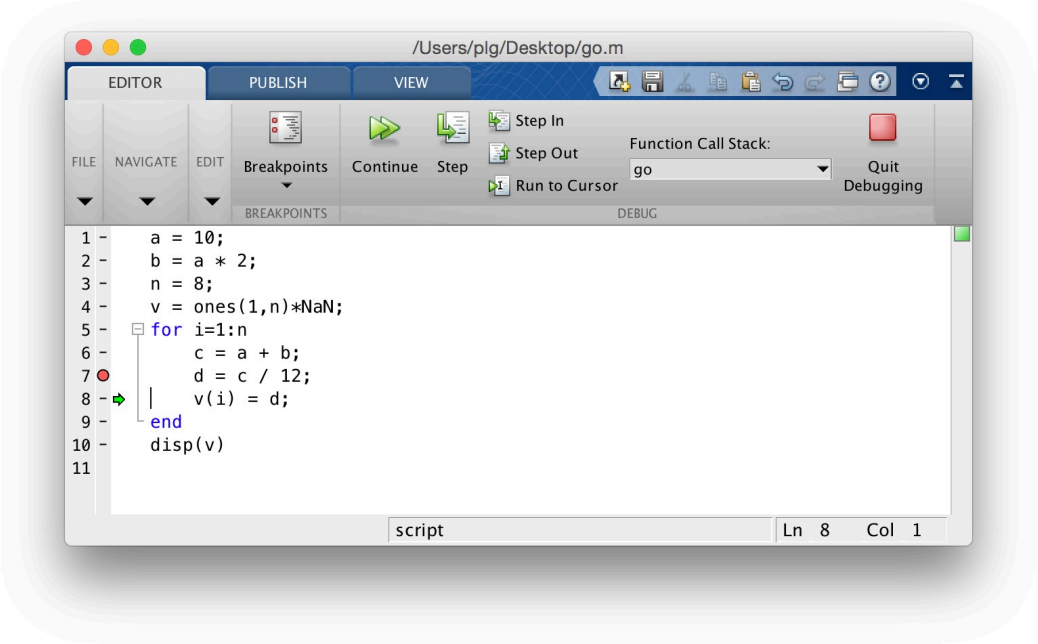


Figure 8.2: Stepping to the next line of code.

button at the top of the editor window to continue. When we do this we see that MATLAB has stopped again, at line 7 again, as shown in Figure 8.3.

At the command prompt we can enter `i` to query the value of `i` and we see that indeed we are now at iteration 2 of the for-loop:

```
K>> i

i =

     2
```

If we click "Continue" again we will stop again at line 7, at the third iteration of the for-loop, and so on. To continue without stopping at the breakpoint each time, we need to remove or disable the breakpoint. Right-click on the little red circle and a pop-up menu gives you these options. Note that there is also an

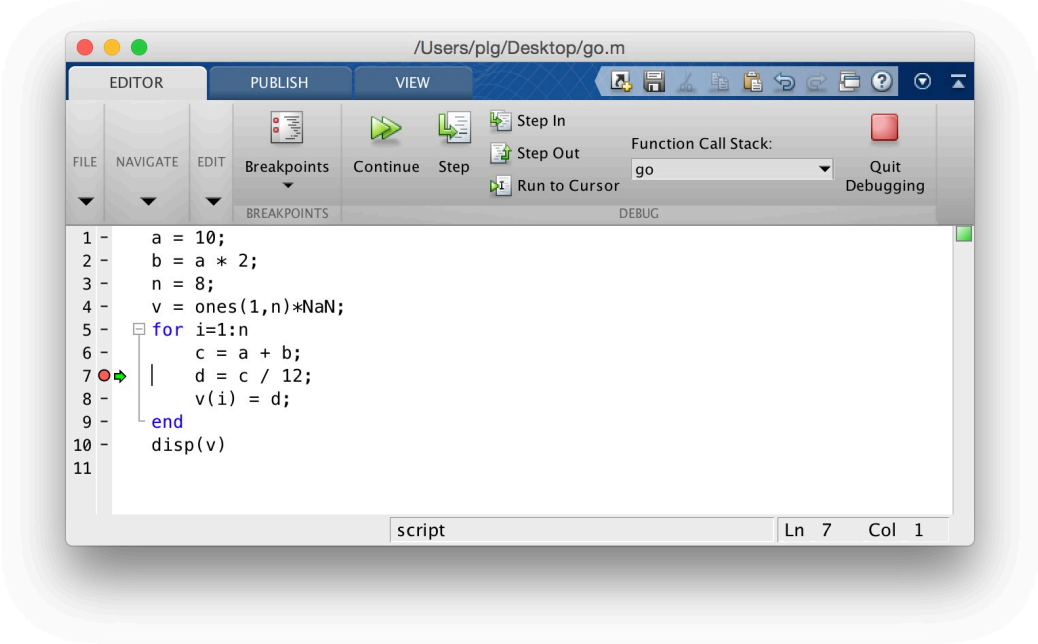


Figure 8.3: After continuing code execution.

option called "Set/Modify Condition..."—this allows you to specify a logical condition which if true, will cause MATLAB to stop at the breakpoint, otherwise not. This is a nice way to set up breakpoints that only stop the code if certain conditions are met—for example if the value of a variable you know should never be negative, is less than zero.

The MathWorks online documentation has a page devoted to debugging here:

Debugging[93]

8.2 Timing and Profiling

One obvious way of speeding up your MATLAB programs is to first identify the pieces of your program that are slowest—and then do what you can to speed up those parts.

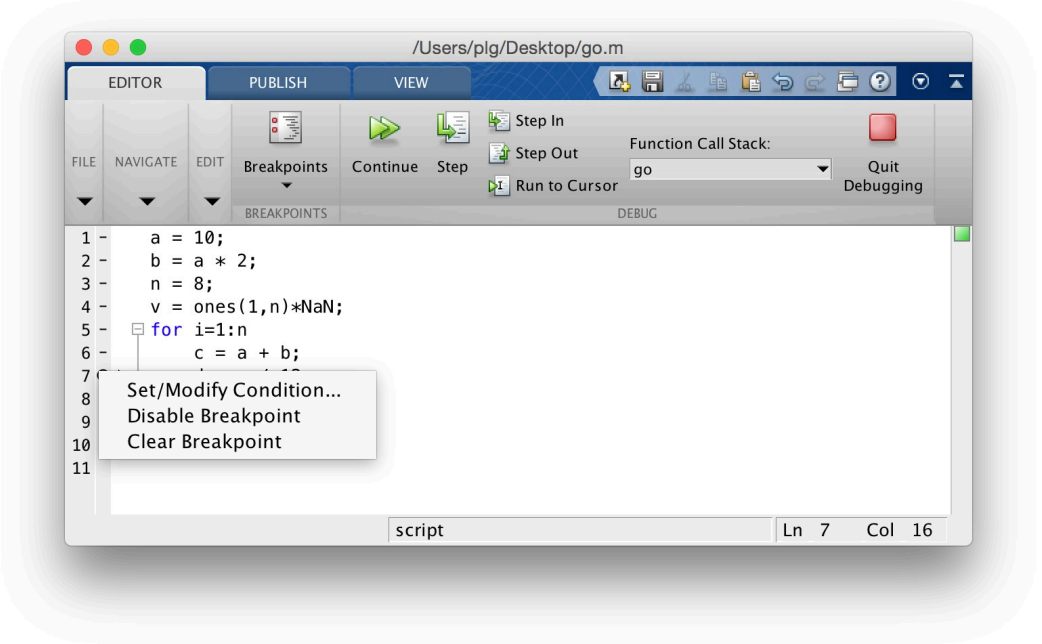


Figure 8.4: Setting a conditional breakpoint.

8.2.1 Timing your code using `tic` and `toc`

One way to time your code is to use the `tic` and `toc` commands in MATLAB.

```
>> help tic
 tic Start a stopwatch timer.
    tic and TOC functions work together to measure elapsed time.
    tic, by itself, saves the current time that TOC uses later to
    measure the time elapsed between the two.

    TSTART = tic saves the time to an output argument, TSTART. The
    numeric value of TSTART is only useful as an input argument
    for a subsequent call to TOC.

    Example: Measure the minimum and average time to compute a sum
             of Bessel functions.

      REPS = 1000; minTime = Inf; nsum = 10;
      tic;
```

```
     for i=1:REPS
       tstart = tic;
       sum = 0; for j=1:nsum, sum = sum + besselj(j,REPS); end
       telapsed = toc(tstart);
       minTime = min(telapsed,minTime);
     end
     averageTime = toc/REPS;

   See also toc, cputime.

   Reference page in Help browser
      doc tic
```

```
>> help toc
 toc Read the stopwatch timer.
    TIC and toc functions work together to measure elapsed time.
    toc, by itself, displays the elapsed time, in seconds, since
    the most recent execution of the TIC command.

    T = toc; saves the elapsed time in T as a double scalar.

    toc(TSTART) measures the time elapsed since the TIC command that
    generated TSTART.

    Example: Measure the minimum and average time to compute a sum
             of Bessel functions.

      REPS = 1000; minTime = Inf; nsum = 10;
      tic;
      for i=1:REPS
        tstart = tic;
        sum = 0; for j=1:nsum, sum = sum + besselj(j,REPS); end
        telapsed = toc(tstart);
        minTime = min(telapsed,minTime);
      end
      averageTime = toc/REPS;

    See also tic, cputime.
```

```
    Reference page in Help browser
       doc toc
```

The typical pattern using `tic` and `toc` is to bracket a chunk of code you want to time with `tic` and `toc`. There are several examples in section 8.3 below in which `tic` and `toc` are used to time MATLAB code execution time.

8.2.2 Using MATLAB Profiler

There is a tool in MATLAB called the *Profiler* that is very useful for showing which parts of your program take the most amount of time to execute. Think of the profiler as a way of automatically timing every part of your program and generating a handy report (which it does also).

The basic way to use the profiler is to first activate it by typing:

```
>> profile on
```

You can then run your MATLAB script, and once it is finished, stop the profiler by typing:

```
>> profile off
```

You can then generate a report by typing:

```
>> profile report
```

Here is an example using a script called `go.m` which calls two other functions, `myfun1` and `myfun2`:

```
n = 1e4;
m = zeros(100,100);
for i=1:n
    m = m + myfun1(m);
    m = m + myfun2(m);
```

```
end
disp(sprintf('grand mean of m is %.6f\n', mean(m(:))/n));
```

```
function out = myfun1(in)
[r,c] = size(in);
tmp = randn(r,c);
for i=1:r
    for j=1:c
        tmp(i,j) = sqrt(tmp(i,j));
    end
end
out = tmp;
end
```

```
function out = myfun2(in)
[r,c] = size(in);
tmp = randn(r,c);
tmp = sqrt(tmp);
out = tmp;
end
```

We turn on the profiler, run the code, stop the profiler, and generate a report, which is shown in Figure 8.5.

We can see that the `go` script overall took 160.726 seconds to run. We also see a list of functions that were called within `go`, and the time they took. We can see immediately that `myfun1` is way slower than `myfun2`. If we click the mouse on `myfun1` in the report, we get a new report of the `myfun2` function itself, which is shown in Figure 8.6.

We get a quite detailed report of the lines of the code where the most time was spent. We also see the time spent, and the number of calls made to each line of code in the function.

In this case we see that line 7 of the `myfun1` function is taking a lot of time to

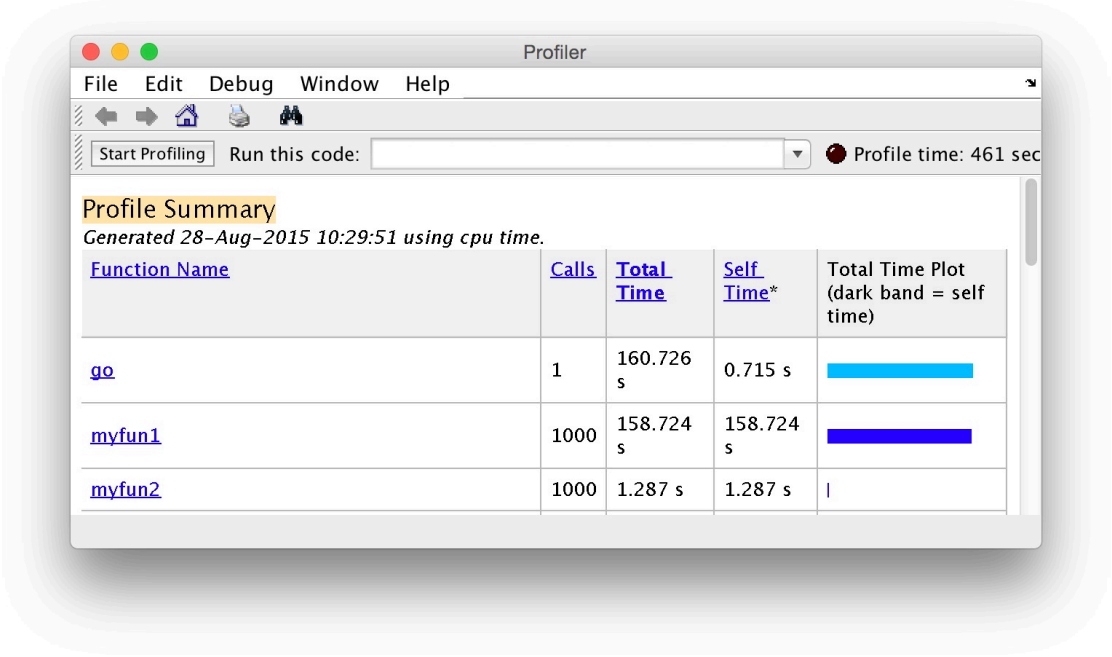


Figure 8.5: Profiler report of `go.m`.

execute—this is where we take the square root of each element of a large matrix, within two nested for-loops. Line 7 represents the innermost part of these two nested for-loops, and so it's no surprise that we are spending a lot of time here. See section 8.3.2 below for more information about how to avoid nested for-loops by using *vectorized* code operations.

The other way of running the profiler is by clicking with your mouse on the "Run and Time" button in the toolbar of the MATLAB code editor. The profiler will run your code, timing each line, and will open up a report window.

The MathWorks online documentation has a page on the profiler here:

Profiling for Improving Performance[94]

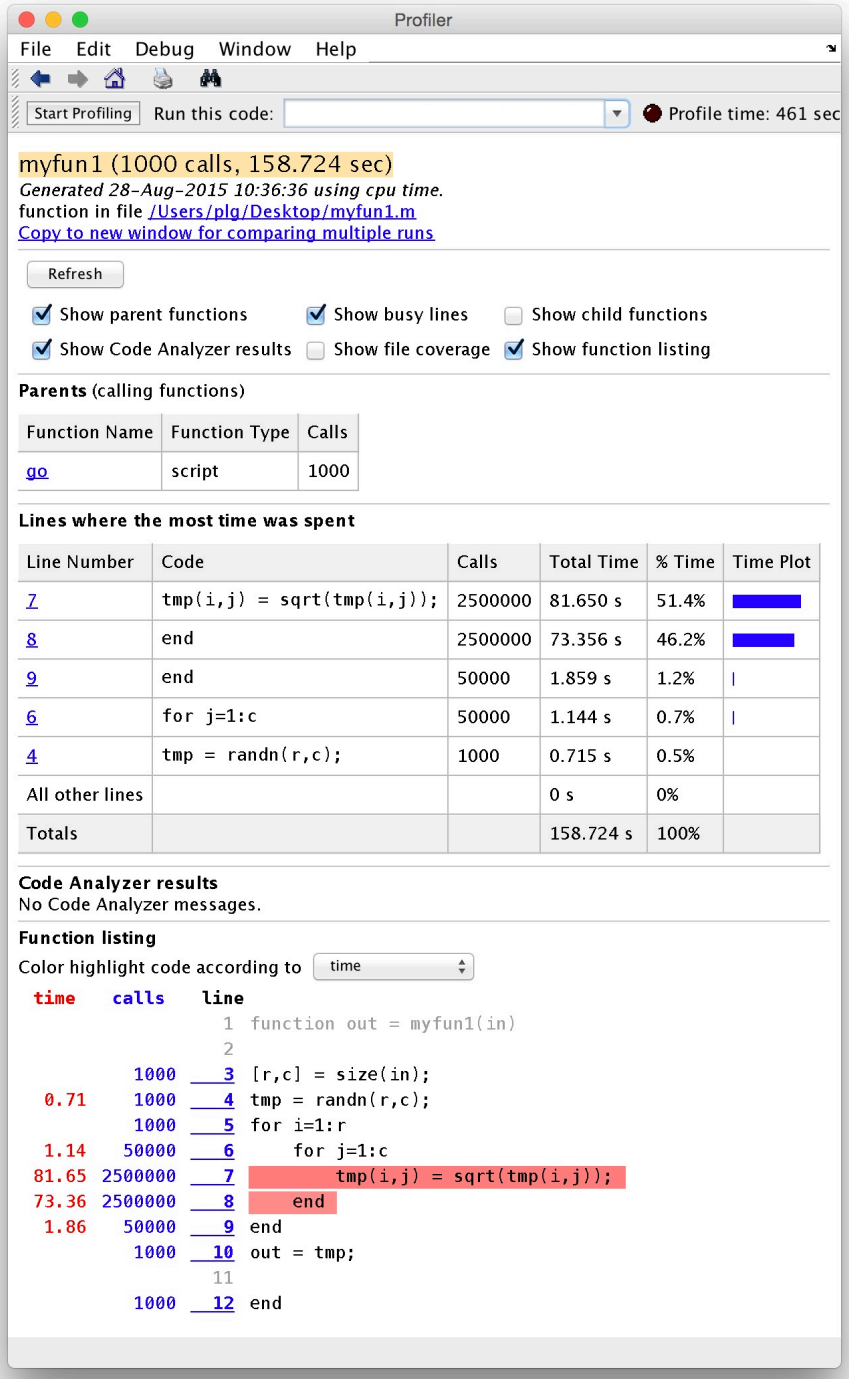


Figure 8.6: Profiler report of `myfun1.m`.

8.3 Speedy Code

8.3.1 Array preallocation

There are many cases in which we want to collect the results of many computations together into a single data structure, e.g. a vector or array. One way of doing this is to start with an empty array, and each time through the loop, add a value to it (and hence lengthening it). It turns out this way is very slow. What's much, much faster is to pre-allocate the array (and fill it with whatever values you want, e.g. `0`s, or `NaN`s), and then set each value as you go through the loop to the result of your computation.

Here is an example in MATLAB:

```
% let's compute the following formula
% for values between 0 and n:
%
% f(i) = (i + f(i-1)) / n

n = 1e5;

% the slow way:
%
tic
c = [0];
for i=2:n
  c = [c, (i + c(i-1)) / n];
end
toc
%
% on my laptop this takes 3.605413 seconds

% the fast way, with array pre-allocation
%
tic
c = zeros(1,n);
for i=2:n
  c(i) = (i + c(i-1)) / n;
```

```
end
toc
%
% on my laptop this takes 0.002819 seconds
% this is over 1,000 times faster than the slow version
```

In the slow version, we start with an array of length 1 containing the number zero. Each time through the loop we concatenate the array with the next value, and in this way we build up the array.

In the fast version, we pre-allocate an array of the required length, fill it with `0`s, and then each time through the loop we simply assign the appropriate value to the appropriate array position.

The reason the slow version is so slow, is that each time we concatenate the array, several steps take place under the hood:

1. a block of memory large enough to hold a new array (of length: one greater than the old array) is found and reserved
2. the new array is created
3. the old array is copied into all elements of the new array (except the last element which is left empty)
4. the new value is copied to the last value in the new array
5. the memory assigned to the old array is freed up (no longer reserved)

As you can imagine, when the array gets large, the copy operation can take a lot of time. It's inefficient to keep copying the array over and over again.

With pre-allocation, there is no copying, only assignment, and only single values are assigned.

8.3.2 Vectorization

Many functions in MATLAB are *vectorized*, that is, they can operate on arrays and matrices as if the function had been applied one by one to each element. An example is the `sqrt()` function.

Here's an example where we have three long arrays, defining 3D points, and our task is compute the length of each vector. We first compute the vector lengths the slow way, using a straightforward for-loop. We then do the same calculations but in a vectorized fashion—in this case by recognizing that arithmetic operations such as squaring, addition and taking the square root can all be applied to vectors as a whole, and MATLAB performs these operations in a vectorized fashion.

```
n = 1e7;        % a big number
x = rand(1,n);  % array of random numbers
y = rand(1,n);  % array of random numbers
z = rand(1,n);  % array of random numbers

% compute the norm of the 3-D vectors (x,y,z)

% the slow way
%
tic
norm_slow = zeros(1,n); % pre-allocate array
for i=1:n
  norm_slow(i) = sqrt(x(i)^2 + y(i)^2 + z(i)^2);
end;
toc
%
% on my laptop this takes 0.594378 seconds

% the vectorized way
%
tic
norm_slow = sqrt(x.^2 + y.^2 + z.^2);
toc
%
% on my laptop this takes 0.040536 seconds
% this is about 15 times faster than the slow version
```

When we implement this in a vectorized way, MATLAB uses pre-compiled, optimized functions to execute that part of the code, instead of running it through

the interpreter. When we use a for-loop, everything happens at the interpreter layer.

Two aspects of the code example are vectorized. First, we use the exponent operator in MATLAB on the entire vector x, y, and z (with the dot notation to denote element-by-element exponentiation). This exponentiates the entire vector using precompiled optimized code under the hood. Then we use the `sqrt()` function which also takes the whole array as an argument. Again, optimized precompiled code is used on the entire array rather than stepping through the array in a for loop, at the interpreter level.

Another salient example of vectorization is matrix algebra. The matrix algebra operators (e.g. matrix multiplication) make use of highly optimized, precompiled routines that are way faster than doing things by hand at the interpreter level, using for loops. Here is an example in code:

```
% matrix multiplication
%
A = rand(400,500);
B = rand(500,600);
C = zeros(400,600);

% the slow way, using for loops at the interpreter level
%
tic
m = size(A,1);
n = size(A,2);
p = size(B,1);
q = size(B,2);
for i=1:m
  for j=1:q
    the_sum = 0;
    for k=1:p
      the_sum = the_sum + A(i,k)*B(k,j);
    end
    C(i,j) = the_sum;
  end
end
```

```
toc
%
% on my laptop this takes 2.552810 seconds

% the fast way (vectorized)
%
C = zeros(400,600);
tic
C = A*B;
toc
%
% on my laptop this takes 0.001998 seconds
% this is over 1,000 times faster than the slow version
```

When we write `A*B` in MATLAB, where `A` and `B` are both matrices, MATLAB uses precompiled, optimized linear algebra routines (written in C and compiled for your CPU) to perform the matrix multiplication calculation.

8.3.3 Suppress output to the screen

This one might seem obvious, but if you are doing something thousands or millions of times, and each time you print something to the screen, that will slow down your code. Here's an example:

```
% suppress output!

% slow version
%
n = 1e5;
x = zeros(1,n);
tic
for i=1:n
  tmp = (i*i) + (i/2)
  x(i) = tmp;
end
toc
%
% on my laptop this takes 2.571819 seconds
```

```
% fast version
%
x = zeros(1,n);
tic
for i=1:n
  tmp = (i*i) + (i/2);
  x(i) = tmp;
end
toc
%
% on my laptop this takes 0.001080 seconds
% this is more than 2,000 times faster than the slow version
```

The *only* difference between the two version of this for-loop is that in the first, we fail to suppress output to the screen when we define the `tmp` variable. In the second version we include a semicolon to suppress output to the screen and our code runs more than 2,000 times as fast. Semicolons are powerful!

Printing values to the screen within a for-loop is not always a bad thing however. Often we want to print values to the screen in a for-loop so that we can keep track of how far along the computation is, or detect errors. One alternative that avoids the slow execution of printing to the screen every time through the loop, is to print more sporadically. Here is an example where we repeat the above code but we only print to the screen every 10,000 iterations. This still allows you to monitor the progress of the computation, but it doesn't eat up precious time displaying stuff on the screen every single time through the loop:

```
% partial suppression of output

% slow version
%
n = 1e6;
x = zeros(1,n);
tic
for i=1:n
  tmp = (i*i) + (i/2);
```

```
  x(i) = tmp;
  disp(tmp);
end
time1=toc
%
% on my laptop this takes 7.689031 seconds

% fast version
%
x = zeros(1,n);
tic
for i=1:n
  tmp = (i*i) + (i/2);
  x(i) = tmp;
  if (mod(i,100000)==0)
    disp(tmp);
  end
end
time2=toc
%
% on my laptop this takes 0.063113 seconds
% this is still more than 100 times faster than the slow version
%
disp(sprintf('time1=%.6f, time2=%.6f\n', time1, time2))
```

8.3.4 Overhead cost of calling a function

We've talked about the benefits of modularizing your code, and sticking commonly used operations inside *functions*. This is absolutely a good idea. It is worth noting however that the act of calling a function does involve some overhead cost in time (and in memory), for various things that happen under the hood.

Functions in general are a very good idea, but if you put *everything* into functions, you can start to experience unneccessary slowdowns due to the overhead in calling functions, passing parameters in, and passing results out. Here is a simple example in which we loop through an array and perform a number of

calculations on each element. In the slow version we put every single calculation into its own function (admittedly this is a bit extreme, but it illustrates the problem). In the fast version we don't use functions at all:

```
% slow version: make everything a function!!
%
n = 1e6;
a = 1:n;
tic
for i=1:n
  tmp1 = mycomp1(i);
  tmp2 = mycomp2(i);
  tmp3 = mycomp3(i);
  tmp4 = mycomp4(i);
  tmp5 = mycomp5(i);
  a(i) = tmp1 + tmp2 + tmp3 + tmp4 + tmp5;
end
toc
%
% on my laptop this takes 1.048836 seconds

% fast version: no functions here
%
n = 1e6;
a = 1:n;
tic
for i=1:n
  tmp1 = i*1;
  tmp2 = i*2;
  tmp3 = i*3;
  tmp4 = i*4;
  tmp5 = i*5;
  a(i) = tmp1 + tmp2 + tmp3 + tmp4 + tmp5;
end
toc
%
% on my laptop this takes 0.010898 seconds
% this is about 100 times faster than the slow version
```

In this case we have defined five functions in separate `.m` files (`mycomp1.m`, `mycomp2.m`, `mycomp3.m`, `mycomp4.m`, `mycomp5.m`,):

```
function out = mycomp1(in)
out = in*1;
```

```
function out = mycomp2(in)
out = in*2;
```

```
function out = mycomp3(in)
out = in*3;
```

```
function out = mycomp4(in)
out = in*4;
```

```
function out = mycomp5(in)
out = in*5;
```

It's a bit of a silly example but it gets the point across.

8.3.5 Passing by reference vs passing by value

In some languages like Python and in C, the default behaviour for passing data structures to functions as arguments, is to *pass by reference*. In MATLAB and R, the default behaviour is to *pass by value*.

Passing by value means that when one calls a function with an input argument (e.g. an array), a *copy* of that array is made—one that is internal to the function—for the function to operate on. When the function exits, that internal copy is deallocated (destroyed). Passing by reference means that instead, a pointer to the array (in other words, the address of the array in memory) is sent to the function, and the function operates on the original array, via its address.

As you can imagine, passing around data structures by value, which involves making copies, can be very inefficient especially if the data structures are large. It takes time to make copies and what's more it eats up memory. On the other hand, there may be times where one specifically wishes to make a copy of a function input, and in that case you might just accept that there is a price to pay.

In fact, MATLAB's behaviour is slightly more complex. If you pass an input argument `x` into a function, and *if inside the function that input argument is never modified*, MATLAB avoids making a copy of it, and passes it by reference. On the other hand, *if inside of the function, input parameter `x` is altered in any way*, MATLAB passes it by value. I suppose this is a good thing, MATLAB is trying to be efficient when it can be. The downside is that you have to remember as a programmer when things might change under the hood.

Here is an example, slightly contrived, but it gets the point across that passing large structures by value is slower than passing them by reference. Here is the slow version, in which MATLAB will pass by value, because inside our function we are changing a value of the input parameter `x`:

```
function out = myfunc_slow(x,y)
  tmp = x(1);
  x(1) = tmp*2;
  out = tmp;
```

and here is the fast version, where we don't change the value of `x`, and so MATLAB will pass by reference:

```
function out = myfunc_fast(x,y)
  tmp = x(1);
  y(1) = tmp*2;
  out = tmp;
```

Here we demonstrate the speed difference:

```
x = rand(1e4,1e4);
y = [1,2,3];

% the slow way
% MATLAB passes x by value
% because it is altered inside myfunc_slow()
%
tic
for i=1:20
  o1 = myfunc_slow(x,y);
end
toc
%
% on my laptop this takes 8.557641 seconds

% the fast way
% MATLAB passes x by reference
% because it is not altered inside myfunc_fast()
%
tic
for i=1:20
  o2 = myfunc_fast(x,y);
end
toc
%
% on my laptop this takes 0.000687 seconds
% this is over 12,000 times faster than the slow version
```

Note that it's not only speed that is a concern here. You will also notice if you pass around large data structures by value, that RAM (random access memory, the internal, temporary memory that your CPU uses) will be eaten up by all of the copies that are made. If your available RAM falls below a certain level, then everything (the entire OS) will slow down. Unix-based operating systems (e.g. Mac OS X, Linux) make use of hard disk space as a temporary scratch pad for situations in which available RAM is scarce. This is known as *swap space*. The problem is, read/write operations on hard disks (especially spinning platters) are orders of magnitude slower than read/write operations in RAM, so you still

suffer the consequences. With new solid-state hard drives (no moving parts) the read/write access is faster, but it's still not as fast as RAM, which has a more direct connection to your CPU.

8.3.6 The algorithm itself

Of course the other thing to consider when writing code that performs some computational task, is to make sure you're using the most efficient algorithm you can (when you have a choice). Sorting is an example. Why use bubblesort when you know quicksort can be orders of magnitude faster, especially for large lists?

Another example is optimization. For certain families of problems, specific optimizers are known to be really fast and efficient. For others, one needs a more generic, more robust optimizer, that may be slower.

Whatver operation you're coding up, do a bit of research to find out if someone has developed an algorithm that solves the problem you're solving, only faster.

8.4 MATLAB Coder

The MATLAB Coder is a toolbox which lets you generate standalone C and C++ code from MATLAB code, and lets you generate binary MEX files which you can call from your own MATLAB code.

Note that there is another MATLAB toolbox called the MATLAB Compiler, which does something different—it lets you share MATLAB programs as standalone applications. We will be talking about the MATLAB Coder here, not the MATLAB Compiler.

Without getting into details (and there are a few, see the documentation) the way to use the MATLAB Coder is to use the `codegen` function to generate a MEX file based on some MATLAB function that you've written, and then to call that compiled version of your function instead of the original MATLAB code version.

So for example let's consider the following function which computes the stan-

dard deviation of means of simulated random data vectors. It's not so important why we are doing these particular calculations—it's just an example of a set of calculations that we can compile to make faster.

```
function out = myfunction(in)
out = zeros(1,in)*NaN;
for i=1:in
    tmp = randn(100,5);
    out(i) = std(mean(tmp));
end
end
```

We can call the function like so:

```
>> tic; out=myfunction(1e5); toc
Elapsed time is 7.873669 seconds.
>> hist(out,50)
```

which produces the figure shown in Figure 8.7.

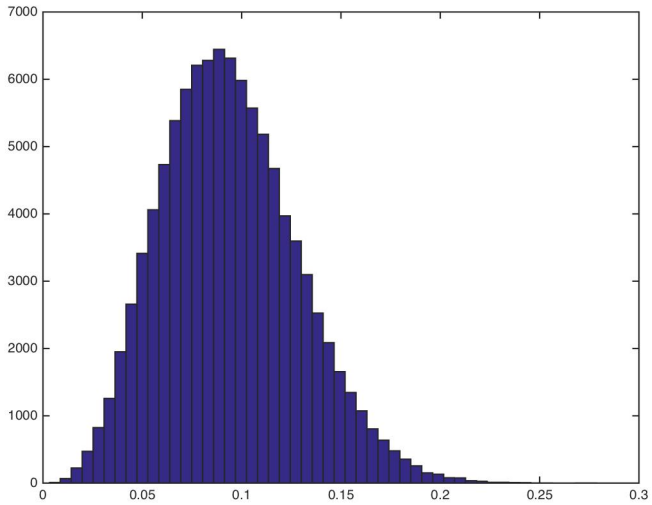


Figure 8.7: Output of `myfunction.m`.

To compile our MATLAB code into a binary MEX file we simply call the `codegen` function:

```
>> codegen myfunction -args {double(0)}
```

The `-args` argument is a list of input parameters to our function `myfunction` and their types, which the MATLAB coder needs to know in advance, in order to produce the C code and then the binary MEX function. The `double(0)` just tells MATLAB that we have a single input argument that is the same type as `double(0)`, in other words a `double`.

Just to unpack this a bit more—if we had a function that took two input arguments, a scalar `double` and a `1x10` array of `doubles` then we could do the following:

```
>> i1 = 0.0;
>> i2 = zeros(1,10);
>> codegen myfunction -args {i1, i2}
```

In this case we have predefined example input variables and passed those on in a cell array (hence the curly brackets).

Now if we look in our current directory we will see a binary MEX file called `myfunction_mex.mexmaci64`:

```
>> !ls -l
total 136
drwxr-xr-x  3 plg  staff    102 26 Aug 11:41 codegen
-rw-r--r--@ 1 plg  staff    126 26 Aug 11:36 myfunction.m
-rwxr-xr-x  1 plg  staff  62540 26 Aug 11:41 myfunction_mex.mexmaci64
```

We also see a directory called `codegen` that contains a subdirectory called `mex` and within that another directory called `myfunction`, that contains all of the various C files and other stuff that's required to build the binary MEX file:

```
>> !ls codegen/mex/myfunction
```

```
_coder_myfunction_api.o         myfunction_initialize.c
_coder_myfunction_info.o        myfunction_initialize.h
_coder_myfunction_mex.o         myfunction_initialize.o
buildInfo.mat                   myfunction_mex.mexmaci64
eml_error.c                     myfunction_mex.mk
eml_error.h                     myfunction_mex.mki
eml_error.o                     myfunction_mex.sh
html                            myfunction_mex_mex.map
interface                       myfunction_terminate.c
mean.c                          myfunction_terminate.h
mean.h                          myfunction_terminate.o
mean.o                          myfunction_types.h
myfunction.c                    randn.c
myfunction.h                    randn.h
myfunction.o                    randn.o
myfunction_data.c               rt_nonfinite.h
myfunction_data.h               rtwtypes.h
myfunction_data.o               setEnv.sh
myfunction_emxutil.c            std.c
myfunction_emxutil.h            std.h
myfunction_emxutil.o            std.o
```

So now to call our compiled version of the function we just call `myfunction_mex` instead of calling `myfunction`:

```
>> tic; out=myfunction_mex(1e5); toc
Elapsed time is 0.981005 seconds.
>> hist(out,50)
```

We can see we already achieved a significant speedup, almost 10x.

The new MEX function produces the figure shown in Figure 8.8, which looks the same as the one produced by the plain MATLAB code, so we have some notion that our compiled MEX file is doing the right thing. Of course we should perform more stringent tests than this just to verify we are getting the expected behaviour out of the binary MEX file.

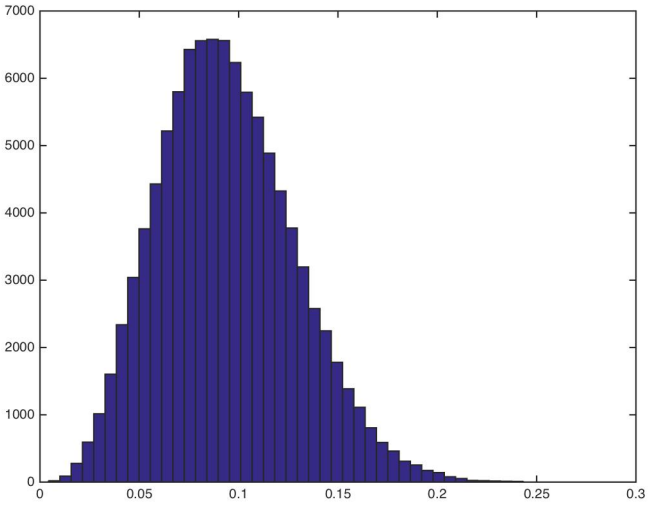


Figure 8.8: Output of `myfunction_mex`.

The MathWorks has a product page devoted to the Coder here:

MATLAB Coder product page[95]

The MathWorks also has a page on their online documentation devoted to the MATLAB Coder here:

MATLAB Coder online documentation[96]

Links

[93] http://www.mathworks.com/help/matlab/debugging-code.html

[94] http://www.mathworks.com/help/matlab/matlab_prog/profiling-for-improving-performance.html

[95] http://www.mathworks.com/products/matlab-coder

[96] http://www.mathworks.com/help/coder/index.html

9 Parallel programming

9.1 What is parallel computing?

Simply put, parallel computing refers to performing multiple computations in *parallel*, i.e. simultaneously. By default most operations that take place on your computer happen in *serial*, that is, one at a time. These days CPU chips (even those on laptops) have multiple cores, which allow for some degree of parallel operations.

In principle, every time you double the number of CPU cores (or CPUs themselves), you can achieve something close to a halving of time to complete the operations. In practice however, there is always some overhead cost in carry-out out the parallel computations. If the operations are at all lengthy however, the overhead cost is always worth it.

There are several types of parallel computing, which we'll talk briefly about (and which are listed below). What we'll get hands-on experience with is symmetric multiprocessing. This is the style of parallel computing where multiple CPUs, or multiple cores on a single CPU, share access to the same memory (RAM) store, and can carry out operations in parallel.

Today (Fall, 2015), it's still the case that not many programs take advantage of multiple cores. Operating systems, however, can take advantage of multiple cores through multithreading (see below), by assigning different threads to their own processing nodes.

Some programs like MATLAB (and some Apple applications) come with the abil-

ity to take advantage of multiple cores built-in. Due to the relative complexity of parallelizing serial code, however, most applications still operate in a serial fashion.

Parallel computing[97] (Wikipedia)

9.2 Multi-threading

Modern operating systems like Mac OSX, Linux, and other Unix variants, provide the ability for programs to spawn multiple threads that execute independently of each other. The advantage of multithreading is that one process can do its work and other processes don't have to wait until the working process is done. This is used extensively for graphical user interfaces.

When you copy a file, you can still move your mouse around, you can still start other programs, you can still browse the web, while other things are happening simultaneously. Multithreading can occur on a single CPU with a single core. This isn't parallel computing per se, as multiple threads still have to share a single CPU processing unit to do their work—but the operating system manages the multiple threads so that the user has the impression that multiple things are happening at once.

See the wikipedia article for more details:

Multithreading[98] (wikipedia)

9.3 Symmetric Multiprocessing (SMP)

These days modern computers ship with CPUs that have multiple cores, or even multiple CPUs each with multiple cores. At the time of writing these notes (Fall 2015) you can for example buy a Mac Pro desktop computer with two 6-core CPUs, for a total of 12 independent processing cores. With hyperthreading (see below) you get 24 processing cores, all for around $5,000—which seems like a lot, but just 10 years ago a computer cluster with 24 nodes would have cost

around $75,000-$100,000.

When multiple CPUs and/or multiple CPU cores live in a single machine, they typically all share access to the same physical RAM (memory). These days all Apple desktops and laptops have CPUs with multiple cores. Generic PCs also ship with multiple CPUs and cores. Even smartphones (e.g. the iPhone, and Google's Nexus phone) come with multiple CPUs and multiple cores.

The great advantage of having multiple computing nodes in a single machine, is that unlike multithreading on a single CPU, where the operating system has to switch back and forth between each thread, with multiple CPUs/cores, each core can execute a different task in parallel with the others (i.e. at the same time).

A good analogy is the following. Imagine someone gives me 10 decks of playing cards, and each deck has been shuffled, and my task is to re-order each deck of cards. A computer with a single CPU/core is like a single person who is tasked with sorting all 10 decks of cards. I would have to sort them all, one at a time, one after the other, i.e. in serial. I could implement "multithreading" by sorting one deck for a few seconds, setting it aside, sorting the next deck for a few seconds, setting it aside, and so on, sorting bits of each one, one by one. It's still happening in serial though.

If I had access to other processing nodes, I could parallelize the task. So imagine instead of me sorting all 10 decks, I found 9 other people to help me. I gave them one of the 10 decks of cards, and I took one. Now we can all sort them, at the same time, in parallel. In theory it should take $\frac{1}{10}^{\text{th}}$ the time compared to me sorting them all myself, in serial. In fact though, there would be some overhead cost, for example at the beginning, when I would have to hand out each deck and give everyone their instructions, and then at the end, when I would have to collect all the sorted decks from each person. If the actual computational task being parallelized is time intensive, however, then these overhead costs would be minimal compared to the gain in speed I would achieve by parallelizing the task.

Symmetric multiprocessing, i.e. having multiple independent processing units

share the same memory store, is advantageous compared to cluster or grid computing, where each processing node has its own memory. In the latter cases, there is a (sometimes relatively major) overhead cost involved in transferring data to the memory store for each processing unit, and back again to a head node. When this transfer happens over a network, as you can imagine, this would be way slower than if it happens on a common logic board on which all processing cores sit (as is with the case of symmetric multiprocessing).

Here is a wikipedia article on symmetric multiprocessing:

Symmetric multiprocessing[99] (wikipedia)

9.4 Hyperthreading

Hyperthreading is a proprietary implementation by Intel for allowing modern CPUs to behave as if they have twice as many logical cores as physical cores. That is, if your CPU has two cores, hyperthreading implements a series of tricks at the operating system level, that interface with a series of tricks at the hardware layer (i.e. in the CPU itself) that results in the ability to address four "logical" cores.

Unlike multithreading, which is simply a software implementation at the operating system level, hyperthreading involves special implementations both at the operating system level and at the hardware level. Current Apple laptops and desktops all implement hyperthreading. Several generic PCs also implement hyperthreading.

For large, time consuming computations, hyperthreading won't actually double the computation speed, since at the end of the day, there are still x physical cores, even though hyperthreading pretends there are $2x$ logical cores. If however each computations is small, and doesn't last a long time, hyperthreading can end up giving you performance gains above and beyond regular multithreading, since it implements a number of efficiencies and tricks at the software and hardware layers.

For our purposes, hyperthreading is either there, or it isn't, and it's not something we will be fiddling with. Here is a wikipedia article on hyperthreading:

Hyper-threading[100] (wikipedia)

9.5 Clusters

So far we have been talking about a single machine with multiple CPUs and/or multiple cores. Another way of implementing parallel computing is to connect together multiple machines, over a specialized local network. In principle one can connect as many machines as one likes, to achieve just about any level of parallelism one wants. Today's fastest supercomputers[101] are in fact clusters of machines hooked together. The world's fastest supercomputer, as of today, October 2015, is the Tianhe-2[102], located in Guangzhou, China. It has 16,000 computer nodes, each one comprising two Intel Ivy Bridge Xeon CPUs and three Xeon Phi chips for a total of 3,120,000 cores (3.12 million cores).

Sharcnet[103] is a Canadian cluster computing facility with several individual clusters, the largest of which has 8,320 cores. Western has access to the Sharcnet clusters, you just have to sign up for an account.

Many individual researchers also operate smaller clusters, for example with 8, or 12, or 24 machines hooked together.

A relatively recent development is the advent of gigantic server farms operated by private companies like Amazon and Google. Amazon's Elastic Compute Cloud[104] allows individuals to spawn multiple "virtual" machines, and hook them together in networks and clusters, and run jobs on them. Cost is per machine and per unit time, and so one can essentially (1) define your own cluster and (2) pay for only those minutes that you actually use. It's a very flexible system that many researchers are beginning to utilize. Rhodri Cusack's lab, for example, uses cloud-based machines for brain imaging data analysis.

The obvious advantage of a cluster over a single SMP machine, is that one can add as many nodes onto the cluster (growing it as you go) to whatever size you

want (provided you can pay for it). The disadvantage is that data transfer over a network can be slower than a SMP machine where CPU cores share the same RAM store. There is also added complexity in managing a cluster of machines, for example in configuring each one, and configuring a head node to manage all of the slave nodes. There is software out there that can organize this for you, for example Oracle Grid Engine[105], and others, but it's still not trivial and takes some investment of time to fully implement.

Computer cluster[106] (wikipedia)

9.6 Grids

A grid is like a cluster, but the individual machines are not on a local network, but they can be anywhere on the internet. Sometimes multiple clusters are hooked together over the internet to form a grid. Sometimes a grid is composed of multiple individual machines, spread out over multiple labs, multiple Departments, Univerisities, or even countries. Sometimes grids are set up so that individual machines can be "taken over" as dedicated computational nodes. In other configurations, individual machines only process grid jobs during their downtime, when for example the user is not using the machine for something else. One way of setting this up is via a specialized screensaver. Whenever the screensaver activates (which is an indication that the machine is not being used), the grid process starts up and processes grid jobs.

Two classic examples of grids are the SETI@home[107] grid (searching for extraterrestrial life in the universe) and the Folding@home[108] grid (simulations of protein folding for disease research). In each case, anyone around the world can sign up their machine to join the grid and donate computer time, install some local software, and then anytime their computer is not busy, it is recruited by the grid to process data. As of now (Oct 2015) the Folding@home website shows that there are 8,067,858 CPUs active right now on the Folding@home grid.

There are also nefarious uses for grids, which are sometimes called Botnet[109]s. In this case, a virus infects a user's machine, installs a nefarious program, which

lies dormant until a central machine somewhere on the internet activates it, for some nasty purpose (like a DDoS attack[110], or for sending spam). Your machine essentially becomes a sleeper cell.

Grid computing[111] (wikipedia)

9.7 GPU Computing

In recent years computer engineers and software developers have teamed up, and have delivered software libraries that allow developers to utilize graphics cards for more general purpose computing (GPGPU Computing).

Graphics cards, unlike CPUs, have hundreds if not thousands of cores, each of which are typically used to process graphics for things like 3D games, video animation and scientific visualization. Each processing unit on a graphics card is a much simpler beast than the cores on CPU chips—but for some computational tasks, one doesn't need much complexity, and massive parallelism can be achieved by farming out general purpose computational tasks to the thousands of cores on a graphics card.

For example, today (Oct 2015) for around $5,000 one can purchase an NVidia Tesla GPU[112], which is a single graphics card, that has 12GB of GPU memory, 2880 cores, and has a processing power of 1.43 Tflops. As you can imagine, if your computational task is well suited to GPU processing, running it on 2880 cores will be quite a bit faster than running on 4, 8 or 12 cores (e.g. that you get with a modern dual 6-core CPU Mac Pro).

There are two major C/C++ software libraries that provide relatively high-level interfaces to performing general purpose computation on graphics cards

- CUDA[113] (Nvidia proprietary)
- OpenCL[114] (open)

MATLAB's Parallel Computing Toolbox has the ability to farm out some computations to NVidia CUDA-enabled GPUs, see this page for more info:

MATLAB GPU Computing Support for NVIDIA CUDA-Enabled GPUs[115]

See this wikipedia page for more general information on GPGPU Computing:

GPGPU Computing[116]

9.8 Types of Parallel problems

Multithreading is an example of *fine-grained parallelism* (many shared operations per second), in which the operating system manages (e.g. switches between) threads at a very fast rate, e.g. with each CPU clock cycle. This can thus happen many times per second. This is what your operating system does in the background, as you are interacting with your graphical user interface, surfing the web, playing music, processing video in the background, all the while copying files from one disk to another.

In another kind of fine-grained parallelism, multiple processes communicate with each other many, many times per second.

In *coarse-grained parallelism*, there are many, many independent threads/tasks, that rarely or never communicate with each other.

Finally, so-called *embarassingly parallel* problems are 100% independent operations, and never communicate with each other. Each process doesn't depend in any way on the result of another operation. This is the kind of parallelism that we will be talking about in this class.

9.9 MATLAB

MATLAB provides parallel computing via its Parallel Computing Toolbox (see below).

- MATLAB Parallel Computing Toolbox[117]
- MATLAB Execute loop iterations in parallel using parfor[118]
- MATLAB Getting Started with parfor[119]
- MATLAB Parallel Computing Toolbox Examples[120]

9.10 Shell scripts

Finally, one can parallelize tasks at the level of the shell, even if the programs you write/run aren't parallelized, using a tool like GNU Parallel (see below). Briefly, with GNU Parallel you can split a list of (ambarassingly parallel) tasks across multiple cores even if the program itself is serial in nature. See the GNU Parallel page below and the tutorial page for some examples. In our lab we use GNU Parallel to distribute subject-level brain imaging processing across multiple cores.

- GNU Parallel[121]
- GNU Parallel tutorial[122]

Exercises

E 9.1 Here is a serial version of a simple MATLAB program that iterates through a for loop, printing to the screen each time. Your task is to parallelize that for loop so that iterations are distributed among available compute cores.

Note that this is an "embarrasingly parallell" problem, i.e. each iteration of the for loop is completely independent of the others.

Also note that you will likely not see the loop iterations appear in sequential order, once the loop is parallelized. When operations are parallelized the order is essentially arbitrary from one run to another. This is why this method of parallelization is only appropriate for computations where each loop iteration is truly independent of the others.

```
for i=1:10
  disp(sprintf('hello from iteration # %d', i))
end
```

E 9.2 **Parallel bootstrap**

As we will find out in my statistics course next semester, we can use *random resampling with replacement* to simulate drawing samples from a population, and we can use this method to quantitatively assess the probability of the null hypothesis in the context of an experiment, and/or some data.

Assume we have the following sample of data x:

```
x = [3 5 4 3 6 7 -1 2 -3 -4 2 -5 3 2 -1]
```

and a second sample, y:

```
y = [2 7 4 7 6 9 -1 3 -2 -1 3 -1 2 4 2]
```

The mean of the sample x is 1.533 and the mean of sample y is 2.933. Let's compute a statistic we'll call d_{samp} which is the difference between means, $\bar{y} - \bar{x}$ which in this case is equal to $d_{samp} = 1.400$.

The null hypothesis is that the samples were taken from a single population with the same mean, and so $d_{pop} = 0.00$, and any departure from this in our sample statistic dsamp is due to random sampling error.

Question 1

Use bootstrapping to compute the probability of the null hypothesis, with one million bootstrap (re)samples. Write your code in the usual serial fashion, using for-loop(s).

Question 2

Rewrite your solution to question 1, and parallelize the bootstrap. In other words execute the one million bootstrap iterations in parallel, with the work spread over your available compute cores.

Links

[97] http://en.wikipedia.org/wiki/Parallel_computing

[98] http://en.wikipedia.org/wiki/Multithreading_(computer_architecture)

[99] http://en.wikipedia.org/wiki/Symmetric_multiprocessing

[100] http://en.wikipedia.org/wiki/Hyper-threading

[101] http://en.wikipedia.org/wiki/Supercomputer

[102] http://en.wikipedia.org/wiki/Tianhe-2

[103] https://www.sharcnet.ca/my/front/

[104] http://aws.amazon.com/ec2/

[105] http://en.wikipedia.org/wiki/Oracle_Grid_Engine

[106] http://en.wikipedia.org/wiki/Cluster_(computing)

[107] http://en.wikipedia.org/wiki/SETI@Home

[108] http://en.wikipedia.org/wiki/Folding@home

[109] http://en.wikipedia.org/wiki/Botnet

[110] http://en.wikipedia.org/wiki/Distributed_denial-of-service_attack#Distributed_attack

[111] http://en.wikipedia.org/wiki/Grid_computing

[112] http://www.nvidia.com/object/tesla-workstations.html

[113] http://www.nvidia.com/object/cuda_home_new.html

[114] http://www.khronos.org/opencl/

[115] http://www.mathworks.com/discovery/matlab-gpu.html

[116] http://en.wikipedia.org/wiki/General-purpose_computing_on_graphics_processing_units

[117] http://www.mathworks.com/products/parallel-computing/

[118] http://www.mathworks.com/help/distcomp/parfor.html

[119] http://www.mathworks.com/help/distcomp/getting-started-with-parfor.html

[120] http://www.mathworks.com/help/distcomp/examples/

[121] http://www.gnu.org/software/parallel/

[122] http://www.gnu.org/software/parallel/parallel_tutorial.html

10 Graphical displays of data

MATLAB comes with lots of built-in functionality for generating both 2-D and 3-D graphics. You will learn a collection of commands (mainly `plot()`) that will enable you do generate plots and configure their appearance with just about any degree of precision you want. The great advantage of generating graphics purely based on scripted commands (as opposed for example to graphical, pointy-clicky approaches based on graphical user interfaces (GUIs)) is that you can easily and instantly re-generate graphics simply by re-running the script(s). In addition making changes to your graphics becomes a simple matter of tweaking commands and scripts.

Rather than writing notes that essentially duplicate the extensive online documentation included with MATLAB, I will instead point you to some intial starting locations where you can learn about generating graphics in MATLAB.

Graphics in MATLAB[123]

Common Graphics Functions in MATLAB[124] (a graphical menu showing different kinds of plots and how to generate them)

2-D and 3-D Plots[125]

The `plot()` command[126]

Creating 2-D Graphs and Customizing Lines[127]

Add Titles, Axis Labels and Legends to Graphs[128]

Figures with multiple axes using subplots[129]

Exercises

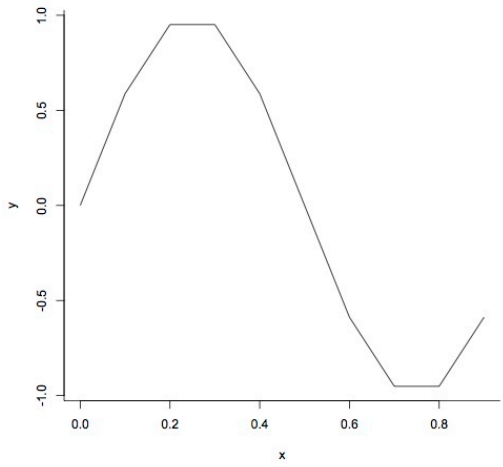
E 10.1 Line Plot

Let x be a vector:

```
[0,0.1,0.2,0.3,0.4,0.5,0.6,0.7,0.8,0.9]
```

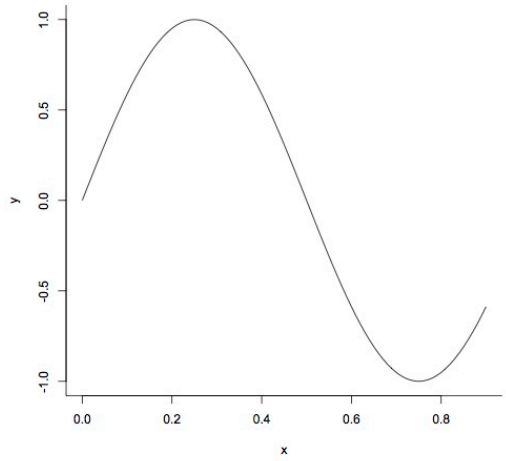
and set y to be equal to sin(2*pi*x).

Generate a line plot that looks like this:



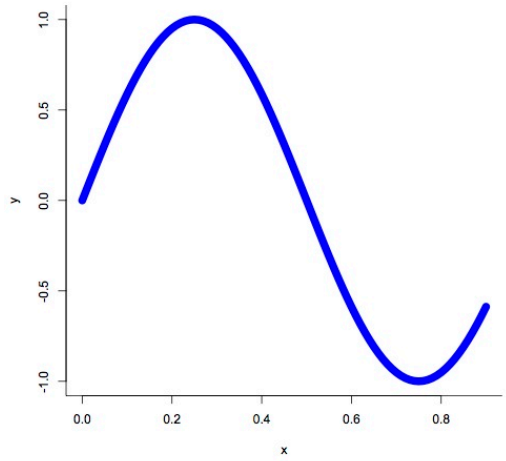
Smoother Line

Redefine x and y to make the curve smoother:



Change Line Colour

Plot it again but make the line blue, and thick:

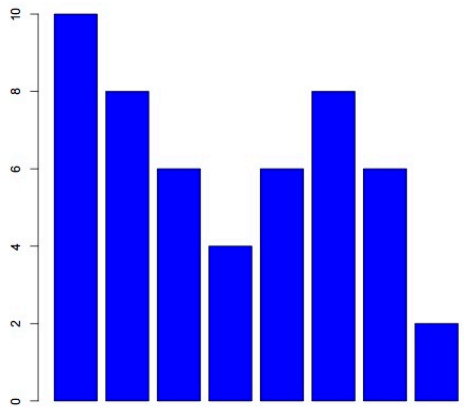


E 10.2 **Bar Plot**

Let y be a vector with the following values:

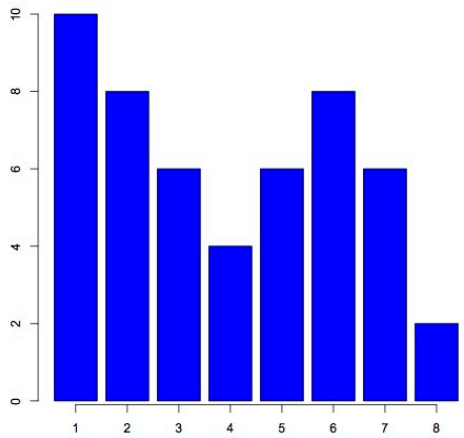
```
[10, 8, 6, 4, 6, 8, 6, 2]
```

Generate the following bar plot:



Again with x labels

Plot it again but this time include labels on the x axis:

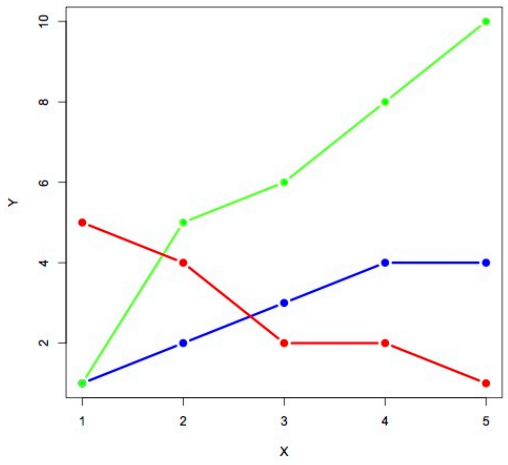


E 10.3 **Multiline plot**

Let x, y1, y2, and y3 be vectors:

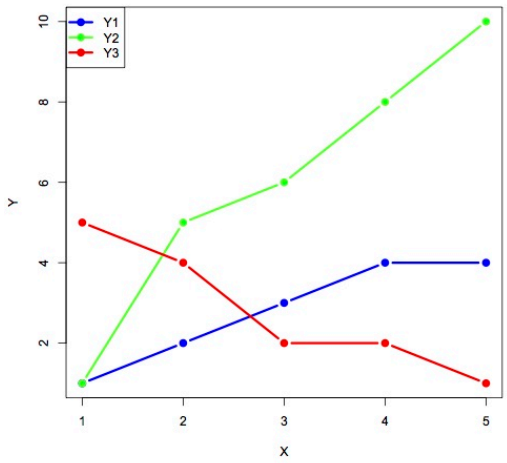
```
x = [1,2,3,4,5]
y1 = [1,2,3,4,4]
y2 = [1,5,6,8,10]
y3 = [5,4,2,2,1]
```

Generate a multi-line plot like this:



Add a Legend

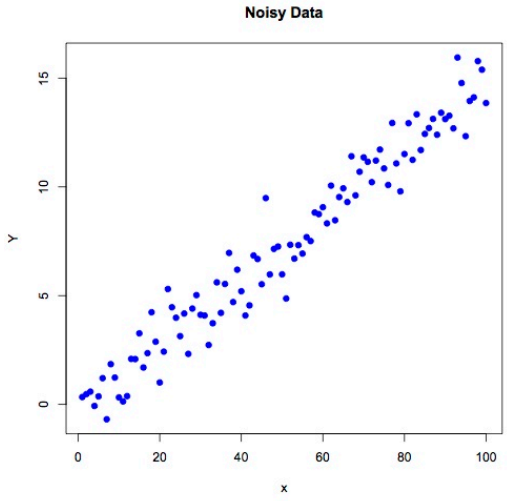
Add a legend to your plot that looks like this:



E 10.4 **Scatterplot**

Let x be a vector starting at 1 and ending at 100. Let y be a vector equal to (x * 0.15) + N where N is a vector of random values chosen from a gaussian distribution with mean 0.0 and standard deviation 1.0.

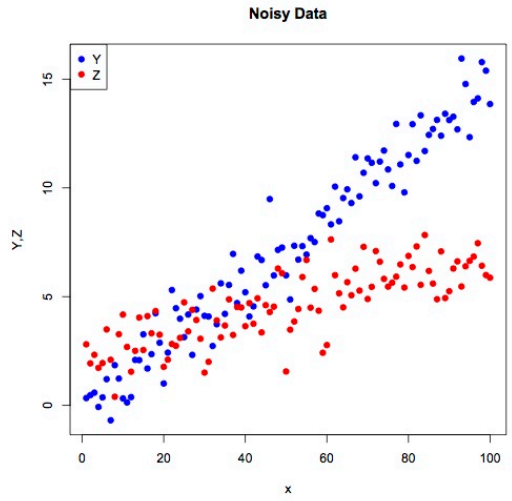
Generate a scatterplot of x vs y:



A second variable

Let z be equal to ((x * 0.05) + 2) + N where N is a vector of random values chosen from a gaussian distribution with mean 0.0 and standard deviation 1.5.

Generate a scatterplot of y and z vs x, including a legend:

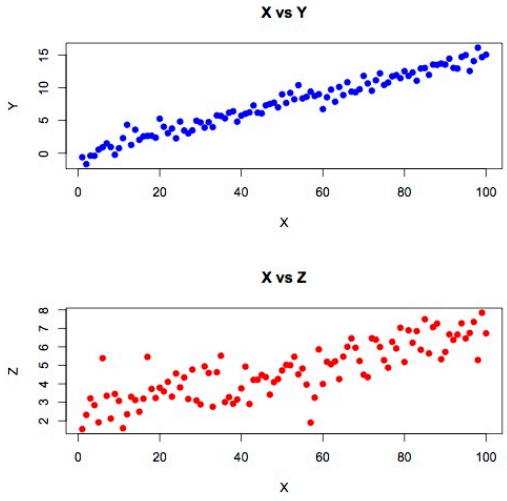


E 10.5 Subplots

Let x be a vector starting at 1 and ending at 100. Let y be a vector equal to (x * 0.15) + N where N is a vector of random values chosen from a gaussian distribution with mean 0.0 and standard deviation 1.0.

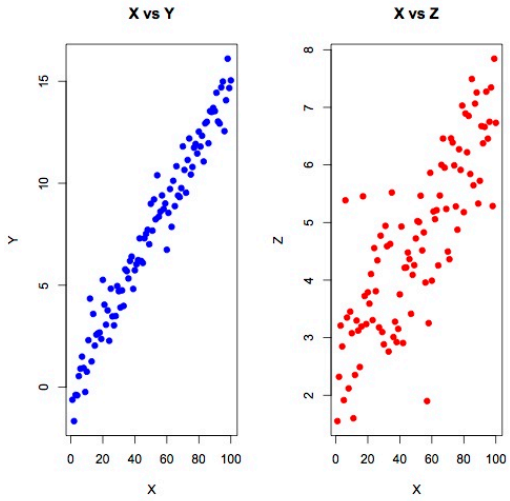
Let z be equal to ((x * 0.05) + 2) + N where N is a vector of random values chosen from a gaussian distribution with mean 0.0 and standard deviation 1.5.

Generate a figure with scatterplots of (x vs y) and (x vs z) in separate subplots, stacked vertically:



horizontally

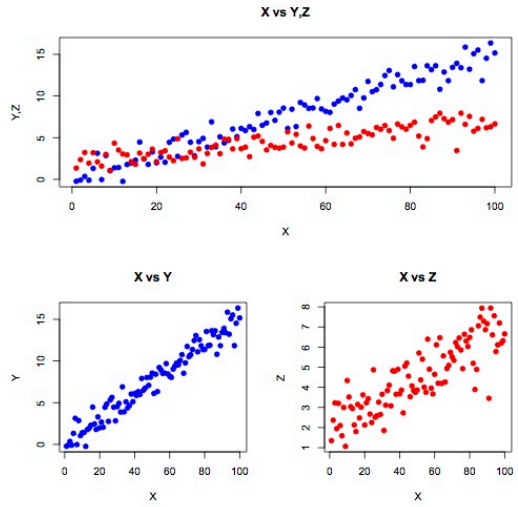
Generate the plot again but stack the subplots horizontally:



more complex arrangements

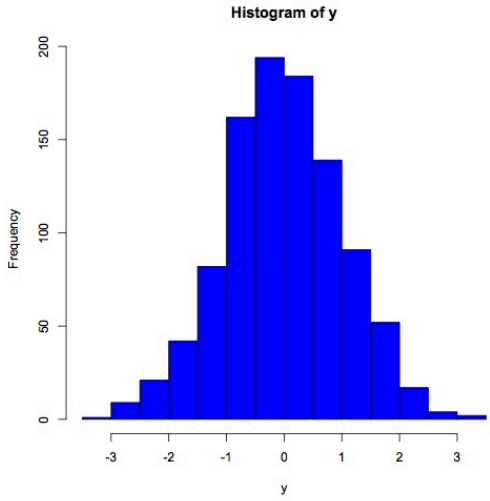
Generate the plot again with 3 subplots: one on the top, occupying the full width of the figure, in which you plot (x vs y) and (x vs z) overlayed, and

two on the bottom, in which you plot (x vs y) in one and (x vs z) in the other:



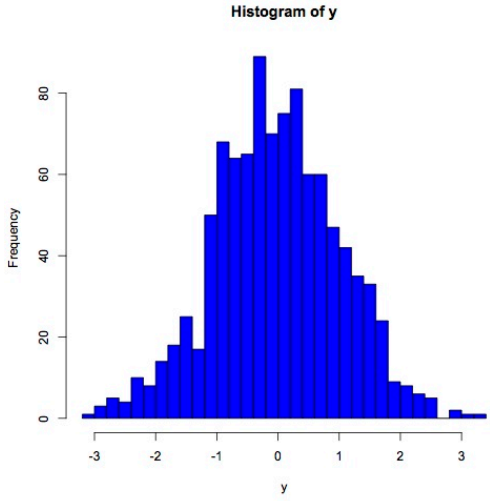
E 10.6 **Histograms**

Define a variable y that contains 1000 values drawn from a gaussian distribution with mean 0.0 and standard deviation 1.0. Plot a histogram of y. For now just use the default settings for whatever function you find that produces a histogram.



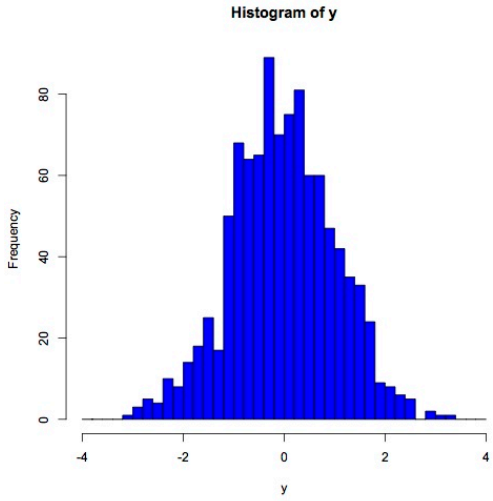
Number of bins

Replot the histogram using 25 bins:



Bin width

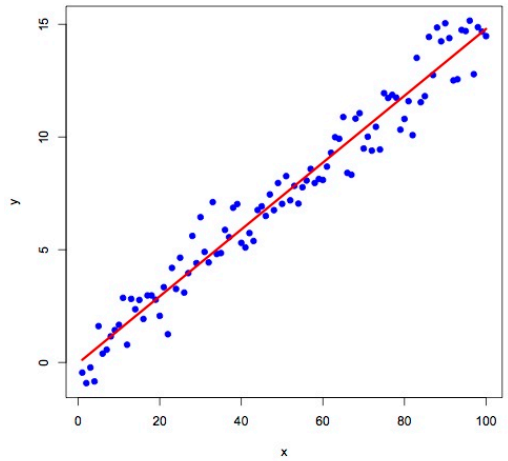
Replot the histogram using a bin width of 0.20:



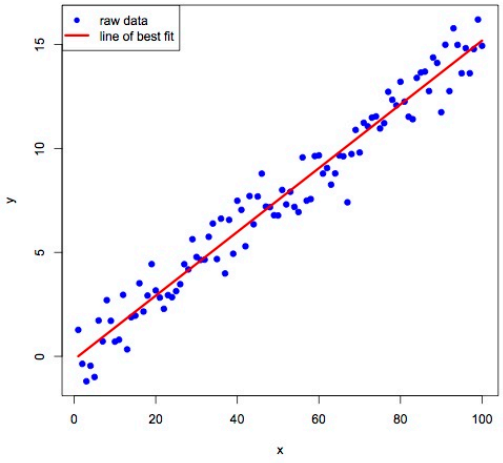
E 10.7 **Line of best fit**

Let x be a vector starting at 1 and ending at 100. Let y be a vector equal to (x * 0.15) + N where N is a vector of random values chosen from a gaussian distribution with mean 0.0 and standard deviation 1.0.

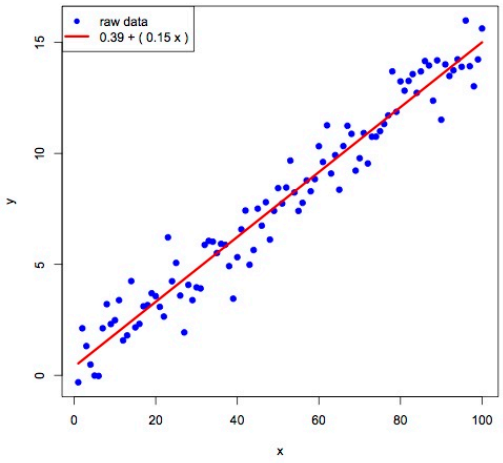
Generate a scatterplot of (x vs y) and overlay on the plot, the line of best fit after fitting a linear model to the data: $\hat{y} = \beta_0 + \beta_1 x$.



Add a legend



Add the equation of the line



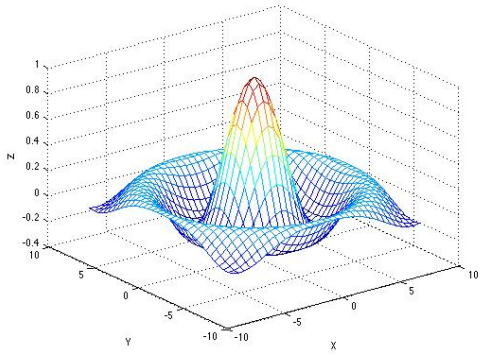
E 10.8 **Surface plot**

Define x and y each over a grid [-8,8] in steps of 0.5.

Define $r = \sqrt{x^2 + y^2 + 0.00001}$.

Define $x = \sin(r)/r$

Generate the following surface plot:



Links

[123] http://www.mathworks.com/help/matlab/graphics.html

[124] http://www.mathworks.com/help/matlab/creating_plots/types-of-matlab-plots.html#btjs9s4-1

[125] http://www.mathworks.com/help/matlab/2-and-3d-plots.html

[126] http://www.mathworks.com/help/matlab/ref/plot.html

[127] http://www.mathworks.com/help/matlab/creating_plots/using-high-level-plotting-functions.html

[128] http://www.mathworks.com/help/matlab/creating_plots/add-title-axis-labels-and-legend-to-graph.html

[129] http://www.mathworks.com/help/matlab/creating_plots/create-graph-with-subplots.html

[130] http://www.mathworks.com/help/matlab/surface-and-mesh-plots-1.html

[131] http://www.mathworks.com/help/matlab/geometry.html

[132] http://www.mathworks.com/help/matlab/graphics-objects.html

11 Signals, sampling & filtering

Whereas signals in nature (such as sound waves, magnetic fields, hand position, electromyograms (EMG), electroencephalograms (EEG), extra-cellular potentials, etc) vary continuously, often in science we measure these signals by *sampling* them repeatedly over time, at some *sampling frequency*. The resulting collection of measurements is a *discretized* representation of the original continuous signal.

Before we get into *sampling theory* however we should first talk about how signals can be represented both in the *time domain* and in the *frequency domain*.

Jack Schaedler has a nice page explaining and visualizing many concepts discussed in this chapter:

Seeing circles, sines and signals[133]

11.1 Time domain representation of signals

This is how you are probably used to thinking about signals, namely how the magnitude of a signal varies over time. So for example a signal s containing a sinusoid with a period T of 0.5 seconds (a frequency of 2 Hz) and a peak-to-peak magnitude b of 2 volts is represented in the time domain t as:

$$s(t) = \left(\frac{b}{2}\right) \sin(wt) \tag{11.1}$$

where

$$w = \frac{2\pi}{T} \tag{11.2}$$

We can visualize the signal by plotting its magnitude as a function of time, as shown in Figure 11.1.

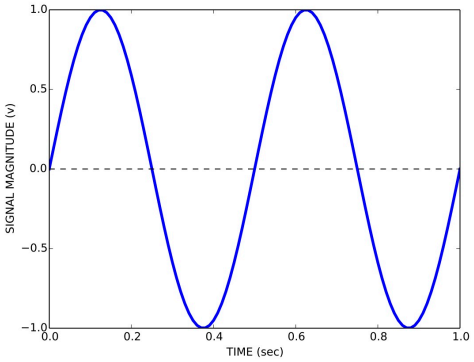


Figure 11.1: Time domain representation of a signal.

11.2 Frequency domain representation of signals

We can also represent signals in the frequency domain. This requires some understanding of the Fourier series[134]. The idea of the Fourier series is that all periodic signals can be represented by (decomposed into) the sum of a set of pure sines and cosines that differ in frequency and period. See the wikipedia link for lots of details and a helpful animation.

$$s(t) = \frac{a_0}{2} + \sum_{n=1}^{\infty} [a_n \cos(nwt) + b_n \sin(nwt)] \tag{11.3}$$

The coefficients a_n and b_n define the weighting of the different sines and cosines at different frequencies. In other words these coefficients represent the strength of the different frequency components in the signal.

We can also represent the Fourier series using only sines:

$$s(t) = \frac{a_0}{2} \sum_{n=1}^{\infty} \left[r_n \cos(nwt - \phi_n) \right] \tag{11.4}$$

Using this formulation we now have *magnitude* coefficients r_n and *phase* coefficients ϕ_n. That is, we are representing the original signal $s(t)$ using a sum of sinusoids of different frequencies and phases.

Here is a web page that lets you play with how sines and cosines can be used to represent different signals: Fourier series visualization[135].

11.3 Fast Fourier transform (FFT)

Given a signal there is a very efficient computational algorithm called the Fast Fourier transform[136] (FFT) for computing the magnitude and phase coefficients. We will not go into the details of this algorithm here, most high level programming languages have a library that includes the FFT algorithm.

Here is a video showing a 100-year-old mechanical computer that does both forward and inverse Fourier transforms:

- Harmonic Analyzer (1/4)[137]
- Harmonic Analyzer (2/4)[138]
- Harmonic Analyzer (3/4)[139]
- Harmonic Analyzer (4/4)[140]

11.4 Sampling

Before we talk about the FFT and magnitude and phase coefficients, we need to talk about discrete versus continuous signals, and sampling. In theory we can derive a mathematical description of the Fourier decomposition of a continuous signal, as we have done above, in terms of an infinite number of sinusoids. In practice however, signals are not continuous, but are *sampled* at some discrete *sampling rate*.

For example, when we use Optotrak to record the position of the fingertip dur-

ing pointing experiments, we choose a sampling rate of 200 Hz. This means 200 times per second the measurement instrument samples and records the position of the fingertip. The interval between any two samples is 5 ms. It turns out that the sampling rate used has a specific effect on the number of frequencies used in a discrete Fourier representation of the recorded signals.

The Shannon-Nyquist sampling theorem[141] states that a signal must be sampled at a rate which is at least twice that of its highest frequency component. If a signal contains power at frequencies higher than half the sampling rate, these high frequency components will appear in the sampled data at lower frequencies and will distort the recording. This is known as the problem of aliasing[142].

Let's look at a concrete example that will illustrate this concept. Let's assume we have a signal that we want to sample, and we choose a sampling rate of 4 Hz. This means every 250 ms we sample the signal. According to the Shannon-Nyquist theorem, the maximum frequency we can uniquely identify is half that, which is 2 Hz. This is called the nyquist frequency[143]. Let's look at a plot and see why this is so.

In Figure 11.2 we see a solid blue line showing a 2 Hz signal, a magenta dashed line showing a 4 Hz signal, and a green dashed line showing a 8 Hz signal. Now imagine we sample these signals at 2 Hz, indicated by the vertical red lines. Notice that at the sample points (vertical red lines), the 2 Hz, 4 Hz and 8 Hz signals overlap with identical values. This means that on the basis of our 2 Hz samples, we cannot distinguish between frequencies of 2, 4 and 8 Hz. What's more, what this means is that if the signal we are actually sampling at 2 Hz has significant signal power at frequencies above the Nyquist (1 Hz) then the power at these higher frequencies will influence our estimates of the magnitude coefficients corresponding to frequencies below the Nyquist... in other words the high-frequency power will be aliased into the lower frequency estimates.

Figure 11.3 shows another example taken from the wikipedia article on aliasing[144]. Here we have two sinusoids—one at 0.1 Hz (blue) and another at 0.9 Hz (red). We sample both at a sampling rate of 1 Hz (vertical green lines). You can

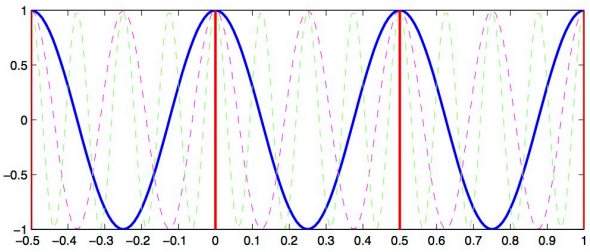


Figure 11.2: Signal aliasing.

see that at the sample points, both the 0.1 Hz and 0.9 Hz sinusoids pass through the sample points and thus both would influence our estimates of the power at the 0.1 Hz frequency. Since the sampling rate is 1 Hz, the Nyquist frequency (the maximum frequency we can distinguish) is 0.5 Hz—and so any power in the signal above 0.5 Hz (such as 0.9 Hz) will be aliased down into the lower frequencies (in this case into the 0.1 Hz band).

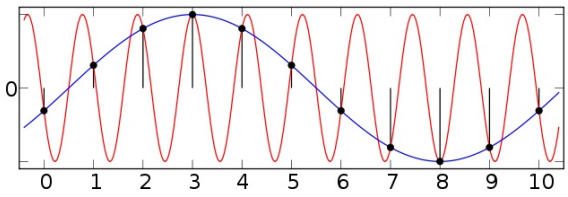


Figure 11.3: Signal aliasing sinusoids.

So the message here is that in advance, before choosing your sampling rate, you should have some knowledge about the highest frequency that you (a) are interested in identifying; and (b) you think is a real component in the signal (as opposed to random noise). In cases where you have no a priori knowledge about the expected frequency content, one strategy is to remove high frequency components *before sampling*. This can be accomplished using low-pass filtering—sometimes called anti-aliasing filters. Once the signal has been sampled, it's too late to perform anti-aliasing.

11.5 Power spectra

Having bypassed completely the computational details of how magnitude and phase coefficients are estimated, we will now talk about how to interpret them.

For a given signal, the collection of magnitude coefficients gives a description of the signal in terms of the strength of the various underlying frequency components. For our immediate purposes these magnitude coefficients will be most important to us and we can for the moment set aside the phase coefficients.

Here is an example of a power spectrum for a pure 10 Hz signal, sampled at 100 Hz.

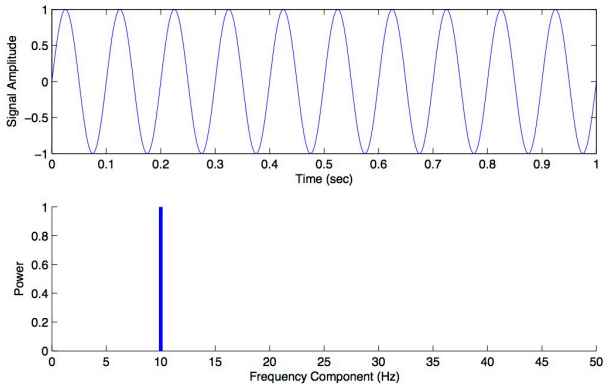


Figure 11.4: Power spectrum for a pure 10 Hz signal.

The magnitude values are zero for every frequency except 10 Hz. We haven't plotted the phase coefficients. The set of magnitude and phase coefficients derived from a Fourier analysis is a complete description of the underlying signal, with one caveat—only frequencies up to the Nyquist are represented. So the idea here is that one can go between the original time-domain representation of the signal and this frequency domain representation of the signal without losing information. As we shall see below in the section on filtering, we can perform operations in the frequency domain and then transform back into the time domain.

Here is some MATLAB code to illustrate these concepts. We construct a one

second signal sampled at 100 Hz that is composed of a 6 Hz, 10 Hz and 13 Hz component. We then use the `fft()` function to compute the Fast Fourier transform, we extract the magnitude information, we set our frequency range (up to the Nyquist) and we plot the spectrum, which is shown in Figure 11.5.

```
t = linspace(0,1,100);
y = sin(2*pi*t*6) + sin(2*pi*t*10) + sin(2*pi*t*13);
figure;
subplot(2,1,1)
plot(t,y)
xlabel('Time (sec)')
ylabel('Signal Amplitude')
subplot(2,1,2)
out = fft(y);
mag = abs(real(out));
plot(0:49, mag(1:50));
set(gca,'xlim',[0 50]);
xlabel('Frequency Component (Hz)')
ylabel('Amplitude')
```

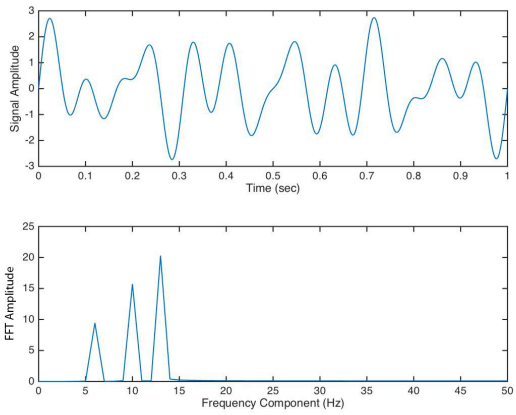


Figure 11.5: A signal with 6, 10 and 13 Hz pure sinusoids, and its spectrum.

We can see that the power spectrum has revealed peaks at 6, 10 and 13 Hz—which we know is correct, since we designed our signal from scratch.

Typically however signals in the real world that we record are not pure sinusoids, but contain random noise. Noise can originate from the actual underlying process that we are interested in measuring, and it can also originate from the instruments we use to measure the signal. For noisy signals, the FFT taken across the whole signal can be noisy as well, and can make it difficult to see peaks.

11.6 Power Spectral Density

One solution is instead of performing the FFT on the entire signal all at once, to instead, split the signal into chunks, take the FFT of each chunk, and then average these spectra to come up with a smoother spectrum. This can be accomplished using a power spectral density[145] function. In MATLAB there is a function `pwelch()` to accomplish this. We won't go into the mathematical details or the theoretical considerations (relating to stochastic processes) but for now suffice it to say that the psd can often give you a better estimate of the power at different frequencies compared to a "plain" FFT.

Here is an example of plotting the power spectral density of a signal in MATLAB. We construct a 50 Hz signal at 1000 Hz sampling rate, and we add some random noise on top:

```
t = linspace(0,1,1000);
y = sin(2*pi*t*50);
yn = y + randn(size(y))*1;
figure
subplot(3,1,1)
plot(t,yn)
xlabel('Time (sec)')
ylabel('Signal Amplitude')
title('TIME SERIES SIGNAL')
subplot(3,1,2)
out = fft(yn);
mag = abs(real(out));
plot(0:499,mag(1:500));
xlabel('Frequency (Hz)')
set(gca,'xlim',[0 100])
```

```
ylabel('Power')
title('RAW FFT')
subplot(3,1,3)
pwelch(yn,[],[],[],1000);
set(gca,'xlim',[0 100])
xlabel('Frequency (Hz)')
ylabel('PSD')
title('PSD')
```

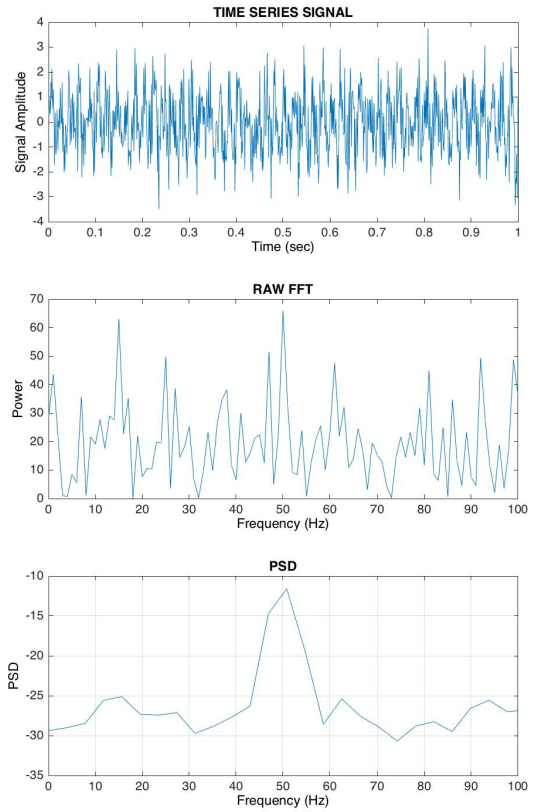


Figure 11.6: Power spectral density of a 50 Hz signal.

In Figure 11.6 you can see that the peak at 50 Hz stands nicely above all the

noise in the power spectral density estimate (bottom panel), while int the raw FFT it's difficult to see the 50 Hz peak against the noise (middle panel).

We have been ignoring the *phase* of the signal here, but just like the magnitude coefficients over frequencies, we can recover the phase coefficients of the signal as well.

11.7 Decibel scale

The decibel (dB) scale is a ratio scale. It is commonly used to measure sound level but is also widely used in electronics and signal processing. The dB is a logarithmic unit used to describe a ratio. You will often see power spectra displayed in units of decibels.

The difference between two sound levels (or two power levels, as in the case of the power spectra above), is defined to be:

$$20(log_{10})\frac{P_2}{P_1}dB \tag{11.5}$$

Thus when P_2 is twice as large as P_1, then the difference is about 6 dB. When P_2 is 10 times as large as P_1, the difference is 20 dB. A 100 times difference is 40 dB.

An advantage of using the dB scale is that it is easier to see small signal components in the presence of large ones. In other words large components don't visually swamp small ones.

Since the dB scale is a ratio scale, to compute absolute levels one needs a reference—a zero point. In acoustics this reference is usually 20 micropascals—about the limit of sensitivity of the human ear.

For our purposes in the absence of a meaningful reference we can use 1.0 as the reference (i.e. as P_1 in the above equation).

11.8 Spectrogram

Often there are times when you may want to examine how the power spectrum of a signal (in other words its frequency content) changes over time. In speech acoustics for example, at certain frequencies, bands of energy called formants[146] may be identified, and are associated with certain speech sounds like vowels and vowel transitions. It is thought that the neural systems for human speech recognition are tuned for identification of these formants.

Essentially a spectrogram is a way to visualize a series of power spectra computed from slices of a signal over time. Imagine a series of single power spectra (frequency versus power) repeated over time and stacked next to each other over a time axis.

MATLAB has a built-in function called `spectrogram()` that will generate a spectrogram. MATLAB has a sample audio file called `mtlb.mat` which can be loaded from the command line:

```
load mtlb
spectrogram(mtlb,256,230,256,Fs,'yaxis')
sound(mtlb)
```

Figure 11.7 shows the resulting spectrogram. Time is on the horizontal axis and frequency is on the vertical axis. The colours indicate the power of the different frequencies at the given time points.

11.9 Filtering

The Fourier series representation and its computational implementation, the FFT and the PSD, are useful not only for determining what frequency com- ponents are present in a signal, but we can also perform operations within frequency space in order to manipulate the strength of different frequency components in the signal. This can be especially effective for eliminating noise sources with known frequency content.

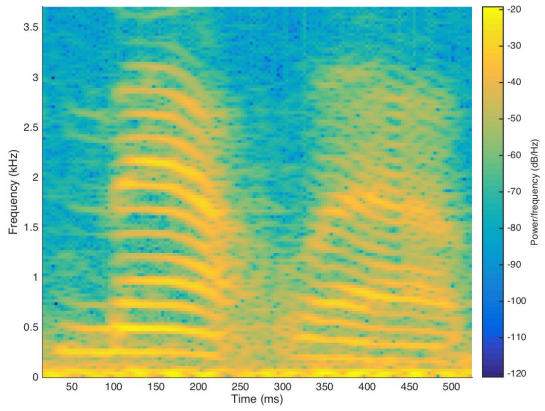


Figure 11.7: Spectrogram of the sound "MATLAB".

Let's look at a concrete example:

```
t = linspace(0,1,1000);
y = sin(2*pi*t*6) + sin(2*pi*t*10) + sin(2*pi*t*13);
yn = y + randn(size(y))*0.5;
[x,y,f] = fft_plus(yn,1000);
semilogx(f,20*log10(x));
xlabel('Frequency (Hz)')
ylabel('Power (dB)')
```

In Figure 11.8 we can see the signal has three signal components: 6, 10 and 13 Hz. Let's say we believe that the frequencies we are interested in are all below 20 Hz. In other words, frequencies above that are assumed to be noise of one sort or another. We can filter the signal so that all frequencies above 20 Hz are essentially zeroed out (or at least reduced in magnitude). One way to do this is simply to take the vector of power coefficients, change all values for frequencies above 20 Hz to zero, and perform an inverse Fourier transform (the inverse of the FFT) to go back to the time domain. We won't go into the mathematical details, but there are also other ways to filter a signal as well.

Here is a short summary of different kinds of filters, and some terminology.

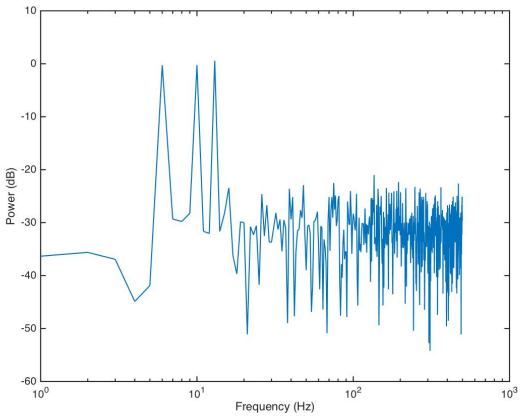


Figure 11.8: A spectrum of a noisy signal with peaks at 6, 10 and 13 Hz.

- *low-pass filters* pass low frequencies without change, but attenuate (i.e. reduce) frequencies above the *cutoff frequency*
- *high-pass filters* pass high frequencies and attenuate low frequencies, below the cutoff frequency
-
- band-pass filters pass frequencies within a *pass band* frequency range and attenuate all others
- *band-stop filters* (sometimes called *band-reject filters* or *notch filters*) attenuate frequencies within the *stop band* and pass all others

In the code example above we use a function called `fft_plus`, which conveniently performs the FFT and converts the results into a format that is useful. Here is the function:

```
function [x, y, f] = fft_plus (xin, rate, winsize)


%
% function [x, y, f] = fft_plus (xin, rate, winsize)
% fft computations - normalized to give 'single-sided' results
%
% inputs:  xin = signal, rate = sampling rate (Hz)
%          winsize (optional) window size for computing FFT
```

```
% outputs: x = magnitude, y = phase, f = frequency
%

if nargin==2
        winsize = length(xin);
end;

fx = fft(xin,winsize);
N=length(fx);
fx(2:N) = fx(2:N)*(2/N);
fx(1)=fx(1)/N;

x=abs(fx);
y=angle(fx); % radians

f=(0:N-1)/N;
f=f*rate;

nq = floor(N/2);
x=x(1:nq);
y=y(1:nq);
f=f(1:nq);

end
```

You might also be interested in a function called `fft_plot`, which generates a nice looking plot of magnitude and phase againt frequency (it calls `fft_plus` to do its work). Here is the code:

```
function fft_plot(xin, rate, logaxis, winsize)

%
% function dum = fft_plot(xin, rate, winsize)
% generates a plot of magnitude and phase against frequency
%
% inputs:  xin = signal, rate = sampling rate (Hz)
%          winsize (optional) window size for computing FFT
% outputs: none
```

```
%

if nargin==2
    logaxis = 1;
end

[X,Y,F] = fft_plus(xin,rate);
subplot(2,1,1)
if logaxis==1
    semilogx(F, 20.*log10(X))
else
    plot(F, 20.*log10(X))
end
grid on
xlabel('Frequency (Hz)')
ylabel('Magnitude (dB)')
drawnow
subplot(2,1,2)
if logaxis==1
    semilogx(F, unwrap(Y))
else
    plot(F, unwrap(Y))
end
grid on
xlabel('Frequency (Hz)')
ylabel('Phase (deg)')
drawnow

end
```

11.9.1 Characterizing filter performance

A useful way of characterizing a filter's performance is in terms of the ratio of the amplitude of the output to the input (the amplitude ratio AR or gain), and the phase shift (ϕ) between the input and output, as functions of frequency. A plot of the amplitude ratio and phase shift against frequency is called a Bode plot[147].

The *pass band* of a filter is the range of frequencies over which signals pass with no change. The *stop band* refers to the range of frequencies over which a filter attenuates signals. The *cutoff frequency* or *corner frequency* of a filter is used to describe the transition point from the pass band to the reject band. This this transition cannot occur instantaneously it is usually defined to be the point at which the filter output is equal to -6 dB of the input in the pass band. The cutoff frequency is sometimes called the -6 dB point or the half-power point since -6 dB corresponds to half the signal power. The *roll-off* refers to the rate at which the filter attenuates the input after the cutoff point. When the roll-off is linear it can be specified as a specific slope, e.g. in terms of dB/decade or dB/octave (an octave is a doubling in frequency).

Let's look at some examples of filter characteristics.

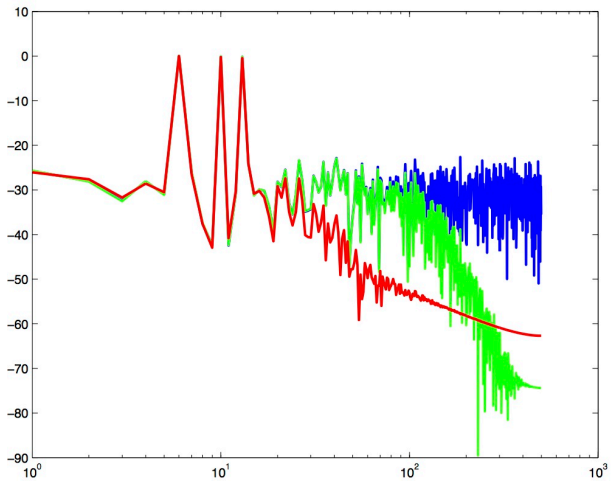


Figure 11.9: Spectrum of three filtered versions of a noisy signal with peaks at 6, 10 and 13 Hz.

In Figure 11.9 the blue trace shows the power spectrum for the unfiltered signal. The red trace shows a lowpass-filtered version of the signal with a cutoff frequency of 30 Hz. The green trace shows a low-pass with a cutoff frequency of 130 Hz. Also notice that the roll-off of the 30 Hz lowpass is not as great as for the 130 Hz lowpass, which has a higher roll-off.

Here is a function in MATLAB to perform low-pass filtering:

```
function newdata = lowpass(data,samprate,cutoff,order)

% newdata = lowpass(data,samprate,cutoff,order)
%
% performs a lowpass filtering of the input data
% using an nth order zero phase lag butterworth filter

if nargin==3 order=2; end; % default to 2nd order

% get filter paramters A and B
[B,A] = butter(order,cutoff/(samprate/2));
% perform filtering
newdata = filtfilt(B,A,data);
```

Here is one to perform high-pass filtering:

```
function newdata = highpass(data,samprate,cutoff,order)

% newdata = highpass(data,samprate,cutoff,order)
%
% performs a highpass filtering of the input data
% using an nth order zero phase lag butterworth filter

if nargin==3 order=2; end;

[B,A] = butter(order,cutoff/(samprate/2),'high');

newdata = filtfilt(B,A,data);
```

Here is one for band-pass filtering:

```
function newdata = bandpass(data,samprate,cutoff,order)

% newdata = bandpass(data,samprate,cutoff,order)
%
% performs a bandpass filtering of the input data
```

```
% using an nth order zero phase lag butterworth filter

if nargin==3 order=2; end;

[B,A] = butter(order/2,cutoff./(samprate/2));

newdata = filtfilt(B,A,data);
```

Here is one for band-stop filtering:

```
function newdata = bandstop(data,samprate,cutoff,order)

% newdata = bandstop(data,samprate,cutoff,order)
%
% performs a bandstop filtering of the input data
% using an nth order zero phase lag butterworth filter

if nargin==3 order=2; end;

[B,A] = butter(order/2,cutoff./(samprate/2),'stop');

newdata = filtfilt(B,A,data);
```

Figure 11.10 shows the corresponding signals shown in the time-domain:

In the code we use a two-pass, bi-directional filter function (called `filtfilt()` in all three languages) to apply the butterworth filter to the signal. One-way single-pass filter functions (e.g. `filter()`) introduce time lags. This is why in real-time applications in which you want to filter signals in real time (e.g. to reduce noise) there are time lags introduced.

So we see a very good example of how low-pass filtering can be used very effectively to filter out random noise. Key is the appropriate choice of cut-off frequency.

11.9.2 Common Filters

There are many different designs of filters, each with their own characteristics (gain, phase and delay characteristics). Some common types:

- *Butterworth Filters* have frequency responses which are maximally flat and have a monotonic roll-off. They are well behaved and this makes them very popular choices for simple filtering applications. For example in my work I use them exlusively for filtering physiological signals. MATLAB has a built-in function called `butter()` that implements the butterworth filter.
- *Tschebyschev Filters* provide a steeper monotonic roll-off, but at the expense of some ripple (oscillatory noise) in the pass-band.
- *Cauer Filters* provide a sharper roll-off still, but at the expense of ripple in both the pass-band and the stop-band, and reduced stop-band attenuation.
- *Bessel Filters* have a phase-shift which is linear with frequency in the pass-band. This corresponds to a pure delay and so Bessel filters preserve the shape of the signal quite well. The roll-off is monotonic and approaches the same slope as the Butterworth and Tschebyschev filters at high frequencies although it has a more gentle roll-off near the corner frequency.

11.9.3 Filter order

In filter design[148] the *order* of a filter is one characteristic that you might come across. Technically the definition of the filter order is the highest exponent in the z-domain[149] (transfer function[150]) of a digital filter[151]. That's helpful isn't it! (not) Another way of describing filter order is the degree of the approximating polynomial for the filter. Yet another way of describing it is that increasing the filter order increases roll-off and brings the filter closer to the ideal response (i.e. a "brick wall" roll-off).

Practically speaking, you will find that a second-order butterworth filter provides a nice sharp roll-off without too much undesirable side-effects (e.g. large time lag, ripple in the pass-band, etc).

See this section[152] of the wikipedia page on low-pass filters for another description.

11.9.4 High-frequency noise and taking derivatives

One of the characteristics of just about any experimental measurement is that the signal that you measure with your instrument will contain a combination of true signal and "noise" (random variations in the signal). A common approach is to take many measurements and average them together. This is what is commonly done in EEG/ERP studies, in EMG studies, with spike-triggered averaging, and many others. The idea is that if the "real" part of the signal is constant over trials, and the "noise" part of the signal is random from trial to trial, then averaging over many trials will average out the noise (which is sometimes positive, sometimes negative, but on balance, zero) and what remains will be the true signal.

You can imagine however that there are downsides to this approach. First of all, it requires that many, many measures be taken so that averages can be computed. Second, there is no guarantee that the underlying "true" signal will in fact remain constant over those many measurements. Third, one cannot easily do analyses on single trials, since we have to wait for the average before we can look at the data.

One solution is to use signal processing techniques such as filtering to separate the noise from the signal. A limitation of this technique however is that when we apply a filter (for example a low-pass filter), we filter out *all* power in the signal above the cutoff frequency—whether "real" signal or noise. This approach thus assumes that we are fairly certain that the power above our cutoff is of no interest to us.

One salient reason to low-pass filter a signal, and remove high-frequency noise, is for cases in which we are interested in taking the temporal derivative of a signal. For example, let's say we have recorded the position of the fingertip as a subject reaches from a start position on a tabletop, to a target located in front

of them on a computer screen. Using a device like Optotrak we can record the (x,y,z) coordinates of the fingertip at a sampling rate of 200 Hz. Figure 11.11 shows an example of such a recording.

In Figure 11.11 the top panel shows position in one coordinate over time. The middle panel shows the result of taking the derivative of the position signal to obtain velocity. I have simply used the `diff()` function here to obtain a numerical estimate of the derivative, taking the forward difference. Note how much noisier it looks than the position signal. Finally the bottom panel shows the result of taking the derivative of the velocity signal, to obtain acceleration. It is so noisy one cannot even see the peaks in the acceleration signal, they are completely masked by noise.

What is happening here is that small amounts of noise in the position signal are amplified each time a derivative is taken. One solution is to *low-pass filter* the position signal. The choice of the cutoff frequency is key—too low and we will decimate the signal itself, and too high and we will not remove enough of the high frequency noise. It happens that we are fairly certain in this case that there isn't much real signal power above 12 Hz for arm movements. Figure 11.12 shows what it looks like when we low-pass filter the position signal at a 12Hz cutoff frequency.

What you can see in Figure 11.12 is that for the position over time, the filtered version (shown in red) doesn't differ that much, at least not visibly, from the unfiltered version (in blue). The velocity and acceleration traces however look vastly different. Differentiating the filtered position signal yields a velocity trace (shown in red in the middle panel) that is way less noisy than the original version. Taking the derivative again of this new velocity signal yields an acceleration signal (shown in red in the bottom panel) that is actually usable. The original version (shown in blue) is so noisy it overwhelms the entire panel. Note the scale change on the ordinate.

11.10 Quantization

Converting an analog signal to a digital form involves the quantization of the analog signal. In this procedure the range of the input variable is divided into a set of class intervals. Quantization involves the replacement of each value of the input variable by the nearest class interval centre.

Another way of saying this is that when sampling an analog signal and converting it to digital values, one is limited by the precision with which one can represent the (analog) signal digitally. Usually a piece of hardware called an analog-to-digital (A/D) board is the thing that performs this conversion. The range of A/D boards are usually specified in terms of *bits*. For example a 12-bit A/D board is capable of specifying $2^{12} = 4096$ unique values. This means that a continuous signal will be represented using only 4096 possible values. A 16-bit A/D board would be capable of using $2^{16} = 65,536$ different values. Obviously the higher the better, in terms of the resolution of the underlying digital representation. Often however in practice, higher resolutions come at the expense of lower sampling rates.

As an example, let's look at a continuous signal and its digital representation using a variety of (low) sample resolutions. Figure 11.13 shows a range of sample resolutions.

Here we see as the number of possible unique values increases, the digital representation of the underlying continuous signal gets more and more accurate. Also notice that in general, quantization adds noise to the representation of the signal.

It is also important to consider the amplitude of the sampled signal compared to the range of the A/D board. In other words, if the signal you are sampling has a very small amplitude compared to the range of the A/D board then essentially your sample will only be occupying a small subset of the total possible values dictated by the resolution of the A/D board, and the effects of quantization will be greatly increased.

For example, let's say you are using an A/D board with 12 bits of resolution and an input range of +/- 5 Volts. This means that you have $2^{12} = 4096$ possible values with which to characterize a signal that ranges maximally over 10 Volts. If your signal is very small compared to this range, e.g. if it only occupies 25 millivolts, then the A/D board is only capable of using $0.0025/10 * 4096 = 10$ (ten) unique values to characterize your signal! The resulting digitized characterization of your signal will not be very smooth.

Whenever possible, amplify your signal to occupy the maximum range of the A/D board you're using. Of course the trick is always to amplify the signal without also amplifying the noise!

11.11 Sources of noise

It is useful to list a number of common sources of noise in physiological signals:

- *Extraneous Signal Noise* arises when a recording device records more than one signal—i.e. signals in addition to the one you as an experimenter are interested in. It's up to you to decide which is signal and which is noise. For example, electrodes placed on the chest will record both ECG and EMG activity from respiratory muscles. A cardiologist might consider the ECG signal and EMG noise, while a respiratory physiologist might consider the EMG signal and the ECG noise.
- *1/f Noise*: Devices with a DC response sometimes show a low frequency trend appearing on their output even though the inputs don't change. EEG systems and EOG systems often show this behaviour. Fourier analyses show that the amplitude of this noise increases as frequency decreases.
- *Power or 60 Hz Noise* is interference from 60 Hz AC electrical power signals. This is one of the most common noise sources that experimental neurophysiologists have to deal with. Often we find, for example, on hot days when the air conditioning in the building is running, we see much more 60 Hz noise in our EMG signals than on other days. Some neurophysiologists like to do their recordings late at night or on weekends when there is

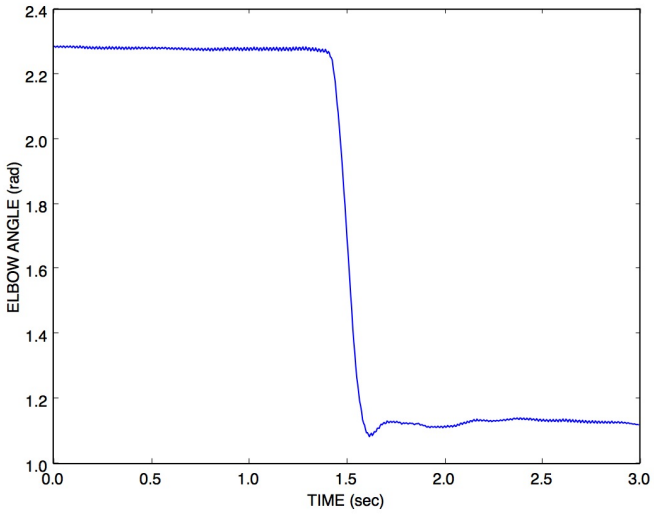
minimal activity on the electrical system in their building.

- *Thermal Noise* arises from the thermal motion of electrons in conductors, is always present and determines the theoretical minimum noise levels for a device. Thermal noise is white (has a Gaussian probability distribution) and thus has a flat frequency content – equal power across all frequencies.

Exercises

E 11.1 Spectrum of a signal

The file e31data.txt[153] contains Optotrak measurements of a single-joint elbow rotation over time. The angle between the upper and lower arm (in radians) was sampled at 200 Hz. Here is a plot of the data file:



Answer the following questions about the data. Use whatever signal processing techniques you wish, to answer each question. Explain the signal processing steps you took, and why.

- What is the Nyquist frequency?
- Compute and plot the spectrum of the signal, showing what the signal power is at different frequencies. I suggest using the `pwelch` function in MATLAB with the following parameters (assume `y` is an array containing the data):

```
pwelch(y,hanning(300),[],[],200);
```

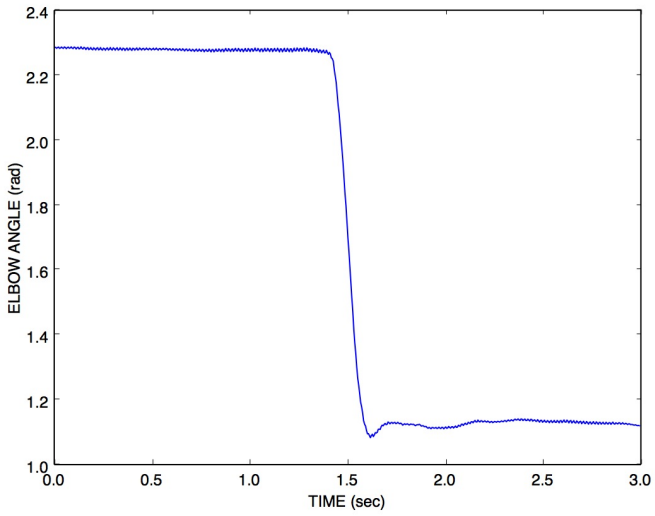
Note that the Hanning function simply returns a vector of weights that

are applied to each window of data used in the `pwelch` function. It provides a smoother spectrum. To visualize the Hanning window you can do this: `plot(hanning(300))`.

- What does the spectrum reveal about this signal?

E 11.2 Scoring kinematics

The file e31data.txt[154] contains Optotrak measurements of a single-joint elbow rotation over time. The angle between the upper and lower arm (in radians) was sampled at 200 Hz. Here is a plot of the data file:



Answer the following questions about the data. Use whatever signal processing techniques you wish, to answer each question. Explain the signal processing steps you took, and why.

- Determine the angle (in degrees) that the elbow rotated over the course of the arm movement.
- Determine the peak velocity, in radians per second, of the elbow movement. Hint: use the built-in MATLAB function `gradient()` to compute the central difference so you don't introduce a time lag and so the derivative has the same number of elements as the position ar-

ray.

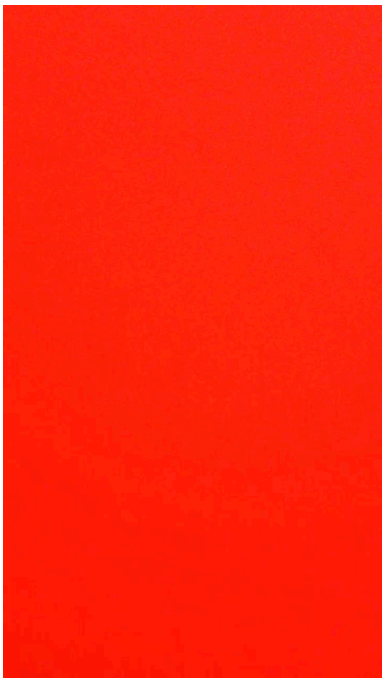
- Determine the peak positive and peak negative accelerations, in radians per second per second.

E 11.3 **Estimating your heart rate using your webcam or smartphone**

In this exercise we will attempt to estimate your heart rate using a video taken with your webcam or your smartphone.

Here's what you will do to generate the data. First, make sure you're in a brightly lit space (i.e. turn on the lights if you're in a dark room!). Better yet, find a light source like a desk lamp and direct it at your webcam or smartphone camera. Now gently rest the tip of your index finger against the lens of your webcam or smartphone camera. Now start recording a video. Record for 30 seconds. Try not to move your finger, keep everything still.

If you used your smartphone, transfer the video file to your computer. Open it up and look at it on the screen. Here's a sample frame from mine, which was approximately 15 seconds in duration:



Here is a link to the example video: IMG_1383.MOV[155]

If you can't make a video of your own, you are free to use my sample video instead, just download it to your machine.

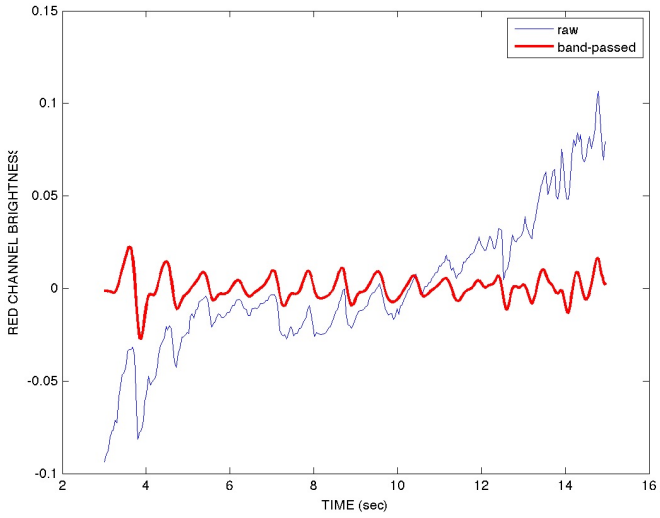
The idea here is that as your heart pumps blood through your arteries and veins, the amount of light that the camera detects, as it comes through your fingertip, will be modulated by the differences in blood flow. The variation in brightness will be subtle, and so your task is to use signal processing techniques to try to detect it.

Your task is to:

1. plot mean brightness over time as below
2. estimate mean heart rate (in beats per minute) during your (or my) video

Here are some suggestions as to how to proceed. Load in your video file, frame by frame. Each frame will have three channels: red, green and blue. Each frame will contain the brightness of each pixel for each of the three channels red, green and blue. You might as well average over all the pixels in the frame to get an average brightness measure. The signal that you ultimately want is probably the brightness over time (i.e. for each frame of the video).

As an example, here is the mean (over pixels) zero-centered brightness over time, for my 15-sec example video (blue) and a band-pass filtered version (in red):



Here are some hints about how to implement this in MATLAB:

The MATLAB function `VideoReader` will load in a .MOV file. Here is some sample code:

```
video = VideoReader('IMG_1383.MOV');
nframes = video.NumberOfFrames;
frameHeight = video.Height;
frameWidth = video.Width;
frameRate = video.FrameRate; % frames per second
duration = video.Duration;   % seconds
time = linspace(0,duration,nframes);
```

To read in a single frame of the video (for example the `i`th frame, you can do the following:

```
frame = read(video, i);
```

To get the mean brightness of the red channel you could do the following:

```
redChannel = frame(:, :, 1);
brt = mean(redChannel(:));
```

or to get the mean brightness across all channels in the frame:

```
brt = mean(frame(:));
```

What you probably want to do is implement a loop, going frame by frame, and in each frame, compute mean brightness, and store that (single) value for each frame, in an array.

Then you could band-pass filter this signal between frequencies of interest (e.g. a frequency range where you expect to see a heartbeat, e.g. 40-200 bpm. Remember to convert beats per minute (bpm) to Hz before using the bandpass function.

The cutting edge (not needed for your assignment, just FYI)

In 2012, some researchers at MIT published a new method for amplifying subtle changes in motion (or other aspects of a video) and visualizing them over time:

Eulerian Video Magnification for Revealing Subtle Changes in the World[156]

It's pretty cool stuff. See example videos:

- Revealing Invisible Changes in the World[157] (layperson version)
- Eulerian Video Magnification[158] (more technical version)

Links

[133] https://jackschaedler.github.io/circles-sines-signals/index.html

[134] http://en.wikipedia.org/wiki/Fourier_series

[135] http://bl.ocks.org/jinroh/7524988

[136] http://en.wikipedia.org/wiki/Fast_Fourier_transform

[137] https://youtu.be/NAsM30MAHLg

[138] https://www.youtube.com/watch?v=8KmVDxkia_w

[139] https://www.youtube.com/watch?v=6dW6VYXp9HM

[140] https://www.youtube.com/watch?v=jfH-NbsmvD4

[141] http://en.wikipedia.org/wiki/Nyquist-Shannon_sampling_theorem

[142] http://en.wikipedia.org/wiki/Aliasing

[143] http://en.wikipedia.org/wiki/Nyquist_frequency

[144] http://en.wikipedia.org/wiki/Aliasing

[145] http://www.mathworks.com/help/signal/ref/dspdata.psd.html

[146] http://en.wikipedia.org/wiki/Formant

[147] http://en.wikipedia.org/wiki/Bode_plot

[148] http://en.wikipedia.org/wiki/Filter_design

[149] http://en.wikipedia.org/wiki/Z-transform

[150] http://en.wikipedia.org/wiki/Transfer_function

[151] http://en.wikipedia.org/wiki/Digital_filter

[152] http://en.wikipedia.org/wiki/Low-pass_filter#Continuous-time_low-pass_filters

[153] http://www.gribblelab.org/scicomp/exercises/e31data.txt

[154] http://www.gribblelab.org/scicomp/exercises/e31data.txt

[155] http://www.gribblelab.org/scicomp/exercises/IMG_1383.MOV

[156] http://people.csail.mit.edu/mrub/vidmag/

[157] http://youtu.be/e9ASH8IBJ2U

[158] http://youtu.be/ONZcjs1Pjmk

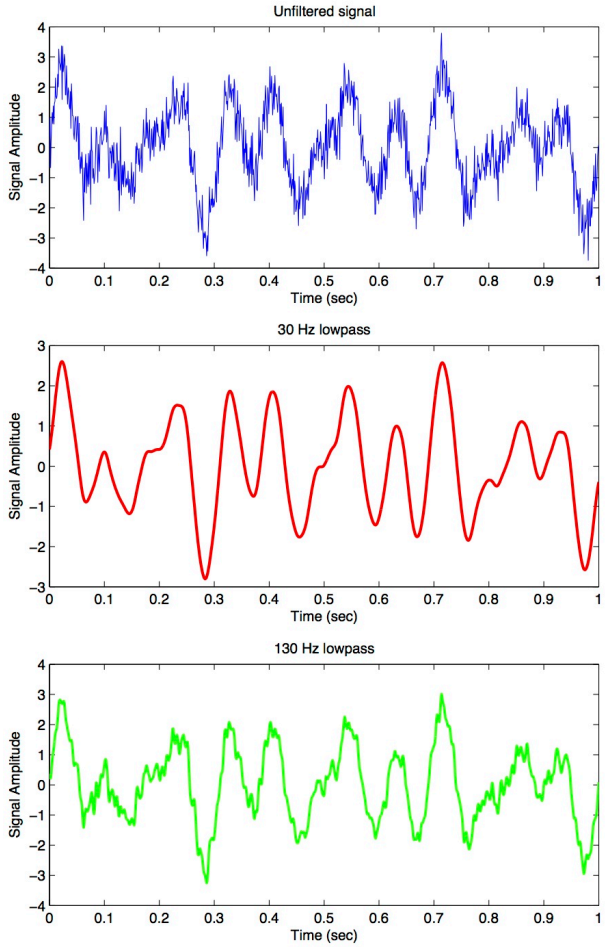


Figure 11.10: Three filtered versions of a noisy signal with peaks at 6, 10 and 13 Hz, in the time domain.

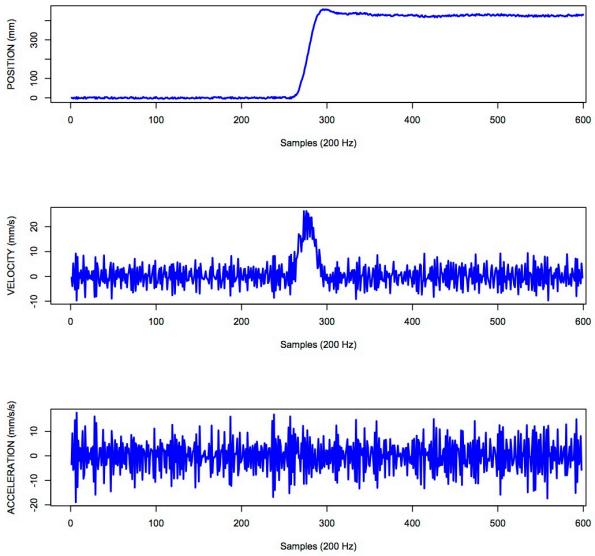


Figure 11.11: Sample 3D movement data recorded from Optotrak at 200 Hz.

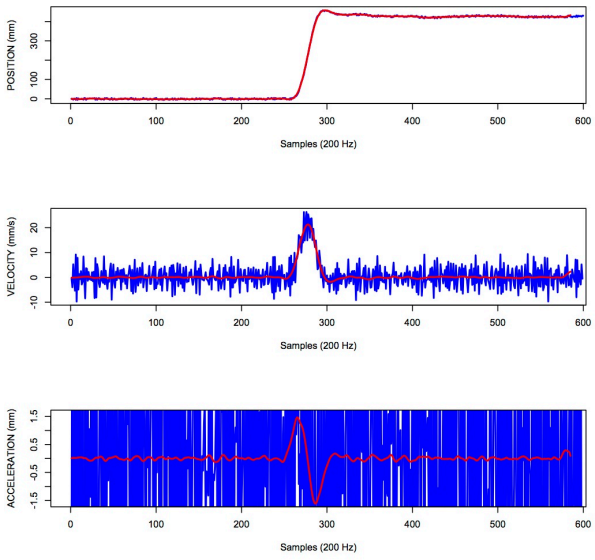


Figure 11.12: Sample 3D movement data recorded from Optotrak at 200 Hz, low-pass filtered using a 12 Hz cutoff frequency.

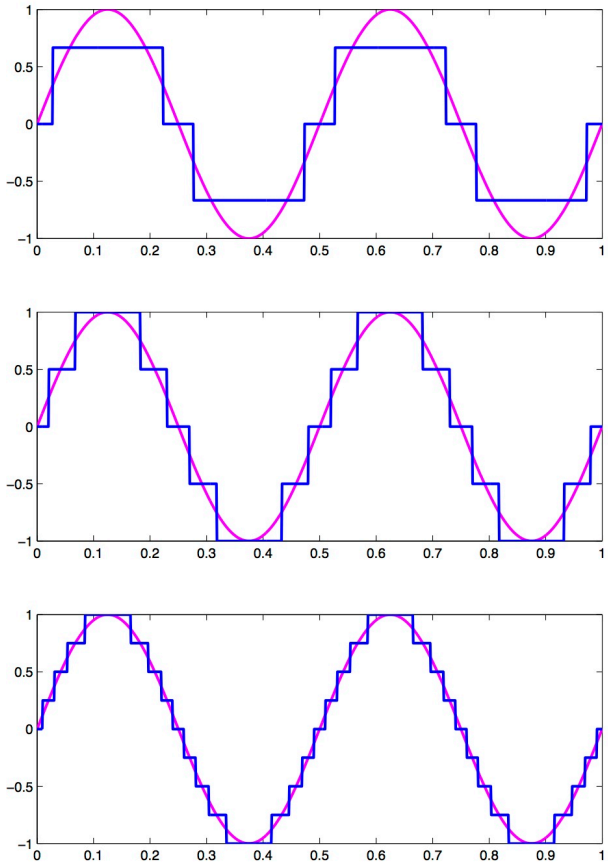


Figure 11.13: A continuous signal sampled at a variety of (low) sampling rates, showing quantization.

12 Optimization & gradient descent

In linear regression, we fit a line of best fit to N samples of (X_i, Y_i) data ($i = 1 \ldots N$) according to a linear equation with two parameters, β_0 and β_1:

$$\hat{Y}_i = \beta_0 + \beta_1 X_i + \varepsilon_i \tag{12.1}$$

To find the β parameters corresponding to the regression line, we can use a formula that's based on a procedure called ordinary least squares (OLS). What OLS does is find the β parameters that minimize the sum of squared deviations of the estimated values of the data Y (using given values of β) and the actual values of Y. That is, the values of β_0 and β_1 that minimize J where:

$$J = \sum_{i=1}^{N} \left(\hat{Y}_i - Y_i \right)^2 \tag{12.2}$$

We can call this function J a *cost function*. The goal then, is to determine, somehow, the values of the *parameters* β_0 and β_1 that *minimize* the cost function J.

This is a classic example of an *optimization problem*. We want to optimize the parameters β so that they minimize the cost function J.

Optimization problems abound in science, data analysis, statistical modeling, and even out there in the real world. Here are a few examples, to help you solidify in your mind what optimization is all about, and how it may be used. For some problems (e.g. the shower example) it is easy to think about how you would find the optimal solution. For others, it is not immediately obvious.

- *Your morning shower*: A simple example of optimization is when you hop in the shower and turn on the hot and cold water taps. What you desire is a water temperature that is not too hot, not too cold, but "just right". The *parameters* to be optimized are the relative amounts of cold and hot water coming out of the shower head. The *cost function* is how uncomfortable (whether too cold or too hot) the water temperature is for you.
- *Tuning a radio*: When you tune a radio (an analog radio) and you're searching for a particular radio station, you are performing an optimization. The parameter you are optimizing is the position of the tuner along the radio spectrum that spans the frequency of the radio station you are trying to listen to. The cost function is the amount of static that you hear overtop of the radio station signal.
- *Controlling rockets*: NASA[159] uses optimization techniques to determine the trajectory of rockets and other spacecraft that will reach their destination using the least amount of fuel. In this case there are parameters that define different trajectories, and a cost function that involves the total amount of fuel burn.
- *Travelling salesman*: A classic example of an optimization problem is the Travelling salesman problem[160]. Given a list of cities and the distances between each pair of cities, what is the shortest possible route that visits each city exactly once and returns to the origin city? In this case the parameters to be optimized are the order of visiting each city, and the cost is the total distance travelled.
- *Finance*: Bankers perform portfolio optimization to determine the mixture of investments that strike the best balance between risk and return. In this case the parameters are the proportions of each type of investment (stocks, bonds, real estate, gold, etc) and the cost function is some (generally secret) equation that balances risk and return.
- *Statistics*: In statistics and data modelling, optimization can be used to find the parameters of a model that best fits the observed data. In this case the parameters to be optimized are the parameters that define the particular model that is being used to model the data (e.g. for linear regression, the β

values), and the cost function is some measure of goodness-of-fit (actually "badness" of fit). In the case of linear regression, the cost function J is given above.

- *Machine Learning*: Many methods in machine learning, including classification, prediction, etc, are based on optimization: finding the values of model parameters that minimize some cost function. In logistic regression, support vector machines, etc, we find the parameter values that minimize the errors in classifying inputs as belonging to one category vs another (e.g. spam vs non-spam email, or benign vs cancerous tumours, etc). In artificial neural network models, we use optimization to find the values of neuron-to-neuron weights that minimize the network's errors on an input-output training set.
- *The Brain?*: Some people theorize that some brain functions (e.g. motor control, perception) can be conceptualized as optimization problems. For example for motor cortex, the parameters to be optimized might be the time-varying pattern of action potentials that arrive at α motoneurons in the spinal cord (and hence activate muscles, and move the body) and the cost function might be the amount of beer that is spilled as you move the beer stein from the tabletop to your mouth.

The big question then, is how to determine the parameters that minimize the cost function? There are two general approaches. The *analytic approach* is to try to find an analytical expression that allows one to directly compute the optimal parameter values. This is wonderful when it can be achieved, because direct calculation is fast. For linear regression using OLS, there exists a matrix equation (shown below) that provides an analytical solution.

For many problems however, it is not possible to find an analytical expression that gives the optimal parameter values. In these cases, one uses a *numerical approach* to estimate the optimal parameter values (the parameter values that minimize the cost function). As long as you can compute the value of the cost function for a given set of parameter guesses, then you can pursue a numerical approach to optimization. The downside of the numerical approach however

is that (1) it can take a long time to converge on the solution, and (2) for some problems, it can be extremely difficult or practically infeasible to converge on the optimal solution.

Optimization is a topic that people can (and have) spent their entire careers studying. It is one of the most important topics in applied mathematics and engineering. We will not attempt to cover the topic in any great breadth. Our goal here is to introduce you to the central idea, and to get some practical experience using numerical approaches to optimization.

12.1 Analytic Approaches

In the case of linear regression, there happens to be an analytical expression that allows us to directly calculate the β values that minimize J. This is the formula, in matrix format:

$$\hat{\beta} = \left(X^\top X\right)^{-1} X^\top Y \tag{12.3}$$

In your undergraduate statistics class(es) you may have seen a simpler looking, non-matrix version of this:

$$\hat{\beta_0} = \bar{Y} - \hat{\beta_1}\bar{X} \tag{12.4}$$

$$\hat{\beta_1} = \frac{\sum \left(Y_i - \bar{Y}\right)\left(X_i - \bar{X}\right)}{\sum \left(X_i - \bar{X}\right)^2} \tag{12.5}$$

How do we come up with analytic expressions like these? The answer is Calculus[161].

It might help to understand the following material by considering a simpler optimization problem, where we have a single paramater β to be optimized, for example the position of a radio tuner as you hone in on your favourite radio station. Call the position of the tuner dial β. What we want is to find the value of β that minimizes the cost function J, where J is, for example, the amount of static

that you hear overtop of the radio station signal. Let's say we're searching the airwaves for Virgin Radio but you've forgotten the frequency (97.5 MHz). We can visualize a hypothetical relationship between β and J graphically, as shown in Figure 12.1.

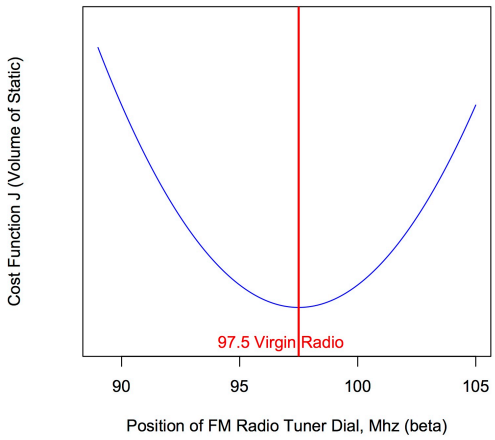


Figure 12.1: Cost function for tuning a radio.

As we move the dial under or over the actual (forgotten) frequency for Virgin Radio, we get static and the cost function J increases. The farther we move the dial away from the 97.5 MHz frequency, the greater the cost function J. What we desire is the frequency (the value of β) corresponding to the bottom (minimum) of the cost function, i.e. the minimum value of J.

We can remember from our high school calculus days that at the minimum of a function f, the first derivative[162] of f equals zero. With respect to our Virgin Radio example, this means that the derivative of J with respect to β is zero at the minimum of J. In equation form with calculus notation, what we want to derive is an expression that gives us the value of β for which the first derivative of β with respect to J is zero:

$$\frac{\partial J}{\partial \hat{\beta}} = 0 \tag{12.6}$$

If we can write an algebraic expression to describe how J varies with β, then there's a chance that we can do the differentiation and arrive at an analytic expression for the minimum. A very simple toy example: let's say we can write $J(\beta)$ as:

$$J = 10 + (\beta - 97.5)^2 \tag{12.7}$$

Now in this little example one doesn't need calculus to see that the way to minimize J is to set $\beta = 97.5$. Let's pretend however that we couldn't see this solution directly (as is often the case with more complex cost functions—for example for linear regression and OLS). If we take the derivative of J with respect to β, we get:

$$\begin{aligned}
\frac{\partial J}{\partial \beta} &= 0 && (12.8)\\
\frac{\partial [10 + (\beta - 97.5)^2]}{\partial \beta} &= 0 && (12.9)\\
2\,(\beta - 97.5) &= 0 && (12.10)\\
2\beta &= 2(97.5) && (12.11)\\
\beta &= 97.5 && (12.12)
\end{aligned}$$

So in this little example the analytical expression for the optimal value of β isn't even an expression per se, it's an actual value.

Note also that technically, that the slope of a function is zero not only at a minimum but also at a peak. If we truly want to find only minima then we should also look for places where the second derivative (the slope of the slope) is positive. Parameter values where the first derivative is zero and the second derivative is positive, correspond to valleys. Parameter values where the first derivative is

zero and the second derivative is negative, correspond to peaks. Draw a function with a peak and a valley, then draw the first and second derivatives, to convince yourself that this is true. See Figure 12.2 for an example of a function with a peak and a valley.

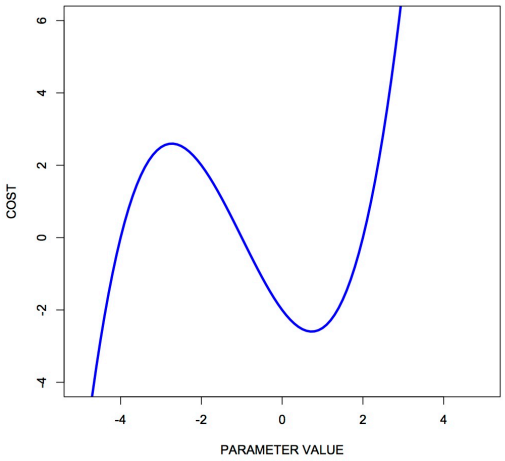


Figure 12.2: Peak and valley.

If you want to see how the solutions for β_0 and β_1 are derived, for linear regression OLS, you can see this summary[163] by Simon Jackman.

For some optimization problems, doing the calculus to find an analytical expression for the optimal parameter values is possible. For many optimization problems however, the calculus simply cannot be done. In this case our only option is to pursue a numerical approach. This is what we will focus on in this course—numerical approaches to optimization.

12.2 Numerical Approaches

In numerical approaches to optimization, the general idea is that you pursue an *iterative* approach in which you guess at optimal parameter values, you evaluate the cost, and then you revise your guess. This loop continues until you decide

you can no longer reduce the cost.

Numerical approaches can be distinguished as *local* versus *global* methods. Local methods use only local information about the relationship between cost and parameter values in the local "neighborhood" of the current guess. Global methods involve multiple guesses over a broad range of parameter values, and revised parameter guesses take into account information from all guesses across the entire parameter range.

12.2.1 Local methods

In local numerical approaches to optimization, the basic idea is to:

1. start with an initial guess at the optimal parameter values
2. compute the cost at hose parameter values
3. is the cost low enough? If yes, stop. If no, continue
4. estimate the local gradient at the current parameter values
5. take a step to new parameter values using the local gradient info
6. go to step 2

Sometimes at step 2, the *stopping rule* looks at not just the current cost but also other values such as the magnitude of the local gradient. For example if the local gradient gets too shallow then the stopping rule might get triggered.

You can think of this all in real-world terms in the following way. Imagine you're heli-skiing in the back-country, and at the end of the day instead of taking you back to Whistler village, your helicopter pilot drops you somewhere on the side of Whistler Mountain[164]. Only problem is, it's extremely foggy and you have no idea where you are, or which way is down to the village. You can only see 3 feet in front of you. All you have on you is an altimeter. What do you do? Probably something akin to the iterative numerical approach of *gradient descent*.

You have to decide which way is downhill, and then ski in that direction. To estimate which way is downhill you could do something like the following: take a step in three directions around a circle, and for each step, check the altime-

ter and compare the altitude to the altitude at the center of the circle. The step corresponding to the greatest altitude decrease represents the steepest "downhill".

Then you have to decide how long to ski in that direction. You could even tailor this ski time to the local gradient of the mountain. The steeper the slope, the smaller the ski time. The shallower the slope, the longer the ski time.

When you determine that moving in any direction doesn't decrease your altitude very much, you conclude that you're at the bottom.

This is essentially how numerical approaches to optimization work, by doing iterative gradient descent. Think about the ski hill example, and what kinds of things can go wrong with this procedure.

12.2.2 Local minima

One common challenge with complex optimization problems, is the issue of local minima. In the bowl-shaped example of a cost function that we plotted above, there is a single global minimum to the cost function—one place on the cost landscape where the slope is zero. It happens often however that there are local minima in the cost function—parameter values that correspond to a flat region of the cost function, where local steps will only increase the cost—but for which the cost is not the global minimum cost. Figure 12.3 shows an example of such a cost function.

You can see that there is a single global minimum at a parameter value of about -1—but there is a second, local minimum at a parameter value of about 2.2. You can see that if our initial parameter guess was between 1.5 and 3.0, that our local gradient descent procedure would put us at the local minimum, not the global minimum.

One strategy to deal with local minima is to run several gradient descent runs, each starting from a different (often randomly chosen) initial parameter guess, and then to take the best one as the global minimum. Ultimately however in

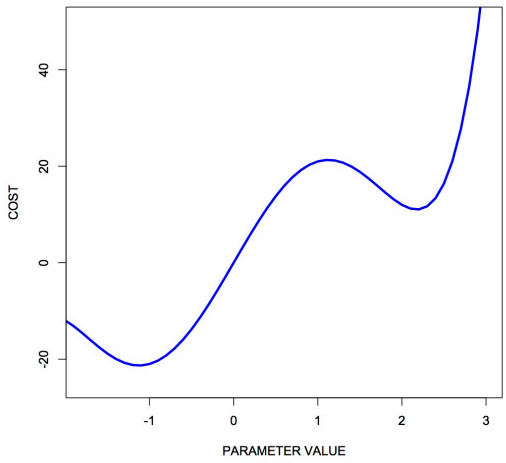


Figure 12.3: Local minimum.

the absence of an analytic solution, or a brute force mapping of the entire cost landscape (which is often infeasible) one can never be sure that one isn't at a local versus a global minimum.

12.2.3 Algorithms

A number of effective algorithms have been developed for finding parameter values that minimize a cost function. Some don't assume any pre-existing knowledge of the gradient—that is, of the derivative of the cost function with respect to the parameters, while some assume that we can compute both the cost and the gradient for a given set of parameter values.

In simple gradient descent[165], the simple idea is as described above, namely to estimate the local gradient and then take a step in the steepest direction. There are all sorts of ways of defining the step size, and adapting the step size to the steepness of the local gradient. There are also terms one can add that implement momentum[166], as a scheme to try to avoid local minima. Another strategy is to include randomness, by implementing stochastic gradient descent[167].

In conjugate gradient descent[168], one requires knowledge of the local gradient, and the idea here is that the algorithm tries to compute a more intelligent guess as to the direction of the cost minimum.

In Newton's method[169], one approximates the local gradient using a quadratic function, and then a step is taken towards the minimum of that quadratic function. You can think of this as a slightly more sophisticated version of simple gradient descent, in which one essentially approximates the local gradient as a straight line.

The Nelder-Mead (simplex) method[170] is an iterative approach that is pretty robust, that has an interesting geometric interpretation (see the animation on the wikipedia page) that is not unlike the old toy called Wacky Wally[171].

There are more complex algorithms such as Levenberg-Marquardt[172] and others, which we won't get into here.

The bottom line is that there are a range of local methods that vary in their complexity, in their memory requirements, in their iteration speed, and their susceptability to getting stuck in local minima. My approach is to start with the simple ones, and add complexity when needed.

12.2.4 Global methods

In global optimization[173], the general idea is instead of making a single guess and descending the local gradient, one instead makes a large number of guesses that broadly span the range of the parameters, and one evaluates the cost for all of them. Then the update step uses the costs of the entire set of guesses to determine a new set of guesses. It's also an iterative procedure, and when the stopping rule is triggered, one takes the guess from the current set of guesses that has the lowest cost, as the best estimate of the global minimum.

Global methods are well suited to problems that involve many local minima. Going back to our ski hill example, imagine instead of dropping one person on the side of Whistler mountain, rather a platoon of paratroopers is dropped from a

plane and scattered all over the entire mountain range. Some will end up in valleys and alpine lakes (local minima) but the chances are good that at least one will end up in whistler village, or close to it. They all radio up to the airplane with their reported altitudes, and on the basis of an analysis of the entire set, a new platoon is dropped, and eventually, someone will end up at the bottom (the global minimum).

Two popular global methods you might come across are simulated annealing[174] and genetic algorithms[175]. Read up on them.

12.3 Optimization in MATLAB

MATLAB has many different functions in the Optimization Toolbox for doing optimization, depending on whether you are doing linear vs nonlinear optimization, whether you have constraints or your problem is unconstrained, and other considerations as well. See the MATLAB documentation for all the details.

Here we will consider unconstrained nonlinear optimization, and later we will look at curve fitting.

12.3.1 Unconstrained nonlinear optimization

There are two main functions to consider in MATLAB for doing unconstrained, nonlinear optimization: `fminsearch` (which usese Nelder-Mead simplex search[176]) and `fminunc` (which uses gradients to search).

The MATLAB documentation contains some guidelines about when to use these different functions:

> "`fminsearch` is generally less efficient than `fminunc` for problems of order greater than two. However, when the problem is highly discontinuous, `fminsearch` might be more robust."

There is also a page in the MATLAB documentation that gives a more comprehensive set of guidelines for when to use different optimization algorithms:

Choosing a Solver[177]

Here is a simple example of a one-dimensional (one parameter) optimization problem. Consider the following function J of a single parameter x:

$$J(x) = xe^{(-x^2)} + \frac{x^2}{20} \tag{12.13}$$

Assume values of x range between -10.0 and +10.0.

Let's first generate a plot of the cost function J over the range of x. The code is shown below and the plot is shown in Figure 12.4.

```
J = @(x) x.*exp(-x.^2) + (x.^2)/20;
x = -10:0.1:10;
y = J(x);
plot(x,y)
```

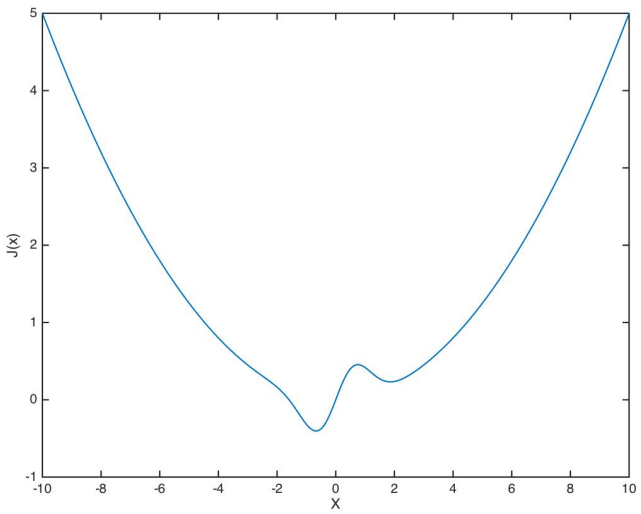


Figure 12.4: A function of a single variable.

We can see that there is a global minimum between -2.0 and 0.0, and there also appears to be a local minimum between 0.0 and 3.0. Let's try using the `fmin-`

`search` function to find the value of x which minimizes $J(x)$:

```
>> [X,FVAL,EXITFLAG] = fminsearch(J,0.0)

X =

   -0.6691


FVAL =

   -0.4052


EXITFLAG =

     1
```

We can see that the optimizer found a minimum at $x = -0.6691$, and that at that value of x, $J(x) = -0.4052$. It appears that the optimizer successfully found the global minimum and did not get fooled by the local minimum.

Let's try a two-dimensional problem:

$$J(x,y) = xe^{(-x.^2-y^2)} + \frac{x^2+y^2}{20} \tag{12.14}$$

Now we have a cost function J in terms of two variables x and y. Our problem is to find the vector (x,y) that minimizes $J(x,y)$.

Let's write a function file for our cost function:

```
function J = mycostfun2d(X)
%
% note use of dot notation on .* and ./ operators
% this enables the computation to happen for
% vector values of x
%
x = X(:,1);
```

```
y = X(:,2);
J = (x .* exp(-(x.*x)-(y.*y))) + (((x.*x)+(y.*y))./20);
```

Let's plot the cost landscape, which is shown in Figure 12.5:

```
x = linspace(-3,3,51);    % sample from -3 to +3 in 50 steps
y = linspace(-3,3,51);
XY = combvec(x,y);
J = mycostfun2d(XY');     % compute cost function over all values
[Y,X] = meshgrid(x,y);    % reshape into matrix form
Z = reshape(J,length(x),length(y));
figure                    % visualize the cost landscape
meshc(X,Y,Z);
shading flat
xlabel('X');
ylabel('Y');
zlabel('J');
```

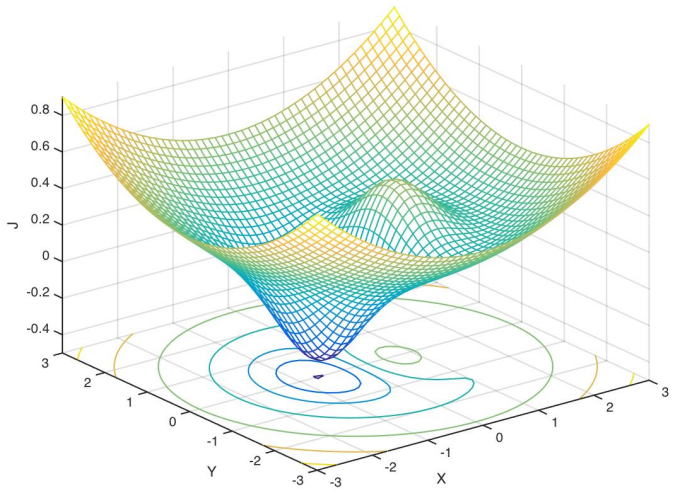


Figure 12.5: Cost function landscape for a 2D problem.

Now let's use `fminsearch` to find the values (x, y) that minimize $J(x, y)$:

```
>> [Xf,FVAL] = fminsearch('mycostfun2d', [5,5])

Xf =

   -0.6690   -0.0000


FVAL =

   -0.4052
```

Let's plot our solution to verify it looks reasonable—this is shown in Figure 12.6:

```
hold on
z0 = get(gca,'zlim');
z0 = z0(1);
plot3([Xf(1),Xf(1)],[get(gca,'ylim')],[z0 z0],'color','r','linewidth',2);
plot3([get(gca,'xlim')],[Xf(2),Xf(2)],[z0 z0],'color','r','linewidth',2);
```

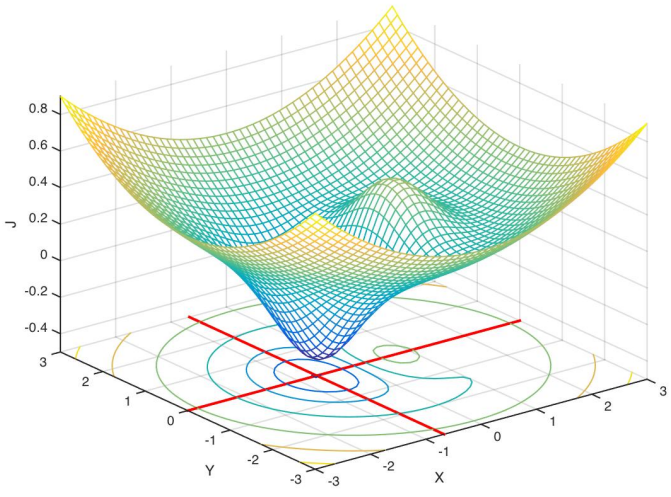


Figure 12.6: Cost function landscape for a 2D problem.

12.3.2 Curve Fitting

We can do nonlinear least squares curve fitting in MATLAB using `lsqcurvefit`. There is also a GUI tool for curve fitting in MATLAB called `cftool`.

Exercises

E 12.1 **Curve Fitting**

Here are 10 pairs of (x,y) data:

```
x = [ 1, 2,  3,  4,  5,   6,   7,   8,   9,  10];
y = [18, 5, 17, 38, 40, 106, 188, 234, 344, 484];
```

Your task is to fit a function to the data. The function has the form:

$$\hat{y}_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \beta_3 x_i^3 \tag{12.15}$$

and the cost function J is:

$$J = \sum_{i=1}^{10} (\hat{y}_i - y_i)^2 \tag{12.16}$$

Use whatever optimizer you wish. Plot the data as a scatter plot of x vs y, and plot the function that corresponds to the parameter values β that minimize J.

E 12.2 **Local Minima**

Generate some noisy (x,y) data using the following MATLAB code:

```
x = 0:0.01:3;
y = sin(2*pi*x) + randn(size(x))*0.5;
```

Generate a scatterplot of the data, plotting x on the abscissa and y on the ordinate.

Your task is to fit a function of the following form to the data:

$$\hat{y} = \sin(\beta x) \tag{12.17}$$

The (single) parameter to be optimized is β. Your cost function J is:

$$J = \sum_{i=1}^{n} (\hat{y}_i - y_i)^2 \tag{12.18}$$

where n is the number of (x,y) pairs in the data.

- Compute the cost function J for values of β ranging from -10.0 to +10.0, and plot the cost landscape (plot J as a function of β)
- Use an optimization method of your choosing to find the value of β that minimizes the cost function J. Plot the data and the overlay the best fitting function. Justify that you have found a global minimum and not a local minimum.

E 12.3 **Egg Carton**

Assume your cost function J is the following function of two parameters (x,y):

$$J(x, y) = -20e^A - e^B + 20 + e \tag{12.19}$$

where

$$A = -0.2\sqrt{0.5(x^2 + y^2)} \tag{12.20}$$

and

$$B = 0.5\left[\cos(2\pi x) + \cos(2\pi y)\right] \tag{12.21}$$

- Compute the cost function J for values of (x, y) ranging from -10.0 to 10.0, and plot the cost landscape (plot J as a function of (x, y)). **hint:** Hint: it should look something like [this[178]
- Use whatever optimization method you wish, to find the values of (x, y) that minimize the cost function J. Justify that you have found the global minimum and not a local minimum

Links

[159] http://www.nasa.gov

[160] http://en.wikipedia.org/wiki/Travelling_salesman_problem

[161] http://en.wikipedia.org/wiki/Calculus

[162] http://en.wikipedia.org/wiki/Derivative

[163] http://jackman.stanford.edu/classes/ssmart/2011/derive1.pdf

[164] http://www.whistlerblackcomb.com/the-mountain/weather-and-mountain-stats.aspx

[165] http://en.wikipedia.org/wiki/Gradient_descent

[166] http://www.willamette.edu/~gorr/classes/cs449/momrate.html

[167] http://en.wikipedia.org/wiki/Stochastic_gradient_descent

[168] http://en.wikipedia.org/wiki/Conjugate_gradient_method

[169] http://en.wikipedia.org/wiki/Newton's_method_in_optimization

[170] http://en.wikipedia.org/wiki/Nelder%E2%80%93Mead_method

[171] http://youtu.be/l8Dbne0wRaE?t=18s

[172] http://en.wikipedia.org/wiki/Levenberg–Marquardt_algorithm

[173] http://en.wikipedia.org/wiki/Global_optimization

[174] http://en.wikipedia.org/wiki/Simulated_annealing

[175] http://en.wikipedia.org/wiki/Genetic_algorithm

[176] https://en.wikipedia.org/wiki/Nelder–Mead_method

[177] http://www.mathworks.com/help/optim/ug/choosing-a-solver.html

[178] http://wolfr.am/85VNivEU

13 Integrating ODEs & simulating dynamical systems

13.1 What is a dynamical system?

Systems can be characterized by the specific relation between their input(s) and output(s). A static system has an output that only depends on its input. A mechanical example of such a system is an idealized, massless spring. The length of the spring depends only on the force (the input) that acts upon it. Change the input force, and the length of the spring will change, and this will happen instantaneously (obviously a massless spring is a theoretical construct). A system becomes dynamical (it is said to have dynamics) when a mass is attached to the spring (Figure 13.1 below). Now the position of the mass (and equivalently, the length of the spring) is no longer directly dependent on the input force, but is also tied to the acceleration of the mass, which in turn depends on the sum of all forces acting upon it (the sum of the input force and the force due to the spring). The net force depends on the position of the mass, which depends on the length of the spring, which depends on the spring force. The property that acceleration of the mass depends on its position makes this a dynamical system.

Dynamical systems can be characterized by differential equations that relate the state derivatives (e.g. velocity or acceleration) to the state variables (e.g. position). The differential equation for the spring-mass system depicted above is:

$$m\ddot{x} = -kx + mg \tag{13.1}$$

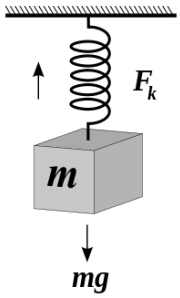


Figure 13.1: A simple mass-spring system

Where x is the position of the mass m (the length of the spring), $\ddot{x}$ is the second derivative of position (i.e. acceleration), k is a constant (related to the stiffness of the spring), and g is the graviational constant (9.81 m/s/s).

The system is said to be a second order system, as the highest derivative that appears in the differential equation describing the system, is two. The position x and its time derivative $\dot{x}$ are called states of the system, and $\dot{x}$ and $\ddot{x}$ are called state derivatives.

Most systems out there in nature are dynamical systems. For example most chemical reactions under natural circumstances are dynamical: the rate of change of a chemical reaction depends on the amount of chemical present, in other words the state derivative is proportional to the state. Dynamical systems exist in biology as well. For example the rate of change of the population size of a certain species likely depends on its population size.

Dynamical equations are often described by a set of coupled differential equations. For example, the reproduction rate of rabbits (state derivative 1) depends on the population of rabbits (state 1) and on the population size of foxes (state 2). The reproduction rate of foxes (state derivative 2) depends on the population of foxes (state 2) and also on the population of rabbits (state 1). In this case we have two coupled first-order differential equations, and hence a system of order two. The so-called predator-prey model is also known as the Lotka-Volterra equations[179]:

$$\dot{x} = x(\alpha - \beta y) \tag{13.2}$$

$$\dot{y} = -y(\gamma - \delta x) \tag{13.3}$$

13.2 Why make models?

There are two main reasons why we would want to model a physical system using mathematical equations, one being practical and one mostly theoretical. The practical use is prediction. A typical example of a dynamical system that is modelled for prediction is the weather. The weather is a very complex, (high-order, nonlinear, coupled and chaotic) system. More theoretically, one reason to make models is to test the validity of a functional hypothesis of an observed phenomenon. A beautiful example is the model made by Hodgkin and Huxley[180] to understand how action potentials arise and propagate in neurons (see Figures 13.2 and 13.3 below). They modelled the different (voltage-gated) ion channels in an axon membrane and showed using mathematical models that indeed the changes in ion concentrations were responsible for the electical spikes observed experimentally 7 years earlier.

A second theoretical reason to make models is that it is sometimes very difficult, if not impossible, to answer a certain question empirically. As an example we take the following biomechanical question: Would you be able to jump higher if your biceps femoris (part of your hamstrings) were two separate muscles each crossing only one joint rather than being one muscle crossing both the hip and knee joint? Not a strange question as one could then independently control the torques around each joint.

In order to answer this question empirically, one would like to do the following experiment:

- measure the maximal jump height of a subject
- change only the musculoskeletal properties in question
- measure the jump height again

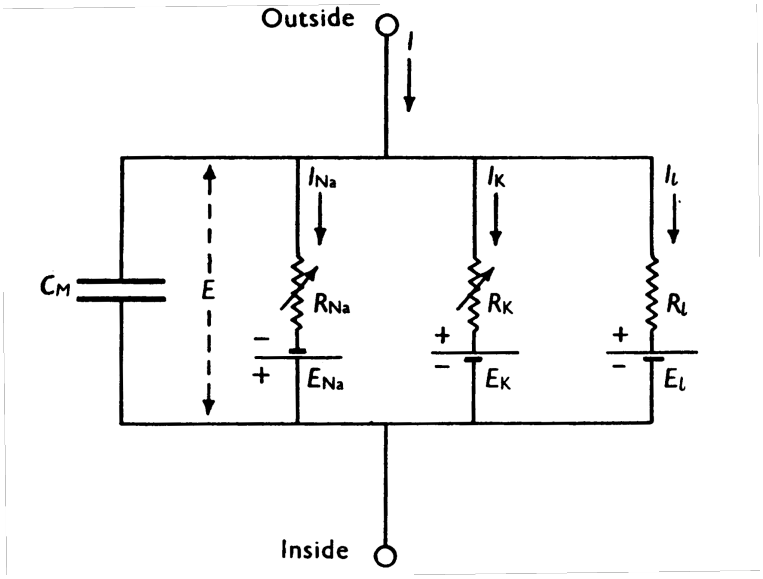


Figure 13.2: Hodgkin-Huxley model of voltage-gated ion channels

Of course, such an experiment would yield several major ethical, practical and theoretical drawbacks. It is unlikely that an ethics committee would approve the transplantation of the origin and insertion of the hamstrings in order to examine its effect on jump height. And even so, one would have some difficulties finding subjects. Even with a volunteer for such a surgery it would not bring us any closer to an answer. After such a surgery, the subject would not be able to jump right away, but would have to undergo significant rehabilitation, and surely during such a period many factors will undesirably change like maximal contractile forces. And even if the subject would fully recover (apart from the hamstrings transplantation), his or her nervous system would have to find the new optimal muscle stimulation pattern.

If one person jumps lower than another person, is that because she cannot jump as high with her particular muscles, or was it just that her CNS was not able to find the optimal muscle activation pattern? Ultimately, one wants to know through what mechanism the subject's jump performance changes. To investigate this, one would need to know, for example, the forces produced by the

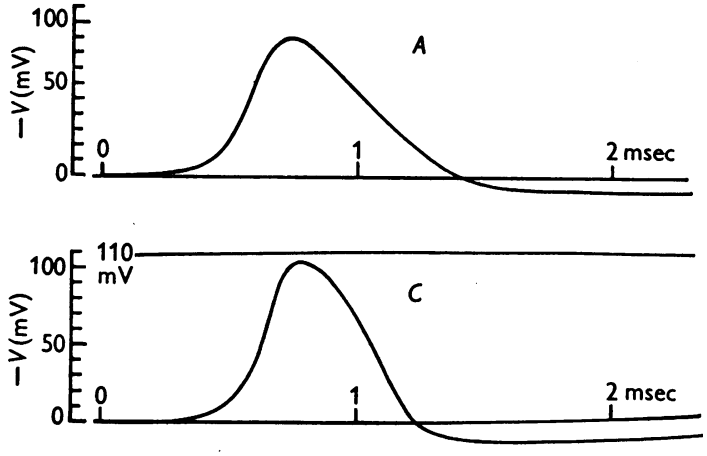


Figure 13.3: Action potentials across the membrane

hamstrings as a function of time, something that is impossible to obtain experimentally. Of course, this example is somewhat ridiculous, but its message is hopefully clear that for several questions a strict empirical approach is not suitable. An alternative is provided by mathematical modelling.

Here we will be examining three systems—a mass-spring system, a two-link double pendulum system, and a system representing weather patterns. In each case we will see how to go from differential equations characterizing the dynamics of the system, to MATLAB code, and run that code to simulate the behaviour of the system over time. We will see the great power of simulation, namely the ability to change aspects of the system at will, and simulate to explore the resulting change in system behaviour.

13.3 Modelling Dynamical Systems

13.3.1 Characterizing a System Using Differential Equations

A dynamical system such as the mass-spring system we saw before, can be characterized by the relationship between state variables s and their (time) derivatives $\dot{s}$. How do we arrive at the correct characterization of this relationship?

The short answer is, we figure it out using our knowledge of physics, or we are simply given the equations by someone else. Let's look at a simple mass-spring system again, shown in Figure 13.4.

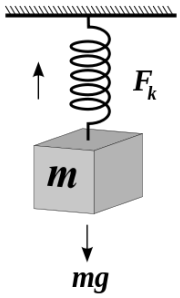


Figure 13.4: A spring with a mass attached

We know a couple of things about this system. We know from Hooke's law[181] of elasticity that the extension of a spring is directly and linearly proportional to the load applied to it. More precisely, the force that a spring applies in response to a perturbation from it's *resting length* (the length at which it doesn't generate any force), is linearly proportional, through a constant k, to the difference in length between its current length and its resting length (let's call this distance x). For convention let's assume positive values of x correspond to lengthening the spring beyond its resting length, and negative values of x correspond to shortening the spring from its resting length.

$$F = -kx \tag{13.4}$$

Let's decide that the *state variable* that we are interested in for our system is x. We will refer to x instead of s from now on to denote our state variable.

We also know from Newton's laws of motion[182] (specifically Newton's second law[183]) that the net force on an object is equal to its mass m multiplied by its acceleration a (the second derivative of position).

$$F = ma \tag{13.5}$$

Instead of using a to denote acceleration let's use a different notation, in terms of the spring's perturbed length x. The rate of change (velocity) is denoted $\dot{x}$ and the rate of change of the velocity (i.e. the acceleration) is denoted $\ddot{x}$.

$$F = m\ddot{x} \tag{13.6}$$

We also know that the mass is affected by two forces: the force due to the spring ($-kx$) and also the gravitational force g. So the equation characterizing the *net forces* on the mass is

$$\sum F = m\ddot{x} = -kx + mg \tag{13.7}$$

or just

$$m\ddot{x} = -kx + mg \tag{13.8}$$

This equation is a *second-order* differential equation, because the highest state derivative is a *second derivative* (i.e. $\ddot{x}$, the second derivative, i.e. the acceleration, of x). The equation specifies the relationship between the state variables (in this case a single state variable x) and its derivatives (in this case a single derivative, $\ddot{x}$).

The reason we want an equation like this, from a practical point of view, is that we will be using numerical solvers in MATLAB to *integrate* this differential equation over time, so that we can *simulate* the behaviour of the system. What these solvers need is a MATLAB function that returns state derivatives, given current states. We can re-arrange the equation above so that it specifies how to compute the state derivative $\ddot{x}$ given the current state $\ddot{x}$.

$$\ddot{x} = \frac{-kx}{m} + g \tag{13.9}$$

Now we have what we need in order to simulate this system in MATLAB. At any time point, we can compute the acceleration of the mass by the formula above.

13.4 Integrating Differential Equations in MATLAB

Here is a MATLAB function that we will be using to simulate the mass-spring system. All it does, really, is compute the equation above: what is the value of $\ddot{x}$, given x? The one addition we have is that we are going to keep track not just of one state variable x but also its first derivative $\dot{x}$ (the rate of change of x, i.e. velocity).

```
function stated = MassSpring(t, state)

  % unpack the state vector
  x  = state(1);
  xd = state(2);

  % these are our constants
  k = 2.5; % Newtons per metre
  m = 1.5; % Kilograms
  g = 9.8; % metres per second

  % compute acceleration xdd
  xdd = ((-k*x)/m) + g;

  stated = [xd, xdd];

end
```

Note that the function we wrote takes two arguments as inputs: `state` and `t`, which corresponds to time. This is necessary for the numerical solver that we will use in MATLAB. The *state variable* is actually an array of two values corresponding to x and $\dot{x}$.

How does numerical integration (simulation) work? Here is a summary of the steps that a numerical solver takes. First, you have to provide the system with two things:

1. initial conditions (what are the initial states of the system?)
2. a time vector over which to simulate

Given this, the numerical solver will go through the following steps to simulate the system:

- calculate state derivatives $\ddot{x}$ at the initial time ($t = 0$) given the initial states $(x, \dot{x})$
- estimate $x(t + \Delta t)$ using $x(t = 0)$, $\dot{x}(t = 0)$ and $\ddot{x}(t = 0)$
- calculate $\ddot{x}(t = t + \Delta t)$ from $x(t = t + \Delta t)$ and $\dot{x}(t = t + \Delta t)$
- estimate $x(t + 2\Delta t)$ and $\dot{x}(t + 2\Delta t)$ using $x(t = t + \Delta t)$, $\dot{x}(t = t + \Delta t)$ and $\ddot{x}(t = t + \Delta t)$
- calculate $\ddot{x}(t = t + 2\Delta t)$ from $x(t = t + 2\Delta t)$ and $\dot{x}(t = t + 2\Delta t)$
- ... etc

In this way the numerical solver can esimate how the system states $(x, \dot{x})$ unfold over time, given the initial conditions, and the known relationship between state derivatives and system states. The details of the "estimate" steps above are not something we are going to dive into now. Suffice it to say that current estimation algorithms are based on the work of two German mathematicians named Runge and Kutta[184] in the beginning of the 20th century. These numerical recipies are readily available in MATLAB and are known as ODE solvers (ODE stands for *ordinary differential equation*).

Here's how we would simulate the mass-spring system above. Assume that we have the function `MassSpring.m` defined as above:

```
state0 = [0.0, 0.0];
t = 0:.1:10;

[t,state] = ode45('MassSpring', t, state0);
```

```
plot(t, state)
xlabel('TIME (sec)')
ylabel('STATES')
title('Mass-Spring System')
legend({'$x$ (m)', '$\dot{x}$ (m/sec)'},'interpreter','latex')
```

A couple of notes about the code. I have simply chosen, out of the blue, values for the constants k and m. The gravitational constant[185] g is of course known. I have also chosen to simulate the system for 10 seconds, and I have chosen a time resolution of 100 milliseconds (0.1 seconds). We will talk later about the issue of what is an appropriate time resolution for simulation.

You should see a plot like the one shown in Figure 13.5 below.

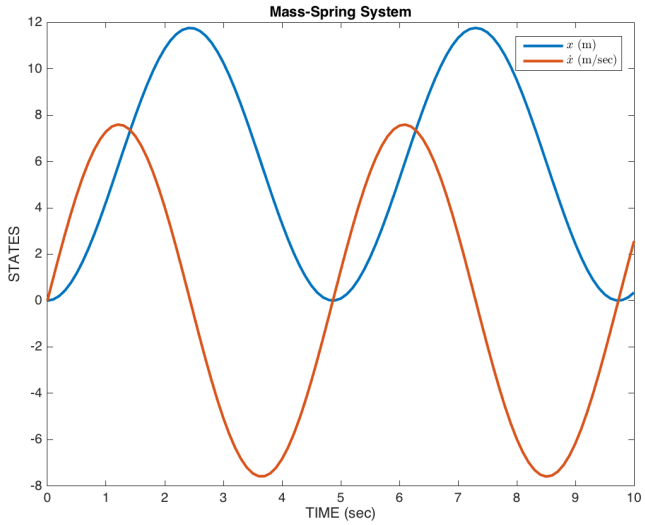


Figure 13.5: Mass-spring simulation

The blue line shows the position x of the mass (the length of the spring) over time, and the orange line shows the rate of change of x, in other words the velocity $\dot{x}$, over time. These are the two states of the system, simulated over time.

The way to interpret this simulation is, if we start the system at $x = 0$ and $\dot{x} = 0$,

and simulate for 10 seconds, this is how the system would behave.

13.5 The power of modelling and simulation

Now you can appreciate the power of mathematical models and simulation: given a model that characterizes (to some degree of accuracy) the behaviour of a system we are interested in, we can use simulation to perform experiments *in simulation* instead of in reality. This can be very powerful. We can ask questions of the model, in simulation, that may be too difficult, or expensive, or time consuming, or just plain impossible, to do in real-life empirical studies. The degree to which we regard the results of simulations as interpretable, is a direct reflection of the degree to which we believe that our mathematical model is a reasonable characterization of the behaviour of the real system.

13.6 Simulating Motion of a Two-Joint Arm

Here is a MATLAB function called `double_pendulum.m` that implements the forward dynamics of a double pendulum[186]. You can look up the equations of motion on the Wikipedia page. The code below simply implements these equations. It's not important right now to understand where the equations came from, but know that they can be derived from a relatively basic knowledge of physics. One property of a double pendulum is that the motion about one joint affects the motion of the adjacent joint, and vice-versa. These interaction forces can result in complex behaviour. Indeed, experimental work has demonstrated that the nervous system is capable of predicting these interaction forces and compensating for them (or in some cases exploiting them) during voluntary movements of the upper limb.

The four state variables are the angle of joint 1, the angle of joint 2, the velocity of joint 1 and the velocity of joint 2.

```
function stated = double_pendulum(t, state)

a1 = state(1);
```

```
a2 = state(2);
a1d = state(3);
a2d = state(4);

damping = 0.0;
g = 9.8;

% inertia matrix
M = [3 + 2*cos(a2), 1+cos(a2); ...
     1+cos(a2), 1];

% coriolis, centripetal and gravitational forces
c1 = a2d*((2*a1d) + a2d)*sin(a2) + ...
     2*g*sin(a1) + g*sin(a1+a2);
c2 = -(a1d^2)*sin(a2) + g*sin(a1+a2);

% passive dynamics
cc = [c1-damping*a1d; ...
      c2-damping*a2d];

% compute accelerations
acc = M\cc;

stated = [a1d a2d acc(1) acc(2)]';

end
```

Now that we have a function that implements the equations of motion, now we can run a simulation, by starting the arm out at some initial condition (initial joint angles and initial joint velocities) and integrating the differential equations over time (using MATLAB's `ode45` function). Here is some MATLAB code for running a simulation from a given set of initial state conditions, and animating the result in a figure window. You'll need this helper function called `a2h.m` as well:

```
function [h0,h1,h2] = a2h(a1,a2)

h0 = [0,0];
h1 = [sin(a1), cos(a1)];
```

```
h2 = [sin(a1) + sin(a1+a2), ...
      cos(a1) + cos(a1+a2)];

end
```

Here is the script for running the simulation and generating the animation:

```
%% run a simulation of a double pendulum

t = 0:.01:10;
x0 = [pi, pi/2, 0, 0];
[t,x] = ode45('double_pendulum', t, x0);

%% plot states over time

figure
plot(t,x)

%% run an animation

figure('position',[62   855   965   333]);
subplot(1,2,1)
plot(t,x(:,1:2))
legend({'a1','a2'})
hold on
s1ylim = get(gca,'ylim');
tline = plot([0 0],s1ylim,'r-','linewidth',1);
subplot(1,2,2)
[h0,h1,h2] = a2h(x(1,1),x(1,2));
l1 = plot([h0(1) h1(1)],[h0(2) h1(2)],'b-');
hold on
l2 = plot([h1(1) h2(1)],[h1(2) h2(2)],'b-');
axis([-2.2 2.2 -2.2 2.2]); axis equal
p0 = plot(h0(1),h0(2),'k.','markersize',15);
p1 = plot(h1(1),h1(2),'b.','markersize',15);
p2 = plot(h2(1),h2(2),'r.','markersize',15);
tp = title(sprintf('%5.1f',t(1)));
skip = 3;
```

```
for i=1:skip:length(t)
    subplot(1,2,1)
    set(tline, 'Xdata', [t(i) t(i)]);
    set(tline, 'Ydata', s1ylim);
    subplot(1,2,2)
    [h0,h1,h2] = a2h(x(i,1), x(i,2));
    set(l1, 'XData', [h0(1) h1(1)]);
    set(l1, 'YData', [h0(2) h1(2)]);
    set(l2, 'XData', [h1(1) h2(1)]);
    set(l2, 'YData', [h1(2) h2(2)]);
    set(p1, 'XData', h1(1));
    set(p1, 'YData', h1(2));
    set(p2, 'XData', h2(1));
    set(p2, 'YData', h2(2));
    set(tp, 'String', sprintf('%5.1f', t(i)));
    axis([-2.2 2.2 -2.2 2.2]);
    drawnow;
end
```

What you see is a window with the time-varying angles on the left panel and an animation of the double pendulum on the right panel, as in Figure 13.6.

Play with the simulation code and see what happens when you start the simulation from different initial conditions, for example different initial joint angles.

The simple model described here has only passive motion, there are no active forces (for example generated by muscles). One can relatively easily add mathematical models of muscle force generation, and other neurophysiologically relevant properties such as muscle mechanics, spinal reflex circuitry, reflex time delays, and so on. One can then use such a model to test hypotheses about how the brain controls voluntary arm movement.

13.7 Lorenz Attractor

The Lorenz system[187] is a dynamical system that we will look at briefly, as it will allow us to discuss several interesting issues around dynamical systems. It

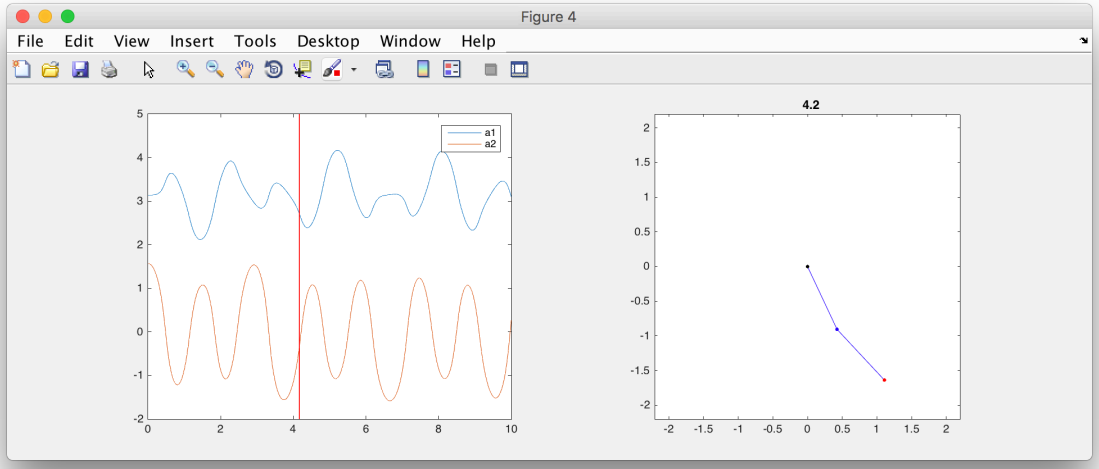


Figure 13.6: Double pendulum

is a system often used to illustrate non-linear systems[188] theory and chaos theory[189]. It's sometimes used as a simple demonstration of the butterfly effect[190] (sensitivity to initial conditions). See here[191] for a YouTube video that explains the meaning of the x, y and z coordinates.

The Lorenz system is a simplified mathematical model for atmospheric convection. Let's not worry about the details of what it represents, for now the important things to note are that it is a system of three /coupled/ differential equations, and characterizes a system with three state variables (x, y, z).

$$\dot{x} = \sigma(y - x) \tag{13.10}$$

$$\dot{y} = (\rho - z)x - y \tag{13.11}$$

$$\dot{z} = xy - \beta z \tag{13.12}$$

If you set the three constants (σ, ρ, β) to specific values, the system exhibits *chaotic behaviour*.

$$\sigma = 10 \tag{13.13}$$

$$\rho = 28 \tag{13.14}$$

$$\beta = \frac{8}{3} \tag{13.15}$$

Let's implement this system in MATLAB. We have been given above the three equations that characterize how the state derivatives $(\dot{x}, \dot{y}, \dot{z})$ depend on (x, y, z) and the constants (σ, ρ, β). All we have to do is write a function that implements this, set some initial conditions, decide on a time array to simulate over, and run the simulation using `ode45()`. First the function `myLorenz.m` that defines the differential equations:

```
function stated = myLorenz(t, state)
 x = state(1);
 y = state(2);
 z = state(3);

 % these are our constants
 sigma = 10.0;
 rho = 28.0;
 beta = 8/3;

 % compute the state derivatives
 xd = sigma * (y-x);
 yd = (rho-z)*x - y;
 zd = x*y - beta*z;

 % return the state derivatives
 stated = [xd, yd, zd]';
end
```

Now the code to run the simulation:

```
state0 = [2.0, 3.0, 4.0];
t = 0:.01:30;
```

```
[t,state] = ode45('myLorenz', t, state0);

% plot the resuling state-space trajectory in 3D
plot(state(:,1), state(:,2), state(:,3))
xlabel('X'); ylabel('Y'); zlabel('Z');
grid on
```

You should see something like the plot shown in Figure 13.7 below.

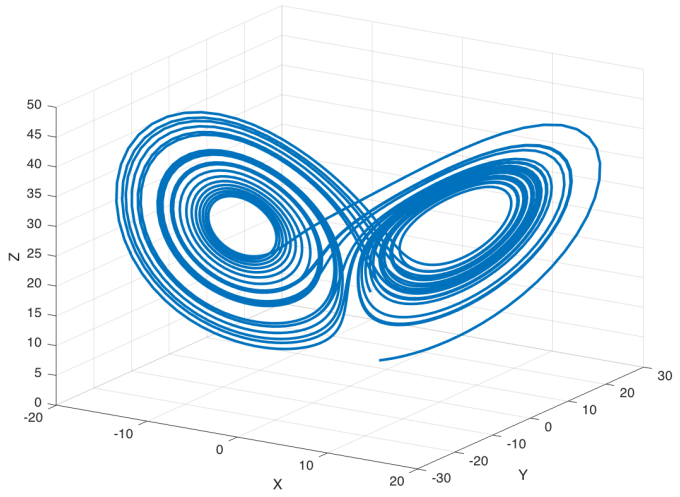


Figure 13.7: Lorenz attractor

The three axes on the plot represent the three states (x, y, z) plotted over the 30 seconds of simulated time. We started the system with three particular values of (x, y, z) (I chose them arbitrarily), and we set the simulation in motion. This is the trajectory, in *state-space*, of the Lorenz system.

You can see an interesting thing ... the system seems to have two stable equilibrium states, or attractors: those circular paths. The system circles around in one "neighborhood" in state-space, and then flips over and circles around the second neighborhood. The number of times it circles in a given neighborhood, and the time at which it switches, displays chaotic behaviour, in the sense that

they are exquisitly sensitive to initial conditions.

For example let's re-run the simulation but change the initial conditions. Let's change them by a very small amount, say 0.0001 ... and let's only change the x initial state by that very small amount. We will simulate again for 30 seconds.

```
state0 = [2.0, 3.0, 4.0];
t = 0:.01:30;

[t,state] = ode45('myLorenz', t, state0);

% plot the resuling state-space trajectory in 3D
plot3(state(:,1), state(:,2), state(:,3), 'b-', 'linewidth', 2)
xlabel('X'); ylabel('Y'); zlabel('Z');
grid on

% re-run with very small change in initial conditions
delta = 0.0001;

state0 = [2.0+delta, 3.0, 4.0];
t = 0:.01:30;

[t2,state2] = ode45('myLorenz', t, state0);

hold on
plot3(state2(:,1), state2(:,2), state2(:,3), 'r-', 'linewidth', 2)
```

You should see something like what is shown in Figure 13.8 below.

You can sort of see that at some point the two state-space trajectories diverge. You can better visualize this by plotting each state against time as shown in Figure 13.9.

But let's go one step further, let's plot the distance between each point in state-space as a function of time:

```
dist = sqrt(sum((state2-state).^2,2));
figure
plot(t,dist,'b-','linewidth',2)
```

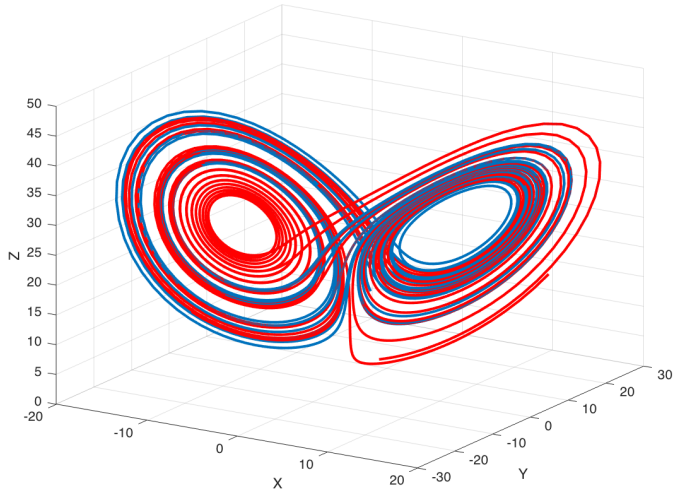


Figure 13.8: Lorenz attractor changing initial conditions

```
xlabel('TIME (sec)')
ylabel('DISTANCE')
grid on
```

You'll see something like what's shown in Figure 13.10.

If you look at the peaks, we see that up until the 15 second mark or so, the two trajectories are basically aligned, and then afterwards, they suddenly diverge, and quite significantly. We have distances in the range of 30, 40 or even 50 units—and remember, this is generated with a difference in initial conditions of only 0.0001. That's a 500,000x change.

Here's some MATLAB code to generate an animation:

```
figure
plot3(state(:,1),state(:,2),state(:,3),'b-');
hold on
plot3(state2(:,1),state2(:,2),state2(:,3),'r-');
p1 = plot3(state(1,1),state(1,2),state(1,3),'b.','markersize',30);
p2 = plot3(state2(1,1),state2(1,2),state2(1,3),'r.','markersize',30);
```

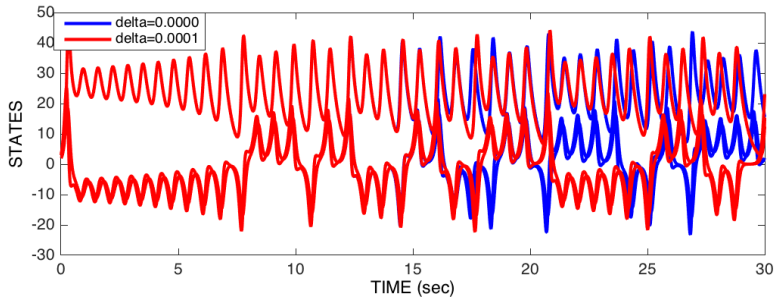


Figure 13.9: Lorenz attractor changing initial conditions

```
tt = title('0.0');
step = 3;
view([32 22])
grid on
xlabel('X'); ylabel('Y'); zlabel('Z');
drawnow
for i=1:step:length(t)
    set(p1,'XData',state(i,1));
    set(p1,'YData',state(i,2));
    set(p1,'ZData',state(i,3));
    set(p2,'XData',state2(i,1));
    set(p2,'YData',state2(i,2));
    set(p2,'ZData',state2(i,3));
    set(tt,'String',sprintf('%6.2f',t(i)));
    drawnow
end
```

You should see an animation of the two state-space trajectories.

The original simulation is shown in blue. The simulation with the altered initial condition is in red. Then an animated filled circle shows the state space over time for the original (blue) and new (red, in which the initial condition of x was increased by 0.0001). The two follow each other quite closely for a long time, and then begin to diverge at about the 16 second mark. At the 20.76 second mark they look like what's shown in Figure 13.11.

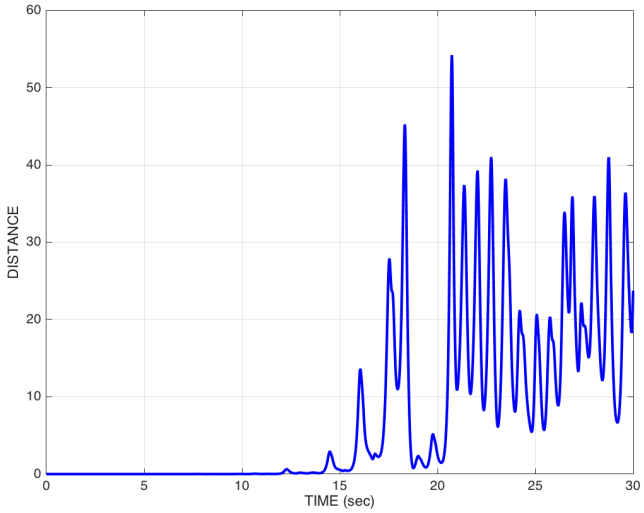


Figure 13.10: Distance between two state space trajectories

Note how the two systems are in different neighborhoods entirely!

This has illustrated how systems with relatively simple differential equations characterizing their behaviour, can turn out to be exquisitely sensitive to initial conditions. Just imagine if the initial conditions of your simulation were gathered from empirical observations (like the weather, for example). Now imagine you use a model simulation to predict whether it will be sunny (left-hand neighborhood of the plot above) or thunderstorms (right-hand neighborhood), 30 days from now. If the answer can flip between one prediction and the other, based on a 1/10,000 different in measurement, you had better be sure of your empirical measurement instruments, when you make a prediction 30 days out! Actually this won't even solve the problem, no matter how precise your measurements. The point is that the system as a whole is very sensitive to even tiny changes in initial conditions. This is one reason why short-term weather forecasts are relatively accurate, but forecasts past a couple of days can turn out to be dead wrong.

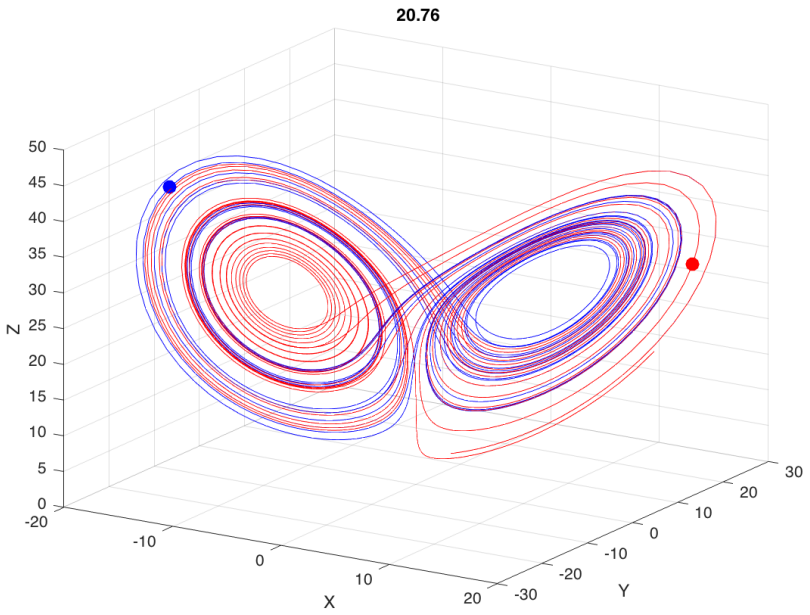


Figure 13.11: Animation of two Lorenz attractors

Exercises

E 13.1 **Mass-Spring simulation**

What is the influence of the sign and magnitude of the stiffness parameter k?

E 13.2 **Mass-Spring simulation**

In physics, damping[192] can be used to reduce the magnitude of oscillations. Damping generates a force that is directly proportional to velocity ($F = -b\dot{x}$). Add damping to the mass-spring system and re-run the simulation. Specify the value of the damping constant $b = -2.0$. What happens?

E 13.3 **Mass-Spring simulation**

What is the influence of the sign and magnitude of the damping coefficient b?

E 13.4 **Mass-Spring simulation**

Double the mass, and re-run the simulaton. What happens?

E 13.5 **Lotka-Volterra Predator-Prey Model**

Above, in Equations 13.3 and 13.3 the lotka-volterra equations are given, which describe a classic predator-prey model. The variable x is the numebr of prey (for example, rabbits), y is the number of predators (e.g. foxes), and $\dot{x}$ and $\dot{y}$ are the growth rates (rate of change over time) of the two populations. Assumptions of the model are:

- prey find ample food at all times
- food supply of predators depends entirely on prey population
- rate of change of population is proportional to its size
- the environment does not change

The values α, β, γ and σ are parameters (constants) that characterize different aspects of the two populations. The parameters can be interpreted as:

- α is the natural growth rate of prey in the absence of predation
- β is the death rate per encounter of prey due to predation
- σ is related to the growth rate of predators
- γ is the natural death rate of predators in the absence of food (prey)

Your task is to simulate this system. Here are some hints about the steps you will have to implement in MATLAB:

- write a MATLAB function that characterizes how the system's state derivatives are related to the system's states (this is given by the equations above)
- decide on values of the system parameters
- decide on values of the initial conditions of the system (the initial values of the states)
- decide on a time span and time resolution for simulating the system
- simulate! (i.e. use `ode45()` to integrate the differential equations over time)

- examine the states, typically by plotting them

Here is some code to help you get started:

```
function stated = lotkaVolterra(t, state)

  x = state(1);
  y = state(2);
  alpha = 0.1;
  beta =  0.1;
  sigma = 0.1;
  gamma = 0.1;
  xd = x*(alpha - beta*y);
  yd = -y*(gamma - sigma*x);
  stated = [xd; yd];

end
```

```
t = 0:1:500;
state0 = [0.5, 0.5];
[t,state] = ode45('lotkaVolterra', t, state0);

figure
plot(t,state(:,1:2))
xlabel('TIME')
ylabel('POPULATION SIZE')
legend({'x (prey)','y (predator)'})
```

Here are some other things to do:

- Plot the trajectory of the system in *state-space* (like we did for the Lorenz attractor). In other words, plot prey population against predator population size. What do these look like?
- increase the α parameter and re-run the simulation. What happens and why?
- set all parameters to 0.2—what happens and why?
- try the following: $(\alpha, \beta, \gamma, \sigma) = (0.20, 0.20, 0.02, 0.0)$. What happens and

why?

Links

[179] http://en.wikipedia.org/wiki/Lotka_Volterra_equation

[180] http://en.wikipedia.org/wiki/Hodgkin-Huxley_model

[181] http://en.wikipedia.org/wiki/Hooke's_law

[182] http://en.wikipedia.org/wiki/Newton's_laws_of_motion

[183] http://en.wikipedia.org/wiki/Newton's_laws_of_motion#Newton.27s_second_law

[184] http://en.wikipedia.org/wiki/Runge–Kutta_methods

[185] http://en.wikipedia.org/wiki/Gravitational_constant

[186] https://en.wikipedia.org/wiki/Double_pendulum

[187] http://en.wikipedia.org/wiki/Lorenz_system

[188] http://en.wikipedia.org/wiki/Nonlinear_system

[189] http://en.wikipedia.org/wiki/Chaos_theory

[190] http://en.wikipedia.org/wiki/Butterfly_effect

[191] https://www.youtube.com/watch?v=YS_xtBMUrJg

[192] http://en.wikipedia.org/wiki/Damping

14 Modelling Action Potentials

In this chapter we will use a model of voltage-gated ion channels in a single neuron to simulate action potentials. The model is based on the work by Hodgkin & Huxley in the 1940s and 1950s. A good reference to refresh your memory about how ion channels in a neuron work is the Kandel, Schwartz & Jessel book "Principles of Neural Science".

- A. L. Hodgkin and A. F. Huxley. A quantitative description of membrane current and its application to conduction and excitation in nerve. J. Physiol. (Lond.), 117(4):500-544, Aug 1952
- A. L. Hodgkin, A. F. Huxley, A. L. Hodgkin, and A. F. Huxley. A quantitative description of membrane current and its application to conduction and excitation in nerve. 1952. Bull. Math. Biol., 52(1-2):25-71, 1990
- O. Ekeberg, P. Wallen, A. Lansner, H. Traven, L. Brodin, and S. Grillner. A computer based model for realistic simulations of neural networks. I. The single neuron and synaptic interaction. Biol Cybern, 65(2):81-90, 1991
- E.R. Kandel, J.H. Schwartz, T.M. Jessell, et al. Principles of neural science, volume 4. McGraw-Hill New York, 2000

To model the action potential we will use an article by Ekeberg et al. (1991) published in Biological Cybernetics (see citation above). When reading the article you can focus on the first three pages (up to paragraph 2.3) and try to find answers to the following questions:

- How many differential equations are there?
- What is the order of the system described in equations 1-9?

- What are the states and state derivatives of the system?

Before we begin coding up the model, it may be useful to remind you of a fundamental law of electricity, one that relates electrical potential V to electric current I and resistance R (or conductance G, the reciprocal of resistance). This of course is known as Ohm's law[193]:

$$V = IR \tag{14.1}$$

or

$$V = \frac{I}{G} \tag{14.2}$$

Our goal here is to code up a dynamical model of the membrane's electric circuit including two types of ion channels: sodium and potassium channels. We will use this model to better understand the process underlying the origin of an action potential.

14.1 The Neuron Model

Figure 14.1 below, adapted from Ekeberg et al., 1991, schematically illustrates the model of a neuron. In panel A we see a soma, and multiple dendrites. Each of these can be modelled by an electrical "compartment" (Panel B) and the passive interactions between them can be modelled as a pretty standard electrical circuit (see Biological Neuron Model[194] for more details about compartmental models of neurons). In panel C, we see an expanded model of the Soma from panel A. Here, a number of active ion channels are included in the model of the soma.

For our purposes here, we will focus on the soma, and we will not include any additional dendrites in our implementation of the model. Thus essentially we will be modelling what appears in panel C, and at that, only a subset.

In panel C we see that the soma can be modelled as an electrical circuit with a

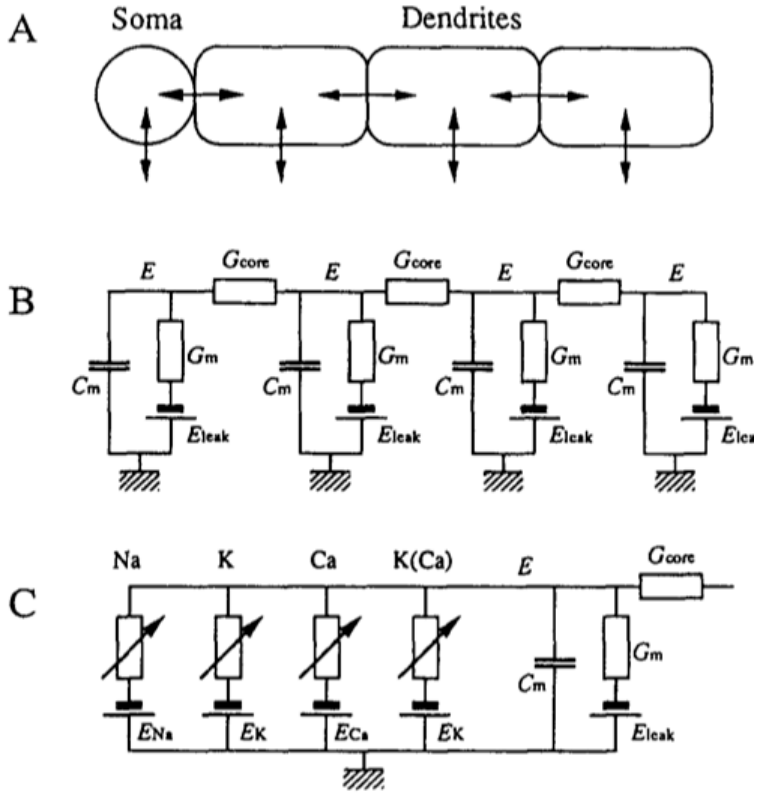


Figure 14.1: Schematic of Ekeberg et al. 1991 neuron model

sodium ion channel (Na), a potassium ion channel (K), a calcium ion channel (Ca), and a calcium-dependent potassium channel (K(Ca)). What we will be concerned with simulating, ultimately, is the intracellular potential E.

14.2 Passive Properties

Equation (1) of Ekeberg is a differential equation describing the relation between the time derivative of the membrane potential E as a function of the passive leak current through the membrane, and the current through the ion channels. Note that Ekeberg uses E instead of the typical V symbol to represent electrical potential.

$$\frac{dE}{dt} = \frac{(E_{leak} - E)G_m + \sum (E_{comp} - E)G_{core} + I_{channels}}{C_m} \tag{14.3}$$

Don't panic, it's not actually that complicated. What this equation is saying is that the rate of change of electrical potential across the current (the left hand side of the equation, $\frac{dE}{dt}$) is equal to the sum of a bunch of other terms, divided by membrane capacitance C_m (the right hand side of the equation). Recall from basic physics that capacitance[195] is a measure of the ability of something to store an electrical charge.

The "bunch of other things" is a sum of three things, actually, (from left to right): a passive leakage current, plus a term characterizing the electrical coupling of different compartments, plus the currents of the various ion channels. Since we are not going to be modelling dendrites here, we can ignore the middle term on the right hand side of the equation $\sum (E_{comp} - E)G_{core}$ which represents the sum of currents from adjacent compartments (we have none).

We are also going to include in our model an external current I_{ext}. This can essentially represent the sum of currents coming in from the dendrites (which we are not explicitly modelling). It can also represent external current injected in a patch-clamp[196] experiment. This is what we as experimenters can manipulate, for example, to see how neuron spiking behaviour changes. So what we will actually be working with is this:

$$\frac{dE}{dt} = \frac{(E_{leak} - E)G_m + I_{channels} + I_{ext}}{C_m} \tag{14.4}$$

What we need to do now is unpack the $I_{channels}$ term representing the currents from all of the ion channels in the model. Initially we will only be including two, the potassium channel (K) and the sodium channel (Na).

14.3 Sodium Channels (Na)

The current through sodium channels that enter the soma are represented by equation (2) in Ekeberg et al. (1991):

$$I_{Na} = (E_{Na} - E_{soma})G_{Na}m^3h \tag{14.5}$$

where m is the activation of the sodium channel and h is the inactivation of the sodium channel, and the other terms are constant parameters: E_{Na} is the reversal potential, G_{Na} is the maximum sodium conductance throught the membrane, and E_{soma} is the membrane potential of the soma.

The activation m of the sodium channels is described by the differential equation (3) in Ekeberg et al. (1991):

$$\frac{dm}{dt} = \alpha_m(1 - m) - \beta_m m \tag{14.6}$$

where α_m represents the rate at which the channel switches from a closed to an open state, and β_m is rate for the reverse. These two parameters α and β depend on the membrane potential in the soma. In other words the sodium channel is voltage-gated. Equation (4) in Ekeberg et al. (1991) gives these relationships:

$$\alpha_m = \frac{A(E_{soma} - B)}{1 - e^{(B - E_{soma})/C}} \tag{14.7}$$

$$\beta_m = \frac{A(B - E_{soma})}{1 - e^{(E_{soma} - B)/C}} \tag{14.8}$$

A tricky bit in the Ekeberg et al. (1991) paper is that the A, B and C parameters above are different for α and β even though there is no difference in the symbols used in the equations.

The inactivation of the sodium channels is described by a similar set of equations: a differential equation giving the rate of change of the sodium channel deactivation, from Ekeberg et al. (1991) equation (5):

$$\frac{dh}{dt} = \alpha_h(1 - h) - \beta_h h \tag{14.9}$$

and equations specifying how α_h and β_h are voltage-dependent, given in Ekeberg et al. (1991) equation (6):

$$\alpha_h = \frac{A(B - E_{soma})}{1 - e^{(E_{soma} - B)/C}} \tag{14.10}$$

$$\beta_h = \frac{A}{1 - e^{(B - E_{soma})/C}} \tag{14.11}$$

Note again that although the terms A, B and C are different for α_h and β_h even though they are represented by the same symbols in the equations.

So in summary, for the sodium channels, we have two state variables: (m, h) representing the activation (m) and deactivation (h) of the sodium channels. We have a differential equation for each, describing how the rate of change (the first derivative) of these states can be calculated: Ekeberg equations (3) and (5). Those differential equations involve parameters (α, β), one set for m and a second set for h. Those (α, β) parameters are computed from Ekeberg equations (4) (for m) and (6) (for h). Those equations involve parameters (A, B, C) that have parameter values specific to α and β and m and h (see Table 1 of Ekeberg et al., 1991).

14.4 Potassium Channels (K)

The potassium channels are represented in a similar way, although in this case there is only channel activation, and no inactivation. In Ekeberg et al. (1991) the three equations (7), (8) and (9) represent the potassium channels:

$$I_k = (E_k - E_{soma}) G_k n^4 \tag{14.12}$$

$$\frac{dn}{dt} = \alpha_n (1 - n) - \beta_n n \tag{14.13}$$

where n is the state variable representing the activation of potassium channels. As before we have expressions for (α, β) which represent the fact that the potassium channel is also voltage-gated:

$$\alpha_n = \frac{A(E_{soma} - B)}{1 - e^{(B - E_{soma})/C}} \quad (14.14)$$

$$\beta_n = \frac{A(B - E_{soma})}{1 - e^{(E_{soma} - B)/C}} \quad (14.15)$$

Again, the parameter values for (A, B, C) can be found in Ekeberg et al., (1991) Table 1.

To summarize, the potassium channel has a single state variable n representing the activation of the potassium channel.

14.5 Summary

We have a model now that includes four state variables:

1. E representing the potential in the soma, given by differential equation (1) in Ekeberg et al., (1991)
2. m representing the activation of sodium channels, Ekeberg equation (3)
3. h representing the inactivation of sodium channels, Ekeberg equation (5)
4. n representing the activation of potassium channels, Ekeberg equation (8)

Each of the differential equations that define how to compute state derivatives, involve (α, β) terms that are given by Ekeberg equations (4) (for m), (6) (for h) and (9) (for n).

So what we have to do in order to simulate the dynamic behaviour of this neuron over time, is simply to implement these equations in MATLAB code, give the system some reasonable initial conditions, and simulate it over time using the `ode45()` function.

14.6 MATLAB code

Here is a MATLAB function called `ekeberg.m` that implements the equations. It looks intimidating but really it's just an implementation of the equations above.

```
function stated = ekeberg(t,state,params)

% Purpose: simulate Hodgkin and Huxley model for the action potential using
% the equations from Ekeberg et al, Biol Cyb, 1991
% Input: state ([E m h n] (ie [membrane potential; activation of
%          Na++ channel; inactivation of Na++ channel; activation of K+
%          channel]),
%          t (time),
%          and the params (parameters of neuron; see Ekeberg et al)
% Output: statep (state derivatives)

E = state(1);
m = state(2);
h = state(3);
n = state(4);

Epar = params.E;
Na   = params.Na;
K    = params.K;

% external current (from "voltage clamp", other compartments, other
% neurons, etc)
I_ext = Epar.I_ext;

% calculate Na rate functions and I_Na
alpha_act = Na.A_alpha_m_act * (E-Na.B_alpha_m_act) / ...
            (1.0 - exp((Na.B_alpha_m_act-E) / Na.C_alpha_m_act));
beta_act = Na.A_beta_m_act * (Na.B_beta_m_act-E) / ...
            (1.0 - exp((E-Na.B_beta_m_act) / Na.C_beta_m_act) );
dmdt = ( alpha_act * (1.0 - m) ) - ( beta_act * m );

alpha_inact = Na.A_alpha_m_inact * (Na.B_alpha_m_inact-E) / ...
             (1.0 - exp((E-Na.B_alpha_m_inact) / Na.C_alpha_m_inact));
beta_inact  = Na.A_beta_m_inact / (1.0 + (exp((Na.B_beta_m_inact-E) / ...
              Na.C_beta_m_inact)));
dhdt = ( alpha_inact*(1.0 - h) ) - ( beta_inact*h );

% Na-current:
I_Na =(Na.Na_E-E) * Na.Na_G * (m^Na.k_Na_act) * h;
```

```
% calculate K rate functions and I_K
alpha_kal = K.A_alpha_m_act * (E-K.B_alpha_m_act) / ...
            (1.0 - exp((K.B_alpha_m_act-E) / K.C_alpha_m_act));
beta_kal = K.A_beta_m_act * (K.B_beta_m_act-E) / ...
           (1.0 - exp((E-K.B_beta_m_act) / K.C_beta_m_act));
dndt = ( alpha_kal*(1.0 - n) ) - ( beta_kal*n );
I_K = (K.k_E-E) * K.k_G * n^K.k_K;

% leak current
I_leak = (Epar.E_leak-E) * Epar.G_leak;

% calculate derivative of E
dEdt = (I_leak + I_K + I_Na + I_ext) / Epar.C_m;
stated = [dEdt; dmdt; dhdt; dndt];

end
```

Here is a MATLAB script called `go_ekeberg.m` that sets up the parameters of the model, and runs a simulation:

```
%% setup parameters

E.E_leak = -7.0e-2;
E.G_leak =  3.0e-09;
E.C_m    =  3.0e-11;
E.I_ext  =  0*1.0e-10;

Na.Na_E            =  5.0e-2;
Na.Na_G            =  1.0e-6;
Na.k_Na_act        =  3.0e+0;
Na.A_alpha_m_act   =  2.0e+5;
Na.B_alpha_m_act   = -4.0e-2;
Na.C_alpha_m_act   =  1.0e-3;
Na.A_beta_m_act    =  6.0e+4;
Na.B_beta_m_act    = -4.9e-2;
Na.C_beta_m_act    =  2.0e-2;
Na.l_Na_inact      =  1.0e+0;
Na.A_alpha_m_inact =  8.0e+4;
Na.B_alpha_m_inact = -4.0e-2;
```

```
Na.C_alpha_m_inact =  1.0e-3;
Na.A_beta_m_inact  =  4.0e+2;
Na.B_beta_m_inact  = -3.6e-2;
Na.C_beta_m_inact  =  2.0e-3;

K.k_E           = -9.0e-2;
K.k_G           =  2.0e-7;
K.k_K           =  4.0e+0;
K.A_alpha_m_act =  2.0e+4;
K.B_alpha_m_act = -3.1e-2;
K.C_alpha_m_act =  8.0e-4;
K.A_beta_m_act  =  5.0e+3;
K.B_beta_m_act  = -2.8e-2;
K.C_beta_m_act  =  4.0e-4;

params.E  = E;
params.Na = Na;
params.K  = K;

%% simulate

% set initial states and time vector
state0 = [-70e-03, 0, 1, 0];
t = 0:0.001:0.2;

% let's inject some external current
params.E.I_ext = 1.0e-10;

% run simulation
ekeberg_f = @(t,state) ekeberg(t,state,params);
[t,state] = ode45(ekeberg_f, t, state0);

%% plot the results

figure('position',[39 268 560 925],'paperposition',[2.4 2.5 3.6 6.0])
subplot(4,1,1)
plot(t, state(:,1))
title('membrane potential')
subplot(4,1,2)
plot(t, state(:,2))
```

```
title('Na2+ channel activation')
subplot(4,1,3)
plot(t, state(:,3))
title('Na2+ channel inactivation')
subplot(4,1,4)
plot(t, state(:,4))
title('K+ channel activation')
xlabel('TIME (sec)')
```

What you will see is a figure as shown in Figure 14.2 below.

Exercises

E 14.1 Alter the code so that the modelled neuron only has the leakage current and external current. In other words, comment out the terms related to sodium and potassium channels. Run a simulation with an initial membrane potential of -70mv and an external current of 0.0mv. What happens and why?

E 14.2 Change the external current to 1.0e-10 and re-run the simulation. What happens and why?

E 14.3 Add in the terms related to the sodium channel (activation and deactivation). Run a simulation with external current of 1.0e-10 and initial states [-70e-03, 0, 1]. What happens and why?

E 14.4 Add in the terms related to the potassium channel. Run a simulation with external current of 1.0e-10 and initial states [-70e-03, 0, 1, 0]. What happens and why?

E 14.5 Play with the external current level (increase it slightly, decrease it slightly, etc). What is the effect on the behaviour of the neuron?

E 14.6 What is the minimum amount of external current necessary to generate an action potential? Why?

Links

[193] http://en.wikipedia.org/wiki/Ohm's_law

[194] http://en.wikipedia.org/wiki/Biological_neuron_model

[195] http://en.wikipedia.org/wiki/Capacitance

[196] http://en.wikipedia.org/wiki/Patch_clamp

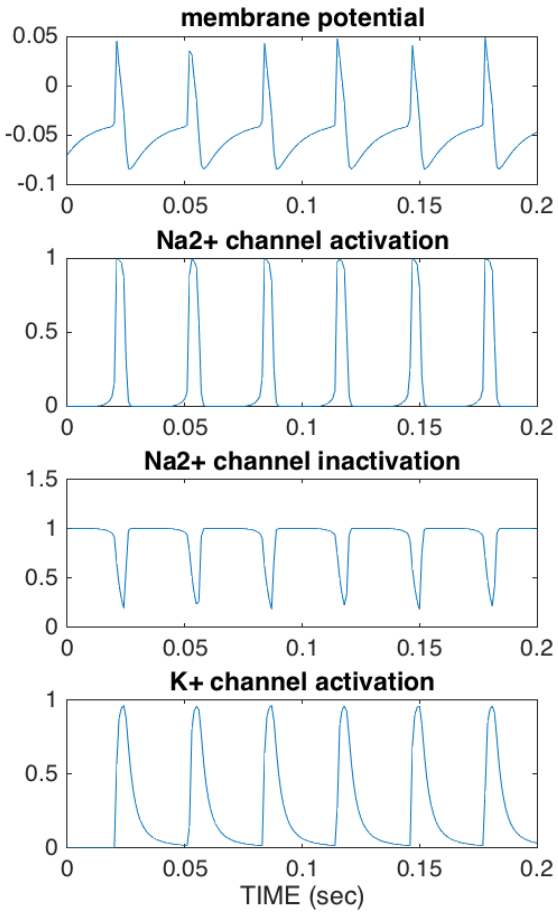


Figure 14.2: Simulation of a neuron using equations from Ekeberg et al., Biol. Cybern. (1991)

15 Basic statistical tests

MATLAB has a toolbox called the Statistics and Machine Learning Toolbox that contains many, many useful functions for statistical analyses.

Statistics and Machine Learning Toolbox[197] documentation.

We will review only a small subset of its functionality here, so you can get a feel for how you might analyse data in MATLAB.

15.1 Probability Distributions

MATLAB has support for a number of common probability distributions including discrete and continuous distributions, including (but not limited to) the following:

- Uniform
- Normal (Gaussian)
- Binomial
- Poisson
- Beta
- Chi-Square
- Exponential
- Gamma
- Lognormal
- Student's t
- Weibull

- F distribution

Each distribution will have functions in MATLAB for the following:

- cumulative distribution function
- probability density function
- inverse cumulative distribution function
- generating random values

So for example for a Normal distribution with mean 100 and standard deviation 15, you could find the area under the curve to the left of the value x=130 using:

```
y = cdf('Normal',130,100,15)
```

```
y =

    0.9772
```

This tells you that 130 is the 97.72 percentile.

To generate random values using a Normal distribution you could use either the `random` function or the more direct `randn` function. To generate 10 random values from a Normal distribution with mean 100 and standard deviation 15:

```
y = randn(1,10)*15 + 100
```

```
y =

  108.0650  127.5083   66.1173  112.9326  104.7815   80.3847   93.4961  105.
    1394  153.6760  141.5416
```

or:

```
>> y = random('Normal', 100, 15, [1,10])
```

```
y =

   79.7517  145.5239  110.8811   99.0542  110.7211   96.9255   98.1378  122.
    3455  121.1355  121.2579
```

15.1.1 Random Seed

An important note about random numbers and computers: The values that are generated are never truly random but only pseudorandom. Remember, computers are deterministic. They can only simulate random numbers. Random number generating algorithms are based on a *seed* value that all subsequent values are based on. This is both good and bad. It's good, because it means if you use the same seed value at the beginning of your program, then each time your program runs, you will get the *same* set of pseudo-random numbers. This is handy for testing and validation purposes. On the other hand if you want different random values each time your program runs, you can still do that, by setting a different seed each time—for example a seed based on the date and/or clock time.

You can test this by closing MATLAB, launching it, and typing:

```
rand(1,5)
```

```
ans =

    0.8147    0.9058    0.1270    0.9134    0.6324
```

Now close MATLAB again and re-open it again, and re-type:

```
rand(1,5)
```

and you ought to get the same random values:

```
ans =

    0.8147    0.9058    0.1270    0.9134    0.6324
```

To set the random seed in MATLAB to a different value, put this line of code at the beginning of your program:

```
rng('shuffle')
```

```
rand(1,5)
```

```
ans =

    0.3672    0.7020    0.8560    0.0797    0.5879
```

15.1.2 Fitting

MATLAB has a function called `fitdist` that will fit a given probability distribution to some data. Here is how to use it. First let's generate 100 data points from a Normal distribution with mean 0 and standard deviation 1:

`fitdist`

```
x = randn(100,1);
```

Now let's use `fitdist` to fit the (2) parameters of a Normal distribution (mean mu, and standard deviation sigma) to the data:

```
d = fitdist(x, 'normal');
```

produces:

```
d =

  NormalDistribution

  Normal distribution
       mu = -0.0726815   [-0.272105, 0.126743]
    sigma =    1.00505   [0.882442, 1.16754]
```

You can use `fitdist` with other distributions besides Normal, just see the documentation in MATLAB.

15.2 Hypothesis Tests

MATLAB has functionality for various kinds of statistical hypothesis tests. Here we outline just a few. See the full documentation for all the details.

15.2.1 t-test

The function `ttest` performs a one-sample or a paired-sample t-test. The function `ttest2` performs an independent samples t-test.

Imagine we have a dependent variable measured from 5 subjects in two conditions:

```
c1 = [1,3,2,3,3];
c2 = [2,5,4,3,5];
```

We can perform a paired-samples t-test:

```
[H,P,CI,STATS] = ttest(c1,c2)
```

```
H =

     1
```

```
P =

    0.0249


CI =

   -2.5106   -0.2894


STATS =

    tstat: -3.5000
       df: 4
       sd: 0.8944
```

The first parameter is whether we reject (1=TRUE) or not (0=FALSE) the null hypothesis that the two groups were sampled from the same population. The second parameter gives the probability of obtaining a value of t as large as the one we did, under the null hypothesis. In this case, p=0.0249. The third parameter is an array containing the 95% confidence interval on the difference between means. The fourth parameter is a `struct` with the t-statistic, the degrees of freedom of the t-test, and the estimate of the standard error of the differences between means. You might report the result of this t-test in a paper like this: t(4)=-3.5, p=0.0249.

There are optional parameters to pass to the `ttest` function for things like one-tailed vs two-tailed tests, and alpha level for rejecting the null hypothesis.

Also have a look at `ttest2` for independent-samples t-tests. Here you also have as an optional parameter whether to assume equal or unequal variances.

15.2.2 Analysis of Variance

MATLAB has a number of functions for performing different kinds of analyses of variance:

- `anova1`: One-way analysis of variance
- `anova2`: Two-way analysis of variance
- `anovan`: N-way analysis of variance
- `aoctool`: Analysis of Covariance
- ANOVA with Random Effects[198]
- `ranova`: Repeated-Measures ANOVA
- `manova`: Multivariate analysis of variance

We are not going to go through all the different kinds of ANOVA here. For now let's just see a simple example of a two-factor, between-subjects ANOVA.

MATLAB includes sample data from a study of popcorn brands and popper types. The columns are brands: (Gourmet, National, Generic) and the rows are popper types (Oil vs Air). The dependent variable is the yield of popped popocorn, measured in cups. The first 3 rows are the oil popper and the last 3 rows are the air popper. Researchers popped a batch of each brand three times with each popper, i.e. the number of replications in each cell of the design is 3.

```
load popcorn
popcorn
```

```
popcorn =

    5.5000    4.5000    3.5000
    5.5000    4.5000    4.0000
    6.0000    4.0000    3.0000
    6.5000    5.0000    4.0000
    7.0000    5.5000    5.0000
    7.0000    5.0000    4.5000
```

To perform a two-way ANOVA and save the output into a cell array called `tbl`:

```
[p,tbl] = anova2(popcorn, 3);
```

```
Source          SS      df     MS       F     Prob>F
-----------------------------------------------------
Columns       15.75      2   7.875     56.7   0
Rows           4.5       1   4.5       32.4   0.0001
Interaction    0.0833    2   0.04167    0.3   0.7462
Error          1.6667   12   0.13889
Total         22        17
```

We get a standard ANOVA table output in a Figure window. We also have these values in our `tbl` variable:

```
>> tbl

tbl =

    'Source'         'SS'         'df'    'MS'        'F'          'Prob>F'
    'Columns'        [15.7500]    [ 2]    [7.8750]    [56.7000]    [7.6790e
    -07]
    'Rows'           [ 4.5000]    [ 1]    [4.5000]    [32.4000]    [1.0037e
    -04]
    'Interaction'    [ 0.0833]    [ 2]    [0.0417]    [ 0.3000]    [    0.
    7462]
    'Error'          [ 1.6667]    [12]    [0.1389]           []
    []
    'Total'          [     22]    [17]          []           []
    []
```

So we see there is a significant main effect of Columns (popper Brand, $F(2,12)=56.7$, $p<.0000001$), a significant main effect of Rows (popper type, $F(1,12)=32.4$, $p<.0001$) and no significant interaction effect ($F(2,12)=0.3$, $p>.7462$).

See the documentation for `multcompare` to see how to run post-hoc multiple comparisons on the data, to see which groups are reliably different.

15.2.3 Multiple Regression

MATLAB comes with a sample dataset called `carsmall`, which contains all sorts of measures of 100 automobiles including:

- acceleration
- number of engine cylinders
- engine displacement
- engine horsepower
- manufacturer
- model
- model year
- miles per gallon
- origin
- weight

Let's say we want to produce a multiple regression model that uses Weight and Acceleration to predict Miles Per Gallon. First store our data in a table:

```
tbl = table(Weight,Acceleration,MPG,'VariableNames',{'Weight','Acceleration
    ','MPG'});
```

We can then use `fitlm` to fit a linear regression model to the data:

```
lm = fitlm(tbl, 'MPG ~ Weight + Acceleration')
```

This says, make a linear model where the MPG variable depends on ( ) Weight and Acceleration.

The regression equation looks like this:

$$\text{MPG} = \beta_0 + \beta_1 \text{Weight} + \beta_2 \text{Acceleration} \tag{15.1}$$

```
lm =


Linear regression model:
    MPG ~ 1 + Weight + Acceleration

Estimated Coefficients:
                     Estimate         SE         tStat       pValue
                    __________    __________    _______    __________

    (Intercept)         45.155        3.4659     13.028    1.6266e-22
    Weight          -0.0082475    0.00059836    -13.783    5.3165e-24
    Acceleration       0.19694       0.14743     1.3359       0.18493


Number of observations: 94, Error degrees of freedom: 91
Root Mean Squared Error: 4.12
R-squared: 0.743,  Adjusted R-Squared 0.738
F-statistic vs. constant model: 132, p-value = 1.38e-27
```

The output tells that $\beta_0 = 45.155$, $\beta_1 = -0.0082475$ and $\beta_2 = 0.19694$. The R-squared on the model as a whole is 0.743.

The tStat and pValue columns in the output tell you the t-statistic and corresponding p-value on a hypothesis test where the null hypothesis is that the value of the corresponding β parameter is zero. This tells us that the Acceleration β value is not reliably different than zero—in other words, perhaps Acceleration doesn't have an impact in the model that includes Weight.

There are also functions for doing Stepwise Regression, which is a procedure where you give MATLAB a list of variables to consider, and it produces a minimal model that includes only the variables that account for a significant (and unique) portion of variance in the dependent variable.

MATLAB can also do generalized regression, for example Logistic Regression. Check the documentation.

15.3 Resampling techniques

Many of the so-called *parametric* tests that we know and love, like the t-test, and ANOVA, and so on, depend on various assumptions, for example that the data come from a Normal distribution, that different groups have the same variance, etc. Sometimes we don't want to have to adhere to these assumptions (and sometimes they are downright false).

Computers are fast, and high-level programming languages like MATLAB have become easier and more convenient to use, and so many people find numerical techniques like resampling (sometimes called bootstrapping) to be a better way to go.

Let's proceed using an example in which we have two groups: a control group and a drug group. Each group has 10 (different) subjects. Each subject contributes one score. Here are the data:

```
g1 = [3,2,2,4,2,1,2,3,3,2]';
g2 = [4,3,3,2,3,5,4,3,6,4]';
```

We could do an independent-samples t-test on the data like this:

```
[h,p,ci,stats] = ttest2(g1,g2)
```

```
h =

     1


p =

    0.0102
```

```
ci =

   -2.2525   -0.3475


stats =

    tstat: -2.8673
       df: 18
       sd: 1.0138
```

And we see we get a p-value of 0.0102. But let's say we don't want to have to make the assumptions that the population data are Normal and the variances are equal. Let's instead do a bootstrap/resampling test.

The idea here is to *simulate* the null hypothesis, namely that both groups are sampled from the same population. Now we don't have access to the stimulated population, all we have are these two samples. What we will do then, is throw both samples into a bucket, and pretend *that* is our stipulated single population. We will then simulate sampling from that bucket, with replacement, to reconstitute two groups. We will then compute a statistic of interest on those two groups (for example, the difference between means). We will then repeat this a large number of time (e.g. 5000) and count how many times we obtained a difference between means *as large as the one in the real data*. If that turns out to be sufficiently rare, we can reject the null hypothesis.

We can use the `datasample` function in MATLAB to accomplish this. The function will re-sample a list of numbers, with replacement. We simply imbed this in a loop and afterwards, compute our statistic of interest—in this case, the difference between means (but it could be anything you want).

```
% shuffle the random number generator seed
%
rng('shuffle')
```

```
N = 5000;
g_all = [g1;g2]; % throw both groups into a bucket

% pre-allocate an array to store our statistic of interest
% and loop N times, each time simulating the null hypothesis
% namely, sampling with replacement from the bucket to
% reconstitute the two groups, then re-computing the
% statistic of interest (the difference between means)
%
boot = ones(N,1);
for i=1:N
  g_resamp = datasample(g_all, 20);
  boot(i) = mean(g_resamp(1:10)) - mean(g_resamp(11:20));
end
```

We get an array `boot` which contains our statistic of interest for each of the 5000 boostrap runs. We can use the `boot` array to ask the question, how many times out of the 5000 bootstrap runs did we obtain a difference between means as large as the one for our actual observed data?

```
% compute actual observed difference between means
%
dm_observed = mean(g1) - mean(g2);
disp(sprintf('actual dm = %.3f', dm_observed))

% how many times in the bootstrap did we get a
% difference between means as large (far from zero)?
%
n_big = length( find( boot <= dm_observed ) );
disp(sprintf('%d times out of %d was dm as extreme as %.3f', ...
   n_big, N, dm_observed))
```

```
actual dm = -1.300
33 times out of 5000 was dm as extreme as -1.300
```

When I ran this I got 33 times out of 5000 was the boostrapped value as extreme as the empirically observed one. You might get something slightly different if your random number generator was seeded using a different value.

We can draw a histogram of the boostrapped distribution of differences between means, and overlay using a vertical red line, our empirically observed difference between means:

```
hist(boot)
hold on
plot([dm_observed dm_observed], get(gca,'ylim'), 'r-', 'linewidth',2)
```

You will see something like what is shown in Figure 15.1 below.

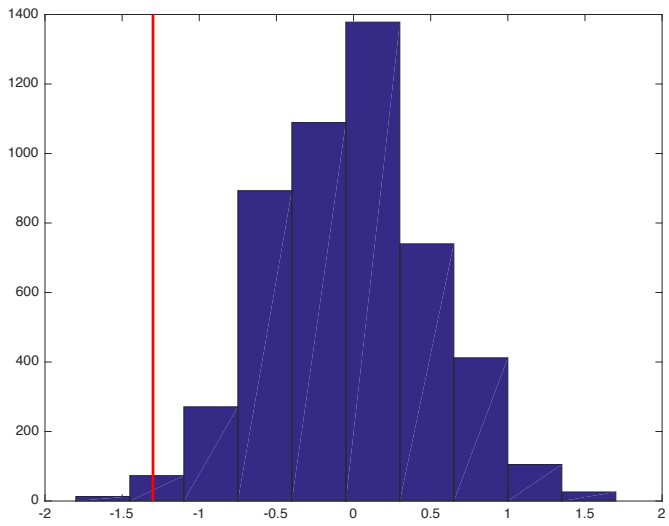


Figure 15.1: Boostrapped distribution of difference between means.

Of the 5000 simulations of the null hypothesis, it's relatively rare that we get a difference between means as extreme as the empirically observed value (the red vertical line). Most of the time, we get a difference between means near zero. This makes sense under the null hypothesis.

Specifically then, 33 times out of 5000 we obtained a difference between means

as extreme as our empirically observed value. This corresponds to p=33/5000 which is 0.0066 (or 0.01 rounded up), about the same as the t-test p-value above. Here though we didn't have to make any assumptions about the underlying distribution, or variances, or anything like that.

If we adopt an alpha level of p=0.05, then our observed p=0.01 might cause us to reject the null hypothesis that the two groups were sampled from the same population.

This approach can be used for just about any statistical test. Some people say that since computers are fast, we might as well do statistical tests this way, since we don't have to make assumptions.

Exercises

E 15.1 **Correlation**

Below you see an array of 10 values in a variable called `x` and another 10 values in `y`:

```
x = [ 1 2 3  4 5  6  7  8  9 10];
y = [12 5 8 12 5 30 27 25 38 26]
```

1. What is the value of the correlation coefficient relating `x` and `y`? Hint: use the MATLAB function `corrcoef`.
2. What is the probability of obtaining such a correlation under the null hypothesis that the data in `x` and `y` were sampled from two populations for which the correlation is in fact zero? Hint: the `corrcoef` function returns a p-value if you ask for one.

E 15.2 **Linear Regression**

Fit an equation of the following form to the `x` and `y` data given above:

$$y_i = \beta_0 + \beta_1 x_i \tag{15.2}$$

Hints: you can use the `fitlm` function. You could also do it by hand using the "slash" operator. You could also do it using `polyfit`. Use whatever method you wish.

1. What are the estimates of β_0 and β_1 that correspond to the best fitting model?
2. Generate a scatterplot with `x` on the ordinate and `y` on the abscissa. Use blue squares. Overlay the linear model prediction. Use a red line.

E 15.3 Here are two data samples `a` and `b`:

```
a = [2 6 6 1 1  4 9 3 5 2];
b = [6 8 9 5 9 12 4 5 4 7];
```

Using resampling, test the hypothesis that the two samples were drawn from populations with the same mean. Use n=10,000 iterations.

- How many times out of 10,000 do you get a difference between means as extreme as the one observed between `a` and `b`?
- What is the corresponding p-value?
- What would be the difference between means that corresponds to a $p = 0.05$ level of significance?

Links

[197] http://www.mathworks.com/help/stats/

[198] http://www.mathworks.com/examples/statistics/2176-anova-with-random-effects