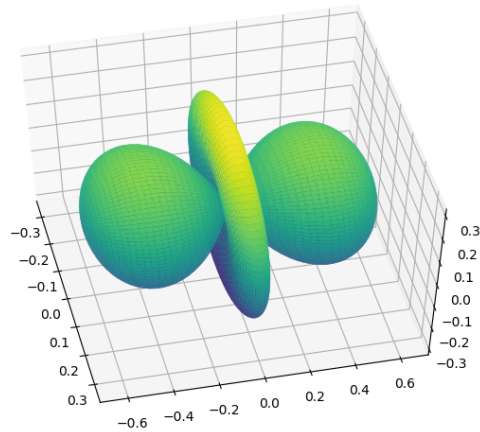


Python for Education



Learning Maths & Science using Python
and
writing them in \LaTeX

Ajith Kumar B.P.
Inter University Accelerator Centre
New Delhi 110067
www.iuac.res.in

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Preface

“Mathematics, rightly viewed, possesses not only truth, but supreme beauty – a beauty cold and austere, like that of sculpture, without appeal to any part of our weaker nature, without the gorgeous trappings of painting or music, yet sublimely pure, and capable of a stern perfection such as only the greatest art can show”, wrote Bertrand Russell about the beauty of mathematics. All of us may not reach such higher planes, probably reserved for Russels and Ramanujans, but we also have beautiful curves and nice geometrical figures with intricate symmetries, like fractals, generated by seemingly dull equations. This book attempts to explore it using a simple tool, the Python programming language.

I started using Python for the Phoenix project (www.iuac.res.in). Phoenix was driven in to Python by Pramode CE (pramode.net) and I followed. Writing this document was triggered by some of my friends who are teaching mathematics at Calicut University.

In the first chapter, a general introduction about computers and high level programming languages is given. Basics of Python language, Python modules for array and matrix manipulation, 2D and 3D data visualization, type-setting mathematical equations using latex and numerical methods in Python are covered in the subsequent chapters. Example programs are given for every topic discussed. This document is meant for those who want to try out these examples and modify them for better understanding. Huge amount of material is already available online on the topics covered, and the references to many resources on the Internet are given for the benefit of the serious reader.

The examples in this book are tested with python3. They are available on the website bpajith.github.io/python

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Ajith Kumar B P

IUAC , New Delhi

[bpajith at gmail dot com](mailto:bpajith@gmail.com)

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Chapter 1

Introduction

Primary objective of this book is to explore the possibilities of using Python language as a tool for learning mathematics and science. The reader is not assumed to be familiar with computer programming. Ability to think logically is good enough. Before getting into Python programming, we will briefly explain some basic concepts and tools required.

Computer is essentially an electronic device like a radio or a television. What makes it different from a radio or a TV is its ability to perform different kinds of tasks using the same electronic and mechanical components. This is achieved by making the electronic circuits flexible enough to work according to a set of instructions. The electronic and mechanical parts of a computer are called the Hardware and the set of instructions is called Software (or computer program). Just by changing the Software, computer can perform vastly different kind of tasks. The instructions are stored in binary format using electronic switches.

1.1 Hardware Components

Central Processing Unit (CPU), Memory and Input/Output units are the main hardware components of a computer. CPU¹ can be called the brain of the computer. It contains a Control Unit and an Arithmetic and Logic Unit, ALU. The control unit brings the instructions stored in the main memory one by one and acts according to it. It also controls the movement of data between memory and input/output units. The ALU can perform arithmetic operations like addition, multiplication and logical operations like comparing two numbers.

Memory stores the instructions and data, that is processed by the CPU. All types of information are stored as binary numbers. The smallest unit of memory is called a binary digit or Bit. It can have a value of zero or one. A group of eight bits are called a Byte. A computer has Main and Secondary types of memory. Before processing, data and instructions are moved into the main memory. Main memory is organized into words of one byte size. CPU can select any memory location by using its address. Main memory is made of semiconductor switches and is very fast. There are two types of Main Memory. Read Only Memory and the Read/Write Memory. The Read/Write Memory is also called Random Access Memory. All computers contains some programs in ROM which start running when you switch on the machine. Data and programs to be stored for future use are saved to Secondary memory, mainly devices like Hard disks, floppy disks, CDROM or removable flash storage like USB drives.

¹The cabinet that encloses most of the hardware is called CPU by some, mainly the computer vendors. They are not referring to the actual CPU chip.

The Input devices are for feeding the input data into the computer. Keyboard is the most common input device. Mouse, scanner etc. are other input devices. The processed data is displayed or printed using the output devices. The monitor screen and printer are the most common output devices.

1.2 Software components

An ordinary user expects an easy and comfortable interaction with a computer, and most of them are least inclined to learn even the basic concepts. To use modern computers for common applications like browsing and word processing, all you need to do is to click on some icons and type on the keyboard. However, to write your own computer programs, you need to learn some basic concepts, like the operating system, editors, compilers, different types of user interfaces etc. This section describes the basics from that point of view.

1.2.1 The Operating System

Operating system (OS) is the software that interacts with the user and makes the hardware resources available to the user. It starts running when you switch on the computer and remains in control. On user request, operating system loads other application programs from disk to the main memory and executes them. OS also provides a file system, a facility to store information on devices like floppy disk and hard disk. In fact the OS is responsible for managing all the hardware resources.

Various distributions of GNU/Linux and MS-Windows are the currently popular operating systems. Based on certain features, operating systems can be classified as:

- Single user, single process systems like MS DOS. Only one process can run at a time. Such operating systems do not have much control over the application programs.
- Multi-tasking systems like MS Windows, where more than one processes can run at a time.
- Multi-user, multi-tasking systems like GNU/Linux, Unix etc. More than one person can use the computer at the same time.
- Real-time systems, mostly used in control applications, where the response time to any external input is maintained under specified limits.

1.2.2 The User Interface

Interacting with a computer involves starting various application programs and managing them on the computer screen. The software that manages these actions is called the user interface. The two most common forms of user interface have historically been the Command-line Interface, where computer commands are typed out line-by-line, and the Graphical User Interface (GUI), where a visual environment (consisting of windows, menus, buttons, icons, etc.) is present.

1.2.2.1 The Command Terminal

To run any particular program, we need to request the operating system to do so. Under a Graphical User Interface, we do this by choosing the desired application from a menu. You need to remember that it is possible only because someone has added it to the menu earlier. When you start writing your own programs, obviously they will not appear in any menu. Another way to request the operating system to execute a program is to enter the name of the program (more


```

ajith@pc230: ~/test
File Edit View Terminal Tabs Help
ajith@pc230:~/test$ ls -l
total 64
-rw----- 1 ajith ajith    3 2010-06-20 17:36 asecret.dat
-rw-r--r-- 1 ajith ajith 47428 2010-05-18 12:00 foo.png
-rwxr-xr-x 1 ajith ajith   589 2010-06-08 06:42 hello.py
-rw-rw-r-- 1 ajith ajith   363 2010-06-18 10:57 share.tex
drwxr-xr-x 2 ajith ajith  4096 2010-06-20 17:34 xdata
ajith@pc230:~/test$
ajith@pc230:~/test$ cd xdata
ajith@pc230:~/test/xdata$ pwd
/home/ajith/test/xdata
ajith@pc230:~/test/xdata$ cd ..
ajith@pc230:~/test$

```

Figure 1.1: A GNU/Linux Terminal.

precisely, the name of the file containing it) at the Command Terminal. On an Ubuntu GNU/Linux system, you can start a Terminal from the menu names Applications->Accessories->Terminal (or by pressing Ctl-Alt-T). Figure 1.1 shows a Terminal displaying the list of files in a directory (output of the command 'ls -l', the -l option is for long listing).

The command processor offers a host of features to make the interaction more comfortable. It keeps track of the history of commands and we can recall previous commands, modify and reuse them using the cursor keys. There is also a completion feature implemented using the Tab key that reduces typing. Use the tab key to complete command and filenames. To run *hello.py* from our test directory, type *python h* and then press the tab key to complete it. If there are more than one file starting with 'h', you need to type more characters until the ambiguity is removed. Always use the up-cursor key to recall the previous commands and re-issue it.

The commands given at the terminal are processed by a program called the *shell*. (The version now popular under GNU/Linux is called bash, the Bourne again shell). Some of the GNU/Linux commands are listed below.

- top : Shows the CPU and memory usage of all the processes started.
- cp filename filename : copies a file to another.
- mv : moves files from one folder to another, or rename a file.
- rm : deletes files or directories.
- man : display manual pages for a program. For example 'man bash' will give help on the bash shell. Press 'q' to come out of the help screen.
- info : A menu driven information system on various topics.

See the manual pages of 'mv', cp, 'rm' etc. to know more about them. Most of these commands are application programs, stored inside the folders /bin or /sbin, that the shell starts for you and displays their output inside the terminal window.

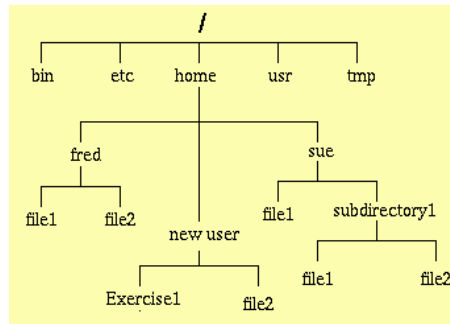


Figure 1.2: The GNU/Linux file system tree.

1.2.3 The File-system

Before the advent of computers, people used to keep documents in files and folders. The designers of the Operating System have implemented the electronic counterparts of the same. The storage space is made to appear as files arranged inside folders (directory is another term for folder). A simplified schematic of the GNU/Linux file system is shown in figure 1.2. The outermost directory is called 'root' directory and represented using the forward slash character. Inside that we have folders named bin, usr, home, tmp etc., containing different type of files.

1.2.3.1 Ownership & permissions

On a multi-user operating system, application programs and document files must be protected against any misuse. This is achieved by defining a scheme of ownerships and permissions. Each and every file on the system will be owned by a specific user. The read, write and execute permissions can be assigned to them, to control the usage. The concept of *group* is introduced to share files between a selected group of users.

There is one special user named *root* (also called the system administrator or the super user), who has permission to use all the resources. Ordinary user accounts, with a username and password, are created for everyone who wants to use the computer. In a multi-user operating system, like GNU/Linux, every user will have one directory inside which he can create sub-directories and files. This is called the 'home directory' of that user. Home directory of one user cannot be modified by another user.

The operating system files are owned by *root*. The `/home` directory contains subdirectories named after every ordinary user, for example, the user *fred* owns the directory `/home/fred` (fig 1.2) and its contents. That is also called the user's home directory. Every file and directory has three types of permissions: read, write and execute. To view them use the `'ls -l'` command. The first character of output line tells the type of the file. The next three characters show the *rw**x* (read, write, execute) permissions for the owner of that file. Next three for the users belonging to the same group and the next three for other users. A hyphen character (-) means the permission corresponding to that field is not granted. For example, the figure 1.1 shows a listing of five files:

1. `asecret.dat` : read & write for the owner. No one else can even see it.
2. `foo.png` : rw for owner, but others can view the file.
3. `hello.py` : *rw**x* for owner, others can view and execute.
4. `share.tex` : rw for owner and other members of the same group.

5. xdata is a directory. Note that execute permission is required to view contents of a directory.

The system of ownerships and permissions also protects the system from virus attacks². The virus programs damage the system by modifying some application program. On a true multi-user system, for example GNU/Linux, the application program and other system files are owned by the root user and ordinary users have no permission to modify them. When a virus attempts to modify an application, it fails due to this permission and ownership scheme.

1.2.3.2 Current Directory

There is a working directory for every user. You can create subdirectories inside that and change your current working directory to any of them. While using the command-line interface, you can use the 'cd' command to change the current working directory. Figure 1.1 shows how to change the directory and come back to the parent directory by using double dots. We also used the command 'pwd' to print the name of the current working directory.

1.3 Text Editors

To create and modify files, we use different application programs depending on the type of document contained in that file. Text editors are used for creating and modifying plain text matter, without any formatting information embedded inside. Computer programs are plain text files and to write computer programs, we need a text editor. 'gedit' is a simple, easy to use text editor available on GNU/Linux, which provides syntax high-lighting for several programming languages.

1.4 High Level Languages

In order to solve a problem using a computer, it is necessary to evolve a detailed and precise step by step method of solution. A set of these precise and unambiguous steps is called an Algorithm. It should begin with steps accepting input data and should have steps which gives output data. For implementing any algorithm on a computer, each of its steps must be converted into proper machine language instructions. Doing this process manually is called Machine Language Programming. Writing machine language programs need great care and a deep understanding about the internal structure of the computer hardware. High level languages are designed to overcome these difficulties. Using them one can create a program without knowing much about the computer hardware.

We already learned that to solve a problem we require an algorithm and it has to be executed step by step. It is possible to express the algorithm using a set of precise and unambiguous notations. The notations selected must be suitable for the problems to be solved. *A high level programming language is a set of well defined notations which is capable of expressing algorithms.*

In general a high level language should have the following features.

1. Ability to represent different data types like characters, integers and real numbers. In addition to this it should also support a collection of similar objects like character strings, arrays etc.
2. Arithmetic and Logical operators that acts on the supported data types.
3. Control flow structures for decision making, branching, looping etc.

²Do not expect this from the MS-Windows system. Even though it allows to create users, any user (by running programs or by viruses) is allowed to modify the system files. This may be because it grew from a single process system like MSDOS and still keeps that legacy.

4. A set of syntax rules that precisely specify the combination of words and symbols permissible in the language.
5. A set of semantic rules that assigns a single, precise and unambiguous meaning to each syntactically correct statement.

Program text written in a high level language is often called the Source Code. It is then translated into the machine language by using translator programs. There are two types of translator programs, the Interpreter and the Compiler. *Interpreter reads the high level language program line by line, translates and executes it. Compilers convert the entire program in to machine language and stores it to a file which can be executed.*

High level languages make the programming job easier. We can write programs that are machine independent. For the same program different compilers can produce machine language code to run on different types of computers and operating systems. BASIC, COBOL, FORTRAN, C, C++, Python etc. are some of the popular high level languages, each of them having advantages in different fields.

To write any useful program for solving a problem, one has to develop an algorithm. The algorithm can be expressed in any suitable high level language. *Learning how to develop an algorithm is different from learning a programming language. Learning a programming language means learning the notations, syntax and semantic rules of that language.* Best way to do this is by writing small programs with very simple algorithms. After becoming familiar with the notations and rules of the language one can start writing programs to implement more complicated algorithms.

1.5 On Free Software

Software that can be used, studied, modified and redistributed in modified or unmodified form without restriction is called Free Software. In practice, for software to be distributed as free software, the human-readable form of the program (the source code) must be made available to the recipient along with a notice granting the above permissions.

The free software movement was conceived in 1983 by Richard Stallman to give the benefit of "software freedom" to computer users. Stallman founded the Free Software Foundation in 1985 to provide the organizational structure to advance his Free Software ideas. Later on, alternative movements like Open Source Software came.

Software for almost all applications is currently available under the pool of Free Software. GNU/Linux operating system, OpenOffice.org office suite, L^AT_EX typesetting system, Apache web server, GIMP image editor, GNU compiler collection, Python interpreter etc. are some of the popular examples. For more information refer to www.gnu.org website.

1.6 Exercises

1. What are the basic hardware components of a computer.
2. Name the working directory of a user named 'ramu' under GNU/Linux.
3. What is the command to list the file names inside a directory (folder).
4. What is the command under GNU/Linux to create a new folder.
5. What is the command to change the working directory.
6. Can we install more than one operating systems on a single hard disk.

7. Name two most popular Desktop Environments for GNU/Linux.
8. How to open a command window from the main menu of Ubuntu GNU/Linux.
9. Explain the file ownership and permission scheme of GNU/Linux.

Chapter 2

Programming in Python

Python is a simple, high level language with a clean syntax. It offers strong support for integration with other languages and tools, comes with extensive standard libraries, and can be learned within few days. Many Python programmers report substantial productivity gains and feel the language encourages the development of higher quality, more maintainable code. To know more visit the Python website.¹

2.1 Getting started with Python

To start programming in Python, we have to learn how to type the source code and save it to a file, using a text editor program. We also need to know how to open a Command Terminal and start the Python Interpreter. The details of this process may vary from one system to another. On an Ubuntu GNU/Linux system, you can open the *Text Editor* and the *Terminal* from the Applications->Accessories menu. You may also choose an Integrated Development Environment. IDEs allows you to edit and run the program, and also has features for managing projects with multiple files. 'geany'² is a simple and lightweight IDE.

The current version of Python3, that differs from the earlier versions in some ways. All the examples given in this book are tested on python3. In case, if you do not have any computer with Python installed try online³

2.1.1 Two modes of using Python Interpreter

If you issue the command 'python3', without any argument, from the command terminal, the Python interpreter will start and display a '>>>' prompt where you can type Python statements. Use this method only for viewing the results of single Python statements, for example to use Python as a calculator. It could be confusing when you start writing larger programs, having looping and conditional statements. The preferred way is to enter your source code in a text editor, save it to a file (with .py extension) and execute it from the command terminal using Python. A screen-shot of the Desktop with Text Editor and Terminal is shown in figure 2.2.

In this document, we will start writing small programs showing the essential elements of the language without going into the details. The reader is expected to run these example programs and also to modify them in different ways. It is like learning to drive a car, you master it by practicing.

¹<http://docs.python.org/tutorial/>

²`sudo apt install geany`

³<https://trinket.io/python3>

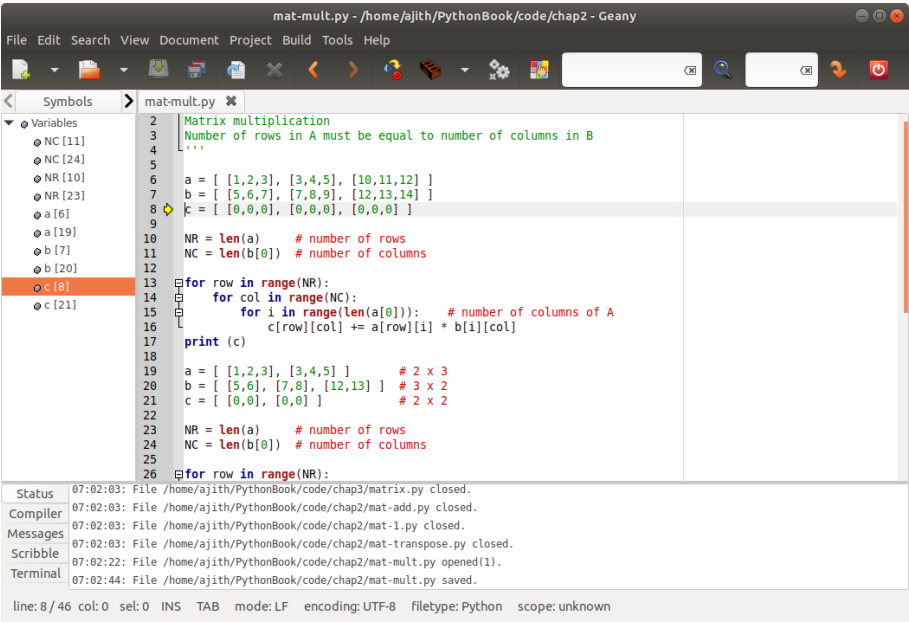


Figure 2.1: Geany IDE

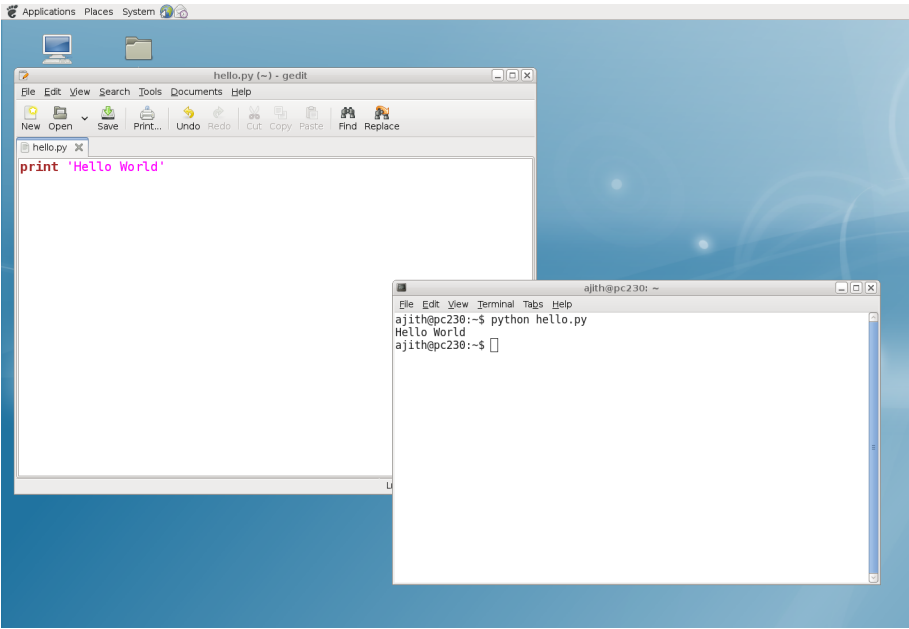


Figure 2.2: Text Editor and Terminal Windows.

Let us start with a program to display the words *Hello World* on the computer screen. This is the customary 'hello world' program. There is another version that prints 'Goodbye cruel world', probably invented by those who give up at this point. The Python 'hello world' program is shown below.

Example. hello.py

```
print ('Hello World')
```

This should be entered into a text file using any text editor. On a GNU/Linux system you may use the text editor like 'gedit' to create the source file, save it as *hello.py*. The next step is to call the Python Interpreter to execute the new program. For that, open a command terminal and (at the \$ prompt) type:

```
$ python3 hello.py
```

The filenames of python programs should not be any of the the keywords of python. For example, naming a file as 'string.py' or 'int.py' may result in hard to track error messages.

2.2 Variables and Data Types

As mentioned earlier, any high level programming language should support several data types. The problem to be solved is represented using variables belonging to the supported data types. Python supports numeric data types like integers, floating point numbers and complex numbers. To handle character strings, it uses the String data type. Python also supports other compound data types like lists, tuples, dictionaries etc.

In languages like C, C++ and Java, we need to explicitly declare the type of a variable. This is not required in Python. The data type of a variable is decided by the value assigned to it. This is called dynamic data typing. The type of a particular variable can change during the execution of the program. If required, one type of variable can be converted in to another type by explicit type casting, like $y = \text{float}(3)$. Strings are enclosed within single quotes or double quotes.

The program *first.py* shows how to define variables of different data types. It also shows how to embed comments inside a program.

Example: first.py

```
'''
A multi-line comment, within a pair of three single quotes.
In a line, anything after a # sign is also a comment
'''
x = 10
print (x, type(x))          # print x and its type
x = 10.4
print (x, type(x))
x = 3 + 4j
print (x, type(x))
x = 'I am a String '
print (x, type(x))
```

The output of the program is shown below. Note that the type of the variable x changes during the execution of the program, depending on the value assigned to it.


```

10 <type 'int'>
10.4 <type 'float'>
(3+4j) <type 'complex'>
I am a String <type 'str'>

```

The program treats the variables like humans treat labelled envelopes. We can pick an envelope, write some name on it and keep something inside it for future use. In a similar manner the program creates a variable, gives it a name and keeps some value inside it, to be used in subsequent steps. So far we have used four data types of Python: int, float, complex and str. To become familiar with them, you may write simple programs performing arithmetic and logical operations using them.

Example: oper.py

```

x = 2 y = 4
print(x + y * 2)
s = 'Hello '
print(s + s)
print(3 * s)
print(x == y)
print(y == 2 * x)
print(5/2 , 5//2)

```

Running the program *oper.py* will generate the following output.

```

10
Hello Hello
Hello Hello Hello
False
True
2.5 2

```

Note that a String can be added to another string and it can be multiplied by an integer. Try to understand the logic behind that and also try adding a String to an Integer to see what is the error message you will get. We have used the logical operator `==` for comparing two variables. The last line demonstrates the nature of division operator on python3. By default it does floating point division. Integer division can be forced by the operator `//`.

2.3 Operators and their Precedence

Python supports a large number of arithmetic and logical operators. They are summarized in the table 2.1. An important thing to remember is their precedence. In the expression $2+3*4$, is the addition done first or the multiplication? According to elementary arithmetics, the multiplication should be done first. It means that the multiplication operator has higher precedence than the addition operator. If you want the addition to be done first, enforce it by using parenthesis like $(2+3)*4$. Whenever there is ambiguity in evaluation, use parenthesis to clarify the order of evaluation.

2.4 Python Strings

So far we have come across four data types: Integer, Float, Complex and String. Out of which, String is somewhat different from the other three. It is a collection of same kind of elements,

| Operator | Description | Expression | Result |
|---|--------------------|-----------------|--------|
| or | Boolean OR | 0 or 4 | 4 |
| and | Boolean AND | 3 and 0 | 0 |
| not x | Boolean NOT | not 0 | True |
| in, not in | Membership tests | 3 in [2,2,3,12] | True |
| <, <=, >, >=, !=, == | Comparisons | 2 > 3 | False |
| | Bitwise OR | 1 2 | 3 |
| ^ | Bitwise XOR | 1 ^ 5 | 4 |
| & | Bitwise AND | 1 & 3 | 1 |
| <<, >> | Bitwise Shifting | 1 << 3 | 8 |
| +, - | Add, Subtract | 6 - 4 | 2 |
| *, / | Multiply, divide | 5 / 2 | 2.5 |
| % | remainder | 5%1 | 1 |
| // | integer division | 3/2 | 1 |
| +x, -x | Positive, Negative | -5*2 | -10 |
| ~ | Bitwise NOT | ~1 | -2 |
| ** | Exponentiation | 2 ** 3 | 8 |
| x[index] | Subscription | a='abcd' ; a[1] | 'b' |

Table 2.1: Operators in Python listed according to their precedence.

characters. The individual elements of a String can be accessed by indexing as shown in *string1.py*. String is a compound, or collection, data type.

Example: string1.py

```
s = 'hello world'
print(s[0])      # print first element, h
print(s[1])      # print e
print(s[-1])     # will print the last character
```

Addition and multiplication is defined for Strings, as demonstrated by *string2.py*.

Example: string2.py

```
a = 'hello'+'world'
print a
b = 'ha' * 3
print b
print a[-1] + b[0]
```

will give the output

```
helloworld
hahaha
dh
```

The last element of *a* and first element of *b* are added, resulting in the string 'dh'

2.4.1 Slicing

Part of a String can be extracted using the slicing operation. It can be considered as a modified form of indexing a single character. Indexing using $s[a : b]$ extracts elements $s[a]$ to $s[b - 1]$. We can skip one of the indices. If the index on the left side of the colon is skipped, slicing starts from the first element and if the index on right side is skipped, slicing ends with the last element.

Example: slice.py

```
a = 'hello world'
print(a[3:5])
print(a[6:])
print(a[:5])
```

The reader can guess the nature of slicing operation from the output of this code, shown below.

```
'lo'
'world'
'hello'
```

Please note that specifying a right side index more than the length of the string is equivalent to skipping it. Modify *slice.py* to print the result of $a[6 : 20]$ to demonstrate it.

2.5 Python Lists

List is an important data type of Python. It is much more flexible than String. The individual elements can be of any type, even another list. Lists are defined by enclosing the elements inside a pair of square brackets, separated by commas. The program *list1.py* defines a list and print its elements.

Example: list1.py

```
a = [2.3, 3.5, 234]    # make a list
print (a[0])
a[1] = 'haha'         # Change an element
print (a)
```

The output is shown below ⁴.

```
2.3
[2.3, 'haha', 234]
```

Lists can be sliced in a manner similar to that if Strings. List addition and multiplication are demonstrated by the following example. We can also have another list as an element of a list.

Example: list2.py

```
a = [1,2]
print (a * 2)
print (a + [3,4])
b = [10, 20, a]
print (b)
```

⁴The floating point number 2.3 showing as 2.2999999999999998 is interesting. This is the very nature of floating point representation of numbers, nothing to do with Python. With the precision we are using, the error in representing 2.3 is around 2.0×10^{-16} . This becomes a concern in operations like inversion of big matrices.

The output of this program is shown below.

```
[1, 2, 1, 2]
[1, 2, 3, 4]
[10, 20, [1, 2] ]
```

2.6 Mutable and Immutable Types

There is one major difference between String and List types, List is mutable but String is not. *We can change the value of an element in a list, add new elements to it and remove any existing element. This is not possible with String type.* Uncomment the last line of *third.py* and run it to clarify this point.

Example: third.py

```
s = [3, 3.5, 234]    # make a list
s[2] = 'haha'        # Change an element
print s
x = 'myname'         # String type
#x[1] = 2             # uncomment to get ERROR
```

The List data type is very flexible, an element of a list can be another list. We will be using lists extensively in the coming chapters. Tuple is another data type similar to List, except that it is immutable. List is defined inside square brackets, tuple is defined in a similar manner but inside parenthesis, like (3, 3.5, 234).

2.7 Input from the Keyboard

Since most of the programs require some input from the user, let us introduce this feature before proceeding further. In python3, the *input()* function gets String type data from the keyboard, that can be converted to integer, float or complex by using *eval()* function. A message to be displayed can be given as an argument while calling these functions.⁵

Example: kin1.py

```
x = eval(input('Enter an integer '))
y = complex(input('Enter a complex number, (like 2+5j) '))
print ('The sum is ', x + y)
s = input('Enter a String ')
print ('You entered ', s)
```

It is also possible to read more than one variable using a single *input()* statement. *String* type data read using *input()* may be converted into *integer* or *float* type if they contain only the valid characters. In order to show the effect of conversion explicitly, we multiply the variables by 2 before printing. Multiplying a String by 2 prints it twice. If the String contains invalid characters then *eval()* will give error.

Example: kin2.py

⁵Functions will be introduced later. For the time being, understand that it is an isolated piece of code, called from the main program with some input arguments and returns some output.

```

x,y = int(input('Enter x and y separated by comma '))
print 'The sum is ', x + y
s = input('Enter a decimal number ')
a = float(s)
print s * 2      # prints string twice
print a * 2      # converted value times 2

```

We have learned about the basic data types of Python and how to get input data from the keyboard. This is enough to try some simple problems and algorithms to solve them.

Example: area.py

```

pi = 3.1416
r = input('Enter Radius ')
a = pi * r ** 2      #  $A = \pi r^2$ 
print ('Area = ', a)

```

The above example calculates the area of a circle. Line three calculates r^2 using the exponentiation operator `**`, and multiply it with π using the multiplication operator `*`. r^2 is evaluated first because `**` has higher precedence than `*`, otherwise the result would be $(\pi r)^2$.

2.8 Iteration: while and for loops

If programs can only execute from the first line to the last in that order, as shown in the previous examples, it would be impossible to write any useful program. For example, we need to print the multiplication table of eight. Using our present knowledge, it would look like the following

Example: badtable.py

```

print (1 * 8)
print (2 * 8)
print (3 * 8)
print (4 * 8)
print (5 * 8)

```

Well, we are stopping here and looking for a better way to do this job.

The solution is to use the *while* loop of Python. The logical expression in front of *while* is evaluated, and if it is True, the body of the while loop (the indented lines below the while statement) is executed. The process is repeated until the condition becomes false. We should have some statement inside the body of the loop that will make this condition false after few iterations. Otherwise the program will run in an infinite loop and you will have to press Control-C to terminate it.

The program *table.py*, defines a variable *x* and assigns it an initial value of 1. Inside the while loop $x * 8$ is printed and the value of *x* is incremented. This process will be repeated until the value of *x* becomes greater than 10.

Example: table.py

```

x = 1
while x <= 10:
    print (x * 8)
    x = x + 1

```

As per the Python syntax, the while statement ends with a colon and the code inside the *while* loop is indented. Indentation can be done using tab or few spaces. In this example, we have demonstrated a simple algorithm.

2.8.1 Python Syntax, Colon & Indentation

Python was designed to be a highly readable language. It has a relatively uncluttered visual layout, uses English keywords frequently where other languages use punctuation, and has notably fewer syntactic constructions than other popular structured languages.

There are mainly two things to remember about Python syntax: indentation and colon. **Python uses indentation to delimit blocks of code.** Both space characters and tab characters are currently accepted as forms of indentation in Python. **Mixing spaces and tabs can create bugs that are hard to track**, since the text editor does not show the difference. There should not be any extra white spaces in the beginning of any line.

The line before any indented block must end with a colon (:) character.

2.8.2 Syntax of 'for loops'

Python *for* loops are slightly different from the for loops of other languages. Python *for* loop iterates over a compound data type like a String, List or Tuple. During each iteration, one member of the compound data is assigned to the loop variable. The flexibility of this can be seen from the examples below.

Example: forloop.py

```
a = 'Hello'
for ch in a: # ch is the loop variable
    print (ch)
b = ['haha', 3.4, 2345, 3+5j]
for item in b:
    print (item)
```

which gives the output :

```
H
e
l
l
o
haha
3.4
2345
(3+5j)
```

For constructing for loops that executes a fixed number of times, we can use the `range()` function and run the for loop over that.

Example: forloop2.py

```
for item in mylist:
    print item
```

The output will look like :

```
0
1
2
3
4
```

In python3 the output of range() function is an object belonging to a class called range. It used to be list type in python2. It is possible to specify the starting point and increment as arguments in the form range(start, end+1, step). The following example prints the table of 5 using this feature.

Example: forloop3.py

```
mylist = range(5,51,5)
for item in mylist:
    print (item , end = ' ')
```

The output is shown below.

```
5 10 15 20 25 30 35 40 45 50
```

The print statement inserts a newline at the end by default. The end = ' ' argument changes this to a space.

In some cases, we may need to traverse the list to modify some or all of the elements. This can be done by looping over a list of indices generated by the range() function. For example, the program forloop4.py zeros all the elements of the list.

Example: forloop4.py

```
a = [2, 5, 3, 4, 12]
size = len(a)
for k in range(size):
    a[k] = 0
print a
```

2.9 Conditional Execution: if, elif and else

In some cases, we may need to execute some section of the code only if certain conditions are true. Python implements this feature using the *if*, *elif* and *else* keywords, as shown in the next example. The indentation levels of *if* and the corresponding *elif* and *else* must be kept the same.

Example: compare.py

```
x = input('Enter a string ')
if x == 'hello':
    print ('You typed ', x)
```

Example: big.py

```
x = eval(input('Enter a number '))
if x > 10:
    print ('Bigger Number')
elif x < 10:
    print ('Smaller Number')
else:
    print ('Same Number')
```

The statement $x > 10$ and $x < 15$ can be expressed in a short form, like $10 < x < 15$.

The next example uses *while* and *if* keywords in the same program. Note the level of indentation when the if statement comes inside the while loop. Remember that, the *if* statement must be aligned with the corresponding *elif* and *else*.

Example: big2.py

```
x = 1
while x < 11:
    if x < 5:
        print ('Small ', x)
    else:
        print ('Big ', x)
    x = x + 1
print ('Done')
```

2.10 Modify loops : break and continue

We can use the *break* statement to terminate a loop, if some condition is met. The *continue* statement is used to skip the rest of the block and go to the beginning again. Both are demonstrated in the program *big3.py* shown below.

Example: big3.py

```
x = 1
while x < 10:
    if x < 3:
        print ('skipping work', x)
        x = x + 1
        continue
    print (x)
    if x == 4:
        print ('Enough of work')
        break
    x = x + 1
print ('Done')
```

The output of big3.py is listed below.

```
skipping work 1
skipping work 2
3
4
Enough of work
Done
```

Now let us write a program to find out the largest positive number entered by the user. The algorithm works in the following manner. To start with, we assume that the largest number is zero. After reading a number, the program checks whether it is bigger than the current value of the largest number. If so the value of the largest number is replaced with the current number. The program terminates when the user enters zero. Modify max.py to work with negative numbers also.

Example: max.py

```
max = 0
while True:      # Infinite loop
    x = eval(input('Enter a number '))
    if x > max:
        max = x
    if x == 0:
        print (max)
        break
```

2.11 Line joining

Python interpreter processes the code line by line. A program may have a long line of code that may not physically fit in the width of the text editor. In such cases, we can split a logical line of code into more than one physical lines, using backslash characters (\), in other words multiple physical lines are joined to form a logical line before interpreting it.

```
if 1900 < year < 2100 and 1 <= month <= 12 :
```

can be split like

```
if 1900 < year < 2100 \
    and 1 <= month <= 12 :
```

Do not split in the middle of words except for Strings. A long String can be split as shown below.

```
longname = 'I am so long and will \
not fit in a single line'
print (longname)
```

2.12 Exercises

We have now covered the minimum essentials of Python; defining variables, performing arithmetic and logical operations on them and the control flow statements. These are sufficient for handling most of the programming tasks. It would be better to get a grip of it before proceeding further, by writing some code.

1. Modify the expression `print 5+3*2` to get a result of 16
2. What will be the output of `print (type(4.5))`
3. Print all even numbers upto 30, suffixed by a * if the number is a multiple of 6. (hint: use % operator)
4. Write Python code to remove the last two characters of 'I am a long string' by slicing, without counting the characters. (hint: use negative indexing)
5. s = '012345' . (a) Slice it to remove last two elements (b) remove first two element.
6. a = [1,2,3,4,5]. Use Slicing and multiplication to generate [2,3,4,2,3,4] from it.

7. Compare the results of $5/2$, $5//2$ and $2.0/3$.
8. Print the following pattern using a while loop

```
++
+++
++++
```
9. Write a program to read inputs like 8A, 10C etc. and print the integer and alphabet parts separately.
10. Write code to print a number in the binary format (for example 5 will be printed as 101)
11. Write code to print all perfect cubes upto 2000.
12. Write a Python program to print the multiplication table of 5.
13. Write a program to find the volume of a box with sides 3,4 and 5 inches in cm^3 (1 inch = 2.54 cm)
14. Write a program to find the percentage of volume occupied by a sphere of diameter r fitted in a cube of side r . Read r from the keyboard.
15. Write a Python program to calculate the area of a circle.
16. Write a program to divide an integer by another without using the $/$ operator. (hint: use - operator)
17. Count the number of times the character 'a' appears in a String read from the keyboard. Keep on prompting for the string until there is no 'a' in the input.
18. Create an integer division machine that will ask the user for two numbers then divide and give the result. The program should give the result in two parts: the whole number result and the remainder. Example: If a user enters 11 / 4, the computer should give the result 2 and remainder 3.
19. Modify the previous program to avoid division by zero error.
20. Create an adding machine that will keep on asking the user for numbers, add them together and show the total after each step. Terminate when user enters a zero.
21. Modify the adding machine to check for errors like user entering invalid characters.
22. Create a script that will convert Celsius to Fahrenheit. The program should ask the users to enter the temperature in Celsius and should print out the temperature in Fahrenheit, using $f = \frac{9}{5}c + 32$.
23. Write a program to convert Fahrenheit to Celsius.
24. Create a script that uses a variable and will write 20 times "I will not talk in class." Make each sentence on a separate line.
25. Define $2 + 5j$ and $2 - 5j$ as complex numbers , and find their product. Verify the result by defining the real and imaginary parts separately and using the multiplication formula.
26. Write the multiplication table of 12 using while loop.

27. Write the multiplication table of a number, from the user, using for loop.
28. Print the powers of 2 up to 1024 using a for loop. (only two lines of code)
29. Define the list `a = [123, 12.4, 'haha', 3.4]`
 - a) print all members using a for loop
 - b) print the float type members (use `type()` function)
 - c) insert a member after 12.4
 - d) append more members
30. Make a list containing 10 members using a for loop.
31. Generate multiplication table of 5 with two lines of Python code. (hint: range function)
32. Write a program to find the sum of five numbers read from the keyboard.
33. Write a program to read numbers from the keyboard until their sum exceeds 200. Modify the program to ignore numbers greater than 99.
34. Write a Python function to calculate the GCD of two numbers
35. Write a Python program to find annual compound interest. Get P,N and R from user

2.13 Functions

Large programs need to be divided into small logical units. A function is generally an isolated unit of code that has a name and performs a well defined job. A function groups several program statements into a unit and gives it a name. This unit can be invoked from other parts of a program. Python allows you to define functions using the *def* keyword. A function may have one or more variables as parameters, which receive their values from the calling program.

In the example shown below, function parameters (a and b) get the values 3 and 4 respectively from the caller. One can specify more than one variables in the return statement, separated by commas. The function will return a tuple containing those variables. Some functions may not have any arguments, but while calling them we need to use an empty parenthesis, otherwise the function will not be invoked. If there is no return statement, a None is returned to the caller.

Example func.py

```
def sum(a,b):    # a trivial function
    return a + b

print (sum(3, 4))
```

The function *factorial.py* calls itself recursively. The value of argument is decremented before each call. Try to understand the working of this by inserting print statements inside the function.

Example factor.py

```
def factorial(n): # a recursive function
    if n == 0:
        return 1
    else:
        return n * factorial(n-1)

print (factorial(10))
```

Example fibonacci.py

```
def fib(n): # print Fibonacci series up to n
    a, b = 0, 1
    while b < n:
        print (b)
        a, b = b, a+b

print fib(30)
```

Running *fibonacci.py* will print

```
1 1 2 3 5 8 13 21
```

Modify the code to replace $a, b = b, a + b$ by two separate assignment statements, if required introduce a third variable.

2.13.1 Scope of variables

The variables defined inside a function are not known outside the function. There could be two unrelated variables, one inside and one outside, having the same name. The program *scope.py* demonstrates this feature.

Example scope.py

```
def change(x):
    counter = x

counter = 10
change(5)
print (counter)
```

The program will print 10 and not 5. The two variables, both named *counter*, are not related to each other. In some cases, it may be desirable to allow the function to change some external variable. This can be achieved by using the *global* keyword, as shown in *global.py*.

Example global.py

```
def change(x):
    global counter # use the global variable
    counter = x

counter = 10
change(5)
print (counter)
```

The program will now print 5. Functions with global variables should be used carefully, to avoid inadvertent side effects.

2.13.2 Optional and Named Arguments

Python allows function arguments to have default values; if the function is called without a particular argument, its default value will be taken. Due to this feature, the same function can be called with different number of arguments. The arguments without default values must appear first in the argument list and they cannot be omitted while invoking the function. The following example shows a function named `power()` that does exponentiation, but the default value of exponent is set to 2.

Example power.py

```
def power(mant, exp = 2.0):
    return mant ** exp

print (power(5., 3))
print (power(4.))      # prints 16
print (power())         # Gives Error
```

Arguments can be specified in any order by using named arguments.

Example named.py

```
def power(mant = 10.0, exp = 2.0):
    return mant ** exp

print (power(5., 3))
print (power(4.))      # prints 16
print (power(exp=3))    # mant gets 10.0, prints 1000
```

2.14 More on Strings and Lists

Before proceeding further, we will explore some of the functions provided for manipulating strings and lists. Python strings can be manipulated in many ways. The following program prints the length of a string, makes an upper case version for printing and prints a help message on the String class.

Example: stringhelp.py

```
s = 'hello world'
print (len(s))
print (s.upper())
help(str)          # press q to exit help
```

Python is an object oriented language and all variables are objects belonging to various classes. The method `upper()` (a function belonging to a class is called a method) is invoked using the dot operator. All we need to know at this stage is that there are several methods that can be used for manipulating objects and they can be invoked like: *variable_name.method_name()*.

2.14.1 split and join

Splitting a String will result in a list of smaller strings. If you do not specify the separator, the space character is assumed by default. To demonstrate the working of these functions, few lines of code and its output are listed below.

Example: split.py

```
s = 'I am a long string'
print (s.split())
a = 'abc.abc.abc'
aa = a.split('.')
print (aa)
mm = '+'.join(aa)
print (mm)
```

The result is shown below

```
['I', 'am', 'a', 'long', 'string']
['abc', 'abc', 'abc']
'abc+abc+abc'
```

The List of strings generated by split is joined using '+' character, resulting in the last line of the output.

2.14.2 Manipulating Lists

Python lists are very flexible, we can append, insert, delete and modify elements of a list. The program *list3.py* demonstrates some of them.

Example: list3.py

```
a = []          # make an empty list
a.append(3)     # Add an element
a.insert(0,2.5) # insert 2.5 as first element
print (a, a[0])
print (len(a))
```

The output is shown below.

```
[2.5, 3] 2.5
2
```

2.14.3 Copying Lists

Lists cannot be copied like numeric data types. The statement $b = a$ will not create a new list b from list a , it just make a reference to a . The following example will clarify this point. To make a duplicate copy of a list, we need to use the *copy* module.

Example: list_copy.py

```

a = [1,2,3,4]
print (a)
b = a          # b refers to a
print (a == b) # True
b[0] = 5       # Modifies a[0]
print (a)
import copy
c = copy.copy(a)
c[1] = 100
print (a is c) # is False
print (a, c)

```

The output is shown below.

```

[1, 2, 3, 4]
True
[5, 2, 3, 4]
False
[5, 2, 3, 4] [5, 100, 3, 4]

```

2.15 Python Modules and Packages

One of the major advantages of Python is the availability of libraries for various applications like graphics, networking and scientific computation. The standard library distributed with Python itself has a large number of modules: time, random, pickle, system etc. are some of them. The site <http://docs.python.org/library/> has the complete reference.

Modules are loaded by using the *import* keyword. Several ways of using *import* is explained below, using the math (containing mathematical functions) module as an example.⁶

2.15.1 Different ways to import

simplest way to use import is shown in *mathsin.py*, where the function is invoked using the form *module_name.function_name()*. In the next example, we use an alias for the module name.

Example mathsin.py

```

import math
print (math.sin(0.5)) # module_name.method_name

```

Example mathsin2.py

```

import math as m # Give another name for math
print (m.sin(0.5)) # Refer by the new name

```

We can also import the functions to behave like local (like the ones within our source file) function, as shown below. The character *** is a wild card for importing all the functions.

⁶While giving names to your Python programs, make sure that you are not directly or indirectly importing any Python module having same name. For example, if you create a program named *math.py* and keep it in your working directory, the *import math* statement from any other program started from that directory will try to import your file named *math.py* and give error. If you ever do that by mistake, delete all the files with .pyc extension from your directory.

Example mathlocal.py

```
from math import sin # sin is imported as local
print (sin(0.5))
```

Example mathlocal2.py

```
from math import * # import everything from math
print (sin(0.5))
```

In the third and fourth cases, we need not type the module name every time. But there could be trouble if two modules imported contains a function with same name. In the program *conflict.py*, the `sin()` from *numpy* is capable of handling a list argument. After importing *math.py*, line 4, the `sin` function from *math* module replaces the one from *numpy*. The error occurs because the `sin()` from *math* can accept only a numeric type argument.

Example conflict.py

```
from numpy import *
x = [0.1, 0.2, 0.3]
print (sin(x))          # numpy's sin can handle lists
from math import *      # sin of math becomes effective
print (sin(x))          # will give ERROR
```

2.15.2 Packages

Packages are used for organizing multiple modules. The module name A.B designates a module named B in a package named A. The concept is demonstrated using the packages Numpy⁷ and Scipy.

Example submodule.py

```
import numpy as np
print (np.random.normal())
import scipy.special
print (scipy.special.j0(.1))
```

In this example *random* is a module inside the package *NumPy*. Similarly *special* is a module inside the package *Scipy*. We use both of them in the `package.module.function()` format. But there is some difference. In the case of Numpy, the *random* module is loaded by default, importing *scipy* does not import the module *special* by default. This behavior can be defined while writing the Package and it is up to the author of the package.

2.16 File Input/Output

Disk files can be opened using the function named `open()` that returns a File object. Files can be opened for reading or writing. There are several methods belonging to the File class that can be used for reading and writing data.

Example wfile.py

⁷NumPy will be discussed later in chapter 3.


```
f = open('test.dat' , 'w')
f.write ('This is a test file')
f.close()
```

Above program creates a new file named 'test.dat' (any existing file with the same name will be deleted) and writes a String to it. The following program opens this file for reading the data.

Example rfile.py

```
f = open('test.dat' , 'r')
print (f.read())
f.close()
```

Note that the data written/read are character strings. read() function can also be used to read a fixed number of characters, as shown below.

Example rfile2.py

```
f = open('test.dat' , 'r')
print (f.read(7))      # get first seven characters
print (f.read())       # get the remaining ones
f.close()
```

Now we will examine how to read a text data from a file and convert it into numeric type. First we will create a file with a column of numbers.

Example wfile2.py

```
f = open('data.dat' , 'w')
for k in range(1,4):
    s = '%3d\n' %(k)
    f.write(s)
f.close()
```

The contents of the file created will look like this.

```
1
2
3
```

Now we write a program to read this file, line by line, and convert the string type data to integer type, and print the numbers.⁸

Example rfile3.py

```
f = open('data.dat' , 'r')
while 1: # infinite loop
    s = f.readline()
    if s == '' :      # Empty string means end of file
        break        # terminate the loop
    m = eval(s)       # Convert to integer
    print (m * 5)
f.close()
```

⁸This will give error if there is a blank line in the data file. This can be corrected by changing the comparison statement to if `len(s) < 1` : , so that the processing stops at a blank line. Modify the code to skip a blank line instead of exiting (hint: use continue).

| Conversion | Conversion | Example | Result |
|------------|----------------------------|-----------------|----------|
| d , i | signed Integer | '%6d'%(12) | ' 12' |
| f | floating point decimal | '%6.4f'%(2.0/3) | 0.667 |
| e | floating point exponential | '%6.2e'%(2.0/3) | 6.67e-01 |
| x | hexadecimal | '%x'%(16) | 10 |
| o | octal | '%o'%(8) | 10 |
| s | string | '%s'__('abcd') | abcd |
| 0d | modified 'd' | '%05d'%(12) | 00012 |

Table 2.2: Formatted Printing in Python

2.17 Formatted Printing

Formatted printing is done by using a format string followed by the % operator and the values to be printed. If format requires a single argument, values may be a single variable. Otherwise, values must be a tuple (just place them inside parenthesis, separated by commas) with exactly the number of items specified by the format string.

Example: format.py

```
a = 2.0 / 3
print (a)
print ('a = %5.3f' %(a)) # upto 3 decimal places
```

Data can be printed in various formats. The conversion types are summarized in the following table. There are several flags that can be used to modify the formatting, like justification, filling etc.

The following example shows some of the features available with formatted printing.

Example: format2.py

```
a = 'justify as you like'
print ('%30s'%a)          # right justified
print ('%-30s'%a)         # minus sign for left justification
for k in range(1,11):     # A good looking table
    print ('5 x %2d = %2d' %(k, k*5))
```

The output of *format2.py* is given below.

```
                justify as you like
justify as you like
5 x  1 =  5
5 x  2 = 10
5 x  3 = 15
5 x  4 = 20
5 x  5 = 25
5 x  6 = 30
5 x  7 = 35
5 x  8 = 40
5 x  9 = 45
5 x 10 = 50
```

2.18 Exception Handling

Errors detected during execution are called exceptions, like divide by zero. If the program does not handle exceptions, the Python Interpreter reports the exception and terminates the program. We will demonstrate handling exceptions using *try* and *except* keywords, in the example `except.py`.

Example: except.py

```
x = input('Enter a number ')
try:
    print (10.0/x)
except:
    print ('Division by zero not allowed')
```

If any exception occurs while running the code inside the try block, the code inside the except block is executed. The following program implements error checking on input using exceptions.

Example: except2.py

```
def get_number():
    while 1:
        try:
            a = input('Enter a number ')
            x = atof(a)
            return x
        except:
            print ('Enter a valid number')

print get_number()
```

2.19 Matrices in pure Python

In this chapter we will explore some matrix operations, using the *list* datatype. Lists inside list will be used to represent 2D matrices. This will be done in pure python with the objective of getting familiar with Python coding. For doing serious scientific computation one should use the packages like numpy and scipy, providing special data types to implement matrices. They will be introduced in the next chapter. Examining the code fragments given below along with their outputs should give some idea about coding in Python. For example, the code

```
x = [1,2]                #1D matrix
a = [ [1,2], [3,4] ]     # 2x2 matrix
print (a[1][0])          # result is 3
print ('NR = ', len(a), 'NC = ', len(a[0]))
```

Prints

```
3
NR = 2 NC = 2
```

It indicates how the row and column are indexed, `y[1][0]` points to element at second row and first column. The number of rows is the number of lists inside `a`, and the number of columns is the size of each list.

According to matrix algebra $cA = c \sum_{ij} A_{ij}$, means all elements should be multiplied by c . Code should have two nested loops to traverse the rows and columns, as shown below.

```

c = 5
for row in range(2):
    for col in range(2):
        a[row][col] *= c    # x *= k is same as x = x * k
print(a)

```

Prints

```
[[5, 10], [15, 20]]
```

How to add two matrices $y = [[1, 2], [3, 4]]$ and $z = [[5, 6], [7, 8]]$. The code required is,

```

a = [ [1,2], [3,4] ]
b = [ [5,6], [7,8] ]
c = [ [0,0], [0,0] ]
for row in range(2):
    for col in range(2):
        c[row][col] = a[row][col] + b[row][col]
print(a)

```

Prints

```
[[6, 8], [10, 12]]
```

2.19.1 Transpose of a matrix

Transpose is obtained by interchanging rows and columns of a matrix.

```

a = [[1,2], [3,4], [5,6] ] # 3x2 matrix
res = [[0,0,0], [0,0,0]]    # 2x3 matrix for results

for i in range(len(a)):
    for j in range(len(a[0])):
        res[j][i] = a[i][j] print (res)

```

2.19.2 Matrix multiplication

Matrix multiplication is a bit more involved. The rule is $c_{ij} = \sum_1^n a_{ik}b_{kj}$. The number of rows in the first matrix should be equal to the number of columns in the second matrix. Examine the program mat-mult.py listed below. For each element c_{ij} is calculated using another loop.

```

# 3 x 3 matrices
a = [ [1,2,3], [3,4,5], [10,11,12] ]
b = [ [5,6,7], [7,8,9], [12,13,14] ]
c = [ [0,0,0], [0,0,0], [0,0,0] ]
NR = len(a)    # number of rows
NC = len(b[0]) # number of columns

for row in range(NR):
    for col in range(NC):
        for i in range(len(a[0])): # number of columns of A
            c[row][col] += a[row][i] * b[i][col]

```

```

print (c)

# 2 x 3 and 3 x 2 matrices
a = [ [1,2,3], [3,4,5] ]      # 2 x 3
b = [ [5,6], [7,8], [12,13] ] # 3 x 2
c = [ [0,0], [0,0] ]          # 2 x 2

NR = len(a)      # number of rows
NC = len(b[0])   # number of columns
for row in range(NR):
    for col in range(NC):
        for i in range(len(a[0])): # number of columns of A
            c[row][col] += a[row][i] * b[i][col]
print (c)

```

2.19.3 Cross product two vectors

Vectors can be represented using matrices and cross product of two vectors is defined by

$$A \times B = \begin{vmatrix} i & j & k \\ A_1 & A_2 & A_3 \\ B_1 & B_2 & B_3 \end{vmatrix} = i(A_2B_3 - A_3B_2) + j(A_3B_1 - A_1B_3) + k(A_1B_2 - A_2B_1) \quad (2.1)$$

The program *cross.py* calculates it using pure python code.

Example cross.py

```

def mycross2(a,b):
    a1, a2, a3 = a
    b1, b2, b3 = b
    return [a2*b3 - a3*b2, a3*b1 - a1*b3, a1*b2 - a2*b1]

def mycross(a,b):
    return [a[1]*b[2]-a[2]*b[1], a[2]*b[0]-a[0]*b[2],
            a[0]*b[1]-a[1]*b[0] ]

a = array([1,2,3])
b = array([4,5,6])
print(mycross(a,b))
print(mycross2(a,b))

```

The output is [-3, 6, -3] in both cases. The function *mycross* and *mycross2* are given to practice Python coding. It is not wise to carry your own cross all the way up to the mountain of scientific computation. Better methods using Numpy will be discussed in the next chapter.

2.19.4 Determinant of a Matrix

Determinant is a scalar value that can be computed from the elements of a square matrix. For 2x2 and 3x3 matrices, they are defined by the equations

$$|A| = \begin{vmatrix} a & b \\ c & d \end{vmatrix} = ad - bc$$

$$|A| = \begin{vmatrix} a & b & c \\ d & e & f \\ g & h & i \end{vmatrix} = a \begin{vmatrix} e & f \\ h & i \end{vmatrix} - b \begin{vmatrix} d & f \\ g & i \end{vmatrix} + c \begin{vmatrix} d & e \\ g & h \end{vmatrix} = aei - afh + bfg - bdi + cdh - ceg$$

The python code given below calculates the determinant of a 3x3 matrix, represented using a list of lists.

```
a = [ [1.,1.,1.], [0.,2.,5.], [2.,5.,-1.] ]
m1, m2, m3 = m[0]
m4, m5, m6 = m[1]
m7, m8, m9 = m[2]
det = m1*(m5*m9-m6*m8) - m2*(m4*m9-m6*m7) + m3*(m4*m8-m5*m7)
```

2.19.5 Inverting a Matrix

There are many ways to invert a matrix. We are using the method of taking the transpose of the matrix of cofactors and dividing it by the determinant.

$$A^{-1} = \frac{1}{|A|} C^T$$

The code listed below does it in a crude manner, applicable only for a 3x3 matrix.

```
def invert(m):
    m1, m2, m3 = m[0]
    m4, m5, m6 = m[1]
    m7, m8, m9 = m[2]
    d = m1*(m5*m9-m6*m8) - m2*(m4*m9-m6*m7) + m3*(m4*m8-m5*m7)
    return [[(m5*m9-m6*m8)/d, (m3*m8-m2*m9)/d, (m2*m6-m3*m5)/d],
            [(m6*m7-m4*m9)/d, (m1*m9-m3*m7)/d, (m3*m4-m1*m6)/d],
            [(m4*m8-m5*m7)/d, (m2*m7-m1*m8)/d, (m1*m5-m2*m4)/d] ]
```

```
a = [ [1.,1.,1.], [0.,2.,5.], [2.,5.,-1.] ]
```

`print (invert(a))`

The output is

```
[[1.2857142857142858, -0.2857142857142857, -0.14285714285714285], [-0.47619047619047616, 0.14285714285714285, 0.2857142857142857],
```

You can verify the result by calculating $A^{-1}A$ using the matrix multiplication program discussed earlier. The result should be an identity matrix, that should look like

```
[[1.0, 0.0, 0.0],
 [0.0, 0.9999999999999999, 0.0],
 [2.220446049250313e-16, -5.551115123125783e-17, 1.0]]
```

The elements are ones and zeros within the precision of our computation.

Examples in this section demonstrates the difficulties in using the list data type for representing arrays and matrices. In the next chapter, we will use Numpy arrays to represent matrices, making coding easier.

2.20 Object Oriented Programming in Python

OOP is a programming paradigm that uses *objects* (Structures consisting of variables and methods) and their interactions to design computer programs. Python is an object oriented language but it does not force you to make all programs object oriented and there is no advantage in making small programs object oriented. In this section, we will discuss some features of OOP.

Before going to the new concepts, let us recollect some of the things we have learned. We have seen that the effect of operators on different data types is predefined. For example $2 * 3$ results in 6 and $2 * 'abc'$ results in `'abcabc'`. This behavior has been decided beforehand, based on some logic, by the language designers. One of the key features of OOP is the ability to create user defined data types. The user will specify, how the new data type will behave under the existing operators like add, subtract etc. and also define methods that will belong to the new data type.

We will design a new data type using the *class* keyword and define the behavior of it. In the program *point.py*, we define a class named *Point*. The variables *xpos* and *ypos* are members of *Point*. The `__init__()` function is executed whenever we create an instance of this class, the member variables are initialized by this function. The way in which an object belonging to this class is printed is decided by the `__str__` function. We also have defined the behavior of add (+) and subtract (-) operators for this class. The + operator returns a new Point by adding the x and y coordinates of two Points. Subtracting a Point from another gives the distance between the two. The method `dist()` returns the distance of a Point object from the origin. We have not defined the behavior of Point under copy operation. We can use the copy module of Python to copy objects.

Example point.py

```
class Point:
    """
    This is documentation comment.
    help(Point) will display this.
    """
    def __init__(self, x=0, y=0):
        self.xpos = x
        self.ypos = y

    def __str__(self): # overloads print
        return 'Point at (%f,%f)'%(self.xpos, self.ypos)

    def __add__(self, other): #overloads +
        xpos = self.xpos + other.xpos
        ypos = self.ypos + other.ypos
        return Point(xpos,ypos)

    def __sub__(self, other): #overloads -
        import math
        dx = self.xpos - other.xpos
        dy = self.ypos - other.ypos
        return math.sqrt(dx**2+dy**2)

    def dist(self):
        import math
        return math.sqrt(self.xpos**2 + self.ypos**2)
```

The program `point1.py` imports the file `point.py` to use the class `Point` defined inside it to demonstrate the properties of the class. A `self.` is prefixed when a method refers to member of the same object. It refers to the variable used for invoking the method.

Example point1.py

```
from point import *
origin = Point()
print origin
p1 = Point(4,4)
p2 = Point(8,7)
print (p1)
print (p2)
print (p1 + p2)
print (p1 - p2)
print (p1.dist())
```

Output of program `point1.py` is shown below.

```
Point at (0.000000,0.000000)
Point at (4.000000,4.000000)
Point at (8.000000,7.000000)
Point at (12.000000,11.000000)
5.0
5.65685424949
```

In this section, we have demonstrated the OO concepts like class, object and operator overloading.

2.20.1 Inheritance, reusing code

Reuse of code is one of the main advantages of object oriented programming. We can define another class that inherits all the properties of the `Point` class, as shown below. The `__init__` function of `colPoint` calls the `__init__` function of `Point`, to get all work except initialization of color done. All other methods and operator overloading defined for `Point` is inherited by `colPoint`.

Example cpoint.py

```
class colPoint(Point): #colPoint inherits Point
    color = 'black'
    def __init__(self,x=0,y=0,col='black'):
        Point.__init__(self,x,y)
        self.color = col

    def __str__(self):
        return '%s colored Point at (%f,%f)'\% \
            (self.color,self.xpos, self.ypos)
```

Example point2.py

```
from cpoint import *
p1 = Point(5,5)
rp1 = colPoint(2,2,'red')
```



```

print (p1)
print (rp1)
print (rp1 + p1)
print (rp1.dist())

```

The output of point2.py is listed below.

```

Point at (5.000000,5.000000)
red colored Point at (2.000000,2.000000)
Point at (7.000000,7.000000)
2.82842712475

```

For a detailed explanation on the object oriented features of Python, refer to the online book <http://openbookproject.net/thinkcs/python/english3e/>

2.21 Turtle Graphics

Turtle Graphics have been noted by many psychologists and educators to be a powerful aid in teaching geometry, spatial perception, logic skills, computer programming, and art. The language LOGO was specifically designed to introduce children to programming, using turtle graphics. An abstract drawing device, called the Turtle, is used to make programming attractive for children by concentrating on doing turtle graphics. It has been used with children as young as 3 and has a track record of 30 years of success in education.

We will use the Turtle module of Python to play with Turtle Graphics and practice the logic required for writing computer programs. Using this module, we will move a *Pen* on a two dimensional screen to generate graphical patterns. The Pen can be controlled using functions like forward(distance), backward(distance), right(angle), left(angle) etc.⁹. Run the program turtle1.py to understand the functions. This section is included only for those who want to practice programming in a more interesting manner.

Example turtle1.py

```

from turtle import *
a = Pen()      # Creates a turtle in a window
a.forward(50)
a.left(45)
a.backward(50)
a.right(45)
a.forward(50)
a.circle(10)
a.up()
a.forward(50)
a.down()
a.color('red')
a.right(90)
a.forward(50)
input('Press Enter')

```

Example turtle2.py

⁹<http://docs.python.org/library/turtle.html>

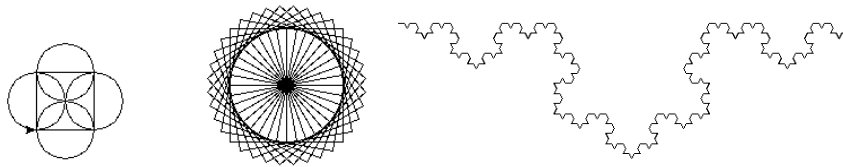


Figure 2.3: Output of turtle2.py (b) turtle3.py (c) turtle4.py

```
from turtle import *
a = Pen()
for k in range(4):
    a.forward(50)
    a.left(90)
    a.circle(25)
input('Press Enter')
```

Outputs of the program turtle2.py and turtle3.py are shown in figure 2.3. Try to write more programs like this to generate more complex patterns.

Example turtle3.py

```
from turtle import *
def draw_rectangle():
    for k in range(4):
        a.forward(50)
        a.left(90)

a = Pen()
for k in range(36):
    draw_rectangle()
    a.left(10)
input('Press Enter')
```

The program turtle3.py creates a pattern by drawing 36 squares, each drawn tilted by 10° from the previous one. The program turtle4.py generates the fractal image as shown in figure 2.3(c).

Example turtle4.py

```
from turtle import *

def f(length, depth):
    if depth == 0:
        forward(length)
    else:
        f(length/3, depth-1)
        right(60)
        f(length/3, depth-1)
        left(120)
        f(length/3, depth-1)
        right(60)
```

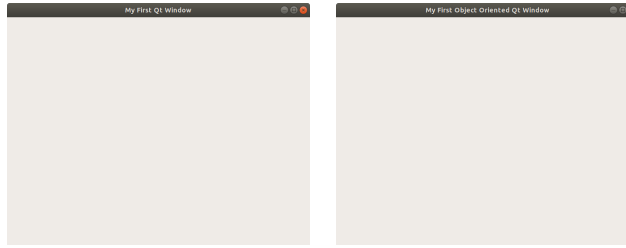


Figure 2.4: Outputs of (a)qt-win.py (b)qt-win-2.py

```
f(length/3, depth-1)

f(500, 4)
input('Press any Key')
```

2.22 Writing GUI Programs

The programs we have written so far do not have any Graphical User Interface. How to write such programs. First thing one should understand is other than the graphics elements there is some fundamental difference. In the text mode programs, the flow of program execution is almost decided by the code. It starts running and waits for user inputs as mentioned in the code. On the other hand, the GUI programs are event driven (movement of mouse, clicking a mouse button, pressing and releasing a key etc. are called events). The execution sequence of the program is decided by these events, generated mostly by the user. For example, when the user clicks on a Button, the code associated with that Button is executed.

Python has several tool kits for creating Graphical User Interfaces. A highly popular toolkit is Qt and PyQt5 is the current python module for that. For more details refer to¹⁰. GUI Programming is about creating Widgets like Button, Label, Canvas etc. on the screen and executing selected functions in response to events. After creating all the necessary widgets and displaying them on the screen, the control is passed on to PyQt toolkit by calling a function named *app.exec_()*. After that the program flow is decided by the events and associated callback functions. You can terminate the program by clicking on the 'x' at the top right corner, or by providing a Button for that purpose.

For writing GUI program using Qt toolkit, the first step is to call the function *QApplication*. After that we create various Widgets. The example program 'qt-win.py' creates a window using *QWidget*, assigns a title to it and then calls *show()* to display it on screen. After that *app_exec()* takes over and waits for events generated within this window by the user. The output of qt-win.py is shown in figure 2.4(a).

While we can code a simple window without using Object Oriented Programming (OOP), it becomes more difficult to as we improve the functionality of our application. We will rewrite the previous application in the object oriented programming styles. The class *MyGUI* inherits all the properties of the parent class *QWidget*. The *__init__* function calls the *super.__init__()* to initialize the parent class. This method becomes handy while writing more complicated programs.

Example qt-win.py

¹⁰<https://pythonspot.com/pyqt5/>
<https://likegeeks.com/pyqt5-tutorial/>

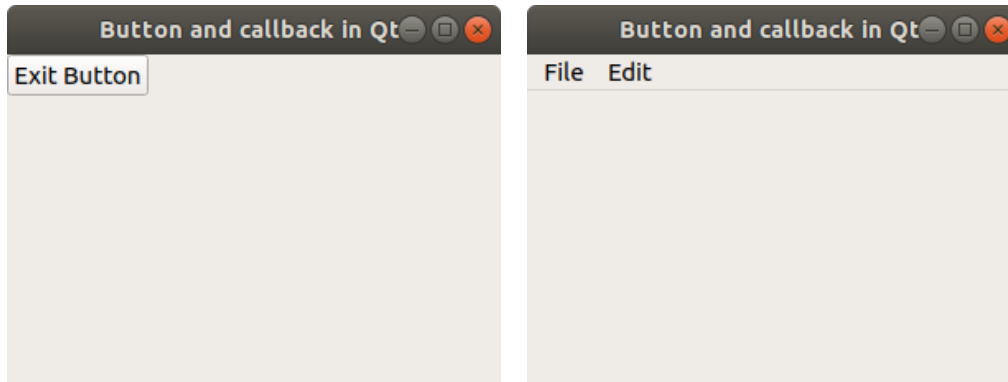


Figure 2.5: Outputs of (a) qt-button.py (b)qt-menu.py

```
import sys
from PyQt5.QtWidgets import QApplication, QWidget

app = QApplication(sys.argv)
w = QWidget()
w.setWindowTitle('My First Qt Window')
w.show()
app.exec_()
```

Example qt-win-2.py

```
import sys
from PyQt5.QtWidgets import QApplication, QWidget

class MyGUI(QWidget):
    def __init__(self):
        super().__init__()
        self.setWindowTitle('My First Object Oriented Qt Window')
        self.show()

app = QApplication(sys.argv)
win = MyGUI()
sys.exit(app.exec_())
```

Button, Menu and Callback

The next example will show how to use a Button widget. A Button widget can have a callback function, *done()* in this case, that gets executed when the user clicks on the Button. The program will display a Button on the screen. When you click on it, the function *done()* will be executed. The output of the program is shown in figure 2.5(a).

Example qt-button.py

```
import sys from PyQt5.QtWidgets
import QApplication, QWidget, QPushButton
```

```

class MyGUI(QWidget):
    def __init__(self):
        super().__init__()
        self.setWindowTitle('Button and callback in Qt')
        self.setGeometry(300, 300, 300, 200)
        btn = QPushButton('Exit Button', self)
        btn.clicked.connect(self.done)
        self.show()

def done(self):
    sys.exit(0)

app = QApplication(sys.argv)
win = MyGUI()
sys.exit(app.exec_())

```

Menu is another commonly used widget. First make a menu bar and add menus to it. Items are added to each menu after that. In order to use the menu widget the class `MyGUI` is subclassed from the `QMainWindow` widget. The output of the code listed below is shown in 2.5(b).

Example qt-menu.py

```

import sys
from PyQt5.QtWidgets import QApplication, QMainWindow, QPushButton

class MyGUI(QMainWindow):
    def __init__(self):
        super().__init__()
        self.setWindowTitle('Button and callback in Qt')
        self.setGeometry(300, 300, 300, 200)
        mainMenu = self.menuBar()
        fileMenu = mainMenu.addMenu('File')
        fileMenu.addAction('Open', self.fileOpen)
        editMenu = mainMenu.addMenu('Edit')
        self.show()

    def fileOpen(self):
        print('File Open called')

app = QApplication(sys.argv)
win = MyGUI()
sys.exit(app.exec_())

```

These examples are not sufficient to get one started in to programming GUIs using Qt, but plenty of documentation is available on the Internet. The objective of this book is different and we will be using a different toolkit for plotting graphs.

2.23 Exercises

1. Generate multiplication table of eight and write it to a file.

2. Make a list and write it to a file using the pickle module.
3. Write a Python program to open a file and write 'hello world' to it.
4. Write a Python program to open a text file and read all lines from it.
5. Write a program to generate the multiplication table of a number from the user. The output should be formatted as shown below
1 x 5 = 5
2 x 5 = 10
6. Write Python code to generate the sequence of numbers
25 20 15 10 5
using the range() function. Delete 15 from the result and sort it. Print it using a for loop.
7. Define a string $s = \text{'mary had a little lamb'}$.
 - a) print it in reverse order
 - b) split it using space character as separator
8. Join the elements of the list ['I', 'am', 'in', 'pieces'] using + character. Do the same using a for loop also.
9. Create a window with five buttons. Each button should have some text on it.
10. Create a program that will put words in alphabetical order. The program should allow the user to enter as many words as he wants to.
11. Create a program that will check a sentence to see if it is a palindrome. A palindrome is a sentence that reads the same backwards and forwards ('malayalam').
12. A text file contains two columns of numbers. Write a program to read them and print the sum of numbers in each row.
13. Read a String from the keyboard. Multiply it by an integer to make its length more than 50. How do you find out the smallest number that does the job.
14. Write a program to find the length of the hypotenuse of a right triangle from the length of other two sides, get the input from the user.
15. Write a program displaying 2 labels and 2 buttons. It should print two different messages when clicked on the two buttons.
16. Write a program using for loop to reverse a string.
17. Write a program to print the values of sine function from 0 to 2π with 0.1 increments. Find the mean value of them.
18. Generate N random numbers using random.random() and find out how many are below 0.5 . Repeat the same for different values of N to draw some conclusions.
19. Use the equation $x = (-b \pm \sqrt{b^2 - 4ac})/2a$ to find the roots of $3x^2 + 6x + 12 = 0$
20. Write a program to calculate the distance between points (x1,y1) and (x2,y2) in a Cartesian plane. Get the coordinates from the user.
21. Write a program to evaluate $y = \sqrt{2.3a} + a^2 + 34.5$ for $a = 1, 2$ and 3 .

22. Print Fibonacci numbers up to 100, without using multiple assignment statement.
23. Draw a chess board pattern using turtle graphics.
24. Find the syntax error in the following code and correct it.

```
x=1  
while x <= 10:  
    print x * 5
```

Chapter 3

Arrays and Matrices

In the previous chapter, we have learned some essential features of Python language and used the *math* module to calculate trigonometric functions. Several matrix operations were carried out in pure Python, using the list data type to store the matrices. The list data type is not really suitable for representing arrays and matrices. In this chapter, we will use Numpy arrays to represent matrices. That will make code much simpler and easy to understand, eliminating enormous number of loops. If your main objective is to apply numerical methods to learn science or mathematics then you should learn to use the well tested and highly efficient modules like NumPy and SciPy.

The two different approaches, coding everything from scratch or using available libraries, is demonstrated by using two examples shown below. The program *sine1.py* generates the coordinates to plot a sine wave and *sine2.py* does the same and also plots it

Example sine1.py

```
import math
x = 0.0
while x < 2 * math.pi:
    print (x , math.sin(x))
    x = x + 0.1
```

The output to the screen can be redirected to a file as shown below, from the command prompt. You can plot the data using some programs.

```
$ python sine1.py > sine.dat
```

Listing of sine2.py below, along with the result in 3.1

```
from pylab import *
x = linspace(0, 2*pi, 100)
plot (sin(x))
show()
```

The need of special tools is evident even from the simple example shown above. Big arrays of numbers and matrices are essential in scientific computation. *NumPy* is a package widely used for scientific computing with Python.¹ . To conclude, we prefer spending more time and energy on learning scientific problems rather than writing complicated python code. In the examples below,

¹<https://www.scipy.org/scipylib/faq.html>

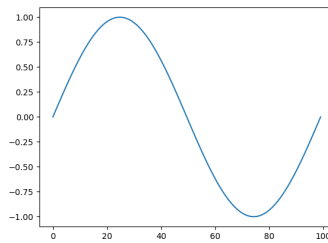


Figure 3.1: Plot of Sine curve

we will import numpy functions as local (*from numpy import **). Since it is the only package used there is no possibility of any function name conflicts. While writing larger program you may use it like *import numpy as np*.

3.1 NumPy Arrays

NumPy is a Python extension module that provides efficient operation on arrays of homogeneous data. *First thing to learn is how to create and manipulate arrays using numpy.* There are several functions that can be used for creating arrays.² The mathematical functions like sine, cosine etc. of numpy accepts array objects as arguments and return the results as arrays objects. NumPy arrays can be indexed, sliced and copied like Python Lists.

The following examples shows how to make a one and two dimensional arrays.

Example numpy1.py

```
from numpy import *
x = array( [1, 2, 3] )    # Make array from list
print (x , type(x))
```

In the above example, we have created a numpy ndarray from a list.

Example numpy2.py

```
from numpy import *
a = [ [1, 2, 3] , [4, 5, 6] ] # make a list of lists
x = array(a)    # and convert to an array
print (a)
```

Other than *array()*, there are several other functions that can be used for creating different types of arrays. Some of them are described below.

<https://numpy.org/devdocs/user/quickstart.html>

<https://docs.scipy.org/doc/scipy/reference/tutorial/index.html>

<https://www.python-course.eu/numpy.php>

http://www.u.arizona.edu/~erdmann/mse350/topics/basic_linear_algebra.html#matrix-powers

²<https://docs.scipy.org/doc/numpy-1.13.0/reference/routines.array-creation.html>

3.1.1 arange(start, stop, step, dtype = None)

Creates an evenly spaced one-dimensional array. Start, stop, step-size and datatype are the arguments. If datatype is not given, it is deduced from the other arguments. Note that, the values are generated within the interval, including start but excluding stop.

```
arange(2.0, 3.0, .1)
makes the array([ 2. , 2.1, 2.2, 2.3, 2.4, 2.5, 2.6, 2.7, 2.8, 2.9])
```

3.1.2 linspace(start, stop, number of elements)

Similar to arange(). Start, stop and number of samples are the arguments.

```
linspace(1, 2, 11) is equivalent to array([ 1. , 1.1, 1.2, 1.3, 1.4, 1.5, 1.6, 1.7, 1.8, 1.9, 2. ])
```

3.1.3 zeros(shape)

Returns a new array of given shape and type, filled zeros. For example `zeros([2,3])` generates a 2 x 3 array filled with zeros

```
[[0,0,0]
 [0,0,0]]
```

3.1.4 ones(shape)

Similar to zeros() except that the elements are initialized to 1.

3.1.5 random.random(shape)

Similar to the functions above, but the matrix is filled with random numbers ranging from 0 to 1, of *float* type. For example, `random.random([3,3])` will generate the 3x3 matrix;

```
array([[ 0.3759652 , 0.58443562, 0.41632997],
       [ 0.88497654, 0.79518478, 0.60402514],
       [ 0.65468458, 0.05818105, 0.55621826]])
```

3.1.6 reshape(array, newshape)

We can also make multi-dimensions arrays by reshaping a one-dimensional array. The function *reshape()* changes dimensions of an array. The total number of elements must be preserved. Working of *reshape()* can be understood by looking at *reshape.py* and its result.

Example reshape.py

```
from numpy import *
a = arange(20)
b = reshape(a, [4,5])
print (b)
```

The result is shown below.

```
array([[ 0,  1,  2,  3,  4],
       [ 5,  6,  7,  8,  9],
       [10, 11, 12, 13, 14],
       [15, 16, 17, 18, 19]])
```

The program *numpy2.py* demonstrates most of the functions discussed so far.

Example numpy2.py

```
from numpy import *
a = arange(1.0, 2.0, 0.1)
print (a)
b = linspace(1,2,11)
print (b)
c = ones(5,'float')
print (c)
d = zeros(5, 'int')
print (d)
e = random.rand(5)
print (e)
```

Output of this program will look like;

```
[ 1.  1.1  1.2  1.3  1.4  1.5  1.6  1.7  1.8  1.9]
[ 1.  1.1  1.2  1.3  1.4  1.5  1.6  1.7  1.8  1.9  2. ]
[ 1.  1.  1.  1.  1.]
[ 0.  0.  0.  0.  0.]
[ 0.89039193  0.55640332  0.38962117  0.17238343  0.01297415]
```

3.1.7 Copying

Numpy arrays can be copied using the copy method, as shown below.

Example array_copy.py

```
from mumpy import *
a = zeros(5)
print a
b = a
c = a.copy()
c[0] = 10
print a, c
b[0] = 10
print a,c
```

The output of the program is shown below. The statement $b = a$ does not make a copy of a . Modifying b affects a , but c is a separate entity.

```
[ 0.  0.  0.]
[ 0.  0.  0.] [ 10.  0.  0.]
[ 10.  0.  0.] [ 10.  0.  0.]
```

3.1.8 Saving and Restoring

There are many ways for reading from file and writing to data files in numpy. We will discuss only the ones saves data in the formatted text form, `savetext()` and `loadtext()` methods, as shown in the code *fileio.py*

Example fileio.py

```

from numpy import *
a = array([[2,3], [4,5]])
print(a)
savetxt('mydata.txt', a, fmt = '%2.3f', delimiter = ' ')
print('Data saved to text file')
b = loadtxt("mydata.txt", delimiter=" ")
print('Data loaded from text file')
print(b)

```

The output of the program will look like

```

[[2 3]
 [4 5]]
Data saved to text file
Data loaded from text file
[[ 2. 3.]
 [ 4. 5.]]

```

The text file 'mydata.txt' will look like

```

2.000 3.000
4.000 5.000

```

3.1.9 Slicing to extract elements and columns

Since slicing is used for extracting columns from a two dimensional array, we need to understand it a bit better.

```
x = reshape(range(12),(4,3))
```

creates the array having 4 rows and 3 columns.

```

[[ 0,  1,  2],
 [ 3,  4,  5],
 [ 6,  7,  8],
 [ 9, 10, 11]]

```

and extract elements from it in different ways, python indexing starts from zero.

```

x[1] extracts the second row to give [3,4,5].
x[2,1] extracts 7, the element at third row and second column.
x[1:3, 1] extracts the elements [4,7] from second column.
x[:, 1] gives the full second column [ 1, 4, 7, 10]
x[:2,:2] gives the array
[[0, 1],
 [3, 4]]

```

You should remember that a statement like $y = x[1]$ does not create a new array. It is only a reference to the second row or x . The statement $y[0] = 100$ changes $x[1,0]$ to 100.

The program *slice.py*

```

from numpy import *
x = reshape(range(12),(4,3))
print(x[1])
print(x[2,1])
print(x[1:3,1])
print(x[:,1])
print(x[:2,:2])

```

will generate the output

```

[3 4 5]
7
[4 7]
[ 1 4 7 10]
[[0 1]
 [3 4]]

```

3.1.10 Arithmetic Operations

Arithmetic operations on array differs from that of ordinary numbers. Adding or multiplying an array object with an ordinary number will multiply all the elements by that number. However, operations involving more than one array could be done in different ways.

```

x = ones((2,2)) makes
[[ 1.,  1.],
 [ 1.,  1.]]

```

`x * 5` multiplies all elements by 5 to give

```

[[ 5.,  5.],
 [ 5.,  5.]]

```

`x * x` will not the matrix multiplication. To perform a proper matrix multiplication try `x@x` , `dot(x,x)` or `x.dot(x)` to get the result

```

[[ 2., 2.],
 [ 2., 2.]]

```

Example aroper.py

```

from numpy import *
x = ones( (2,2,))
print(x*5)
print(x * x)
print(x @ x)

```

Modifying this program for more operations is left as an exercise to the reader.

3.1.11 Pauli spin matrices

We use the Pauli spin matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \text{ and } \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

to demonstrate some matrix operations using numpy, with the program *pauli.py* listed below

```
from numpy import *
sx = array( [ [0+0j, 1+0j], [1+0j, 0+0j] ]) # sigma x
sy = array( [ [0+0j, 0-1j], [0+1j, 0+0j] ]) # sigma y
sz = array( [ [1+0j, 0+0j], [0+0j, -1+0j] ]) # sigma z
print ('sx\n', sx)
print ('Transpose(sx)\n', transpose(sx))
commutexy = sx.dot(sy) - sy.dot(sx)
print ('[sx,sy]\n',commutexy)
sz2i = 2 * (0+1j) * sz
print ('2 i sz\n',sz2i)
print (sz2i == commutexy)
```

The output of the program is given below. The last result shows that $[\sigma_x, \sigma_y] = 2i\sigma_z$. Refer to Wikipedia³ for more information.

```
sx
[[ 0.+0.j  1.+0.j]
 [ 1.+0.j  0.+0.j]]
Transpose(sx)
[[ 0.+0.j  1.+0.j]
 [ 1.+0.j  0.+0.j]]
[sx,sy]
[[ 0.+2.j  0.+0.j]
 [ 0.+0.j  0.-2.j]]
2 i sz
[[ 0.+2.j  0.+0.j]
 [ 0.+0.j  0.-2.j]]
[[ True  True]
 [ True  True]]
```

3.2 Vectorizing Functions

The functions like sine, log etc. from NumPy are capable of accepting arrays as arguments. This eliminates the need of writing loops in our Python code.

Example vfunc.py

```
from numpy import *
a = array([1,10,100,1000])
print (log10(a))
```

³https://en.wikipedia.org/wiki/Pauli_matrices

The output of the program is `[0. 1. 2. 3.]` , where the log of each element is calculated and returned in an array. This feature simplifies the programs a lot. Numpy also provides a function to vectorize functions written by the user.

Example vectorize.py

```
from numpy import *

def spf(x):
    return 3*x

vspf = vectorize(spf)
a = array([1,2,3,4])
print (vspf(a))
```

The output will be `[3 6 9 12]` .

3.3 Exercises

1. Write code to make a one dimensional matrix with elements 5,10,15,20 and 25. make another matrix by slicing the first three elements from it.
2. Create a 3×2 matrix and print the sum of its elements using for loops.
3. Create a 2×3 matrix and fill it with random numbers.
4. Use `linspace` to make an array from 0 to 10, with step-size of 0.1
5. Use `arange` to make an 100 element array ranging from 0 to 10
6. Make an array `a = [2,3,4,5]` and copy it to `b`. change one element of `b` and print both.
7. Make a 3x3 matrix and multiply it by 5.
8. Create two 3x3 matrices and add them.
9. Write programs to demonstrate the dot and cross products.
10. Using matrix inversion, solve the system of equations

$$\begin{aligned} 4x_1 - 2x_2 + x_3 &= 11 \\ -2x_1 + 4x_2 - 2x_3 &= -16 \\ x_1 - 2x_2 + 4x_3 &= 17 \end{aligned}$$
11. Find the new values of the coordinate (10,10) under a rotation by angle $\pi/4$.
12. Write a vectorized function to evaluate $y = x^2$ and print the result for `x=[1,2,3]`.

Chapter 4

Data visualization

A graph or chart is used to present numerical data in visual form. A graph is one of the easiest ways to compare numbers. They should be used to make facts clearer and more understandable. Results of mathematical computations are often presented in graphical format. In this chapter, we will explore the Python modules used for generating two and three dimensional graphs of various types.

4.1 The Matplotlib Module

Matplotlib¹ is a python package that produces publication quality figures in a variety of hardcopy formats. It also provides many functions for matrix manipulation. You can generate plots, histograms, power spectra, bar charts, error-charts, scatter-plots, etc, with just a few lines of code and have full control of line styles, font properties, axes properties, etc. The data points to the plotting functions are supplied as Python lists or Numpy arrays.

If you import matplotlib as *pylab*, the plotting functions from the submodules *pyplot* and matrix manipulation functions from the submodule *mlab* will be available as local functions. Pylab also imports Numpy for you.

4.1.1 2D plots

Let us start with some simple plots to become familiar with matplotlib.

Example plot1.py

```
from pylab import *  
data = [1,2,5]  
plot(data)  
show()
```

In the above example, the x-axis of the three points is taken from 0 to 2. We can specify both the axes as shown below.

Example plot2.py

¹https://www.tutorialspoint.com/matplotlib/matplotlib_quick_guide.htm
<https://matplotlib.org/>
<https://matplotlib.org/tutorials/introductory/pyplot.html#sphx-glr-tutorials-introductory-pyplot-py>

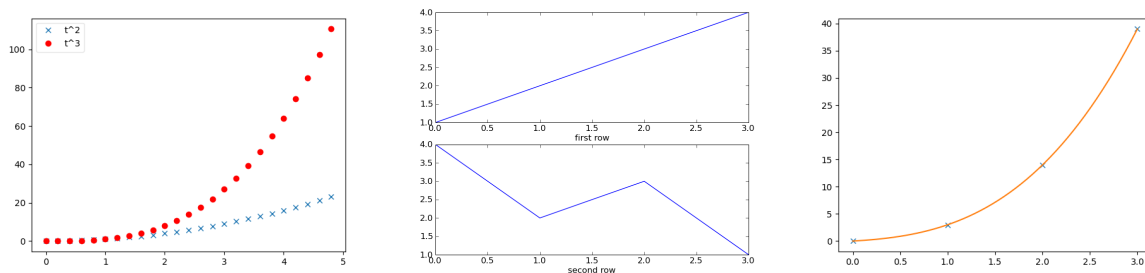


Figure 4.1: Output of (a) plot4.py (b) subplot1.py (c) piechart.py

```
from pylab import *
x = [1,2,5]
y = [4,5,6]
plot(x,y)
show()
```

By default, the color is blue and the line style is continuous. This can be changed by an optional argument after the coordinate data, which is the format string that indicates the color and line type of the plot. The default format string is 'b-' (blue, continuous line). Let us rewrite the above example to plot using red circles. We will also set the ranges for x and y axes and label them, as shown in *plot3.py*.

Example plot3.py

```
from pylab import *
x = [1,2,5]
y = [4,5,6]
plot(x,y,'ro')
xlabel('x-axis')
ylabel('y-axis')
axis([0,6,1,7])
show()
```

The figure 4.1 shows two different plots in the same window, using different markers and colors. It also shows how to use legends.

Example plot4.py

```
from pylab import *
t = arange(0.0, 5.0, 0.2)
plot(t, t**2, 'x', label='t^2')      # t^2
plot(t, t**3, 'ro', label='t^3')    # t^3
legend(framealpha=0.5)
show()
```

We have just learned how to draw a simple plot using the pylab interface of matplotlib. Another way to call numpy and matplotlib is like,

```
import numpy as np
import matplotlib.pyplot as plt
t = np.arange(0.0, 5.0, 0.2)
plt.plot(t, t**2, 'x', label='t^2')
show()
```

4.1.2 Polar plots

Polar coordinates locate a point on a plane with one distance and one angle. The distance ‘r’ is measured from the origin. The angle θ is measured from some agreed starting point. Use the positive part of the x – axis as the starting point for measuring angles. Measure positive angles anti-clockwise from the positive x – axis and negative angles clockwise from it.

Matplotlib supports polar plots, using the `polar(θ , r)` function. Let us plot a circle using `polar()`. For every point on the circle, the value of *radius* is the same but the polar angle θ changes from 0 to 2π . Both the coordinate arguments must be arrays of equal size. Since θ is having 100 points, r also must have the same number. This array can be generated using the `ones()` function. The `axis([θ_{min} , θ_{max} , r_{min} , r_{max}])` function can be used for setting the scale.

Example polar.py

```
from pylab import *
th = linspace(0,2*pi,100)
r = 5 * ones(100) # radius = 5
polar(th,r)
show()
```

4.1.3 Pie Charts

An example of a pie chart is given below. The percentage of different items and their names are given as arguments. The output is shown in figure 4.1(c).

Example piechart.py

```
from pylab import *
labels = 'Frogs', 'Hogs', 'Dogs', 'Logs'
fracs = [25, 25, 30, 20]
pie(fracs, labels=labels)
show()
```

4.1.4 Multiple plots

Matplotlib allows you to have multiple plots in the same window, using the `subplot()` command as shown in the example `subplot1.py`, whose output is shown in figure 4.1(b).

Example subplot1.py

```
from pylab import *
subplot(2,1,1)           # the first subplot
plot([1,2,3,4])
subplot(2,1,2)           # the second subplot
plot([4,2,3,1])
show()
```

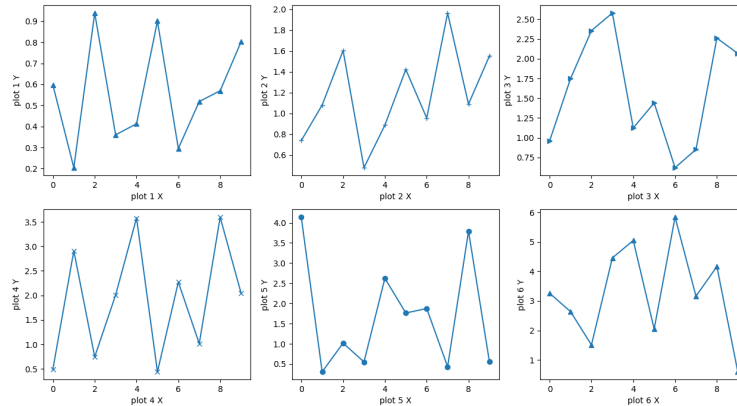


Figure 4.2: Multiple plots

The arguments to subplot function are NR (number of rows) , NC (number of columns) and a figure number, that ranges from 1 to $NR * NC$. The commas between the arguments are optional if $NR * NC < 10$, ie. subplot(2,1,1) can be written as subplot(211).

Another example of subplot is given is *subplot2.py*. You can modify the variable NR and NC to watch the results. Please note that the % character has different meanings. In $(pn+1)\%5$, it is the remainder operator resulting in a number less than 5. The % character also appears in the String formatting.

Example subplot2.py

```
from pylab import *
mark = ['x','o','^','+', '>']
NR = 2 # number of rows
NC = 3 # number of columns
pn = 1
for row in range(NR):
    for col in range(NC):
        subplot(NR, NC, pn)
        a = rand(10) * pn
        plot(a, marker = mark[(pn+1)%5])
        xlabel('plot %d X'%pn)
        ylabel('plot %d Y'%pn)
        pn = pn + 1
show()
```

The output is shown in figure4.2.

4.2 Plotting mathematical functions

One of our objectives is to understand different mathematical functions better, by plotting them graphically. We will use the *arange*, *linspace* and *logspace* functions from *numpy* to generate the input data and also the vectorized versions of the mathematical functions. For *arange()*, the third

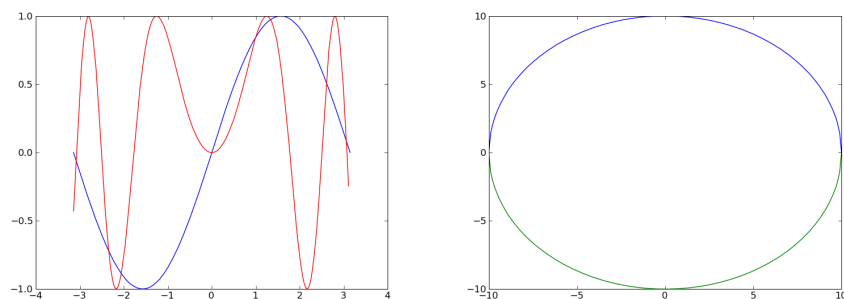


Figure 4.3: (a) Output of npsin.py (b) Output of circ.py .

argument is the step-size. The total number of elements is calculated from start, stop and step-size. In the case of `linspace()`, we provide start, stop and the total number of points. The step size is calculated from these three parameters. Please note that to create a data set ranging from 0 to 1 (including both) with a step-size of 0.1, we need to specify `linspace(0,1,11)` and not `linspace(0,1,10)`.

4.2.1 Sine function and friends

Let the first example be the familiar sine function. The input data is from $-\pi$ to $+\pi$ radians². To make it a bit more interesting we are plotting $\sin x^2$ also. The objective is to explain the concept of odd and even functions. Mathematically, we say that a function $f(x)$ is even if $f(x) = f(-x)$ and is odd if $f(-x) = -f(x)$. Even functions are functions for which the left half of the plane looks like the mirror image of the right half of the plane. From the figure 4.3(a) you can see that $\sin x$ is odd and $\sin x^2$ is even.

Example npsin.py

```
from pylab import *
x = linspace(-pi, pi , 200)
y = sin(x)
y1 = sin(x*x)
plot(x,y)
plot(x,y1,'r')
show()
```

Exercise: Modify the program *npsin.py* to plot $\sin^2 x$, $\cos x$, $\sin x^3$ etc.

4.2.2 Trouble with Circle

Equation of a circle is $x^2 + y^2 = a^2$, where a is the radius and the circle is located at the origin of the coordinate system. In order to plot it using Cartesian coordinates, we need to express y in terms of x , and is given by

$$y = \sqrt{a^2 - x^2}$$

We will create the x-coordinates ranging from $-a$ to $+a$ and calculate the corresponding values of y . This will give us only half of the circle, since for each value of x , there are two values of y

²Why do we need to give the angles in radians and not in degrees. Angle in radian is the length of the arc defined by the given angle, with unit radius. Degree is just an arbitrary unit.

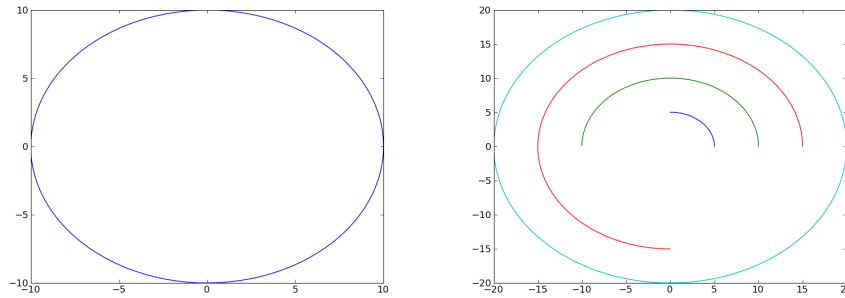


Figure 4.4: (a)Output of circpar.py. (b)Output of arcs.py

(+y and -y). The following program *circ.py* creates both to make the complete circle as shown in figure 4.3(b). Any multi-valued function will have this problem while plotting. Such functions can be plotted better using parametric equations or using the polar plot options, as explained in the coming sections.

Example circ.py

```
from pylab import *
a = 10.0
x = linspace(-a, a , 200)
yupper = sqrt(a**2 - x**2)
ylower = -sqrt(a**2 - x**2)
plot(x,yupper)
plot(x,ylower)
show()
```

4.2.3 Parametric plots

The circle can be represented using the equations $x = a \cos \theta$ and $y = a \sin \theta$. To get the complete circle θ should vary from zero to 2π radians. The output of circpar.py is shown in figure 4.4(a).

Example circpar.py

```
from pylab import *
a = 10.0
th = linspace(0, 2*pi, 200)
x = a * cos(th)
y = a * sin(th)
plot(x,y)
show()
```

Changing the range of θ to less than 2π radians will result in an arc. The following example plots several arcs with different radii. The *for* loop will execute four times with the values of radius 5,10,15 and 20. The range of θ also depends on the loop variable. For the next three values it will be π , 1.5π and 2π respectively. The output is shown in figure 4.4(b).

Example arcs.py

```

from pylab import *
a = 10.0
for a in range(5,21,5):
    th = linspace(0, pi * a/10, 200)
    x = a * cos(th)
    y = a * sin(th)
    plot(x,y)
show()

```

4.3 Simple 2D animation

Matplotlib supports some animation functions. Program *animate.py* uses `FuncAnimation()` to do a basic animation of a sine wave. A matplotlib *figure* object is created and a *line* is drawn. The `FuncAnimation` function periodically calls *update* with frame number sequentially incremented from 0 to 99, that is used for adding a phase increment to the plot. You may change the variable 'interval' to adjust the update rate.

```

from matplotlib.animation import FuncAnimation as fa
from pylab import *

x = linspace(-2*pi, 2*pi, 100)
fig1 = figure()
L, = plot(x, sin(x))

def update(fnum):
    L.set_data(x, sin(x+ 0.1 *fnum))
    return L,
anim = fa(fig1, update, frames=100, interval=50)
show()

```

4.4 Famous Curves

Connection between different branches of mathematics like trigonometry, algebra and geometry can be understood by geometrically representing the equations. You will find a large number of equations generating geometric patterns having interesting symmetries. A collection of them is available on the Internet [2][?]. We will select some of them and plot here. Exploring them further is left as an exercise to the reader.³

4.4.1 Astroid

The astroid was first discussed by Johann Bernoulli in 1691-92. It also appears in Leibniz's correspondence of 1715. It is sometimes called the tetracuspid for the obvious reason that it has four cusps. A circle of radius 1/4 rolls around inside a circle of radius 1 and a point on its circumference traces an astroid. The Cartesian equation is

$$x^{\frac{2}{3}} + y^{\frac{2}{3}} = a^{\frac{2}{3}} \quad (4.1)$$

The parametric equations are

³https://en.wikipedia.org/wiki/List_of_curves

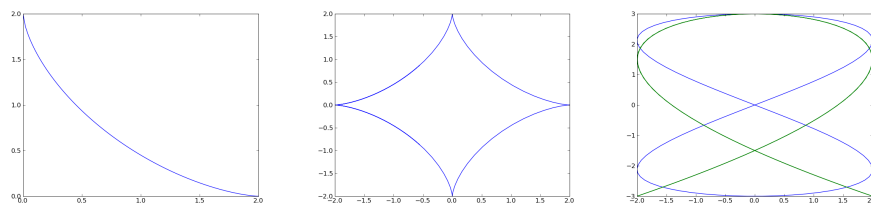


Figure 4.5: (a) Output of astro.py (b) astropar.py (c) lissa.py

$$x = a \cos^3(t), y = a \sin^3(t) \quad (4.2)$$

In order to plot the curve in the Cartesian system, we rewrite equation 4.1 as

$$y = (a^{\frac{2}{3}} - x^{\frac{2}{3}})^{\frac{3}{2}}$$

The program *astro.py* plots the part of the curve in the first quadrant. The program *astropar.py* uses the parametric equation and plots the complete curve. Both are shown in figure 4.5

Example astro.py

```
from pylab import *
a = 2
x = linspace(0,a,100)
y = ( a**(2.0/3) - x**(2.0/3) )**(3.0/2)
plot(x,y)
show()
```

Example astropar.py

```
from pylab import *
a = 2
t = linspace(-2*a,2*a,101)
x = a * cos(t)**3
y = a * sin(t)**3
plot(x,y)
show()
```

4.4.2 Ellipse

The ellipse was first studied by Menaechmus [?] . Euclid wrote about the ellipse and it was given its present name by Apollonius. The focus and directrix of an ellipse were considered by Pappus. Kepler, in 1602, said he believed that the orbit of Mars was oval, then he later discovered that it was an ellipse with the sun at one focus. In fact Kepler introduced the word *focus* and published his discovery in 1609.

The Cartesian equation is

$$\frac{x^2}{a^2} + \frac{y^2}{b^2} = 1 \quad (4.3)$$

The parametric equations are

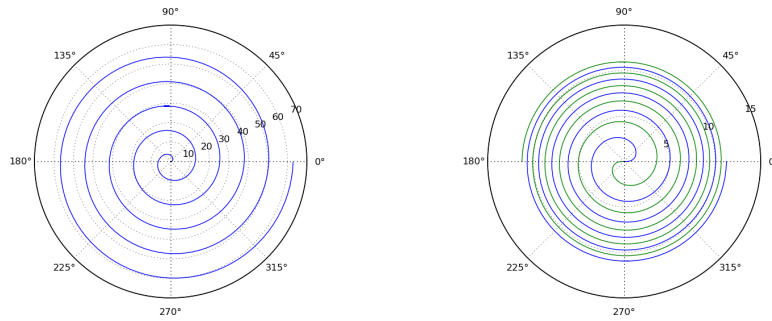


Figure 4.6: (a)Archimedes Spiral (b)Fermat's Spiral (c)Polar Rose

$$x = a \cos(t), y = b \sin(t) \quad (4.4)$$

The program *ellipse.py* uses the parametric equation to plot the curve. Modifying the parametric equations will result in Lissajous figures. The output of *lissa.py* are shown in figure 4.5(c).

Example ellipse.py

```
from pylab import *
a = 2
b = 3
t = linspace(0, 2 * pi, 100)
x = a * sin(t)
y = b * cos(t)
plot(x,y)
show()
```

Example lissa.py

```
from pylab import *
a = 2
b = 3
t= linspace(0, 2*pi,100)
x = a * sin(2*t)
y = b * cos(t)
plot(x,y)
x = a * sin(3*t)
y = b * cos(2*t)
plot(x,y)
show()
```

The Lissajous curves are closed if the ratio of the arguments for sine and cosine functions is an integer. Otherwise open curves will result, both are shown in figure 4.5(c).

4.4.3 Spirals of Archimedes and Fermat

The spiral of Archimedes is represented by the equation $r = a\theta$. Fermat's Spiral is given by $r^2 = a^2\theta$. The output of *archi.py* and *fermat.py* are shown in figure 4.6.

Example archi.py

```
from pylab import *
a = 2
th= linspace(0, 10*pi,200)
r = a*th
polar(th,r)
axis([0, 2*pi, 0, 70])
show()
```

Example fermat.py

```
from pylab import *
a = 2
th= linspace(0, 10*pi,200)
r = sqrt(a**2 * th)
polar(th,r)
polar(th, -r)
show()
```

4.5 Spirograph

Spirograph is a geometric drawing device that produces mathematical roulette curves of the variety technically known as hypotrochoids and epitrochoids. Consider a fixed outer circle of radius R , centered at the origin, and a smaller inner circle of radius r inside it, as shown in figure4.7(a). When the small circle rolls inside the big circle, the trajectory of a point located inside the small circle at a distance $\rho < R$ from it's center is given by the equations,

$$x(t) = R \left[(1 - k) \cos t + lk \cos \frac{1 - k}{k} t \right]$$

$$y(t) = R \left[(1 - k) \sin t + lk \sin \frac{1 - k}{k} t \right]$$

where $k = \frac{r}{R}$; $l = \frac{\rho}{r}$ and t is the angle of rotation. The python code *spiro.py* plots the output for some values of R , r and ρ .4.7(b). You may try changing the values of these parameters.

```
# spiro.py
from pylab import *
t = linspace(0, 10*pi, 500)
r = 3.
R = 10.0
k = r/R
l = 1.4
x = R*((1-k)*cos(t) + l*k*cos((1-k)*t/k))
y = R*((1-k)*sin(t) - l*k*sin((1-k)*t/k))
plot(x,y)
show()
```

<https://en.wikipedia.org/wiki/Spirograph>

<https://www.geeksforgeeks.org/fractal-using-spirograph-python>

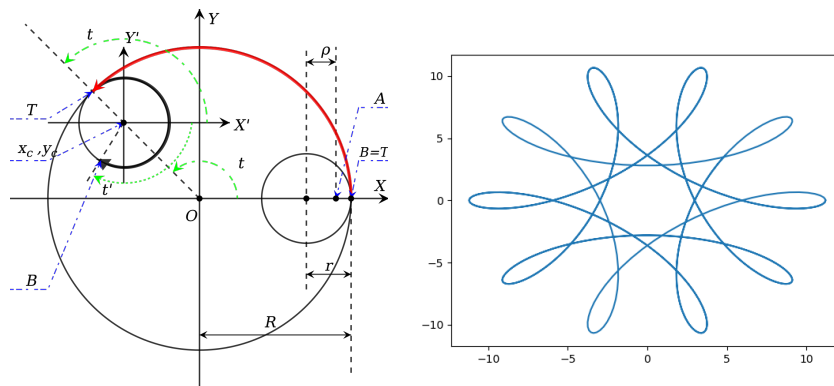
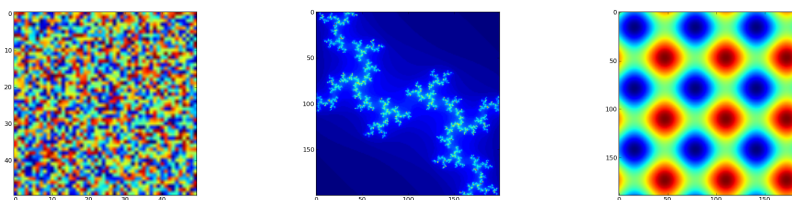


Figure 4.7: Spirograph.(a) mathematical basis (b) trajecory plot

Figure 4.8: Outputs of (a) `imshow1.py` (b) `julia.py` (c) `mgrid2.py`

4.6 2D plot using colors

A two dimensional matrix can be represented graphically by assigning a color to each point proportional to the value of that element. The program `imshow1.py` makes a 50×50 matrix filled with random numbers and uses `imshow()` to plot it. The result is shown in figure 4.8(a).

Example `imshow1.py`

```
from pylab import *
m = random([50,50])
imshow(m)
show()
```

4.6.1 Fractals

Fractals⁴ are a part of fractal geometry, which is a branch of mathematics concerned with irregular patterns made of parts that are in some way similar to the whole (e.g.: twigs and tree branches). A fractal is a design of infinite details. It is created using a mathematical formula. No matter how closely you look at a fractal, it never loses its detail. It is infinitely detailed, yet it can be contained in a finite space. Fractals are generally self-similar and independent of scale. The theory of fractals was developed from Benoit Mandelbrot's study of complexity and chaos. Complex numbers are required to compute the Mandelbrot and Julia Set fractals and it is assumed that the reader is familiar with the basics of complex numbers.

⁴<http://en.wikipedia.org/wiki/Fractal>

To compute the basic Mandelbrot (or Julia) set one uses the equation $f(z) \rightarrow z^2 + c$, where both z and c are complex numbers. The function is evaluated in an iterative manner, ie. the result is assigned to z and the process is repeated. The purpose of the iteration is to determine the behavior of the values that are put into the function. If the value of the function goes to infinity (practically to some fixed value, like 1 or 2) after few iterations for a particular value of z , that point is considered to be outside the Set. A Julia set can be defined as the set of all the complex numbers (z) such that the iteration of $f(z) \rightarrow z^2 + c$ is bounded for a particular value of c .

To generate the fractal the number of iterations required to diverge is calculated for a set of points in the selected region in the complex plane. The number of iterations taken for diverging decides the color of each point. The points that did not diverge, belonging to the set, are plotted with the same color. The program *julia.py* generates a fractal using a julia set. The program creates a 2D array (200 x 200 elements). For our calculations, this array represents a rectangular region on the complex plane centered at the origin whose lower left corner is (-1,-j) and the upper right corner is (1+j). For 200x200 equidistant points in this plane the number of iterations are calculated and that value is given to the corresponding element of the 2D matrix. The plotting is taken care by the *imshow* function. The output is shown in figure 4.8(b). Change the value of c and run the program to generate more patterns. The equation also may be changed.

Example julia.py

```

'''
Region of a complex plane ranging from -1 to +1 in both real
and imaginary axes is represented using a 2D matrix
having X x Y elements. For X and Y equal to 200, the step-size
in the complex plane is 2.0/200 = 0.01.
The nature of the pattern depends much on the value of c.
'''

from pylab import *
X = 200
Y = 200
MAXIT = 100
MAXABS = 2.0
c = 0.02 - 0.8j    # The constant in equation z**2 + c
m = zeros([X,Y])  # A two dimensional array

def numit(x,y):    # number of iterations to diverge
    z = complex(x,y)
    for k in range(MAXIT):
        if abs(z) <= MAXABS:
            z = z**2 + c
        else:
            return k    # diverged after k trials
    return MAXIT    # did not diverge,

for x in range(X):
    for y in range(Y):
        re = 0.01 * x - 1.0    # complex number for
        im = 0.01 * y - 1.0    # this (x,y) coordinate
        m[x][y] = numit(re,im) # get the color for (x,y)
imshow(m) # Colored plot using the 2D matrix
show()
```

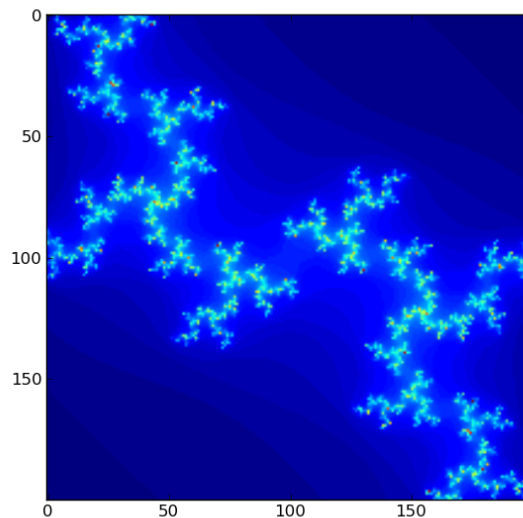


Figure 4.9: Julia fractal

4.7 3D Plots

Matplotlib supports several types of 3D plots, using the `Axes3D` class. The following three lines of code are required in every program making 3D plots using matplotlib.⁵

```
from pylab import *
from mpl_toolkits.mplot3d import Axes3D
ax = Axes3D.figure()
```

4.7.1 Line Plots

Example of a line plot is shown in `line3d.py` along with the output in figure 4.7.3(b).

Example line3d.py

```
from pylab import *
from mpl_toolkits.mplot3d import Axes3D
ax = Axes3D.figure()
phi = linspace(0, 2*pi, 400)
x = cos(phi)
y = sin(phi)
z = 0
ax.plot(x, y, z, label = 'x') # plot a circle
z = sin(4*phi) # modulated in z plane
ax.plot(x, y, z, label = 'x')
ax.set_xlabel('X')
ax.set_ylabel('Y')
```

⁵<https://jakevdp.github.io/PythonDataScienceHandbook/04.12-three-dimensional-plotting.html>

```
ax.set_zlabel('Z')
show()
```

Modify the code to make $x = \sin(2\phi)$ to observe Lissajous figures

4.7.2 Meshgrids

in order to make contour and 3D plots, we need to understand the concept of meshgrid. Consider a rectangular area on the X-Y plane. Assume there are m divisions in the X direction and n divisions in the Y direction. We now have a $m \times n$ mesh. A meshgrid is the coordinates of a grid in a 2D plane, x coordinates of each mesh point is held in one matrix and y coordinates are held in another.

The NumPy function `meshgrid()` creates two 2x2 matrices from two 1D arrays, as shown in the example below. This can be used for plotting surfaces and contours, by assigning a Z coordinate to every mesh point.

Example mgrid1.py

```
from numpy import *
x = arange(0, 3, 1)
y = arange(0, 3, 1)
gx, gy = meshgrid(x, y)
print gx
print gy
```

The outputs are as shown below, `gx(i,j)` contains the x-coordinate and `gy(i,j)` contains the y-coordinate of the point `(i,j)`.

```
[[0 1 2]
 [0 1 2]
 [0 1 2]]
[[0 0 0]
 [1 1 1]
 [2 2 2]]
```

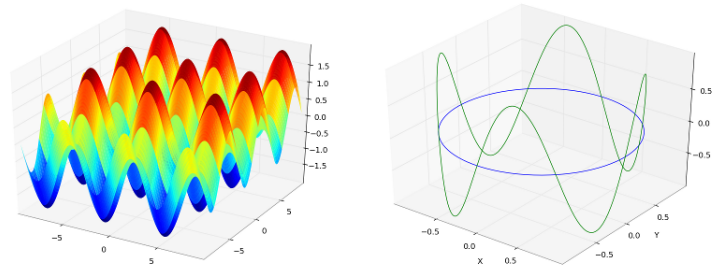
We can evaluate a function at all points of the meshgrid by passing the meshgrid as an argument. The program `mgrid2.py` plots the sum of sines of the x and y coordinates, using `imshow` to get a result as shown in figure 4.8(c).

Example mgrid2.py

```
from pylab import *
x = arange(-3*pi, 3*pi, 0.1)
y = arange(-3*pi, 3*pi, 0.1)
xx, yy = meshgrid(x, y)
z = sin(xx) + sin(yy)
imshow(z)
show()
```

4.7.3 Contour Plots

The example `mgrid2.py` is re-written to make a surface plot using the same equation in `surface3d.py` and the result is shown in figure 4.7.3(a).



Output of (a)surface3d.py (b)line3d.py

Example surface3d.py

```
from pylab import *
from mpl_toolkits.mplot3d import Axes3D
ax = Axes3D.figure()
x = arange(-3*pi, 3*pi, 0.1)
y = arange(-3*pi, 3*pi, 0.1)
xx, yy = meshgrid(x, y)
z = sin(xx) + sin(yy)
ax.plot_surface(xx, yy, z, cmap=cm.jet, cstride=1)
show()
```

4.7.4 Wire-frame Plots

Data for a sphere is generated using the outer product of matrices and plotted, by sphere.py.

```
from pylab import *
from mpl_toolkits.mplot3d import Axes3D
ax = Axes3D.figure()
phi = linspace(0, 2 * pi, 100)
theta = linspace(0, pi, 100)
x = 10 * outer(cos(phi), sin(theta))
y = 10 * outer(sin(phi), sin(theta))
z = 10 * outer(ones(size(phi)), cos(theta))
ax.plot_wireframe(x,y,z, rstride=2, cstride=2)
show()
```

4.8 Spherical harmonics

Program ylm20.py plots the spherical harmonics Y_m^l for $l = 2, m = 0$. The plot of $Y_2^0 = \frac{1}{4}\sqrt{\frac{5}{\pi}}(3\cos^2\phi - 1)$ is shown in figure4.10.

Example ylm20.py

```
from numpy import *
from pylab import * from mpl_toolkits.mplot3d import Axes3D ax = Axes3D.figure()
polar = linspace(0,pi,100)
```

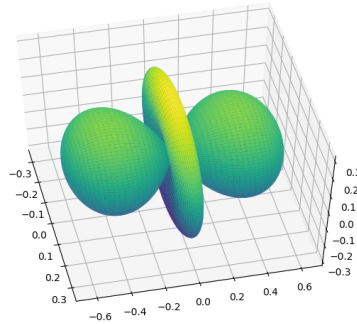


Figure 4.10: Output of ylm20.py

```
azimuth = linspace(0, 2*pi,100)
phi,th = meshgrid(polar, azimuth)
r = 0.25 * sqrt(5.0/pi) * (3*cos(phi)**2 - 1)
x = r*sin(phi)*cos(th)
y = r*cos(phi)
z = r*sin(phi)*sin(th)
ax.plot_surface(x,y,z, rstride=1, cstride=1,cmap='viridis', edgecolor='none') show()
```

4.9 Exercises

1. Plot a sine wave using markers +, o and x using three different colors.
2. Plot $\tan \theta$ from θ from -2π to 2π , watch for singular points.
3. Plot a circle using the polar() function.
4. Plot the following from the list of Famous curves at reference [?]
 - a) $r^2 = a^2 \cos 2\theta$, Lemniscate of Bernoulli
 - b) $y = \sqrt{2\pi}e^{-x^2/2}$ Frequency curve
 - c) $a \cosh(x/a)$ catenary
 - d) $\sin(a\theta)$ for $a = 2, 3$, and 4 . Rhodonea curves
5. Generate a triangular wave using Fourier series.
6. Evaluate $y = \sum_{n=1}^{n=\infty} \frac{(-1)^n x^{2n+1}}{(2n+1)!}$ for 10 terms.
7. Write a Python program to calculate sine function using series expansion and plot it.
8. Write a Python program to plot $y = 5x^2 + 3x + 2$ (for x from 0 to 5, 20 points),using pylab, with axes and title. Use red colored circles to mark the points.
9. Write a Python program to plot a Square wave using Fourier series, number of terms should be a variable.
10. Write a Python program to read the x and y coordinates from a file, in a two column format, and plot them.

11. Plot $x^2 + y^2 + z^2 = 25$ using mayavi.
12. Make a plot $z = \sin(x) + \sin(y)$ using `imshow()` , from -4π to 4π for both x and y .
13. Write Python code to plot $y = x^2$, with the axes labelled

Chapter 5

Numerical methods

Numerical analysis is the area of mathematics and computer science that creates, analyzes, and implements algorithms for solving the problems of continuous mathematics numerically. Solving mathematical equations is an important requirement for various branches of science for several reasons. Many equations evade an analytic solution and in some cases the input could be numerical data from an experiment. Even when we have an analytical solution, for all practical purposes we need to evaluate the numeric value of the result, with the desired accuracy.

Numerical solution of systems of linear or non-linear equations, differential or integral equations, interpolation etc., are some of the major applications. In this book, we are not going in to the theoretical details but will focus on developing simple working programs to illustrate the concept. Detailed theory of numerical analysis can be found in text books.¹ Since the Taylor series and the polynomial interpolation forms the mathematical basis of many numerical methods, we start with a brief introduction of them.

It should be noted that almost all the example programs given in this chapter are for learning purpose only. They can be made much smaller and efficient by using library functions from numpy or scipy. You may cross check the results of you code with the output of standard library functions.

5.1 Taylor's Series

All of you are familiar with the sine function, starting from the high school days. You know how to differentiate it, integrate it and do so many other things with it. Now, how do we find the value of $\sin(\theta)$, where $\theta = 1^0$, without using the tables or a calculator. The childhood friend becomes a bit unfamiliar at this point, I guess. But we know the value of $\sin(\theta)$ and all it's derivatives at $\theta = 0$. Suppose we know the position, velocity and acceleration of a car at some point $t = t_0$, we can calculate it's position after a time interval Δt . The situation is similar in the case of $\sin(1^0)$ also, we use something called the Taylor series.

The Taylor series provides an algorithm for connecting the value of a function at two points to the derivatives that function. If a function and its derivatives are known at some point $x = x_0$, we can express $f(x)$ in the vicinity of that point using a polynomial. The Taylor series expansion is given by,

$$f(x) = f(x_0) + (x - x_0)f'(x_0) + \frac{(x - x_0)^2}{2!}f''(x_0) + \cdots + \frac{(x - x_0)^n}{n!}f^n(x_0) \quad (5.1)$$

¹Introductory methods of numerical analysis by S.S.Sastry.

In the case of $f(x) = \sin(\theta)$, we know that $f(0) = 0$. The other terms involve the derivatives of $\sin(x)$. The first, second and third derivatives of $\sin(x)$ are $\cos(x)$, $-\sin(x)$ and $-\cos(x)$, respectively. Evaluating each of these at zero, we get 1, 0 and -1 respectively. The terms with even powers vanish. taking $x_0 = 0$, results in,

$$\sin(x) = x - \frac{x^3}{3!} + \frac{x^5}{5!} + \cdots = \sum_{n=0}^{\infty} (-1)^n \frac{x^{2n+1}}{(2n+1)!} \quad (5.2)$$

The program `sine-1deg.py` listed below calculates five terms to get the value

```
from numpy import *

x = 1./360
sinx = 0
for n in range(3):
    term = (-1)**(n) * (x**(2*n+1)) / math.factorial(2*n+1)
    sinx = sinx + term
    print (sinx,term)
print(sin(x))
```

The results are shown below. For comparison the value from the built-in sine function also is printed. It can be seen that it agrees very well, even with just three terms. Modify the program to calculate for higher angles to observe the effect of accuracy. Also increase the number of terms to see the effect of it on accuracy.

```
0.002777777777777778 0.002777777777777778
0.002777774205532693 -3.5722450845907643e-09
0.0027777742055340713 1.3781809739933504e-15
0.00277777420553
```

5.2 Polynomial Interpolation

For any single valued and continuous function $y = f(x)$, we can calculate the value of y for any value of x in an interval $a < x < b$, where it is defined. Now, consider the problem that is just opposite of it.

We have a set of tabular values (x_0, y_0) (x_1, y_1) ... (x_i, y_i) satisfying a function $y = f(x)$ but we do not know what the function is. We construct a function $\phi(x)$ that satisfies all the given data points, obtained $\phi(x)$ may be only an approximation of $y = f(x)$. When a set of polynomials are used for constructing such a function like

$$y_n(x) = a_0 + a_1(x - x_0) + \cdots + a_n(x - x_0)(x - x_1) \cdots (x - x_{n-1}) \quad (5.3)$$

is called polynomial interpolation. We can construct a polynomial of degree n from $n+1$ distinct data points. The coefficients a_i can be evaluated in the following manner. Since the polynomial passes through all the data points, when $x = x_0$, all the terms in 5.3 except a_0 should vanish due to the presence of $(x - x_0)$.

$$a_0 = y_0$$

Similarly for $x = x_1$, only the first two terms will be non-zero.

$$y_1 = a_0 + a_1(x_1 - x_0)$$

$$a_1 = \frac{(y_1 - y_0)}{(x_1 - x_0)}$$

and for $x = x_2$,

$$y_2 = a_0 + a_1(x_2 - x_0) + a_2(x_2 - x_0)a_1(x_2 - x_1)$$

$$a_2 = \frac{\frac{y_2 - y_1}{x_2 - x_1} - \frac{y_1 - y_0}{x_1 - x_0}}{x_2 - x_0}$$

This procedure can be continued to evaluate all the coefficients. Before proceeding with the general case, first let us consider a special case where the data points (x_i, y_i) are equally spaced. It is possible to construct difference tables and use them for interpolation.

5.2.1 Difference Table

For a set of given values $(x_0, y_0) (x_1, y_1) \dots (x_i, y_i)$, the differences are

$$\Delta y_0 = y_1 - y_0$$

$$\Delta y_1 = y_2 - y_1$$

$$\Delta y_2 = y_3 - y_2 \text{ etc.}$$

And

$$\Delta^2 y_0 = \Delta y_1 - \Delta y_0 = (y_2 - y_1) - (y_1 - y_0)$$

Similarly

$$\Delta^3 y_0 = \Delta^2 y_1 - \Delta^2 y_0$$

They can be expressed in the tabular form as shown below, to make manual computation easier. For numerical computation, we will use the data sets $[0, 2, 4, 6]$ and $[0, 8, 64, 216]$, that are derived from the equation $y = x^3$. This will help make verification of the interpolated results by comparing with the analytic value.

| x | y | Δ | Δ^2 | Δ^3 |
|-----|-----|----------|------------|------------|
| 0 | 0 | | | |
| | | 8 | | |
| 2 | 8 | | 48 | |
| | | 56 | | 48 |
| 4 | 64 | | 96 | |
| | | 152 | | |
| 6 | 216 | | | |

The Differences are available from the table. We can use Newton's formula for interpolation to calculate the value of y for an unknown value of x .

5.2.2 Newton's forward difference formula

On the equation

$$y_n(x) = a_0 + a_1(x - x_0) + \dots + a_n(x - x_0)(x - x_1) \dots (x - x_{n-1}) \quad (5.4)$$

applying the condition of equal spacing $x_1 = x_0 + h$, $x_2 = x_0 + 2h$ etc. results in

$$y_n(x) = y_0 + p\Delta y_0 + \frac{p(p-1)}{2!}\Delta^2 y_0 + \frac{p(p-1)(p-2)}{3!}\Delta^3 y_0 + \dots \quad (5.5)$$

where $p = \frac{x-x_0}{h}$ and $h = x_1 - x_0$. This is Newton's forward difference interpolation formula. Using it, let us calculate $y(x)$ for $x = 2.5$
 $h = 2 - 0 = 2$, $p = (2.5 - 0)/2 = 1.25$

$$y(2.5) = 0 + 1.25 \times 8 + \frac{1.25(1.25 - 1)48}{2} + \frac{1.25(1.25 - 1)(1.25 - 2)48}{6} = 15.625$$

The calculations could be done manually and the result agrees with the analytical result $2.5^3 = 15.625$. It is left as an exercise to the reader to use the function $y = x^4$ and repeat the exercise. The result would not agree, add one more point to observe the difference.

Next step is to write a Python program to do the same. The code should work for any number of input points. We need to create two arrays to store the x and y values. The the table we can see that the differences require arrays of different sizes and the number of difference arrays depends on the number of data points. A better approach is to make a single difference array. After each iteration, we store the first element calculated in that iteration to a list, to be used in the interpolation formula. The program *forward-diff-table.py* listed below prints the forward difference table.

```
from numpy import *
x = [0,2,4,6]
y = [0,8,64,216]
n = len(x)
for a in x: print('%10.0f'%a, end = '')
print()
for a in y: print('%10.0f'%a, end = '')
print()
deltas = []    # list to store the required Delta values

diff = copy(y)
for k in range(0, n-1):
    tmp = copy(diff)
    print((k+1)*5*' ', end = '') # adjust spacing
    for i in range(k,n-1):
        tmp[i+1] = (diff[i+1] - diff[i])
        print('%10.0f'%tmp[i+1], end = '')
    print()
    deltas.append(tmp[k+1]) # store delta
    diff = copy(tmp)
print ('Delta values ',Delta)
```

The algorithm works in the following manner. y is the starting value of difference array. Inside the loop the difference array is copied into a temporary array. Inside the inner loop, the next set of differences are calculated. The element required for future use is appended to a list. The output of the program is given below.

| | | | |
|--------------|-------------|----|-----|
| 0 | 2 | 4 | 6 |
| 0 | 8 | 64 | 216 |
| | 8 | 56 | 152 |
| | 48 | 96 | |
| | | 48 | |
| Delta values | [0 8 48 48] | | |

The code shown below uses the Delta to calculate the value of y for $x=2.5$.

```

nx = 2.5
h = x[1] - x[0]
p = (nx-x[0])/h
print('p = ', p)
ny = y[0] + p*deltas[0] + p*(p-1)*deltas[1]/2 + p*(p-1)*(p-2)*deltas[2]/6
print (ny)

```

Look for similarities between Taylor's series discussed in section 5.1 that and polynomial interpolation process. The derivative of a function represents an infinitesimal change in the function with respect to one of its variables. The finite difference is the discrete analog of the derivative. Using the divided difference method, we are in fact calculating the derivatives in the discrete form.

5.2.3 Newton's forward difference formula

By taking the final point as reference, the polynomial can be expressed as

$$y_n(x) = a_0 + a_1(x - x_n) + \cdots + a_n(x - x_n)(x - x_{n-1}) \cdots (x - x_1) \quad (5.6)$$

Applying similar conditions on this equation, we arrive at the Backward Difference Interpolation Formula.

$$y_n(x) = y_n + p\nabla y_n + \frac{p(p+1)}{2!}\nabla^2 y_n + \cdots + \frac{p(p+1)\cdots(p+n-1)}{n!}\nabla^n y_n \quad (5.7)$$

In this method also, the table is prepared in the same manner but it uses values from the end of the table. The program *backward-diff-table.py*, listed below, is identical to the previous program, except for statement `deltas.append(tmp[-1])` that stores the last element from the k^{th} difference array.

```

from numpy import *
x = [0,2,4,6]
y = [0,8,64,216]
n = len(x)
for a in x: print('%10.0f'%a, end = '')
print()
for a in y: print('%10.0f'%a, end = '')
print()
deltas = []    # list to store the required Delta values

diff = copy(y)
for k in range(0, n-1):
    tmp = copy(diff)
    print((k+1)*5*' ', end = '') # adjust spacing
    for i in range(k,n-1):
        tmp[i+1] = (diff[i+1] - diff[i])
        print('%10.0f'%tmp[i+1], end = '')
    print()
    deltas.append(tmp[-1]) # store delta
    diff = copy(tmp)
print ('Delta values ',Delta)

```

The code given below can be used to verify the table.

```

nx = 2.5
h = x[1] - x[0]
p = (nx-x[-1])/h
print('p = ', p)
ny = y[-1] + p*deltas[0] + p*(p+1)*deltas[1]/2 + p*(p+1)*(p+2)*deltas[2]/6
print (ny, nx**3)

```

The program diff-table-test.py listed below plots the results from both the interpolations and the input data points along with $y = x^3$.

```

from pylab import *
x = [0,2,4,6]
y = [0,8,64,216]
n = len(x)

nx = linspace(0,6,11) # 11 values of x from 0 to 3
h = x[1] - x[0]
p = (nx-x[0])/h

deltas = [8, 48, 48] #from difference table, forward
ny = y[0] + p*deltas[0] + p*(p-1)*deltas[1]/2 +
    p*(p-1)*(p-2)*deltas[2]/6
plot(nx,ny, 'x', label='Forward') # interpolated by FD method
p = (nx-x[-1])/h
deltas = [152, 96, 48] #from difference table, backward
ny = y[-1] + p*deltas[0] + p*(p+1)*deltas[1]/2 + p*(p+1)*(p+2)*deltas[2]/6
plot(nx,ny, '+', label='Backward') # interpolated by BD method
plot(x,y, 'o', label='Data points') # given data points
plot(nx, nx**3, label = '$y=x^3$') # analytical value
legend(framealpha=0.5)
show()

```

The output of the program is given in figure 5.1

5.2.4 Lagrange's Interpolation formula

This method can be used for interpolating non-uniformly spaced data points. A set of tabular values (x_0, y_0) (x_1, y_1) ... (x_i, y_i) can be represented as

$$L_n(x) = \sum_{i=0}^n l_i(x) y_i$$

where $l_i(x)$ are polynomials in x of degree n .

$$l_i(x) = \frac{(x-x_0)(x-x_1)\dots(x-x_{i-1})(x-x_{i+1})\dots(x-x_n)}{(x_i-x_0)(x_i-x_1)\dots(x_i-x_{i-1})(x_i-x_{i+1})\dots(x_i-x_n)}$$

program lagrange-poly.py uses a non-uniformly spaced data set. We have generated this from equation $y = x^3$ to cross check the results of interpolation. The evaluation of the coefficients is simple, the i^{th} data point is excluded while calculating the i^{th} term.

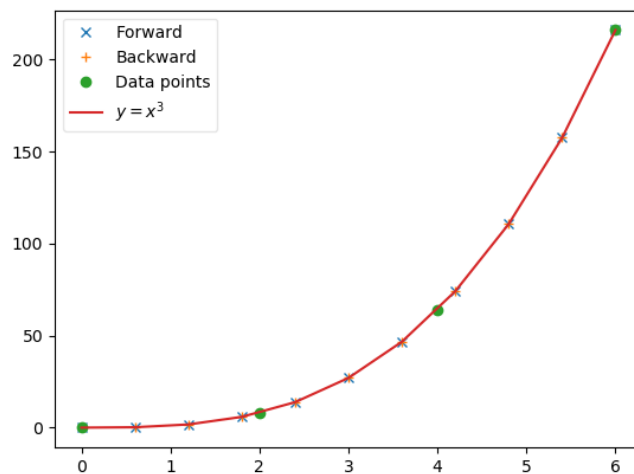


Figure 5.1: Newton's forward and backward interpolation results.

```

xa = [0, .5, 1.5, 3]
ya = [0, .125, 3.375, 27]
N = len(xa)

def lagra(x):
    res = 0.0
    for i in range(N):
        term = 1
        for k in range(N):
            if i != k:
                #print (x, xa[k], xa[i], xa[k])
                term = term * (x - xa[k]) / (xa[i]-xa[k])
        #print (term)
        res += term * ya[i]
    return res

print (lagra(2.5), 2.5**3)

```

The output is 15.625 15.625. The result tallies with the analytical value. Remove the comments to print each term.

5.2.5 Newton's General Interpolation Formula

Suppose the the given set is $(x_i, y_i), i = 0, 1 \dots n - 1$ and the polynomial is

$$y_n(x) = a_0 + a_1(x - x_0) + \dots + a_n(x - x_0)(x - x_1) \dots (x - x_{n-1}) \quad (5.8)$$

We have already seen that the coefficients can be calculated from equations;

$$a_0 = y_0$$

$$a_1 = \frac{(y_1 - y_0)}{(x_1 - x_0)}$$

$$a_2 = \frac{\frac{y_2 - y_1}{x_2 - x_1} - \frac{y_1 - y_0}{x_1 - x_0}}{x_2 - x_0}$$

They can be expressed better using the divided difference notation as shown below.

$$[y_0] = y_0$$

$$[y_0, y_1] = \frac{(y_1 - y_0)}{(x_1 - x_0)}$$

$$[y_0, y_1, y_2] = \frac{\frac{y_2 - y_1}{x_2 - x_1} - \frac{y_1 - y_0}{x_1 - x_0}}{x_2 - x_0} = \frac{[y_1, y_2] - [y_0, y_1]}{(x_2 - x_0)}$$

Using these notation, the polynomial can be re-written as;

$$\begin{aligned} y(x) = & [y_0] + [y_0, y_1](x - x_0) + [y_0, y_1, y_2](x - x_0)(x - x_1) + \\ & \dots + [y_0, \dots, y_n](x - x_0) \dots (x - x_{n-1}) \end{aligned} \quad (5.9)$$

The preparation of the forward difference table or equation 5.9 does not assume uniformly spaced data points. We will demonstrate it using a non-uniformly spaced data set, using the program *newton-general.py* listed below. Note the term $x(i - k)$ in the denominator, that decides the x interval. We have generated the input data using the equation $y = x^3$.

```
from numpy import *
x = [0, .5, 1.5, 3]
y = [0, .125, 3.375, 27]
n = len(x)

for a in x: print('%10.2f'%a, end= '') print()
for a in y: print('%10.2f'%a, end = '') print()
for k in range(0,n-1):
    tmp = copy(y)
    for i in range(k,n-1):
        tmp[i+1] = (y[i+1] - y[i]) / (x[i+1]-x[i-k])
        print('%10.2f'%tmp[i+1], end = '')
    print()
    y = copy(tmp)
print ('coefficients ',y)

#Verification
a = y
nx = 2.5
ny = a[0] + (nx - x[0])*a[1] + (nx - x[0])*(nx - x[1])*a[2] +
      (nx - x[0])*(nx - x[1])*(nx - x[2])*a[3]
print(ny, nx**3)
```


The program prints the difference table and the coefficients. We verify the validity of all these equations by calculating the value of y for any arbitrary value of x using equation 5.9 and comparing it with x^3 . Let us take $x = 2.5$ as an example.

$$y(2.5) = 0 + 1(2.5 - 0) + 3(2.5 - 0)(2.5 - 1) + 1(2.5 - 0)(2.5 - 1)(2.5 - 2) = 15.625$$

The result tallies with the exact value of $2.5^3 = 15.625$.

5.3 Numerical Integration

The general problem of numerical integration is to compute

$$I = \int_a^b f(x) dx \quad (5.10)$$

where a set of tabular values (x_0, y_0) (x_1, y_1) ... (x_i, y_i) satisfying a function $y = f(x)$ are given. To evaluate the integral 5.10, we divide it into n equal intervals each having a width h . Then $x_n = x_0 + nh$ and $I = \int_{x_0}^{x_0+nh} f(x) dx$

According to Newton's forward difference formula,

$$f(x) = y_0 + p\Delta y_0 + \frac{p(p-1)}{2!}\Delta^2 y_0 + \frac{p(p-1)(p-2)}{3!}\Delta^3 y_0 + \dots$$

will lead to the Newton Cote's Quadrature formula²,

$$I = nh \left[y_0 + \frac{n}{2}\Delta y_0 + \frac{n(2n-3)}{3!}\Delta^2 y_0 + \frac{n(n-1)^2}{4!}\Delta^3 y_0 + \dots \right] \quad (5.11)$$

For different values of n this will result in different quadrature formulae.

5.3.1 Trapezoidal Rule

Truncating equation 5.11 at $n = 1$ results in Trapezoidal rule. The sum of the areas .

$$\int_{x_0}^{x_0+h} f(x)dx = h\left(y_0 + \frac{\Delta y_0}{2}\right) = h \left[y_0 + \frac{1}{2}(y_1 - y_0) \right] = \frac{h}{2}(y_0 + y_1)$$

Similarly

$$\int_{x_0+h}^{x_0+2h} ydx = \frac{h}{2}(y_1 + y_2)$$

Adding all the areas give

$$\int_{x_0}^{x_0+nh} f(x)dx = \frac{h}{2} [y_0 + 2(y_1 + y_2 + \dots + y_{n-1}) + y_n] \quad (5.12)$$

This is known as trapezoidal formula. The area under the curve, as shown in figure 5.2, is calculated by dividing it into n sections. Each section is a trapezoid in this case. The program *trapez.py* does integration of a given function using equation 5.12. We will choose an example where the results can be cross checked easily, the value of π is calculated by evaluating the area of a unit circle by integrating the equation of a circle.

²<https://theengineeringmaths.com/wp-content/uploads/2017/11/num-diff-integ-web.pdf>

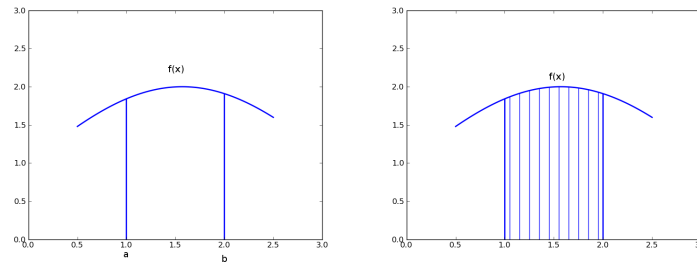


Figure 5.2: Area under the curve is divided it in to a large number of intervals. Area of each of them is calculated by assuming them to be trapezoids.

Example trapez.py

```
from math import *
def y(x): # equation of a circle
    return sqrt(1.0 - x**2)

def trapez(f, a, b, n):
    h = (b-a) / n
    sum = 0
    x = 0.5 * h # f(x) at middle of the slice
    for i in range (1,n):
        sum = sum + h * f(x)
        x = x + h
    return sum

print 4 * trapez(y, 0.0, 1.0,1000)
print 4 * trapez(y, 0.0, 1.0,10000)
```

The output is shown below. The result gets better by increasing n thus resulting in smaller h .

```
3.140417031779045
3.141555466911023
```

5.3.2 Simpson's 1/3-Rule

Truncating equation 5.11 at $n = 2$ results in a second degree polynomial. The total curve will be divided into $\frac{n}{2}$ arcs, that also implies that n must be an even number. Area of sections will be given by,

$$\int_{x_0}^{x_2} y dx = 2h(y_0 + \Delta y_0 + \frac{1}{6}\Delta^2 y_0) = \frac{h}{3}(y_0 + 4y_1 + y_2)$$

similarly

$$\int_{x_2}^{x_4} y dx = \frac{h}{3}(y_2 + 4y_3 + y_4)$$

etc. Summing all terms will give.

$$\int_{x_0}^{x_n} y dx = \frac{h}{3} [y + 4(y_1 + y_3 + \cdots + y_{n-1}) + 2(y_2 + y_4 + \cdots + y_{n-2}) + y_n] \quad (5.13)$$

This is known as Simpson's 1/3 rule.

```
from math import *
def sqr(a):
    return sqrt(1.0 - a**2)

def simp13(f, a, b, n):
    h = (b-a) / n
    result = f(a)    # first point
    for i in range (1,n,2):
        result = result + 4 * f(a + h * i)
    for i in range (2,n-1,2):
        result = result + 2 * f(a + h * i)
    result = result + f(b) # last point
    return h/3 * result

print(4*simp13(sqr,0.,1.,100))
print(4*simp13(sqr,0.,1.,1000))
```

The program prints

```
3.1411332053392274
3.1415781302139867
```

5.4 Derivatives from the Interpolation Formula

The Forward Difference Interpolation formula is expressed as

$$y_n(x) = a_0 + p\Delta y_0 + \frac{p(p-1)}{2!}\Delta^2 y_0 + \frac{p(p-1)(p-2)}{3!}\Delta^3 y_0 + \cdots \quad (5.14)$$

where $p = \frac{x-x_0}{h}$ giving $\frac{dp}{dx} = \frac{1}{h}$

$$\frac{dy}{dp} = \Delta y_0 + \frac{(2p-1)}{2!}\Delta^2 y_0 + \frac{(3p^2-6p+2)}{3!}\Delta^3 y_0 + \cdots \quad (5.15)$$

$$\frac{dy}{dx} = \frac{dy}{dp} \times \frac{dp}{dx}$$

$$\frac{dy}{dx} = \frac{1}{h} \left[\Delta y_0 + \frac{2p-1}{2!}\Delta^2 y_0 + \frac{(3p^2-6p+2)}{3!}\Delta^3 y_0 + \cdots \right] \quad (5.16)$$

At $x = 0, p = 0$

$$\frac{dy}{dx} = \frac{1}{h} \left[\Delta y_0 + \frac{\Delta^2 y_0}{2!} + \frac{\Delta^3 y_0}{3!} + \cdots \right] \quad (5.17)$$

To verify these equations again we use data generated from $y = x^3$. The program *fd-derivative-test.py* uses the results from the forward difference table and calculates the value of the derivative at $x = 1.5$ by using equation 5.16. The result is cross checked against $3x^2$, the derivative of x^3 .

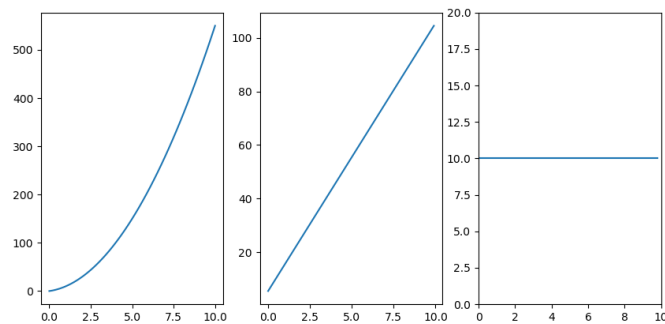


Figure 5.3: Numpy gradient function demonstration

```

from pylab import *
x = [0,1,2,3]
y = [0,1,8,27]
a = [0,1,3,1]    #coefficients from FD table

h = x[1] - x[0]
nx = 1.5    # new point
p = (nx-x[0])/h
dny = a[1] + (2*p-1)*a[2] + (3*p**2-6*p+2)*a[3]
print (dny, 3*nx**2)

```

5.4.1 Numpy gradient function

The numpy module provides functions to differentiate data sets available in numerical form. Program *diff-data.py* loads two columns of data, x and y, from a file, calculates the first and second derivatives and plots them. The program is shown below.

```

from pylab import *
x,y = loadtxt("diff-data.txt", delimiter=' ')    # read 2 column data
dx = x[1] - x[0]
dy = diff(y)/dx
d2y = diff(dy)/dx
subplot(1,3,1)
plot(x,y)
subplot(1,3,2)
plot(x[:-1],dy)
subplot(1,3,3)
axis([0,10,0,20])
plot(x[:-2],d2y)
show()

```

Output of the program is shown in figure 5.3. The input data looks like a parabola, first derivative has constant slope and the second derivative is a constant. The data is generated by the following lines of code.

```

t = linspace(0,10,11)
s = 5 * t**2    #S = ut + 1/2 at^2
savetxt('diff-data.txt', array([t,s]), delimiter = ' ')

```

5.5 First Order Ordinary Differential Equations

Differential equations are one of the most important mathematical tools used in producing models for physical and biological processes. In this section, we will discuss the numerical methods for solving the initial value problem for first-order ordinary differential equations. Consider the equation,

$$\frac{dy}{dx} = f(x, y); \quad y(x_0) = y_0 \quad (5.18)$$

where the derivative of the function $f(x, y)$ is known and the value of the function at some value of $x = x_0$ also is known. The objective is to find out the value of the function for other values of x . The underlying idea of any routine for solving the initial value problem is to rewrite the dy and dx as finite steps Δy and Δx , and multiply the equations by Δx , and use the Taylor series as explained in the previous section.

Implementation of this procedure as such results in the Euler's method. Euler method is very simple and demonstrates the concept of using Taylor series. The method is not accurate due to the following reasons. The derivative at the starting point is used for computing the function during the interval Δx , that may not be true. The higher order derivatives are ignored. Later we will explore some methods that remedy this drawbacks.

5.5.1 Euler method

The equations of Euler's method can be obtained as follows. By the definition of derivative,

$$y'(x_n, y_n) = \lim_{h \rightarrow 0} \frac{y(x_n + h) - y(x_n)}{h} \quad (5.19)$$

For sufficiently small values of h , we can write,

$$y(x_n + h) = y(x_n, y_n) + hy'(x_n) \quad (5.20)$$

The above equations implies that, if the value of the function $y(x)$ is known to be y_n at the point x_n , its value at a nearby point x_{n+1} is given by $y_n + h \times y'$. The program *euler.py* calculates the value of sine function using its derivative, ie. the cosine function. We start from $x = 0$, where $\sin(x) = 0$ and compute the subsequent values using the derivative, $\cos(x)$, and compare the result with the actual sine function. The requirement is to calculate the value of a function during a given interval. The values of the function and it's derivative is given at the starting point. We will define a numpy array of the values of the independent variable x during the interval with a spacing of Δx between two adjacent points. An empty array of the same size is created to fill in the computed values of the function.

Example euler-sine.py

```

from pylab import *
def f1(x,y):
    return cos(x)
def euler(x, y, fxy, h):

```

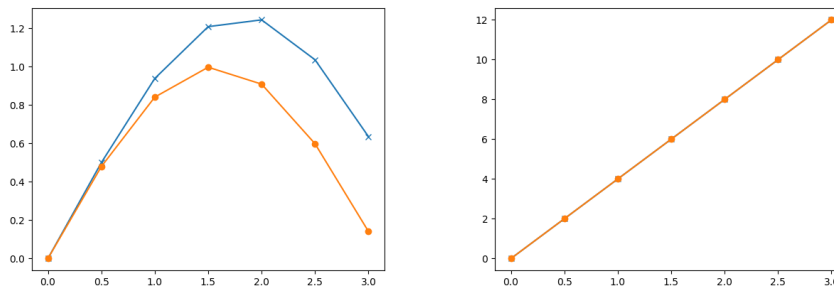


Figure 5.4: Outputs of (a)euler-sine.py.(b)modified for line

```

    return y + h * fxy(x,y)    # Euler method

dx = .5    # step size
xmin = 0   # initial value
xmax = pi  # calculate up to this only
xa = np.arange(xmin, xmax, dx)
N = len(xa)
ya = np.empty(N) # numpy array to store results
ya[0] = 0.0      # given initial value

for i in range(N-1):
    ya[i+1] = euler(xa[i], ya[i], f1, dx)
plot(xa, ya, 'x-')
plot(xa, np.sin(xa), 'o-')
show()

```

The output of *euler-sine.py* is shown in figure 5.4. A large step size is chosen to highlight the error. Modify the code to reduce dx to see the result. To understand the source of error, modify the function $f1$ to return a number, like *return 4*. This represents a straight line with a slope of 4. The results are shown in figure .

5.5.2 Second order Runge-Kutta method

The formula 5.19 used by Euler method which advances a solution from x_n to x_{n+1} is not symmetric, it advances the solution through an interval h , but uses derivative information at the beginning of that interval. Better results are obtained if we take *trial* step to the midpoint of the interval and use the value of both x and y at that midpoint to compute the *real* step across the whole interval. This is called the second-order Runge-Kutta method or the midpoint method. The only changes required in the code are replacing the function *euler* by *rk2*, as shown below.

```

def rk2(x, y, fxy, h):
    k1 = fxy(x, y)
    k2 = fxy(x + h, h*k1)
    return y + h * ( k1/2 + k2/2)

```

The result is shown in figure 5.5(a).

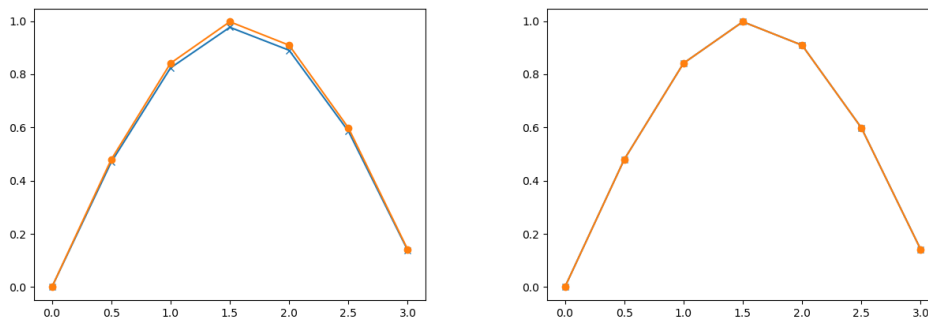
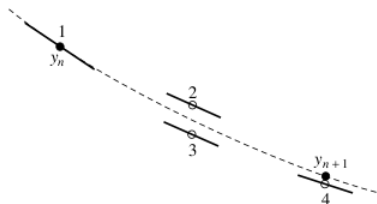


Figure 5.5: Outputs of (a) rk2.py (b) rk4.py

5.5.3 Fourth order Runge-Kutta method

The fourth order Runge-Kutta method is the most popular one and is commonly referred as the Runge-Kutta method. In each step the derivative is evaluated four times, once at the initial point, twice at trial midpoints, and once at a trial endpoint, as shown below.



Every trial evaluation uses the value of the function from the previous trial point, ie. k_2 is evaluated using k_1 and not using y_n . From these derivatives the final function value is calculated, The calculation is done using the equations,

$$\begin{aligned}
 k_1 &= hf(x_n, y_n) \\
 k_2 &= hf(x_n + \frac{h}{2}, y_n + \frac{k_1}{2}) \\
 k_3 &= hf(x_n + \frac{h}{2}, y_n + \frac{k_2}{2}) \\
 k_4 &= hf(x_n + h, y_n + k_3) \\
 y_{n+1} &= y_n + \frac{1}{6} (k_1 + 2k_2 + 2k_3 + k_4)
 \end{aligned} \tag{5.21}$$

The program rk4-sine.py is obtained by repacing function rk2 by rk4, as listed below.

```
def rk4(x, y, fxy, h):    # x, y , f(x,y)
    k1 = h * fxy(x, y)
    k2 = h * fxy(x + h/2.0, y+k1/2)
    k3 = h * fxy(x + h/2.0, y+k2/2)
    k4 = h * fxy(x + h, y+k3)
    return y + ( k1/6 + k2/3 + k3/3 + k4/6 )
```

From the results 5.4(a) ,5.5(a) and 5.5(b) one can see the superiority of fourth order Runge-Kutta method. The program *compare-euler-RK4.py* evaluates sine function using both Euler and RK4

methods. The error is compared by plotting the differences with `sin()` function. It can be seen that the error is much less in the case of RK4

Example compare-euler-RK4.py

```
from pylab import *

def f1(x,y):
    return cos(x)

def euler(x, y, fxy, h):
    return y + h * fxy(x,y)    # Euler method

def rk4(x, y, fxy, h):    # x, y , f(x,y)
    k1 = h * fxy(x, y)
    k2 = h * fxy(x + h/2.0, y+k1/2)
    k3 = h * fxy(x + h/2.0, y+k2/2)
    k4 = h * fxy(x + h, y+k3)
    return y + ( k1/6 + k2/3 + k3/3 + k4/6 )

dx = .1    # step size
xmin = 0    # initial value
xmax = pi # calculate up to this only
xa = np.arange(xmin, xmax, dx)
# array of the independent variable N =len(xa)
ya = np.empty(N) # numpy array to store results
sf = sin(xa) # sine function

ya[0] = 0.0 # given initial value
for i in range(N-1):
    ya[i+1] = euler(xa[i], ya[i], f1, dx)
plot(xa, ya-sf, 'x')

for i in range(N-1):
    ya[i+1] = rk4(xa[i], ya[i], f1, dx)
plot(xa, ya-sf, 'o')
show()
```

5.5.4 Function depending on the integral

In the previous examples, the function depends on the independent variable only. Let us consider an example where it depends on y also. *The program rk4-xy.py* listed below evaluates the function $f(x,y) = 2(y - x^2) + 1$. Readers may verify the results by manual computing.

Example rk4-xy.py

```
from pylab import *

def f1(x,y):
    return 2*(y-x**2) + 1    # derivative
```



```

def rk4(x, y, fxy, h):    # x, y , f(x,y)
    k1 = h * fxy(x, y)
    k2 = h * fxy(x + h/2.0, y+k1/2)
    k3 = h * fxy(x + h/2.0, y+k2/2)
    k4 = h * fxy(x + h, y+k3)
    ny = y + ( k1/6 + k2/3 + k3/3 + k4/6 )
    return ny

dx = 0.1    # stepsize
xa = arange(0,1,dx)
N = len(xa)
ya = empty(N)    # to store y values
ya[0] = 0.0    # initial value

for k in range(N-1):
    ya[k+1] = rk4(xa[k], ya[k], f1, dx)

for k in range(N):
    print (xa[k], ya[k], xa[k]**2 + xa[k])

```

The results are shown below. The last column is the exact value, from $y = x^2 + x$. We have used the derivative of this equation with some rearrangement.

```

0.0 0.0 0.0
0.1 0.109998333333 0.11
0.2 0.239996297667 0.24
0.3 0.389993811303 0.39
0.4 0.559990774459 0.56
0.5 0.749987065258 0.75
0.6 0.959982534839 0.96
0.7 1.18997700139 1.19
0.8 1.43997024283 1.44
0.9 1.70996198792 1.71

```

5.6 Second Order Ordinary Differential Equations

In order to solve a second order differential equation using numerical methods we need to convert it in to two coupled first order equations, as shown below. The equation

$$\frac{d^2 y}{dx^2} = \frac{d}{dx} \left(\frac{dy}{dx} \right) = f(x, y)$$

can be converted in to two coupled equations

$$\frac{dy_1}{dx} = f_1(y_1, y_2, x) = y_2 \text{ and } \frac{dy_2}{dx} = f_2(y_1, y_2, x)$$

The program *second-ode-rk4.py* listed below. It integrates the equation $\frac{d^2 y}{dx^2} = -y$, with the initial conditions $y = 0$ and $\frac{dy}{dx} = 2$ at $x = 0$. The variable x is passed on to the functions f_1 and f_2 , even though they don't use it in this example. The result plotted shows that the solution is sine function, where the initial value of $\frac{dy}{dx}$ decides the amplitude.

```

from pylab import *
dx = 0.1
xa = arange(0, 10, dx)    # array of x

```

```

N =len(xa)

def f1(y1,y2,x):
    return y2    # derivative of y1 is y2

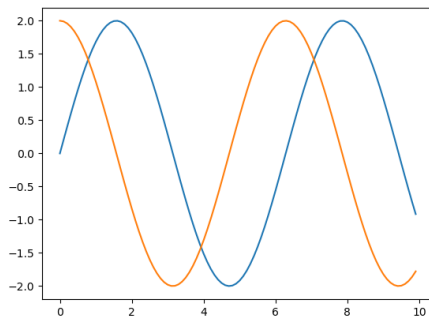
def f2(y1,y2,x):
    return -y1    # as per the equation

def rk4(y1,y2, f1, f2, x, h):
    k11 = h*f1(y1,y2,x);
    k21 = h*f2(y1,y2,x);
    k12 = h*f1(y1+0.5*k11,y2+0.5*k21,x+0.5*h);
    k22 = h*f2(y1+0.5*k11,y2+0.5*k21,x+0.5*h);
    k13 = h*f1(y1+0.5*k12,y2+0.5*k22,x+0.5*h);
    k23 = h*f2(y1+0.5*k12,y2+0.5*k22,x+0.5*h);
    k14 = h*f1(y1+k13,y2+k23,x+h);
    k24 = h*f2(y1+k13,y2+k23,x+h);
    y1 += (k11+2*k12+2*k13+k14)/6;
    y2 += (k21+2*k22+2*k23+k24)/6;
    return y1,y2

y1a = np.zeros(N)    # array to store the computed y1
y2a = np.zeros(N)    # and y2
y1a[0] = 0 # initial values
y2a[0] = 2 # of y1 and y2

for i in range(N-1):
    y1a[i+1], y2a[i+1] = rk4(y1a[i], y2a[i], f1, f2, xa[i], dx)
plot(xa, y1a) plot(xa, y2a) show()

```



5.7 Solution of Algebraic Equations

In general, an equation may have any number of roots, or no roots at all. For example $f(x) = x^2$ has a single root whereas $f(x) = \sin(x)$ has an infinite number of roots. The roots can be located visually, by looking at the intersections with the x-axis. Another useful tool for detecting and bracketing roots is the incremental search method. The basic idea behind the incremental search method is simple: if $f(x_1)$ and $f(x_2)$ have opposite signs, then there is at least one root in the

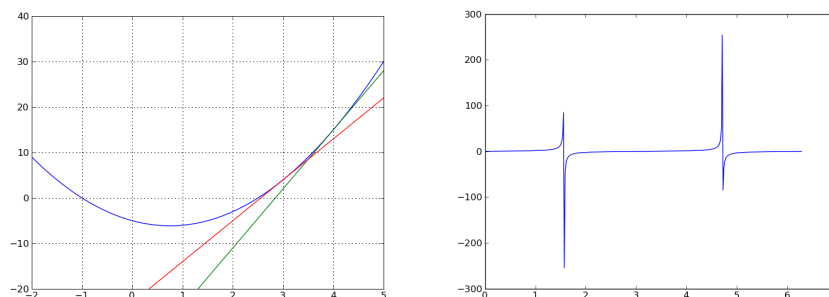


Figure 5.6: (a) Function $2x^2 - 3x - 5$ and its tangents at $x = 4$ and $x = 3$ (b) $\tan(x)$.

interval (x_1, x_2) . If the interval is small enough, it is likely to contain a single root. Thus the zeroes of $f(x)$ can be detected by evaluating the function at intervals of Δx and looking for change in sign.

There are several potential problems with the incremental search method: It is possible to miss two closely spaced roots if the search increment Δx is larger than the spacing of the roots. Certain singularities of $f(x)$ can be mistaken for roots. For example, $f(x) = \tan(x)$ changes sign at odd multiples of $\pi/2$, but these locations are not true zeroes as shown in figure 5.6 (b).

Program *rootsearch.py* listed below implements the function *root()* that searches the roots of a function $f(x)$ from $x = a$ to $x = b$, increasing it by dx .

```
def func(x):
    return x**3-10.0*x*x + 5

def root(f,a,b,dx):
    x = a
    while True:
        f1 = f(x)
        f2 = f(x+dx)
        if f1*f2 < 0:
            return x, x + dx
        x = x + dx
    if x >= b:
        return (None, None)

x,y = root(func, 0.0, 1.0, .1)
print x,y
```

The program finds that the root is between .7 and .8. Let us explore other methods like Bisection method, Newton-Raphson method etc., to find the root with a specified accuracy.

5.7.1 The Bisection method

The method of bisection finds the root by successively halving the interval until it becomes sufficiently small. Bisection is not the fastest method available for computing roots, but it is the most reliable. Once a root has been bracketed, bisection will always find it. The method of bisection works in the following manner. If there is a root between x_1 and x_2 , then $f(x_1) \times f(x_2) < 0$.

Next, we compute $f(x_3)$, where $x_3 = (x_1 + x_2)/2$. If $f(x_2) \times f(x_3) < 0$, then the root must be in (x_2, x_3) and we replace the original bound x_1 by x_3 . Otherwise, the root lies between x_1 and x_3 , in that case x_2 is replaced by x_3 . This process is repeated until the interval has been reduced to the specified value, say ε .

The number of bisections required to reach a prescribed limit, ε , is given by equation 5.22.

$$n = \frac{\ln(|\Delta x|)/\varepsilon}{\ln 2} \quad (5.22)$$

The program *bisection.py* finds the root of the equation $x^3 - 10x^2 + 5$. The starting values are found using the program *rootsearch.py*. The results are printed for two different values of accuracy.

Example bisection.py

```
import math
def func(x):
    return x**3 - 10.0* x*x + 5

def bisect(f, x1, x2, epsilon=1.0e-9):
    f1 = f(x1)
    f2 = f(x2)
    if f1*f2 > 0.0:
        print 'x1 and x2 are on the same side of x-axis'
        return
    n = math.ceil(math.log(abs(x2 - x1)/epsilon)/math.log(2.0))
    n = int(n)
    for i in range(n):
        x3 = (x1 + x2) / 2.0    # take the midpoint
        f3 = f(x3)
        if f3 == 0.0:    # found the root
            return x3
        if f2*f3 < 0.0:    # root is in second half
            x1 = x3        # change start to midpoint
            f1 = f3
        else:
            x2 = x3        # root is in first half
            f2 = f3        # change end to midpoint
    return x3

x = bisect(func, 0., 1., 1.0e-4)
print (x, func(x))
x = bisect(func, .7, .8, 1.0e-4)
print (x, func(x))
x = bisect(func, .7, .8, 1.0e-6)
print (x, func(x))
```

The output is shown below. Second column indicates amount of the error.

```
0.73455810546875 0.0005935349679475621
0.73466796875 -0.0008427397655319524
0.7346031188964843 5.08405033805559e-06
```

5.7.2 Regula Falsi (method of Chords)

In the bisection method the new interval depends only on the choice of end points, the function $f(x)$ is not used for finding the next interval. A better approximation would be obtained by taking the straight line joining the points $(a, f(a))$ and $(b, f(b))$ intersecting the x -axis. This is given by

$$x = \frac{af(b) - bf(a)}{f(b) - f(a)}$$

The program `regula-falsi.py` implements this. Only one line of code is different from the code for bisection method. The line

```
x3 = (x1*f2 - x2*f1)/(f2-f1)
```

replaces

```
x3 = 0.5 * (x1 + x2)
```

The results after this change are

```
0.7346035077884963 1.0549783269198088e-11
0.7346035077893032 8.881784197001252e-16
0.7346035077893032 8.881784197001252e-16
```

It can be seen that the Regula Falsi is giving better results.

5.7.3 Newton-Raphson Method

The Newton-Raphson algorithm requires the derivative of the function also to evaluate the roots. Therefore, it is usable only in problems where $f'(x)$ can be readily computed. It does not require the value at two points to start with. We start with an initial guess which is reasonably close to the true root. Then the function is approximated by its tangent line and the x -intercept of the tangent line is calculated. This value is taken as the next guess and the process is repeated. The Newton-Raphson formula is shown below.

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)} \quad (5.23)$$

Figure 5.6(a) shows the graph of the quadratic equation $2x^2 - 3x - 5 = 0$ and its two tangents. It can be seen that the zeros are at $x = -1$ and $x = 2.5$, and we use the program *newraph.py* shown below to find the roots. The function `nr()` is called twice, and we get the roots nearer to the corresponding starting values.

Example newraph.py

```
from pylab import *
def f(x):
    return 2.0 * x**2 - 3*x - 5

def df(x):
    return 4.0 * x - 3

def nr(x, tol = 1.0e-9):
    for i in range(30):
```

```

        dx = -f(x)/df(x)
        #print x
        x = x + dx
        if abs(dx) < tol:
            return x

    print nr(4)
    print nr(0)

```

The output is shown below.

```

2.5
-1.0

```

Uncomment the print statement inside `nr()` to view how fast this method converges, compared to the bisection method. The program *newraph_plot.py*, listed below is used for generating the figure 5.6.

Example newraph_plot.py

```

from pylab import *
def f(x):
    return 2.0 * x**2 - 3*x - 5

def df(x):
    return 4.0 * x - 3

vf = vectorize(f)
x = linspace(-2, 5, 100)
y = vf(x)
# Tangents at x=3 and 4, using one point slope formula
x1 = 4
tg1 = df(x1)*(x-x1) + f(x1)
x1 = 3
tg2 = df(x1)*(x-x1) + f(x1)
grid(True)
plot(x,y)
plot(x,tg1)
plot(x,tg2)
ylim([-20,40])
show()

```

We have defined the function $f(x) = 2x^2 - 3x - 5$ and vectorized it. The derivative $4x^2 - 3$ also is defined by $df(x)$, which is the slope of $f(x)$. The tangents are drawn at $x = 4$ and $x = 3$, using the point slope formula for a line $y = m(x - x_1) + y_1$.

5.8 System of Linear Equations

How to solve a system of linear equations. Let us start with a simple example.

$$3y + 2x = 7$$

$$5y + 2x = 9$$

Elimination and substitution are the two methods generally used. We can eliminate x from the second by subtracting the first from it, like.

$$3y + 2x = 7$$

$$2y - 0 = 2$$

Now multiply second by $3/2$ and subtract it from first gives

$$0 + 2x = 4$$

$$2y - 0 = 2$$

Dividing both equations by 2, we get the solutions $x = 2$ and $y = 1$. For large systems it is much easier to formulate the problem using matrices and solve by standard methods.

5.8.1 Gauss-Jordan Elimination method

The system of equations

$$\begin{array}{rrrr} 2x & +y & -z & = & 9 \\ -3x & -y & +2z & = & -11 \\ -2x & +y & +2z & = & -3 \end{array}$$

can be represented by an augmented matrix as shown below.

$$A = \left(\begin{array}{ccc|c} 2 & 1 & -1 & 9 \\ -3 & -1 & 2 & -11 \\ -2 & 1 & 2 & -3 \end{array} \right)$$

Our objective is to reduce the 3×3 matrix on the left side to an identity matrix. Then the right most column will contain the solutions. The permitted row operations are

1. Swap the positions of two rows.
2. Multiply a row by a non-zero scalar.
3. Add to one row a scalar multiple of another.

The first step is to convert the matrix in to an upper triangular form by performing the following operations.

- Find the ratio $r_{21} = \frac{A_{21}}{A_{11}}$. If A_{11} is zero we will swap two rows.
- Perform $Row2 \rightarrow Row2 - r_{21} \times Row1$. This will make a_{21} zero.
- Similarly find $r_{31} = \frac{A_{31}}{A_{11}}$ and make a_{31} zero.

- Repeat the same for all remaining rows.
- Move one step along the diagonal.
- Find the ratio $r_{23} = \frac{A_{32}}{A_{22}}$
- Perform $Row3 \leftarrow Row3 - r_{21} \times Row2$. This will make a_{32} zero.

The result will look like

$$A = \left(\begin{array}{ccc|c} 2 & 1 & -1 & 8 \\ 0 & .5 & .5 & 1 \\ 0 & 0 & -1 & 1 \end{array} \right)$$

Next step is to repeat the same procedure, starting from A_{33} and eliminate the upper half of the matrix. After that each row will be divided by the value of the diagonal element in that row so that we get an identity matrix in the left part of the augmented matrix. The Python code *gauss-jordan.py* (contains comments) listed below implements the algorithm explained.

```
from numpy import *
a = array( [ [2,1,-1,8], [-3,-1,2,-11], [-2,1,2,-3] ],dtype='float')
NR = len(a)
NC = NR + 1      # one more column, Augmented matrix

for anchor in range(NR-1):
    for row in range(anchor, NR-1):
        ratio = a[row+1,anchor]/a[anchor,anchor]
        a[row+1] = subtract(a[row+1],a[anchor]*ratio)
        print (a,'\n')

for anchor in range(NR-1, 0,-1):    # looping for 2, 1,
    for row in range(anchor):
        ratio = a[row,anchor]/a[anchor,anchor]
        a[row] = subtract(a[row],a[anchor]*ratio)
        print (a,'\n')
```

The final output is

```
[[ 1.  0.  0.  2.]
 [ 0.  1.  0.  3.]
 [-0. -0.  1. -1.]]
```

implies $x = 2$, $y = 3$ and $z = -1$. In the code above, we have not considered the case of any diagonal element being zero in the beginning. This will result in a division by zero error. One can check for this and do a swapping of rows using

```
def swapRow(a, r1, r2): # swap rows r1 an r2 in a
    tmp = copy(a[r2])
    a[r2] = a[r1]
    a[r1] = tmp
```


5.8.2 Matrix Inversion method

Non-homogeneous matrix equations of the form $Ax = b$ can be solved by matrix inversion to obtain $x = A^{-1}b$. The system of equations

$$\begin{aligned} 4x + y - 2z &= 0 \\ 2x - 3y + 3z &= 9 \\ -6x - 2y + z &= 0 \end{aligned}$$

can be represented in the matrix form as

$$\begin{pmatrix} 4 & 1 & -2 \\ 2 & -3 & 3 \\ -6 & -2 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} 0 \\ 9 \\ 0 \end{pmatrix}$$

and can be solved by finding the inverse of the coefficient matrix.

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} 4 & 1 & -2 \\ 2 & -3 & 3 \\ -6 & -2 & 1 \end{pmatrix}^{-1} \begin{pmatrix} 0 \\ 9 \\ 0 \end{pmatrix}$$

If you want to practice your python skills try using the methods described earlier, as listed in the program solve-eqn.py.

```
def invert(m):
    m1, m2, m3 = m[0]
    m4, m5, m6 = m[1]
    m7, m8, m9 = m[2]
    d = m1*(m5*m9-m6*m8) - m2*(m4*m9-m6*m7) + m3*(m4*m8-m5*m7)
    return [[(m5*m9-m6*m8)/d, (m3*m8-m2*m9)/d, (m2*m6-m3*m5)/d],
            [(m6*m7-m4*m9)/d, (m1*m9-m3*m7)/d, (m3*m4-m1*m6)/d],
            [(m4*m8-m5*m7)/d, (m2*m7-m1*m8)/d, (m1*m5-m2*m4)/d] ]

a = invert(a)
b = [ [0], [9], [0] ] # 3 x 1
c = [ [0], [0], [0] ] # 3 x 1
NR = len(a) # number of rows
NC = len(b[0]) # number of columns
for row in range(NR):
    for col in range(NC):
        for i in range(len(a[0])): # number of columns of A
            c[row][col] += a[row][i] * b[i][col]
print (c)
```

Using numpy we can solve the same problem in a much simpler manner

Example solve-eqn-numpy.py

```
from numpy import *
b = array([0,9,0])
A = array([ [4,1,-2], [2,-3,3], [-6,-2,1]])
print (linalg.inv(A) @ b)
```

The result will be $\begin{bmatrix} 0.75 & -2. & 0.5 \end{bmatrix}$, that means $x = 0.75, y = -2, z = 0.5$. This can be verified by substituting them back in to the equations.

Exercise: solve $x+y+3z = 6; 2x+3y-4z=6; 3x+2y+7z=0$

5.9 Inverse of Matrix by Gauss-Jordan method

If the matrix X is the inverse of matrix A , then $AX = I$. We form an augmented matrix AI and apply the Gauss-Jordan elimination process to all the columns. In the end of it, when the first half A becomes I , the second half will be A^{-1} . The program *gauss-jordan-invert.py* demonstrates the process.

```
from numpy import *
a = array( [[2,1,-1,1,0,0],[-3,-1,2, 0,1,0],[-2,1,2,0,0,1] ], dtype='float')
NR = len(a)
NC = NR + 3 # three more columns, Augmented matrix

for anchor in range(NR-1):
    for row in range(anchor, NR-1):
        ratio = a[row+1,anchor]/a[anchor,anchor]
        a[row+1] = subtract(a[row+1],a[anchor]*ratio)
    print (a,'\n')

for anchor in range(NR-1, 0,-1): # looping for 2, 1,
    for row in range(anchor):
        ratio = a[row,anchor]/a[anchor,anchor]
        a[row] = subtract(a[row],a[anchor]*ratio)
    print (a,'\n')

ia = a[:,3:6] # extract columns 3,4,5
print (ia)
```

The program prints

```
[[ 4.  3. -1.]
 [-2. -2.  1.]
 [ 5.  4. -1.]]
```

5.10 Least Squares Fitting

A mathematical procedure for finding the best-fitting curve $f(x)$ for a given set of points (x_n, y_n) by minimizing the sum of the squares of the vertical offsets of the points from the curve is called least squares fitting. The least square fit is obtained by minimizing the function,

$$S(a_0, a_1, \dots, a_m) = \sum_{i=0}^n [y_i - f(x_i)]^2 \quad (5.24)$$

with respect to each a_i and the condition for that is

$$\frac{\partial S}{\partial a_i} = 0, \quad i = 0, 1, \dots, m \quad (5.25)$$

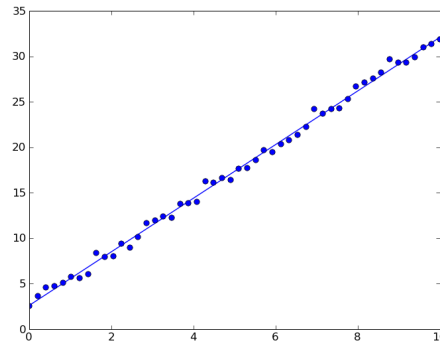


Figure 5.7: Output of lsfit.py

For a linear fit, the equation is

$$f(a, b) = a + bx$$

Solving the equations $\frac{\partial S}{\partial a} = 0$ and $\frac{\partial S}{\partial b} = 0$ will give the result,

$$b = \frac{\sum y_i(x - \bar{x})}{\sum x_i(x - \bar{x})}, \quad \text{and} \quad a = \bar{y} - \bar{x}b \quad (5.26)$$

where \bar{x} and \bar{y} are the mean values defined by the equations,

$$\bar{x} = \frac{1}{n+1} \sum_{i=0}^n x_i, \quad \bar{y} = \frac{1}{n+1} \sum_{i=0}^n y_i \quad (5.27)$$

The program lsfit.py demonstrates the usage of equations 5.26 and 5.27.

Example lsfit.py

```
from pylab import *
NP = 50
r = 2*ranf([NP]) - 0.5
x = linspace(0,10,NP)
data = 3 * x + 2 + r

xbar = mean(x)
ybar = mean(data)
b = sum(data*(x-xbar)) / sum(x*(x-xbar))
a = ybar - xbar * b
print a,b
y = a + b * x
plot(x,y)
plot(x,data,'ob')
show()
```

The raw data is made by adding random numbers (between -1 and 1) to the y coordinates generated by $y = 3*x + 2$. The Numpy functions `mean()` and `sum()` are used. The output is shown in figure 5.7.

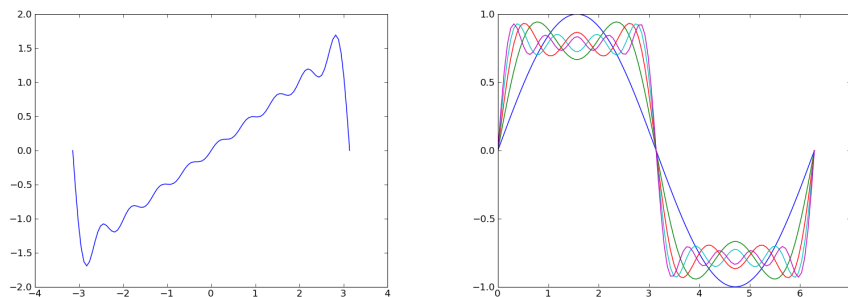


Figure 5.8: Sawtooth and Square waveforms generated using Fourier series.

5.11 Monte Carlo methods

We only provide a glimpse of this method using an example program to calculate the value of π . We consider a square shaped area ranging from the coordinates (0,0) to (1,1), and a quarter of a circle centered at (0,0). We randomly generate points in the range 0 to 1, representing the x and y coordinates of a random point inside the square. We calculate the distance to the point from the origin to find out whether it falls inside the circle. This probability is decided by the area of the circle (one fourth of it) and that of the square. The program *pi-value.py* is listed below. Accuracy of the result depends on the number of trials.

```
from random import random
from math import sqrt

NP = 100000
inside = 0
for k in range(NP):
    x = random()
    y = random()
    r = sqrt(x**2 + y**2)
    if r <= 1:
        inside += 1

ratio = inside / NP
print (4*ratio)
```

5.12 Fourier Series

A Fourier series is an expansion of a periodic function $f(x)$ in terms of an infinite sum of sines and cosines. The computation and study of Fourier series is known as harmonic analysis and is extremely useful as a way to break up an arbitrary periodic function into a set of simple terms that can be plugged in, solved individually, and then recombined to obtain the solution to the original problem or an approximation to it to whatever accuracy is desired or practical.

The examples below shows how to generate a square wave and sawtooth wave using this technique. To make the output better, increase the number of terms by changing the argument of the range() function, used in the for loop. The output of the programs are shown in figure 5.8.

Example fourier_square.py

```
from pylab import *
N = 100      # number of points
x = linspace(0.0, 2 * pi, N)
y = zeros(N)
for n in range(5):
    term = sin((2*n+1)*x) / (2*n+1)
    y = y + term
    plot(x,y)
show()
```

Example fourier_sawtooth.py

```
from pylab import *
N = 100      # number of points
x = linspace(-pi, pi, N)
y = zeros(N)
for n in range(1,10):
    term = (-1)**(n+1) * sin(n*x) / n
    y = y + term
plot(x,y)
show()
```

5.13 Exercises

1. Differentiate $5x^2 + 3x + 5$ numerically and evaluate at $x = 2$ and $x = -2$.
2. Write code to numerically differentiate $\sin(x^2)$ and plot it by vectorizing the function. Compare with the analytical result.
3. Integrate $\ln x$, e^x from $x = 1$ to 2 .
4. Solve $2x + y = 3$; $-x + 4y = 0$; $3 + 3y = -1$ using matrices.
5. Modify the program `julia.py`, $c = 0.2 - 0.8j$ and $z = z^6 + c$
6. Write Python code, using `numpy`, to solve the following equations using matrices

$$\begin{aligned} 4x + y - 2z &= 0 \\ 2x - 3y + 3z &= 9 \\ -6x - 2y + z &= 0 \end{aligned}$$
7. Find the roots of $5x^2 + 3x - 6$ using bisection method.
8. Find the all the roots of $\sin(x)$ between 0 and 10 , using Newton-Raphson method.

Chapter 6

Type setting using L^AT_EX

L^AT_EX is a powerful typesetting system, used for producing scientific and mathematical documents of high typographic quality. L^AT_EX is not a word processor! Instead, L^AT_EX encourages authors not to worry too much about the appearance of their documents but to concentrate on getting the right content. You prepare your document using a plain text editor, and the formatting is specified by commands embedded in your document. The appearance of your document is decided by L^AT_EX, but you need to specify it using some commands. In this chapter, we will discuss some of these commands mainly to typeset mathematical equations.¹

6.1 Document classes

L^AT_EX provides several predefined document classes (book, article, letter, report, etc.) with extensive sectioning and cross-referencing capabilities. Title, chapter, section, subsection, paragraph, subparagraph etc. are specified by commands and it is the job of L^AT_EX to format them properly. It does the numbering of sections automatically and can generate a table of contents if requested. Figures and tables are also numbered and placed without the user worrying about it.

The latex source document (the .tex file) is compiled by the latex program to generate a device independent (the .dvi file) output. From that you can generate postscript or PDF versions of the document. We will start with a simple example *hello.tex* to demonstrate this process. In a line, anything after a % sign is taken as a comment.

Example hello.tex

```
\documentclass{article}
\begin{document}
Small is beautiful.    % I am just a comment
\end{document}
```

Compile, view and make a PDF file using the following commands:

```
$ latex hello.tex
$ xdvi hello.dvi
$ dvi2pdf hello.dvi
```

The output will look like : Small is beautiful.

¹<http://www.latex-project.org/>
<http://mirror.ctan.org/info/lshort/english/lshort.pdf>
<http://en.wikibooks.org/wiki/L^AT_EX>

6.2 Modifying Text

In the next example *texts.tex* we will demonstrate different types of text. We will `\newline` or `\\` to generate a line break. A blank line will start a new paragraph.

Example texts.tex

```
\documentclass{article}
\begin{document}
This is normal text.
\newline
\textbf{This is bold face text.}
\textit{This is italic text.}\\
\tiny{This is tiny text.}
\large{This is large text.}
\underline{This is underlined text.}
\end{document}
```

Compiling *texts.tex*, as explained in the previous example, will generate the following output.

This is normal text.
This is bold face text. *This is italic text.*
This is tiny text. This is large text. This is underlined text.

6.3 Dividing the document

A document is generally organized in to sections, subsections, paragraphs etc. and Latex allows us to do this by inserting commands like section subsection etc. If the document class is book, you can have chapters also. There is a command to generate the table of contents from the sectioning information.²

Example sections.tex

```
\documentclass{article}
\begin{document}
\tableofcontents
\section{Animals}
This document defines sections.
\subsection{Domestic}
This document also defines subsections.
\subsubsection{cats and dogs}
Cats and dogs are Domestic animals.
\end{document}
```

The output of sections.tex is shown in figure 6.1.

²To generate the table of contents, you may have to compile the document two times.

Contents

| | | |
|----------|-------------------------|----------|
| 1 | Animals | 1 |
| 1.1 | Domestic | 1 |
| 1.1.1 | cats and dogs | 1 |

1 Animals

This document defines sections.

1.1 Domestic

This document also defines subsections.

1.1.1 cats and dogs

Cats and dogs are domestic animals.

Figure 6.1: Output of sections.tex

6.4 Environments

Environments decide the way in which your text is formatted : numbered lists, tables, equations, quotations, justifications, figure, etc. are some of the environments. Environments are defined like :

```
\begin{environment_name} your text \end{environment_name}
```

The example program *environ.tex* demonstrates some of the environments.

Example environ.tex

```
\documentclass{article}
\begin{document}
\begin{flushleft} A bulleted list. \end{flushleft}
\begin{itemize} \item dog \item cat \end{itemize}
\begin{center} A numbered List. \end{center}
\begin{enumerate} \item dog \item cat \end{enumerate}
\begin{flushright} This text is right justified. \end{flushright}
\begin{quote}
Any text inside quote\\ environment will appe-\\ ar as typed.\\
\end{quote}
\begin{verbatim}
x = 1
while x <= 10:
    print x * 5
    x = x + 1
\end{verbatim}
```



```
\end{document}
```

The `enumerate` and `itemize` are used for making numbered and non-numbered lists. `Flushleft`, `flushright` and `center` are used for specifying text justification. `Quote` and `verbatim` are used for portions where we do not want L^AT_EX to do the formatting. The output of `environs.tex` is shown below.

A bulleted list.

- dog
- cat

A numbered List.

1. dog
2. cat

This text is right justified.

Any text inside quote
environment will appear
as typed.

```
x = 1      # a Python program
while x <= 10:
    print x * 5
    x = x + 1
```

6.5 Typesetting Equations

There are two ways to typeset mathematical formulae: in-line within a paragraph, or in a separate line. In-line equations are entered between *two \$ symbols*. The equations in a separate line can be done within the *equation* environment. Both are demonstrated in `math1.tex`. *We use the `amsmath` package in this example.*

Example `math1.tex`

```
\documentclass{article}
\usepackage{amsmath}
\begin{document}
The equation  $a^2 + b^2 = c^2$  is typeset as inline.
```

```

The same can be done in a separate line using
\begin{equation}
a^2 + b^2 = c^2
\end{equation}
\end{document}

```

The output of this file is shown below.

The equation $a^2 + b^2 = c^2$ is typeset as inline. The same can be done in a separate line using

$$a^2 + b^2 = c^2 \tag{6.1}$$

The equation number becomes 5.1 because this happens to be the first equation in chapter 5.

6.5.1 Building blocks for typesetting equations

To typeset equations, we need to know the commands to make constructs like fraction, sqareroot, integral etc. The following list shows several commands and corresponding outputs. For each item, the output of the command, between the two \$ signs, is shown on the right side. The reader is expected to insert then inside the body of a document, compile the file and view the output for practicing.

1. Extra space³ : $\$A \quad B \quad C\$$ $A \quad B \quad C$
2. Greek letters : $\$ \alpha \beta \gamma \pi \$$ $\alpha \beta \gamma \pi$
3. Subscript and Exponents : $\$A_n \quad A^m \$$ $A_n \quad A^m$
4. Multiple Exponents : $\$a^b \quad a^{b^c} \$$ $a^b \quad a^{b^c}$
5. Fractions : $\$\frac{3}{5} \$$ $\frac{3}{5}$
6. Dots : $\$n! = 1 \cdot 2 \cdot \dots (n-1) \cdot n \$$ $n! = 1 \cdot 2 \cdot \dots (n-1) \cdot n$
7. Under/over lines : $\$0.\overline{3} = \underline{1/3} \$$ $0.\overline{3} = \underline{1/3}$
8. Vectors : $\$\vec{a} \$$ \vec{a}
9. Functions : $\$\sin x + \arctan y \$$ $\sin x + \arctan y$
10. Square root : $\$\sqrt{x^2 + y^2} \$$ $\sqrt{x^2 + y^2}$
11. Higher roots : $\$z = \sqrt[3]{x^2} + \sqrt{y} \$$ $z = \sqrt[3]{x^2} + \sqrt{y}$

³\quad is for inserting space, the size of a \quad corresponds to the width of the character ‘M’ of the current font. Use \qquad for larger space.

12. Equalities : $A \neq B \quad A \approx C$ $A \neq B$ $A \approx C$
13. Arrows : $\Leftrightarrow \quad \Downarrow$ \Leftrightarrow \Downarrow
14. Partial derivative : $\frac{\partial^2 A}{\partial x^2}$ $\frac{\partial^2 A}{\partial x^2}$
15. Summation : $\sum_{i=1}^n$ $\sum_{i=1}^n$
16. Integration : $\int_0^{\frac{\pi}{2}} \sin x$ $\int_0^{\frac{\pi}{2}} \sin x$
17. Product : \prod_{ϵ} \prod_{ϵ}
18. Big brackets : $\Big((x+1)(x-1)\Big)^2$ $\Big((x+1)(x-1)\Big)^2$
19. Integral : $\int_a^b f(x) dx$ $\int_a^b f(x) dx$
20. Operators : $\pm \div \times \cup *$ $\pm \div \times \cup *$

6.6 Arrays and matrices

To typeset arrays, use the array environment, that is similar to the tabular environment. Within an array environment, & character separates columns, \\ starts a new line. The command \hline inserts a horizontal line. Alignment of the columns is shown inside braces using characters (lcr) and the | symbol is used for adding vertical lines. An example of making a table is shown below.

```
$ \begin{array}{|l|cr|} \hline
person & sex & age \\
John & male & 20 \\
Mary & female & 10 \\
Gopal & male & 30 \\
\hline
\end{array} $
```

| <i>person</i> | <i>sex</i> | <i>age</i> |
|---------------|---------------|------------|
| <i>John</i> | <i>male</i> | 7 |
| <i>Mary</i> | <i>female</i> | 20 |
| <i>Gopal</i> | <i>male</i> | 30 |

The first column is left justified, second is centered and the third is right justified (decided by the {l|cr}). If you insert a | character between c and r, it will add a vertical line between second and third columns.

Let us make a matrix using the same command.

```
$ A = \left(
\begin{array}{ccc}
x_1 & x_2 & \ldots
\end{array}
\right)
```

```

y_1 & y_2 & \ldots \\
\vdots & \vdots & \ddots \\
\end{array}
\right) $

```

The output is shown below. The `\left(` and `\right)` provides the enclosure. All the columns are centered. We have also used horizontal, vertical and diagonal dots in this example.

$$A = \begin{pmatrix} x_1 & x_2 & \dots \\ y_1 & y_2 & \dots \\ \vdots & \vdots & \ddots \end{pmatrix}$$

6.7 Floating bodies, Inserting Images

Figures and tables need special treatment, because they cannot be broken across pages. One method would be to start a new page every time a figure or a table is too large to fit on the present page. This approach would leave pages partially empty, which looks very bad. The easiest solution is to *float* them and let L^AT_EX decide the position. (You can influence the placement of the floats using the arguments [htbp], here, top, bottom or special page). Any material enclosed in a figure or table environment will be treated as floating matter. The *graphicsx* packages is required in this case.

```

\usepackage{graphicx}
\text{Learn how to insert pictures with caption inside the figure environment.}
\begin{figure}[h]
\centering
\includegraphics[width=0.2\textwidth]{pics/arcs.eps}
\includegraphics[width=0.2\textwidth]{pics/sawtooth.eps}
\caption{Picture of Arc and Sawtooth, inserted with [h] option.}
\end{figure}

```

The result is shown below.

Learn how to insert pictures with caption inside the figure environment.

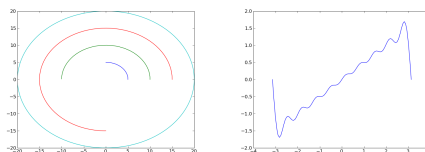


Figure 6.2: Picture of Arc and Sawtooth, inserted with [h] option.

6.8 Example Application

Latex source code for a simple question paper listed below.

Example qpaper.tex

```

\documentclass{article}
\usepackage{amsmath}
begin{document}
\begin{center}
\large{\textbf{Sample Question Paper\\for\\
Mathematics using Python}}
\end{center}
\begin{tabular}{p{8cm}r}
\textbf{Duration:3 Hrs} & \textbf{30 weightage}
\end{tabular}
\section{Answer all Questions. $4\times 1\frac{1}{2}$}
\begin{enumerate}
\item What are the main document classes in LATEX.
\item Typeset  $\sin^2 x + \cos^2 x = 1$  using LATEX.
\item Plot a circle using the polar() function.
\item Write code to print all perfect cubes upto 2000.
\end{enumerate}
\section{Answer any two Questions. $3\times 5$}
\begin{enumerate}
\item Set a sample question paper using LATEX.
\item Using Python calculate the GCD of two numbers
\item Write a program with a Canvas and a circle.
\end{enumerate}
\begin{center}\text{End}\end{center}
\end{document}

```

The formatted output is shown below.

Sample Question Paper for Mathematics using Python

Duration: 3 Hrs

30 weightage

1 Answer all Questions. $4 \times 1\frac{1}{2}$

1. What are the main document classes supported by L^AT_EX.
2. Typeset $\sin^2 x + \cos^2 x = 1$ using L^AT_EX.
3. Plot a circle using the `polar()` function.
4. Write code to print all perfect cubes upto 2000.

2 Answer any two Questions. 3×5

1. Set a sample question paper using L^AT_EX.
2. Write a Python function to calculate the GCD of two numbers
3. Write a program with a Canvas and a circle drawn on it.

End

6.9 Exercises

1. What are the main document classes supported by L^AT_EX.
2. How does Latex differ from other word processor programs.
3. Write a .tex file to typeset 'All types of Text Available' in tiny, large, underline and italic.
4. Rewrite the previous example to make the output a list of numbered lines.
5. Generate an article with section and subsections with table of contents.
6. Typeset 'All types of justifications' to print it three times; left, right and centered.
7. Write a .tex file that prints 12345 in five lines (one character per line).
8. Typeset a Python program to generate the multiplication table of 5, using verbatim.
9. Typeset $\sin^2 x + \cos^2 x = 1$

10. Typeset $\left(\sqrt{x^2+y^2}\right)^2 = x^2 + y^2$

11. Typeset $\sum_{n=1}^{\infty} \left(1 + \frac{1}{n}\right)^n$

12. Typeset $\frac{\partial A}{\partial x} = A$

13. Typeset $\int_0^{\pi} \cos x . dx$

14. Typeset $x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$

15. Typeset $A = \begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix}$

16. Typeset $R = \begin{pmatrix} \sin \theta & \cos \theta \\ \cos \theta & \sin \theta \end{pmatrix}$

Appendix A : Installing GNU/Linux

Programming can be learned better by practicing and it requires an operating system, and Python interpreter along with some library modules. The following section explains how to install GNU/Linux on a computer. We have selected the Ubuntu distribution due to its relatively simple installation procedure, ease of maintenance and support for most of the hardware available in the market.

6.10 Where to get Ubuntu

Download the ISO image of the latest distribution from <https://ubuntu.com/download/desktop>, preferably the latest Long Term Support (LTS) version. At the time of writing this, Ubuntu-20.04 is currently the latest. A startup disk need to be created from this ISO image, using a USB pendrive. MS-Windows users may download the program Rufus(from <https://rufus.ie/>) and use that to make a USB pendrive bootable with this ISO image.

After making the bootable pendrive, shut down the PC, insert the pendrive and select the boot device while starting again. The keys to press to enter BIOS depends on the brand of the PC you have (for HP it is ESC key, for Lenovo Fn+F2 and Fn+F12 to select the boot device, more info <http://www.disk-image.com/faq-bootmenu.htm>). The system will boot in to Ubuntu Desktop and you can use it in the live mode, without even installing it. However, to install additional software and to save data, you need to install it in to a hard disk partition.

6.11 Installing Ubuntu

Most of the users prefer a dual boot system, to keep their MSWindows working. We will explain the installation process keeping that handicap in mind. All we need is an empty partition of minimum 20 GB size to install Ubuntu. Free space inside a Windows partition will not do, we need to format the partition to install Ubuntu. The Ubuntu installer will make the system multi-boot by searching through all the partitions for installed operating systems.

The System

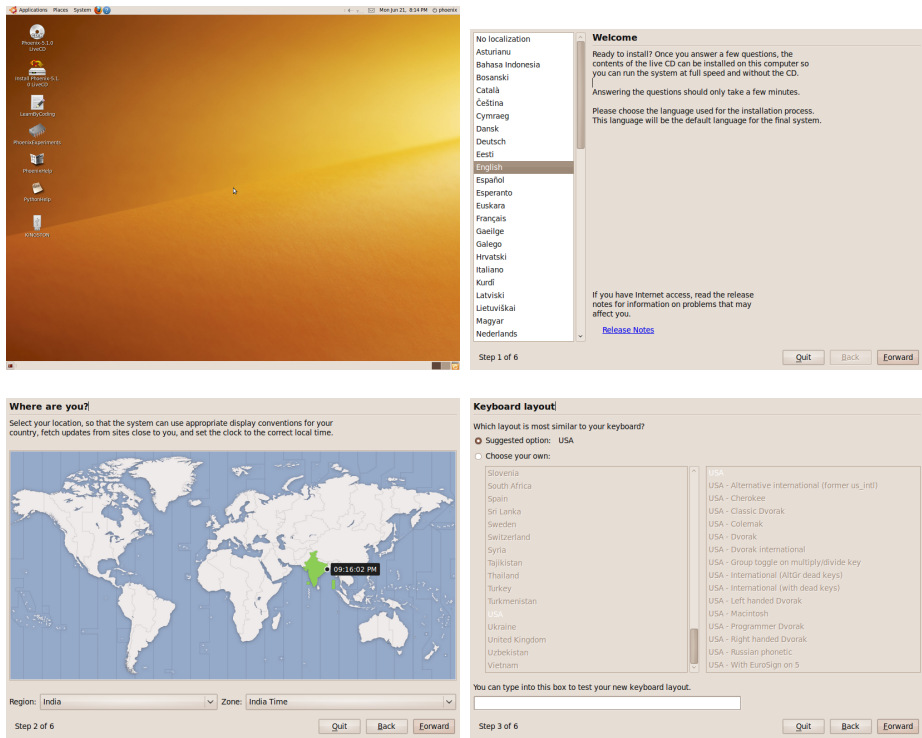
This section will describe how Ubuntu was installed on a system, with MSWindows, having the following partitions:

- C: (GNU/Linux calls it /dev/sda1) 200 GB
- D: (/dev/sda5) 200 GB
- E: (/dev/sda6) 100 GB

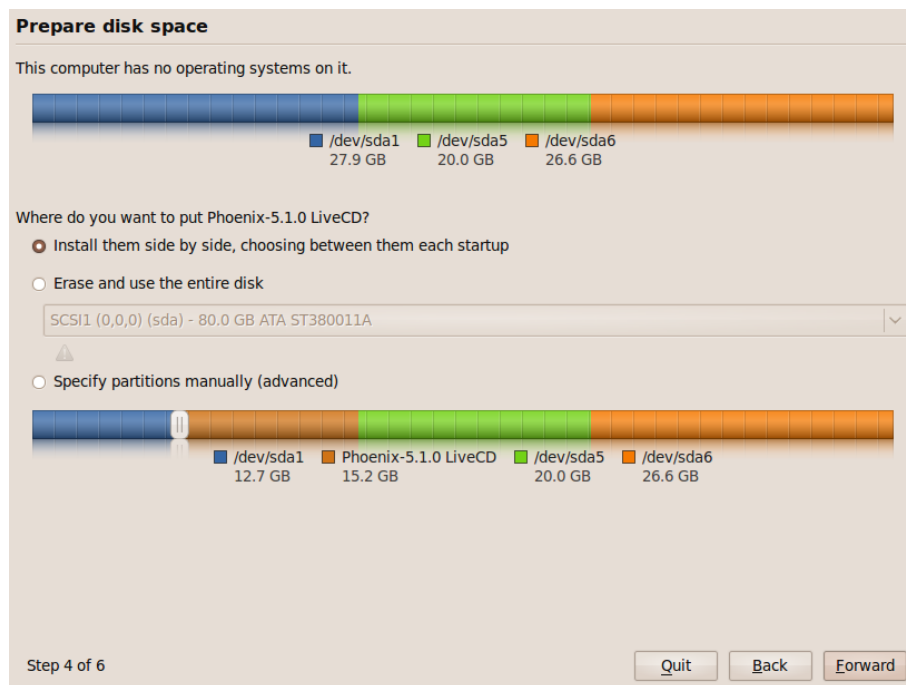
We will use the partition E: to install Ubuntu, it will be formatted.

The Procedure

Click on the Installer icon, the window shown next will pop up. Screens will appear to select the language, time zone and keyboard layout as shown in the figures below.



Now we proceed to the important part, choosing a partition to install Ubuntu.

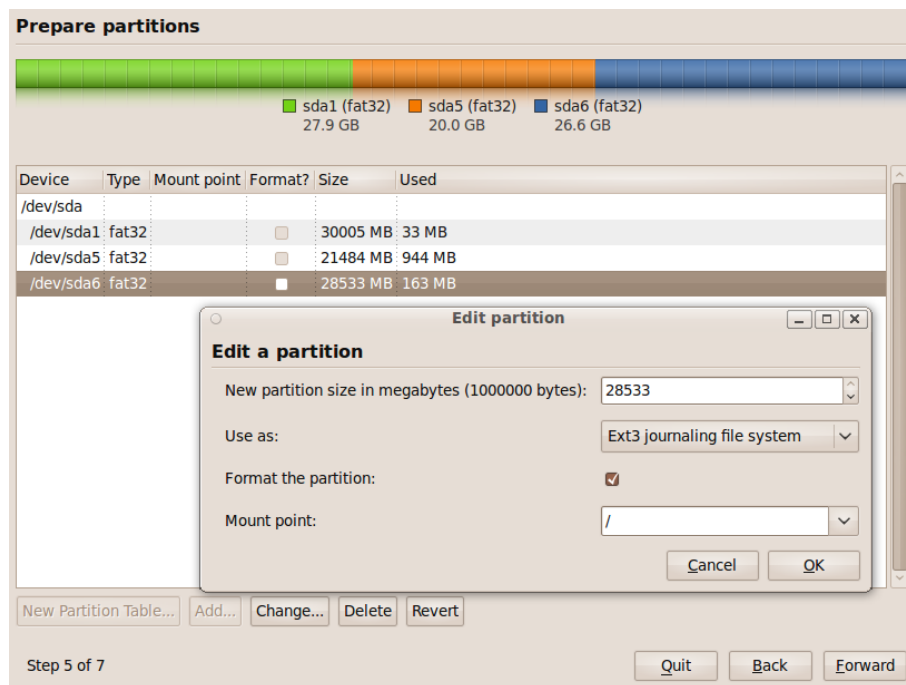


The bar on the top graphically displays the existing partitions. Below that there are three options provided :

1. Install them side by side.
2. Erase and use the entire disk.
3. Specify partitions manually.

If you choose the first option, the Installer will resize and repartition the disk to make some space for the new system. By default this option is marked as selected. The bar at the bottom shows the proposed partition scheme. In the present example, the installer plans to divide the C: drive in to two partitions to put Ubuntu on the second.

We are going to choose the third option, choose the partition manually. We will use the last partition (drive E:) for installing Ubuntu. Once you choose that and click forward, a screen will appear where we can add, delete and change partitions. We have selected the third partition and clicked on Change. A pop-up window appeared. Using that we selected the file-system type to ext3, marked the format option, and selected the mount point as /. The screen with the pop-up window is shown below.



If we proceed with this, a warning will appear complaining about the absence of swap partitions. The swap partition is used for supplementing the RAM with some virtual memory. When RAM is full, processes started but not running will be swapped out. One can install a system without swap partition but it is a good idea to have one.

We decide to go back on the warning, to delete the E: drive, create two new partitions in that space and make one of them as swap. This also demonstrates how to make new partitions. The screen after deleting E: , with the pop-up window to make the swap partition is shown below.

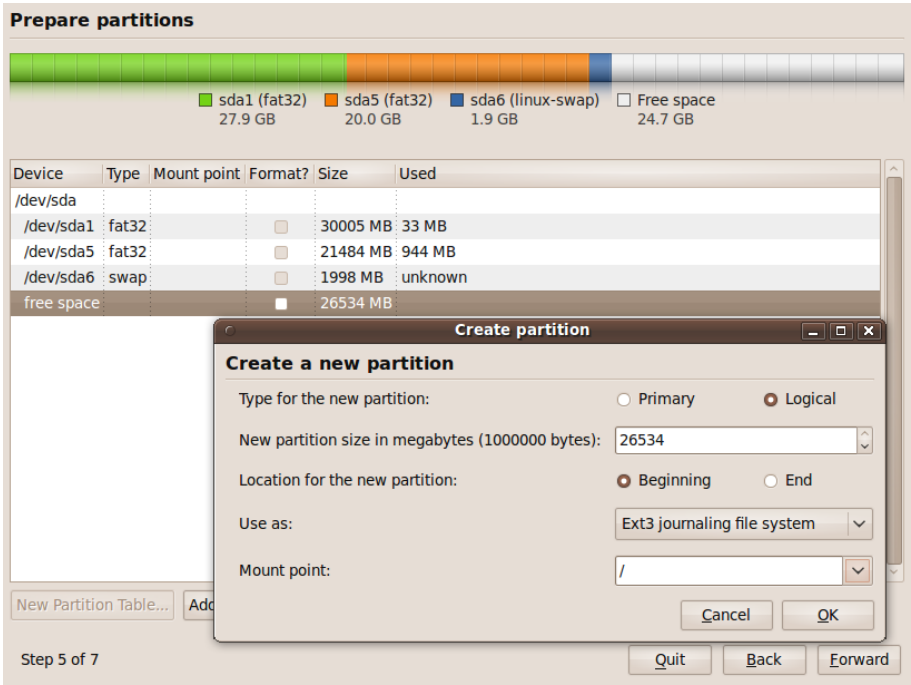
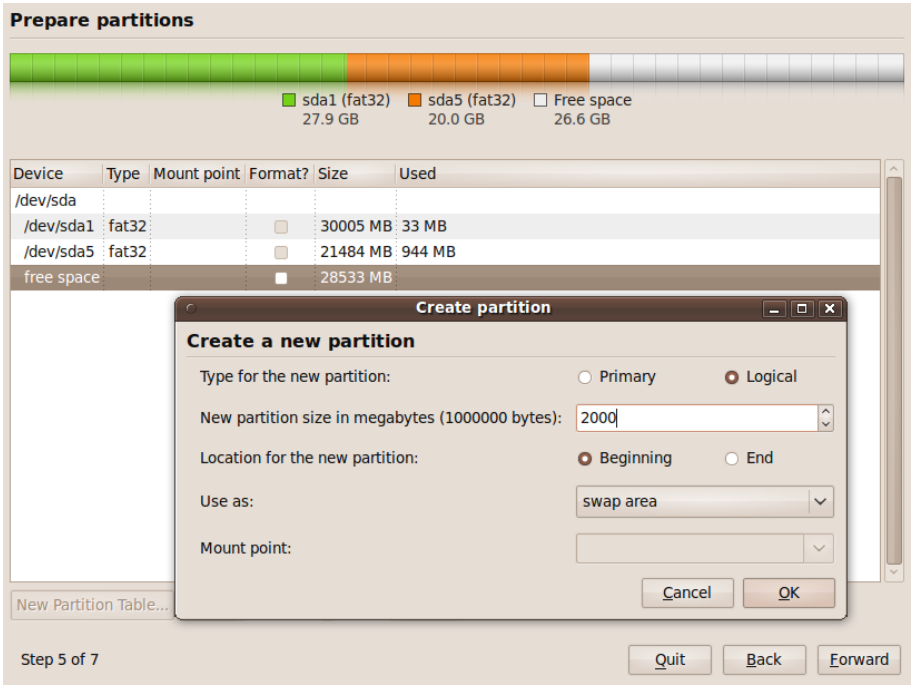


Figure 6.3: Making the partition to install Ubuntu.



We made a 4 GB swap. The remaining space is used for making one more partition, as shown in the figure 6.3.

Once disk partitioning is over, you will be presented with a screen to enter a user name and password.⁴ A warning will be issued if the password is less than 8 characters in length. You will be given an option to import desktop settings from other installations already on the disk, choose this if you like. The next screen will confirm the installation. After the installation is over, it takes 10 to 15 minutes, you will be prompted to reboot the system. On rebooting you will be presented with a menu, to choose the operating system to boot. First item in the menu will be the newly installed Ubuntu.

6.12 Installing Additional Software

The ISO image used for installation contains a selected set from the packages, like web browser, office package, document viewer etc., from the Ubuntu repository. The repository contains tens of thousands of packages, that can be installed very easily. You need to have a reasonably fast Internet connection for this purpose. Additional packages can be installed using command line tools or by using package management programs with a GUI.

For example to install python3-matplotlib issue the following commands

```
$ sudo apt update          # do this once
$ sudo apt install python3-matplotlib
```

This will also install all the packages required for python3-matplotlib. The package management system handles all the dependencies.

6.13 Synaptic Package Manager

```
$ sudo apt install synaptic
```

will install the synaptic package manager. Once installed, it can be started from the Desktop. The synaptic window will popup as shown in figure 6.4.

Select Settings->Repositories to get a pop-up window as shown below. Tick the four repositories, close the pop-up window and Click on Reload. Synaptic will now try to download the index files from all these repositories. It may take several minutes.

⁴All GNU/Linux installations ask for a root password during installation. For simplicity, Ubuntu has decided to hide this information. The first user created during installation has special privileges and that password is asked, instead of the root password, for all system administration jobs, like installing new software.

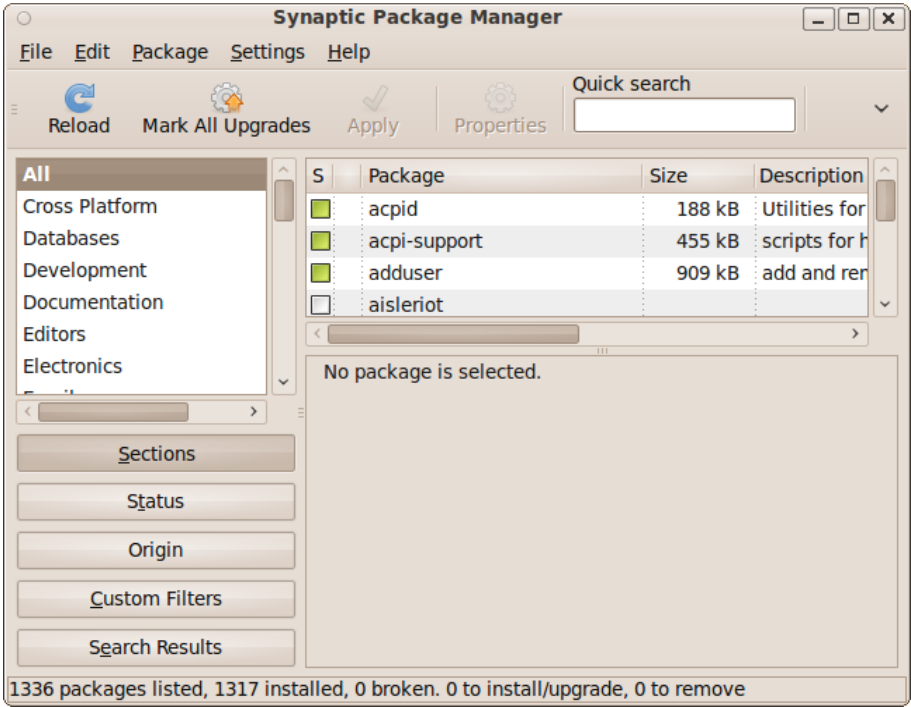
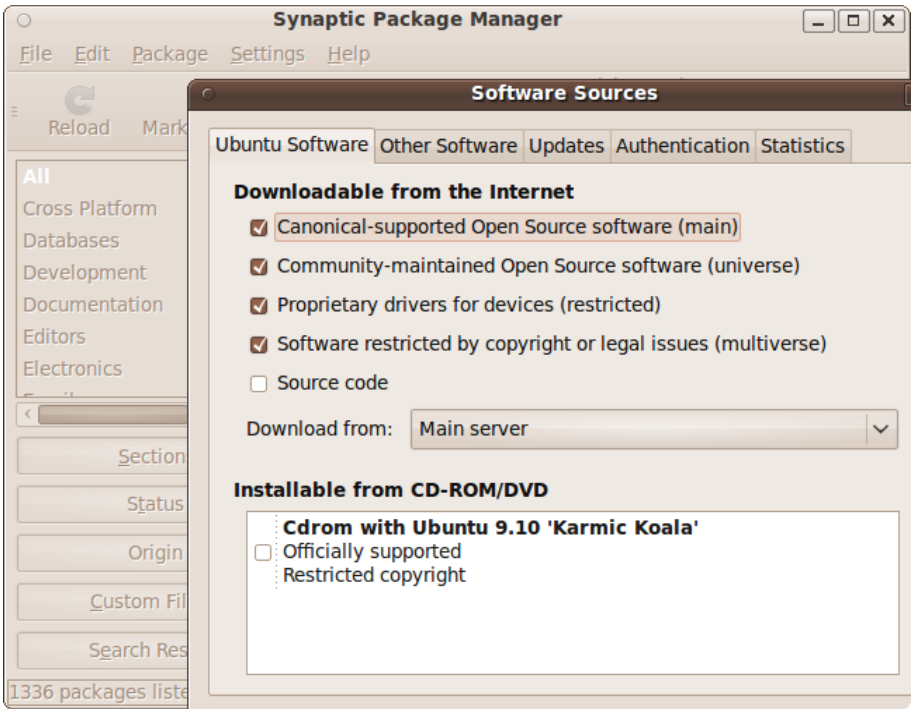


Figure 6.4: Synaptic package manager window



Now, you are ready to install any package from the Ubuntu repository. Search for

any package by name, from these repositories, and install it. The added advantage is that you need not remember the exact name of the package.

6.13.1 Behind the scene

Even though there are installation programs that performs all these steps automatically, it is better to know what is really happening. Installing an operating system involves;

- Partitioning of the hard disk
- Formatting the partitions
- Copying the operating system files
- Installing a boot loader program

The storage space of a hard disk drive can be divided into separate data areas, known as partitions. You can create primary partitions and extended partitions. Logical drives (secondary partitions can be created inside the extended partitions). On a disk, you can have up to 4 partitions, where one of them could be an extended partition. You can have many logical drives inside the extended partition.

On a MSWindows system, the primary partition is called the C: drive. The logical drives inside the extended partition are named from D: onwards. GNU/Linux uses a different naming convention. The individual disks are named as `/dev/sda`, `/dev/sdb` etc. and the partitions inside them are named as `/dev/sda1`, `/dev/sda2` etc. The numbering of secondary partitions inside the logical drive starts at `/dev/sda5`. (1 to 4 are reserved for primary and extended). Hard disk partitioning can be done using the `fdisk` program. The installation program also does this for you.

The process of making a file system on a partition is called formatting. There are many different types of file systems. MSWindows use file systems like FAT32, NTFS etc. and GNU/Linux mostly uses file systems like `ext3`, `ext4` etc.

The operating system files are kept in directories named `boot`, `sbin`, `bin`, etc etc. The kernel that loads while booting the system is kept in `/boot`. The configuration files are kept in `/etc`. `/sbin` and `/bin` holds programs that implements many of the shell commands. Most of the application programs are kept in `/usr/bin` area.

The boot loader program is the one provides the selection of OS to boot, when you power on the system. GRUB is the boot loader used by most of the GNU/Linux systems.

Bibliography

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