$\begin{array}{ccc} \textbf{Introduction to Numerical Analysis with} \\ \textbf{Python} \end{array}$

Shobhit Mahajan shobhit.mahajan@gmail.com

Contents

1	Get	ting Started	7
	1.1	Introduction	7
		1.1.1 Algorithm	8
		1.1.2 Computer Languages	9
	1.2	Python	10
	1.3	Setting up Python	11
		1.3.1 Using Python on Linux based machines	11
		1.3.2 Python Integrated Development Environment	13
		1.3.3 Installing Pycharm IDE	14
	1.4	Using Python	18
		Using Python	18
_	_	¥	
2		ic Python Structures	24
	2.1	Introduction	24
	2.2	Python Variables	24
	2.3	Variable Types	25
		2.3.1 Strings	25
		2.3.2 Python Numbers	29
	2.4	Arithmetic Operations	32
	2.5	The if statement	36
		2.5.1 Else used with If	37
		2.5.2 elif statement	38
		2.5.3 Nested if	39
	2.6	Iteration	40
		2.6.1 While loop	40
		2.6.2 For Loop	41
	2.7	Python Functions	46
		2.7.1 Lambda Functions	48
		2.7.2 Recursive functions	49
	2.8	Lists	51

	2.9	Arrays	53
	2.10	Least Square Fitting	56
	2.11	Reading & Writing into a data file	59
	2.12	Random Numbers	62
	2.13	Exercises	67
3	Gra	phics with Matplotlib	71
	3.1	Introduction	71
	3.2	Using Matplotlib	71
		3.2.1 Plotting the results of a computation	73
		3.2.2 Subplots	75
		3.2.3 Plotting using data file	77
		3.2.4 Error Bars	80
		3.2.5 Interpolation	84
		3.2.6 Polar Plots	87
		3.2.7 Histograms with Matplotlib	88
	3.3	Contours	92
	3.4	3-d Plotting	95
	3.5	Exercises	97
4	Fini	te & Infinite Series	101
	4.1	Introduction	101
	4.2	Finite Series	101
	4.3	Infinite Series	105
	4.4	Exercises	109
5	Roo	ot Finding	113
	5.1	Introduction	113
	5.2	Bisection Method	115
	5.3	Secant Method	118
	5.4	Newton-Raphson Method	120
	5.5	Exercises	121
6	Inte	erpolation	125
	6.1	Introduction	125
	6.2	Interpolation Techniques	125
		6.2.1 Newton Polynomial Interpolation	126
		6.2.2 Lagrange Polynomial Interpolation	130
	6.3	Exercises	136

7	Ord	inary Differential Equations	138
	7.1	Introduction	138
	7.2	Euler's Formula	139
	7.3	Runge-Kutta Methods	141
	7.4	Simultaneous Equations of First-Order	146
	7.5	Use of Scipy for solving Differential Equations	149
		7.5.1 Spread of information	152
	7.6	Boundary Value Problems	155
		7.6.1 Shooting Method	156
	7.7	Exercises	158
8	Inte	$_{ m egration}$	165
	8.1	Introduction	165
	8.2	Methods Based on Intervals of Equal Width	166
		8.2.1 Trapezoidal Rule	166
		8.2.2 Simpson's Rule	168
	8.3	Methods Based on Intervals of Unequal Width	171
		8.3.1 Gauss Quadrature	171
		8.3.2 Gauss-Laguerre Quadrature	173
		8.3.3 Gauss-Hermite Quadrature	174
	8.4	Integration in Python using Scipy.integrate module	174
	8.5	Exercises	176
9	Mat	crices	181
	9.1	Introduction	181
	9.2	Use of arrays and loops for matrix manipulation	181
		9.2.1 Inputting Matrices	181
	9.3	Matrix operations	183
	9.4	Using in-built libraries for Matrix Operations	184
		9.4.1 Eigenvalues & Eigenvectors	185
	9.5	Linear Equations	187
	9.6	Exercises	189
10	Line	ear Regression	192
	10.1	Introduction	192
	10.2	Least Square Regression	192
		Using Python for regression	198
		10.3.1 Using Numpy.linalg	198
		10.3.2 Using curve_fit	200

11 Time Independent Schrodinger Equation	203
11.1 Introduction	203
11.2 Shooting + RK4 method	204
11.3 Exercises	206
12 Introduction to Monte Carlo	207
12.1 Introduction	207
12.2 Monte Carlo methods for Integration	207
12.2.1 One-dimensional Integration	209
12.2.2 Multi dimensional Integration	212
12.3 Exercises	214
13 Monte Carlo Simulations	216
13.1 Introduction	216
13.2 One-Dimensional Random Walk	216
13.3 Two dimensional Random Walk	219
13.4 Simulating the Spread of Disease	226
13.5 Simulation of Bending of a Beam	
Index	240

A Note to the Reader

This Manual was written for use in the Numerical Analysis Lab of MSc Physics course at Dept. of Physics & Astrophysics, University of Delhi. However, it can be used at the undergraduate level too or in other courses since it does not assume any knowledge of either Numerical Analysis or Python.

Like any lab manual, it is not a place where you can learn the theory of Numerical Analytic methods, though at various places we have tried to give a brief introduction to them. Instead, it is primarily a Manual focussed on using the numerical methods in programming in Python.

The Manual is organized into 13 Chapters. The first three chapters are about Python language and the others discuss various topics in Numerical Programming.

After an introductory chapter with a brief introduction to algorithms and computer languages as well some very basic Python commands, the second chapter discusses Python language in somewhat more detail. This includes Python variables, operations with variable, conditional statements and iteration, python arrays, user defined functions and manipulating data files. The idea behind this is not to provide exhaustive details of the language but instead to serve as an introduction which allows the reader to explore further. Thus, apart from describing the various structures and constructs in Python, there are several sample programs which illustrate the use of these structures. There are also exercises in programming after each chapter which the reader should do.

Chapter 3 is an introduction to graphics in Python. We discuss various options available for plotting with Matplotlib library of routines.

The rest of the chapters are basically the use of Python to solve various Numerical problems using Numerical analysis. The techniques discussed include summing of finite and infinite series, finding roots of a function, solving ordinary differential equations, integration of functions and matrices. We also discuss numerical solutions to time independent Schrodinger equation, interpolation and regression. There are two introductory chapters on Monte Carlo methods as used for integration and simulation.

Each chapter follows the same format of briefly describing the numerical method and then using it to show how programs in Python can implement that method.

Programming, like swimming or cycling can only be learnt by actually doing it. Python is a very exhaustive language which is very versatile. In addition, there are many structures and options in

Python which we have not listed. The reader is encouraged to use the vast resources on the Internet on Python to explore these. The programs described in the book are not necessarily written in the most efficient way nor using the full power of Python. Instead the idea is to convey the logic in the simplest possible way and encourage the reader to modify the programs using other structures and learn about them. The exercises are an essential component of the Manual and the reader is advised to attempt all of them in the Manual.

We would very much like to get your suggestions regarding how to improve this Manual. In addition, if there are any errors or misprints that are spotted in the Manual, we would like to hear from you. Please send a mail with the suggestions/errors etc. to shobhit.mahajan@gmail.com making sure you quote the version number of the Manual as well as the Modification date of the Manual you are using. The version number and date are on the title page of the Manual.

October 1, 2025

Index

while loop, 35
while True, 38
Least Squares Regression, 173 linear regression, 51 Lists, 46
Matplotlib, 66
3-d plotting, 90
Contours, 87
Error Bars, 75
Histograms, 83
Interpolation, 79
plotting from data, 72
Plotting in program, 68
Polar Plots, 81
Subplots, 70
Using, 66
Matrices, 163
Diagonalization, 168
Eigenvalues & Eigenvectors, 167
Inputting Matrices, 163
Linear equations, 169
Matrix operations, 165
Numpy libraries, 166
Use of arrays, 163
Monte Carlo Methods, 188
Integration, 188
Multi dimensional integration, 193
One dimensional integration, 190
Ordinary Differential Equations, 128
Boundary Value Problems, 141
Euler's Method, 129

Fourth Order Runge-Kutta, 132 Runge-Kutta Methods, 131 second order equations, 137 Second Order Runge Kutta, 132 Shooting Method, 142 Simultaneous Equations of first order, 136 Using Scipy, 139

Programming Languages, 9 Python IDE, 16

random numbers, 57
Reading & Writing data file, 54
Roots, 105
Bisection Method, 107
Newton-Raphson Method, 113

Secant Method, 111

Schrodinger Equation, 184 Shooting +RK4 Method, 185 Series, 95

> Finite Series, 95 Infinite Series, 99 Partial Sum, 96 ratio, 96

Simulations, 197

One Dimensional Random Walk, 197 Bending of a beam, 207 Two dimensional Random Walk, 200

variables, 19
Boolean, 26
complex numbers, 25
floating point numbers, 25
numbers, 24
strings, 20

Variable types, 20