

Contents

List of Figures	xv
Preface	xix
Acknowledgements	xxiii

PART 1 INTRODUCTION TO PYTHON PROGRAMMING

CHAPTER 1	Python Basics	3
1.1	Getting Started With Python	3
1.1.1	Setting Up Your Working Environment	3
1.1.2	Three Ways to Run Python Code	7
1.2	Python as a Calculator	9
1.3	Managing Packages	15
1.3.1	Managing Packages Using Package Managers	15
1.3.2	Install Packages From Source	18
1.4	Introduction to Jupyter Notebook	18
1.4.1	Starting the Jupyter Notebook	18
1.4.2	Within the Notebook	19
1.4.3	How Do I Close a Notebook?	20
1.4.4	Shutting Down the Jupyter Notebook Server	20
1.5	Logical Expressions and Operators	20
1.6	Summary and Problems	23
1.6.1	Summary	23
1.6.2	Problems	23
CHAPTER 2	Variables and Basic Data Structures	27
2.1	Variables and Assignment	27
2.2	Data Structure – String	30
2.3	Data Structure – List	35
2.4	Data Structure – Tuple	38
2.5	Data Structure – Set	40
2.6	Data Structure – Dictionary	42
2.7	Introducing NumPy Arrays	44
2.8	Summary and Problems	52
2.8.1	Summary	52
2.8.2	Problems	52
CHAPTER 3	Functions	55
3.1	Function Basics	55
3.1.1	Built-In Functions in Python	55
3.1.2	Define Your Own Function	56
3.2	Local Variables and Global Variables	63

3.3	Nested Functions	67
3.4	Lambda Functions	69
3.5	Functions as Arguments to Functions	70
3.6	Summary and Problems	72
3.6.1	Summary	72
3.6.2	Problems	72
CHAPTER 4	Branching Statements	77
4.1	If-Else Statements	77
4.2	Ternary Operators	84
4.3	Summary and Problems	85
4.3.1	Summary	85
4.3.2	Problems	85
CHAPTER 5	Iteration	91
5.1	For-Loops	91
5.2	While Loops	97
5.3	Comprehensions	100
5.3.1	List Comprehension	100
5.3.2	Dictionary Comprehension	101
5.4	Summary and Problems	101
5.4.1	Summary	101
5.4.2	Problems	101
CHAPTER 6	Recursion	105
6.1	Recursive Functions	105
6.2	Divide-and-Conquer	110
6.2.1	Tower of Hanoi	110
6.2.2	Quicksort	113
6.3	Summary and Problems	114
6.3.1	Summary	114
6.3.2	Problems	114
CHAPTER 7	Object-Oriented Programming	121
7.1	Introduction to OOP	121
7.2	Class and Object	123
7.2.1	Class	123
7.2.2	Object	124
7.2.3	Class vs Instance Attributes	125
7.3	Inheritance, Encapsulation, and Polymorphism	127
7.3.1	Inheritance	127
7.3.2	Encapsulation	130
7.3.3	Polymorphism	132
7.4	Summary and Problems	132
7.4.1	Summary	132
7.4.2	Problems	132

CHAPTER 8	Complexity	135
8.1	Complexity and Big-O Notation	135
8.2	Complexity Matters	137
8.3	The Profiler	139
8.3.1	Using the Magic Command	139
8.3.2	Use Python Profiler	140
8.3.3	Use Line Profiler	141
8.4	Summary and Problems	142
8.4.1	Summary	142
8.4.2	Problems	142
CHAPTER 9	Representation of Numbers	145
9.1	Base-N and Binary	145
9.2	Floating Point Numbers	147
9.3	Round-Off Errors	151
9.3.1	Representation Error	151
9.3.2	Round-Off Error by Floating-Point Arithmetic	152
9.3.3	Accumulation of Round-Off Errors	152
9.4	Summary and Problems	153
9.4.1	Summary	153
9.4.2	Problems	153
CHAPTER 10	Errors, Good Programming Practices, and Debugging	157
10.1	Error Types	157
10.2	Avoiding Errors	160
10.2.1	Plan Your Program	160
10.2.2	Test Everything Often	161
10.2.3	Keep Your Code Clean	161
10.3	Try/Except	163
10.4	Type Checking	166
10.5	Debugging	168
10.5.1	Activating Debugger After Running Into an Exception	168
10.5.2	Activating Debugger Before Running the Code	171
10.5.3	Add a Breakpoint	172
10.6	Summary and Problems	173
10.6.1	Summary	173
10.6.2	Problems	173
CHAPTER 11	Reading and Writing Data	175
11.1	TXT Files	175
11.1.1	Writing to a File	176
11.1.2	Appending a File	176
11.1.3	Reading a File	177
11.1.4	Dealing With Numbers and Arrays	178
11.2	CSV Files	180
11.2.1	Writing and Opening a CSV File	180

	11.2.2 Reading a CSV File	180
	11.2.3 Beyond NumPy	181
11.3	Pickle Files	182
	11.3.1 Writing to a Pickle File	182
	11.3.2 Reading a Pickle File	182
	11.3.3 Reading in Python 2 Pickle File	182
11.4	JSON Files	183
	11.4.1 JSON Format	183
	11.4.2 Writing a JSON File	184
	11.4.3 Reading a JSON File	184
11.5	HDF5 Files	185
	11.5.1 Reading an HDF5 File	186
11.6	Summary and Problems	187
	11.6.1 Summary	187
	11.6.2 Problems	188
CHAPTER 12	Visualization and Plotting	189
12.1	2D Plotting	189
12.2	3D Plotting	199
12.3	Working With Maps	205
12.4	Animations and Movies	212
12.5	Summary and Problems	215
	12.5.1 Summary	215
	12.5.2 Problems	215
CHAPTER 13	Parallelize Your Python	225
13.1	Parallel Computing Basics	225
	13.1.1 Process and Thread	226
	13.1.2 Python's GIL Problem	227
	13.1.3 Disadvantages of Using Parallel Computing	227
13.2	Multiprocessing	227
	13.2.1 Visualize the Execution Time	229
13.3	Using Joblib	230
13.4	Summary and Problems	231
	13.4.1 Summary	231
	13.4.2 Problems	232

PART 2 INTRODUCTION TO NUMERICAL METHODS

CHAPTER 14	Linear Algebra and Systems of Linear Equations	235
14.1	Basics of Linear Algebra	235
	14.1.1 Sets	235
	14.1.2 Vectors	236
	14.1.3 Matrices	239
14.2	Linear Transformations	244
14.3	Systems of Linear Equations	245

14.4	Solutions to Systems of Linear Equations	246
14.4.1	Gauss Elimination Method	248
14.4.2	Gauss–Jordan Elimination Method	250
14.4.3	LU Decomposition Method	251
14.4.4	Iterative Methods – Gauss–Seidel Method	253
14.5	Solving Systems of Linear Equations in Python	256
14.6	Matrix Inversion	258
14.7	Summary and Problems	260
14.7.1	Summary	260
14.7.2	Problems	261
CHAPTER 15	Eigenvalues and Eigenvectors	265
15.1	Eigenvalues and Eigenvectors Problem Statement	265
15.1.1	Eigenvalues and Eigenvectors	265
15.1.2	The Motivation Behind Eigenvalues and Eigenvectors	265
15.1.3	The Characteristic Equation	268
15.2	The Power Method	269
15.2.1	Finding the Largest Eigenvalue	269
15.2.2	The Inverse Power Method	272
15.2.3	The Shifted Power Method	273
15.3	The QR Method	273
15.4	Eigenvalues and Eigenvectors in Python	275
15.5	Summary and Problems	276
15.5.1	Summary	276
15.5.2	Problems	276
CHAPTER 16	Least Squares Regression	279
16.1	Least Squares Regression Problem Statement	279
16.2	Least Squares Regression Derivation (Linear Algebra)	280
16.3	Least Squares Regression Derivation (Multivariate Calculus)	281
16.4	Least Squares Regression in Python	283
16.4.1	Using the Direct Inverse Method	283
16.4.2	Using the Pseudo-Inverse	285
16.4.3	Using <code>numpy.linalg.lstsq</code>	285
16.4.4	Using <code>optimize.curve_fit</code> From SciPy	285
16.5	Least Squares Regression for Nonlinear Functions	286
16.5.1	Log Tricks for Exponential Functions	286
16.5.2	Log Tricks for Power Functions	288
16.5.3	Polynomial Regression	288
16.5.4	Using <code>optimize.curve_fit</code> From SciPy	289
16.6	Summary and Problems	290
16.6.1	Summary	290
16.6.2	Problems	291
CHAPTER 17	Interpolation	295
17.1	Interpolation Problem Statement	295

17.2	Linear Interpolation	296
17.3	Cubic Spline Interpolation	297
17.4	Lagrange Polynomial Interpolation	301
17.4.1	Using the Lagrange Function From SciPy	304
17.5	Newton's Polynomial Interpolation	305
17.6	Summary and Problems	308
17.6.1	Summary	308
17.6.2	Problems	309
CHAPTER 18	Taylor Series	315
18.1	Expressing Functions Using a Taylor Series	315
18.2	Approximations Using Taylor Series	316
18.3	Discussion About Errors	320
18.3.1	Truncation Errors for Taylor Series	320
18.3.2	Estimating Truncation Errors	321
18.3.3	Round-Off Errors for Taylor Series	322
18.4	Summary and Problems	323
18.4.1	Summary	323
18.4.2	Problems	323
CHAPTER 19	Root Finding	325
19.1	Root Finding Problem Statement	325
19.2	Tolerance	326
19.3	Bisection Method	327
19.4	Newton–Raphson Method	330
19.5	Root Finding in Python	332
19.6	Summary and Problems	333
19.6.1	Summary	333
19.6.2	Problems	333
CHAPTER 20	Numerical Differentiation	337
20.1	Numerical Differentiation Problem Statement	337
20.2	Using Finite Difference to Approximate Derivatives	338
20.2.1	Using Finite Difference to Approximate Derivatives With Taylor Series	338
20.3	Approximating of Higher Order Derivatives	344
20.4	Numerical Differentiation With Noise	345
20.5	Summary and Problems	347
20.5.1	Summary	347
20.5.2	Problems	348
CHAPTER 21	Numerical Integration	353
21.1	Numerical Integration Problem Statement	353
21.2	Riemann Integral	354
21.3	Trapezoid Rule	356
21.4	Simpson's Rule	359
21.5	Computing Integrals in Python	363

21.6	Summary and Problems	365
21.6.1	Summary	365
21.6.2	Problems	365
CHAPTER 22	Ordinary Differential Equations (ODEs) Initial-Value Problems	371
22.1	ODE Initial Value Problem Statement	371
22.2	Reduction of Order	374
22.3	The Euler Method	375
22.4	Numerical Error and Instability	380
22.5	Predictor–Corrector and Runge–Kutta Methods	382
22.5.1	Predictor–Corrector Methods	382
22.5.2	Runge–Kutta Methods	383
22.6	Python ODE Solvers	384
22.7	Advanced Topics	389
22.7.1	Multistep Methods	389
22.7.2	Stiffness ODE	389
22.8	Summary and Problems	390
22.8.1	Summary	390
22.8.2	Problems	391
CHAPTER 23	Boundary-Value Problems for Ordinary Differential Equations (ODEs)	399
23.1	ODE Boundary Value Problem Statement	399
23.2	The Shooting Method	401
23.3	The Finite Difference Method	406
23.4	Numerical Error and Instability	411
23.5	Summary and Problems	412
23.5.1	Summary	412
23.5.2	Problems	412
CHAPTER 24	Fourier Transform	415
24.1	The Basics of Waves	415
24.1.1	Modeling a Wave Using Mathematical Tools	415
24.1.2	Characteristics of a Wave	417
24.2	Discrete Fourier Transform (DFT)	421
24.2.1	DFT	422
24.2.2	The Inverse DFT	426
24.2.3	The Limit of DFT	427
24.3	Fast Fourier Transform (FFT)	428
24.3.1	Symmetries in the DFT	428
24.3.2	Tricks in FFT	428
24.4	FFT in Python	432
24.4.1	FFT in NumPy	432
24.4.2	FFT in SciPy	434
24.4.3	More Examples	435
24.5	Summary and Problems	441
24.5.1	Summary	441

24.5.2	Problems	441
Appendix A	Getting Started With Python in Windows	445
A.1	Getting Started With Python in Windows	445
A.1.1	Setting Up Your Working Environment in Windows	445
A.1.2	Three Ways to Run Python Code	447
Index		453