



SERIES IN COMPUTATIONAL PHYSICS

Introduction to Python for Science and Engineering

David J. Pine



CRC Press
Taylor & Francis Group

Contents

| | |
|--|------------|
| <i>Preface</i> | <i>xv</i> |
| <i>About the Author</i> | <i>xix</i> |
| 1 Introduction | 1 |
| 1.1 Introduction to Python for Science and Engineering | 1 |
| 2 Launching Python | 3 |
| 2.1 Interacting with Python | 3 |
| 2.2 Installing Python on Your Computer | 4 |
| 2.3 The Spyder Window | 4 |
| 2.4 The IPython Pane | 4 |
| 2.4.1 Magic commands | 6 |
| 2.4.2 System shell commands | 8 |
| 2.4.3 Tab completion | 8 |
| 2.4.4 Recap of commands | 9 |
| 2.5 Interactive Python as a Calculator | 9 |
| 2.5.1 Binary arithmetic operations in Python | 10 |
| 2.5.2 Types of numbers | 10 |
| 2.5.3 Important note on integer division in Python | 12 |
| 2.6 Variables | 13 |
| 2.6.1 Names and the assignment operator | 13 |
| 2.6.2 Legal and recommended variable names | 14 |
| 2.6.3 Reserved words in Python | 15 |
| 2.7 Script Files and Programs | 16 |
| 2.7.1 First scripting example: The Editor pane | 16 |
| 2.8 Python Modules | 18 |
| 2.8.1 Python modules and functions: A first look | 20 |
| 2.8.2 Some NumPy functions | 22 |
| 2.8.3 Scripting Example 2 | 23 |
| 2.8.4 Different ways of importing modules | 24 |
| 2.9 Getting Help: Documentation in IPython | 26 |

| | | |
|--------|---|----|
| 2.10 | Stand-alone IPython | 26 |
| 2.10.1 | Writing Python scripts in a text editor | 27 |
| 2.11 | Programming Errors | 28 |
| 2.11.1 | Pyflakes | 28 |
| 2.11.2 | Error checking | 29 |
| 2.12 | Exercises | 29 |
| 3 | Strings, Lists, Arrays, and Dictionaries | 33 |
| 3.1 | Strings | 34 |
| 3.2 | Lists | 35 |
| 3.2.1 | Slicing lists | 37 |
| 3.2.2 | The <code>range</code> function: Sequences of numbers | 38 |
| 3.2.3 | Tuples | 39 |
| 3.2.4 | Multidimensional lists and tuples | 40 |
| 3.3 | NumPy Arrays | 41 |
| 3.3.1 | Creating arrays (1-d) | 41 |
| 3.3.2 | Mathematical operations with arrays | 43 |
| 3.3.3 | Slicing and addressing arrays | 46 |
| 3.3.4 | Fancy indexing: Boolean masks | 47 |
| 3.3.5 | Multi-dimensional arrays and matrices | 49 |
| 3.3.6 | Differences between lists and arrays | 52 |
| 3.4 | Dictionaries | 53 |
| 3.5 | Objects | 55 |
| 3.6 | Exercises | 57 |
| 4 | Input and Output | 61 |
| 4.1 | Keyboard Input | 61 |
| 4.2 | Screen Output | 64 |
| 4.2.1 | Formatting output with <code>str.format()</code> | 64 |
| 4.2.2 | Printing arrays | 68 |
| 4.3 | File Input | 69 |
| 4.3.1 | Reading data from a text file | 69 |
| 4.3.2 | Reading data from an Excel file: CSV files | 71 |
| 4.4 | File Output | 73 |
| 4.4.1 | Writing data to a text file | 73 |
| 4.4.2 | Writing data to a CSV file | 76 |
| 4.5 | Exercises | 76 |

| | | |
|-------|---|-----|
| 5 | Conditionals and Loops | 81 |
| 5.1 | Conditionals | 82 |
| 5.1.1 | if, elif, and else statements | 82 |
| 5.1.2 | Logical operators | 86 |
| 5.2 | Loops | 87 |
| 5.2.1 | for loops | 87 |
| 5.2.2 | while loops | 91 |
| 5.2.3 | Loops and array operations | 93 |
| 5.3 | List Comprehensions | 94 |
| 5.4 | Exercises | 96 |
| 6 | Plotting | 99 |
| 6.1 | An Interactive Session with PyPlot | 100 |
| 6.2 | Basic Plotting | 102 |
| 6.2.1 | Specifying line and symbol types and colors | 106 |
| 6.2.2 | Error bars | 108 |
| 6.2.3 | Setting plotting limits and excluding data | 110 |
| 6.2.4 | Subplots | 113 |
| 6.3 | Logarithmic Plots | 116 |
| 6.3.1 | Semi-log plots | 116 |
| 6.3.2 | Log-log plots | 118 |
| 6.4 | More Advanced Graphical Output | 118 |
| 6.4.1 | An alternative syntax for a grid of plots | 122 |
| 6.5 | Plots with multiple axes | 125 |
| 6.6 | Mathematics and Greek symbols | 126 |
| 6.7 | The Structure of matplotlib: OOP and All That | 131 |
| 6.7.1 | The backend layer | 132 |
| 6.7.2 | The artist layer | 135 |
| 6.7.3 | The PyPlot (scripting) layer | 137 |
| 6.8 | Contour and Vector Field Plots | 139 |
| 6.8.1 | Making a 2D grid of points | 139 |
| 6.8.2 | Contour plots | 140 |
| 6.8.3 | Streamline plots | 144 |
| 6.9 | Three-Dimensional Plots | 149 |
| 6.10 | Exercises | 152 |
| 7 | Functions | 155 |
| 7.1 | User-Defined Functions | 156 |
| 7.1.1 | Looping over arrays in user-defined functions | 158 |

| | | |
|-------|--|-----|
| 7.1.2 | Fast array processing for user-defined functions | 160 |
| 7.1.3 | Functions with more than one input or output | 161 |
| 7.1.4 | Positional and keyword arguments | 162 |
| 7.1.5 | Variable number of arguments | 163 |
| 7.1.6 | Passing function names and parameters as arguments | 164 |
| 7.2 | Passing data (objects) to and from functions | 167 |
| 7.2.1 | Variables and arrays created entirely within a function | 167 |
| 7.2.2 | Passing lists and arrays to functions: Mutable and immutable objects | 169 |
| 7.3 | Anonymous Functions: Lambda Expressions | 171 |
| 7.4 | NumPy Object Attributes: Methods and Instance Variables | 173 |
| 7.5 | Example: Linear Least Squares Fitting | 175 |
| 7.5.1 | Linear regression | 177 |
| 7.5.2 | Linear regression with weighting: χ^2 | 179 |
| 7.6 | Exercises | 182 |
| 8 | Curve Fitting | 187 |
| 8.1 | Using Linear Regression for Fitting Nonlinear Functions | 187 |
| 8.1.1 | Linear regression for fitting an exponential function | 187 |
| 8.1.2 | Linear regression for fitting a power-law function | 192 |
| 8.2 | Nonlinear Fitting | 193 |
| 8.3 | Exercises | 198 |
| 9 | Numerical Routines: SciPy and NumPy | 205 |
| 9.1 | Special Functions | 206 |
| 9.2 | Random Numbers | 209 |
| 9.2.1 | Uniformly distributed random numbers | 210 |
| 9.2.2 | Normally distributed random numbers | 210 |
| 9.2.3 | Random distribution of integers | 211 |
| 9.3 | Linear Algebra | 212 |
| 9.3.1 | Basic computations in linear algebra | 212 |
| 9.3.2 | Solving systems of linear equations | 213 |
| 9.3.3 | Eigenvalue problems | 214 |

| | | |
|--------|---|-----|
| 9.4 | Solving Nonlinear Equations | 216 |
| 9.4.1 | Single equations of a single variable | 217 |
| 9.4.2 | Solving systems of nonlinear equations | 221 |
| 9.5 | Numerical Integration | 221 |
| 9.5.1 | Single integrals | 222 |
| 9.5.2 | Double integrals | 226 |
| 9.6 | Solving ODEs | 227 |
| 9.7 | Discrete (Fast) Fourier Transforms | 231 |
| 9.7.1 | Continuous and discrete Fourier transforms | 231 |
| 9.7.2 | The SciPy FFT library | 232 |
| 9.8 | Exercises | 234 |
| 10 | Data Manipulation and Analysis: Pandas | 239 |
| 10.1 | Reading Data from Files Using Pandas | 240 |
| 10.1.1 | Reading from Excel files saved as csv files | 240 |
| 10.1.2 | Reading from text files | 247 |
| 10.1.3 | Reading from an Excel file | 250 |
| 10.2 | Dates and Times in Pandas | 251 |
| 10.3 | Data Structures: Series and DataFrame | 253 |
| 10.3.1 | Series | 253 |
| 10.3.2 | DataFrame | 256 |
| 10.4 | Getting Data from the Web | 261 |
| 10.5 | Extracting Information from a DataFrame | 263 |
| 10.6 | Plotting with Pandas | 267 |
| 10.7 | Grouping and Aggregation | 272 |
| 10.7.1 | The <code>groupby</code> method | 273 |
| 10.7.2 | Iterating over groups | 274 |
| 10.7.3 | Reformatting DataFrames | 277 |
| 10.7.4 | Custom aggregation of DataFrames | 280 |
| 10.8 | Exercises | 281 |
| 11 | Animation | 287 |
| 11.1 | Animating a Sequence of Images | 287 |
| 11.1.1 | Simple image sequence | 288 |
| 11.1.2 | Annotating and embellishing videos | 292 |
| 11.2 | Animating Functions | 294 |
| 11.2.1 | Animating for a fixed number of frames | 295 |
| 11.2.2 | Animating until a condition is met | 300 |
| 11.3 | Combining Videos with Animated Functions | 306 |

| | | |
|--------|---|-----|
| 11.3.1 | Using a single animation instance | 307 |
| 11.3.2 | Combining multiple animation instances | 308 |
| 11.4 | Exercises | 311 |
| 12 | Python Classes and GUIs | 315 |
| 12.1 | Defining and Using a Class | 316 |
| 12.1.1 | The <code>__init__()</code> method | 319 |
| 12.1.2 | Defining methods for a class | 320 |
| 12.1.3 | Calling methods from within a class | 321 |
| 12.1.4 | Updating instance variables | 322 |
| 12.2 | Inheritance | 323 |
| 12.3 | Graphical User Interfaces (GUIs) | 326 |
| 12.3.1 | Event-driven programming | 327 |
| 12.3.2 | PyQt | 328 |
| 12.3.3 | A basic PyQt dialog | 328 |
| 12.3.4 | Summary of PyQt5 classes used | 337 |
| 12.3.5 | GUI summary | 337 |
| A | Installing Python | 339 |
| A.1 | Installing Python | 339 |
| A.1.1 | Setting preferences | 340 |
| A.1.2 | Pyflakes | 340 |
| A.1.3 | Updating your Python installation | 341 |
| A.2 | Testing Your Installation of Python | 341 |
| A.3 | Installing FFMpeg for Saving Animations | 343 |
| B | Jupyter Notebooks | 345 |
| B.1 | Launching a Jupyter Notebook | 345 |
| B.2 | Running Programs in a Jupyter Notebook | 347 |
| B.3 | Annotating a Jupyter Notebook | 348 |
| B.3.1 | Adding headings and text | 349 |
| B.3.2 | Comments with mathematical expressions | 350 |
| B.4 | Terminal commands in a Jupyter notebook | 351 |
| B.5 | Plotting in a Jupyter Notebook | 351 |
| B.6 | Editing and Rerunning a Notebook | 353 |
| B.7 | Quitting a Jupyter Notebook | 353 |
| B.8 | Working with an Existing Jupyter Notebook | 353 |
| C | Glossary | 355 |

| | |
|---|------|
| Contents | xiii |
| D Python Resources | 359 |
| D.1 Python Programs and Data Files Introduced in This Text | 359 |
| D.2 Web Resources | 359 |
| D.3 Books | 361 |
| <i>Index</i> | 363 |