

Contents

<i>Preface</i>	<i>page xiii</i>
<i>List of codes</i>	<i>xvii</i>
1 Idiomatic Python	1
1.1 Why Python?	2
1.2 Code Quality	3
1.3 Summary of Python Features	4
1.3.1 Basics	4
1.3.2 Control Flow	5
1.3.3 Data Structures	6
1.3.4 User-Defined Functions	8
1.4 Core-Python Idioms	10
1.4.1 List Comprehensions	10
1.4.2 Iterating Idiomatically	11
1.5 Basic Plotting with <code>matplotlib</code>	13
1.6 NumPy Idioms	15
1.7 Project: Visualizing Electric Fields	21
1.7.1 Electric Field of a Distribution of Point Charges	21
1.7.2 Plotting Field Lines	22
1.8 Problems	25
2 Numbers	28
2.1 Motivation	28
2.2 Errors	29
2.2.1 Absolute and Relative Error	30
2.2.2 Error Propagation	32
2.3 Representing Real Numbers	38
2.3.1 Basics	38
2.3.2 Overflow	39
2.3.3 Machine Precision	40
2.3.4 Revisiting Subtraction	41
2.3.5 Comparing Floats	44
2.4 Rounding Errors in the Wild	45
2.4.1 Are Roundoff Errors Random?	45
2.4.2 Compensated Summation	47
2.4.3 Naive vs Manipulated Expressions	49

2.4.4	Computing the Exponential Function	50
2.4.5	An Even Worse Case: Recursion	55
2.4.6	When Rounding Errors Cancel	58
2.5	Project: the Multipole Expansion in Electromagnetism	60
2.5.1	Potential of a Distribution of Point Charges	60
2.5.2	Expansion for One Point Charge	65
2.5.3	Expansion for Many Point Charges	71
2.6	Problems	76
3	Derivatives	85
3.1	Motivation	85
3.1.1	Examples from Physics	85
3.1.2	The Problem to Be Solved	86
3.2	Analytical Differentiation	86
3.3	Finite Differences	87
3.3.1	Noncentral-Difference Approximations	87
3.3.2	Central-Difference Approximation	91
3.3.3	Implementation	93
3.3.4	More Accurate Finite Differences	95
3.3.5	Second Derivative	96
3.3.6	Points on a Grid	97
3.3.7	Richardson Extrapolation	101
3.4	Automatic Differentiation	105
3.4.1	Dual Numbers	105
3.4.2	An Example	106
3.4.3	Special Functions	107
3.5	Project: Local Kinetic Energy in Quantum Mechanics	109
3.5.1	Single-Particle Wave Functions in One Dimension	109
3.5.2	Second Derivative	114
3.6	Problems	117
4	Matrices	121
4.1	Motivation	121
4.1.1	Examples from Physics	121
4.1.2	The Problems to Be Solved	123
4.2	Error Analysis	125
4.2.1	From <i>a posteriori</i> to <i>a priori</i> Estimates	126
4.2.2	Magnitude of Determinant?	127
4.2.3	Norms for Matrices and Vectors	129
4.2.4	Condition Number for Linear Systems	131
4.2.5	Condition Number for Simple Eigenvalues	135
4.2.6	Sensitivity of Eigenvectors	141
4.3	Solving Systems of Linear Equations	146
4.3.1	Triangular Matrices	147

4.3.2	Gaussian Elimination	152
4.3.3	LU Method	159
4.3.4	Pivoting	165
4.3.5	Jacobi Iterative Method	171
4.4	Eigenproblems	175
4.4.1	Power Method	177
4.4.2	Inverse-Power Method with Shifting	181
4.4.3	QR Method	187
4.4.4	All Eigenvalues and Eigenvectors	204
4.5	Project: the Schrödinger Eigenvalue Problem	206
4.5.1	One Particle	206
4.5.2	Two Particles	211
4.5.3	Three Particles	223
4.5.4	Implementation	226
4.6	Problems	233
5	Roots	243
5.1	Motivation	243
5.1.1	Examples from Physics	243
5.1.2	The Problem(s) to Be Solved	244
5.2	Nonlinear Equation in One Variable	246
5.2.1	Conditioning	247
5.2.2	Order of Convergence and Termination Criteria	248
5.2.3	Fixed-Point Iteration	250
5.2.4	Bisection Method	256
5.2.5	Newton's Method	260
5.2.6	Secant Method	265
5.2.7	Ridders' Method	269
5.2.8	Summary of One-Dimensional Methods	272
5.3	Zeros of Polynomials	272
5.3.1	Challenges	273
5.3.2	One Root at a Time: Newton's Method	274
5.3.3	All the Roots at Once: Eigenvalue Approach	277
5.4	Systems of Nonlinear Equations	279
5.4.1	Newton's Method	280
5.4.2	Discretized Newton Method	282
5.4.3	Broyden's Method	283
5.5	Minimization	287
5.5.1	One-Dimensional Minimization	287
5.5.2	Multidimensional Minimization	289
5.5.3	Gradient Descent	292
5.5.4	Newton's Method	295
5.6	Project: Extremizing the Action in Classical Mechanics	297
5.6.1	Defining and Extremizing the Action	297

5.6.2	Discretizing the Action	298
5.6.3	Newton's Method for the Discrete Action	299
5.6.4	Implementation	301
5.7	Problems	304
6	Approximation	311
6.1	Motivation	311
6.1.1	Examples from Physics	311
6.1.2	The Problems to Be Solved	313
6.2	Polynomial Interpolation	317
6.2.1	Monomial Basis	319
6.2.2	Lagrange Interpolation	322
6.2.3	Error Formula	329
6.2.4	Hermite Interpolation	331
6.3	Cubic-Spline Interpolation	333
6.3.1	Three Nodes	333
6.3.2	General Case	335
6.3.3	Implementation	338
6.4	Trigonometric Interpolation	341
6.4.1	Fourier Series	342
6.4.2	Finite Series: Trigonometric Interpolation	343
6.4.3	Discrete Fourier Transform	348
6.5	Least-Squares Fitting	361
6.5.1	Chi Squared	362
6.5.2	Straight-Line Fit	364
6.5.3	General Linear Fit: Normal Equations	368
6.6	Project: Testing the Stefan–Boltzmann Law	376
6.6.1	Beyond Linear Fitting	377
6.6.2	Total Power Radiated by a Black Body	378
6.6.3	Fitting to the Lummer and Pringsheim Data	380
6.7	Problems	387
7	Integrals	393
7.1	Motivation	393
7.1.1	Examples from Physics	393
7.1.2	The Problem to Be Solved	394
7.2	Newton–Cotes Methods	396
7.2.1	Rectangle Rule	397
7.2.2	Midpoint Rule	400
7.2.3	Integration from Interpolation	401
7.2.4	Trapezoid Rule	402
7.2.5	Simpson's Rule	407
7.2.6	Summary of Results	411
7.2.7	Implementation	412

7.3	Adaptive Integration	414
7.3.1	Doubling the Number of Panels	415
7.3.2	Thoughts before Implementing	416
7.3.3	Implementation	417
7.4	Romberg Integration	419
7.4.1	Richardson Extrapolation	419
7.4.2	Romberg Recipe	421
7.4.3	Implementation	425
7.5	Gaussian Quadrature	427
7.5.1	Gauss–Legendre: $n = 2$ Case	428
7.5.2	Gauss–Legendre: General Case	429
7.5.3	Other Gaussian Quadratures	439
7.6	Complicating the Narrative	441
7.6.1	Periodic Functions	441
7.6.2	Singularities	442
7.6.3	Infinite Intervals	444
7.6.4	Multidimensional Integrals	446
7.6.5	Evaluating Different Integration Methods	448
7.7	Monte Carlo	448
7.7.1	Random Numbers	449
7.7.2	Monte Carlo Quadrature	453
7.7.3	Monte Carlo beyond the Uniform Distribution	458
7.7.4	Implementation	463
7.7.5	Monte Carlo in Many Dimensions	465
7.8	Project: Variational Quantum Monte Carlo	473
7.8.1	Hamiltonian and Wave Function	474
7.8.2	Variational Method	479
7.9	Problems	486
8	Differential Equations	494
8.1	Motivation	494
8.1.1	Examples from Physics	494
8.1.2	The Problems to Be Solved	496
8.2	Initial-Value Problems	498
8.2.1	Euler’s Method	499
8.2.2	Second-Order Runge–Kutta Methods	506
8.2.3	Fourth-Order Runge–Kutta Method	511
8.2.4	Simultaneous Differential Equations	522
8.3	Boundary-Value Problems	529
8.3.1	Shooting Method	530
8.3.2	Matrix Approach	532
8.4	Eigenvalue Problems	536
8.4.1	Shooting Method	537
8.4.2	Matrix Approach	541

8.5	Project: Poisson's Equation in Two Dimensions	545
8.5.1	Examples of PDEs	545
8.5.2	Poisson's Equation via FFT	546
8.6	Problems	552
Appendix A	Installation and Setup	559
Appendix B	Number Representations	560
B.1	Integers	560
B.2	Real Numbers	561
B.2.1	Single-Precision Floating-Point Numbers	562
B.2.2	Double-Precision Floating-Point Numbers	564
B.3	Problems	565
Appendix C	Math Background	566
C.1	Taylor Series	566
C.2	Matrix Terminology	567
C.3	Probability	570
C.3.1	Discrete Random Variables	570
C.3.2	Continuous Random Variables	572
	<i>Bibliography</i>	<i>573</i>
	<i>Index</i>	<i>577</i>