

Contents

Preface *xi*

About the Companion Website *xv*

1	Problem Solving in Engineering	<i>1</i>
1.1	Equation Identification and Categorization	<i>4</i>
1.1.1	Algebraic versus Differential Equations	<i>4</i>
1.1.2	Linear versus Nonlinear Equations	<i>5</i>
1.1.3	Ordinary versus Partial Differential Equations	<i>6</i>
1.1.4	Interpolation versus Regression	<i>8</i>
	Problems	<i>10</i>
	Additional Resources	<i>11</i>
	References	<i>11</i>
2	Programming with Python	<i>12</i>
2.1	Why Python?	<i>12</i>
2.1.1	Compiled versus Interpreted Computer Languages	<i>13</i>
2.1.2	A Note on Python Versions	<i>14</i>
2.2	Getting Python	<i>15</i>
2.2.1	Installation of Python	<i>17</i>
2.2.2	Alternative to Installation: SageMathCloud	<i>18</i>
2.3	Python Variables and Operators	<i>19</i>
2.3.1	Updating Variables	<i>21</i>
2.3.2	Containers	<i>23</i>
2.4	External Libraries	<i>25</i>
2.4.1	Finding Documentation	<i>27</i>
	Problems	<i>28</i>
	Additional Resources	<i>29</i>
	References	<i>30</i>
3	Programming Basics	<i>31</i>
3.1	Comparators and Conditionals	<i>31</i>
3.2	Iterators and Loops	<i>34</i>

3.2.1	Indentation Style	39
3.3	Functions	39
3.3.1	Pizza Example	43
3.3.2	Print Function	44
3.4	Debugging or Fixing Errors	45
3.5	Top 10+ Python Error Messages	45
	Problems	47
	Additional Resources	49
	References	49
4	External Libraries for Engineering	51
4.1	Numpy Library	51
4.1.1	Array and Vector Creation	51
4.1.2	Array Operations	55
4.1.3	Getting Helping with Numpy	55
4.1.4	Numpy Mathematical Functions	56
4.1.5	Random Vectors with Numpy	57
4.1.6	Sorting and Searching	57
4.1.7	Polynomials	58
4.1.8	Loading and Saving Arrays	59
4.2	Matplotlib Library	60
4.3	Application: Gillespie Algorithm	63
	Problems	66
	Additional Resources	68
	References	68
5	Symbolic Mathematics	70
5.1	Introduction	70
5.2	Symbolic Mathematics Packages	71
5.3	An Introduction to SymPy	72
5.3.1	Multiple Equations	75
5.4	Factoring and Expanding Functions	76
5.4.1	Equilibrium Kinetics Example	77
5.4.2	Partial Fraction Decomposition	78
5.5	Derivatives and Integrals	78
5.5.1	Reaction Example	79
5.5.2	Symbolic Integration	80
5.5.3	Reactor Sizing Example	80
5.6	Cryptography	81
	Problems	83
	References	86
6	Linear Systems	87
6.1	Example Problem	88
6.2	A Direct Solution Method	91

6.2.1	Distillation Example	95
6.2.2	Blood Flow Network Example	95
6.2.3	Computational Cost	98
6.3	Iterative Solution Methods	100
6.3.1	Vector Norms	100
6.3.2	Jacobi Iteration	100
6.3.3	Gauss–Seidel Iteration	103
6.3.4	Relaxation Methods	105
6.3.5	Convergence of Iterative Methods	105
	Problems	107
	References	112
7	Regression	113
7.1	Motivation	113
7.2	Fitting Vapor Pressure Data	114
7.3	Linear Regression	115
7.3.1	Alternative Derivation of the Normal Equations	118
7.4	Nonlinear Regression	119
7.4.1	Lunar Disintegration	122
7.5	Multivariable Regression	126
7.5.1	Machine Learning	127
	Problems	129
	References	134
8	Nonlinear Equations	135
8.1	Introduction	135
8.2	Bisection Method	137
8.3	Newton's Method	140
8.4	Broyden's Method	143
8.5	Multiple Nonlinear Equations	146
8.5.1	The Point Inside a Square	149
	Problems	151
9	Statistics	156
9.1	Introduction	156
9.2	Reading Data from a File	156
9.2.1	Numpy Library	157
9.2.2	CVS Library	159
9.2.3	Pandas	159
9.2.4	Parsing an Array	162
9.3	Statistical Analysis	162
9.4	Advanced Linear Regression	164
9.5	U.S. Electrical Rates Example	168
	Problems	172
	References	175

10	Numerical Differentiation and Integration	176
10.1	Introduction	176
10.2	Numerical Differentiation	176
10.2.1	First Derivative Approximation	177
10.2.2	Second Derivative Approximation	180
10.2.3	Scipy Derivative Approximation	181
10.3	Numerical Integration	183
10.3.1	Trapezoid Rule	185
10.3.2	Numerical Integration Using Scipy	186
10.3.3	Error Function	187
	Problems	190
	Reference	192
11	Initial Value Problems	193
11.1	Introduction	193
11.2	Biochemical Reactors	193
11.3	Forward Euler	195
11.4	Modified Euler Method	198
11.5	Systems of Equations	199
11.5.1	The Lorenz System and Chaotic Solutions	200
11.5.2	Second-Order Initial Value Problems	203
11.6	Stiff Differential Equations	203
	Problems	206
	References	210
12	Boundary Value Problems	211
12.1	Introduction	211
12.2	Shooting Method	212
12.3	Finite Difference Method	216
12.3.1	Reactions in Spherical Catalysts	220
	Problems	224
	Reference	226
13	Partial Differential Equations	227
13.1	Finite Difference Method for Steady-State PDEs	227
13.1.1	Setup	228
13.1.2	Matrix Assembly	230
13.1.3	Solving and Plotting	232
13.2	Convection	233
13.3	Finite Difference Method for Transient PDEs	236
	Problems	241
	Reference	244

14	Finite Element Method	<i>245</i>
14.1	A Warning	<i>245</i>
14.2	Why FEM?	<i>246</i>
14.3	Laplace's Equation	<i>246</i>
14.3.1	The Mesh	<i>246</i>
14.3.2	Discretization	<i>247</i>
14.3.3	Wait! Why Are We Doing This?	<i>248</i>
14.3.4	FEniCS Implementation	<i>248</i>
14.4	Pattern Formation	<i>249</i>
	Additional Resources	<i>253</i>
	References	<i>254</i>
	Index	<i>255</i>