

Contents

Preface *xiii*

Foreword *xvii*

About the Authors *xix*

1	Preliminary Notions	1
1.1	Introduction	1
1.2	Versions of Mathematica	1
1.3	Getting Started	2
1.4	Simple Calculations	2
1.4.1	Arithmetic Operations	2
1.4.2	Approximate Numerical Results	3
1.4.3	Algebraic Calculations	3
1.4.4	Defining Variables	4
1.4.5	Using the Previous Results	5
1.4.6	Suppressing the Output	6
1.4.7	Sequences of Operations	6
1.5	Built-in Functions	7
1.6	Additional Features	9
1.6.1	Arbitrary-Precision Calculations	9
1.6.2	Value for Symbols	10
1.6.3	Defining Naming and Evaluating Functions	10
1.6.4	Composition of Functions	11
1.6.5	Conditional Assignment	12
1.6.6	Warnings and Messages	13
1.6.7	Interrupting Calculations	13
1.6.8	Using Symbols to Tag Objects	13
2	Basic Mathematical Operations	15
2.1	Introduction	15
2.2	Basic Algebraic Operations	15
2.3	Basic Trigonometric Operations	20
2.4	Basic Operations with Complex Numbers	21

3	Lists and Tables	25
3.1	Introduction	25
3.2	Lists	25
3.3	Arrays	26
3.4	Tables	26
3.5	Extracting the Elements from the Arrays/Tables	29
4	Two-Dimensional Graphics	31
4.1	Introduction	31
4.2	Plotting Functions of a Single Variable	31
4.3	Additional Commands	34
4.4	Plot Styles	44
4.5	Probability Distribution	58
4.5.1	Binomial Distribution	58
4.5.2	Poisson Distribution	58
4.5.3	Normal or Gaussian Distribution	59
4.6	Some More Useful Commands	61
5	Parametric, Polar, Contour, Density, and List Plots	65
5.1	Introduction	65
5.2	Parametric Plotting	65
5.3	Polar Plots	72
5.3.1	Polar Plots of Circles	72
5.3.2	Polar Plots of Ellipse, Parabola, and Hyperbola	72
5.4	Implicit Plot	80
5.5	Contour Plots	81
5.6	Density Plot	85
5.7	ListPlot and ListLinePlot	85
5.8	LogPlot, LogLogPlot, ErrorListPlot	88
5.9	Least Square Fit	89
5.10	Plotting of Complex Numbers	92
6	Three-Dimensional Graphics	97
6.1	Introduction	97
6.2	Plotting Function of Two Variables	97
6.3	Parametric Plots	101
6.4	3D Plots in Cylindrical and Spherical Coordinates	102
6.5	ContourPlot3D	105
6.6	ListContourPlot3D	108
6.7	ListSurfacePlot3D	110
6.8	Surface of Revolution	112
6.9	Conicoids	114

7	Matrices	123
7.1	Introduction	123
7.2	Properties of Matrices	123
7.2.1	Matrix Multiplication	123
7.3	Types of Matrices	123
7.4	The Rank of the Matrix	124
7.5	Special Matrices	124
7.6	Creation of a Matrix and Matrix Operations	125
7.6.1	Extraction of the Submatrices or the Elements of the Matrices	126
7.7	Properties of the Special Matrices	133
7.8	Direct Sum of Matrices	137
7.9	Direct Product of Matrices	137
7.10	Examples from Group Theory	138
7.10.1	SO(3) Group	138
7.10.2	SU(n) Group	139
7.10.3	SU(2) Group	140
7.10.4	SU(3) Group	141
8	Solving Algebraic and Transcendental Equations	143
8.1	Introduction	143
8.2	Solving System of Linear Equations	143
8.2.1	Number of Equations Equal to Number of Unknowns	144
8.2.2	Number of Equations Less than the Number of Unknowns	146
8.2.3	Number of Equations More than Number of Unknowns	146
8.3	Nonlinear Algebraic Equations	147
8.4	Solving Complex Equations	149
8.5	Solving Transcendental Equations	153
9	Eigenvalues and Eigenvectors of a Matrix	161
9.1	Introduction	161
9.2	Eigenvalues and Eigenvectors	161
9.2.1	Distinct Eigenvalues Having Independent Eigenvectors	162
9.2.2	Multiple Eigenvalues Having Independent Eigenvectors	163
9.2.3	Multiple Eigenvalues Not Having Independent Eigenvectors	165
9.3	Cayley–Hamilton Theorem	166
9.4	Diagonalization of a Matrix	167
9.4.1	Gram–Schmidt Orthogonalization Method	167
9.4.2	Diagonalizability of a Matrix	169
9.4.3	Case of a Non-diagonalizable Matrix	170
9.5	Some More Properties of the Special Matrices	172
9.6	Power of a Matrix	173
9.6.1	Roots of a Matrix	174

9.6.2	Exponential of a Matrix	174
9.6.3	Logarithm of a Matrix	174
9.6.4	Matrix Power Series	174
9.7	Power of a Matrix by Diagonalization	174
9.8	Bilinear, Quadratic, and Hermitian Forms	177
9.9	Principal Axes Transformation	178
10	Differential Calculus	183
10.1	Introduction	183
10.2	Limits	183
10.2.1	Evaluation of the Limits Using L'Hospital's Rule	184
10.2.2	Application of L'Hospital's Rule for the "Indeterminate Form" $\frac{\infty}{\infty}$	185
10.2.3	Evaluation of the Limit Using Taylor's Theorem of Mean	186
10.3	Differentiation	188
10.3.1	Computation of Partial Derivatives	191
10.3.2	Total Derivative	193
10.4	Derivatives of Functions in Parametric Forms	195
10.4.1	Chain Rule for a Function of Two Independent Variables	196
10.4.2	Chain Rule for a Function of Three Independent Variables	196
10.5	Rolle's Theorem	198
10.6	Mean Value Theorem	198
10.7	Series	200
10.8	Maxima and Minima	209
10.8.1	First Derivative Test	210
10.8.2	Second Derivative Test	211
10.8.3	Maximum and Minimum Values of a Function in a Closed Interval	213
10.8.4	Maxima and Minima of Two Variables	218
10.9	Differential Equations	222
10.9.1	Simple Harmonic Oscillator	225
10.9.2	LCR Circuit – Discharging of a Capacitor Through an LR Circuit	227
11	Integral Calculus	235
11.1	Introduction	235
11.1.1	Indefinite Integral	235
11.1.2	Definite Integral	235
11.1.3	Numerical Value of the Integral	235
11.1.4	Assumptions While Evaluating the Integral	236
11.1.5	Multiple Integrals	236
11.1.6	Triple Integral	236
11.2	Evaluation of Indefinite Integrals	236
11.3	Evaluation of Definite Integrals	238
11.3.1	Numerical Value of the Integral	238
11.3.2	Options for Integration	239
11.4	Two and Three-Dimensional Integrals	240
11.5	Evaluation of the Integral in Polar Coordinates	242

11.6	Evaluation of Special Integrals	242
11.7	Orthogonal Polynomials	248
11.8	Area Between Curves	252
11.9	Application of Green's Theorem in a Plane	256
11.10	Area of Surfaces of Revolution	257
12	Dirac Delta Function	263
12.1	Introduction	263
12.2	The Limiting Form of the Dirac Delta Function	263
12.3	Integral Representation of the Dirac Delta Function	265
12.4	Some Important Properties of the Dirac Delta Function	267
12.5	The Three-Dimensional Dirac Delta Function	270
13	Fourier Transforms	273
13.1	Introduction	273
13.2	Fourier Transforms	273
13.3	Scaling Property	280
13.4	Shifting Property	280
13.5	Fourier Sine and Cosine Transforms	281
13.6	Fourier Transform of the Derivative	282
13.7	Inverse Fourier Transform	282
13.8	Convolution	283
13.9	Convolution Theorem for Fourier Transforms	291
13.10	Parseval's Theorem	293
14	Laplace Transforms	295
14.1	Introduction	295
14.2	Some Simple Examples	296
14.3	Properties of the Laplace Transforms	297
14.3.1	Linearity	297
14.3.2	Shifting Property	297
14.3.3	Scaling Property	297
14.4	Laplace Transform of the Derivative	298
14.5	Laplace Transform of Certain Special Functions	299
14.6	The Laplace Transform of Error and Complementary Error Functions	300
14.7	The Evaluation of a Certain Class of Definite Integrals Using Laplace Transforms	300
14.8	The Inverse Laplace Transform	302
14.8.1	Inverse Laplace Transform of Standard Functions	303
14.8.2	Shifting Properties	303
14.8.3	Inverse Laplace Transforms of Derivatives	305
14.9	Solving the Differential Equation by Laplace Transform	306
14.10	Convolution Theorem	307
14.11	Graphical Treatment of the Convolution	308

15	Vectors	315
15.1	Introduction	315
15.2	Properties	315
15.3	Vector Differentiation	319
15.4	Directional Derivative	320
15.5	Unit Vector Normal to the Surface	320
15.6	Gradient, Divergence, and Curl in the Cartesian Coordinate System	320
15.6.1	Gradient	320
15.6.2	Divergence	321
15.6.3	Curl	321
15.6.4	Laplacian Operator (∇^2)	321
15.6.5	Examples	322
15.7	Expressing the Gradient, Divergence, and Curl in Other Coordinate Systems	326
15.7.1	Spherical Coordinate System	326
15.7.2	Cylindrical Coordinate System	330
15.8	Vector Plots	337
16	Linear Vector Spaces and Quantum Mechanics	343
16.1	Introduction	343
16.2	Linear Independence, Basis, and Dimension	343
16.3	Dimension of the Vector Space	343
16.4	Basis of the Vector Space	343
16.5	Completeness	344
16.6	Scalar Product in a Linear Vector Space	344
16.7	Norm of the Vector	344
16.8	Orthonormal Basis	344
16.9	Linear Independence of Functions	348
16.10	Hilbert Space	349
16.11	Completeness in Functional Space	350
16.12	The Dirac Ket and Bra Notation	351
16.12.1	The Scalar Product of Kets and Bras	351
16.12.2	Schwartz Inequality	352
16.12.3	The Orthonormal States	352
16.12.4	Basis	352
16.12.5	Probability Density	352
16.13	The Hermitian and Skew-Hermitian Operators in Dirac Ket and Bra Notation	352
16.14	Expectation Values	353
16.15	Matrix Representation of the Linear Operator	359
17	Application of Mathematica to Quantum Mechanics	361
17.1	Introduction	361
17.2	A Particle in a One-Dimensional Box	361
17.3	A Particle in a Two-Dimensional Box	365

17.4	The Hydrogen Atom Problem	368
17.4.1	The Orthonormal Property of the Hydrogen Atom Wave Functions	371
17.5	The One-Dimensional Linear Harmonic Oscillator Atom Problem	373
17.6	Three-Dimensional Harmonic Oscillator	377
17.7	Miscellaneous Problems	382
References		385
Index		387