

## Applying Maths in the Chemical and Biomolecular Sciences

An example-based-approach

**Godfrey Beddard** 

Universitäts- und Landesbibliothek Darmstadt Bibliothek Biologie

Inv-Nr. 1688



## **Contents**

|                             | Glossary of Selected Mathematical Symb<br>Table of Scientific Constants | ols              |             |           | . xv<br>xvi     |
|-----------------------------|---|------------------|-------------|-----------|-----------------|
|                             | Conversion Table: Energy Units and Relat                                | ed Quantities    |             |           | χvi             |
|                             | Table of Derived Units and Quantities                                   |                  |             |           | xvii            |
|                             | Table of Prefixes   |                  |             | * •       | xvii            |
|                             |   |                  |             |           |                 |
| 1                           | Numbers, Equations, Operators, and                                      | d Algorithms     |             | .,        | ·               |
| 1.1                         | Symbols and basics  | ·                |             |           | 1               |
| 1.2                         | Integers, real and irrational numbers                                   |                  | •           |           | 5               |
| 1.3                         | The exponential $e$ and $e^x$   |                  |             |           | 13              |
| 1.4                         | Logarithms  |                  |             |           | 15              |
| 1.5                         | Trigonometric functions   |                  |             |           | 18              |
| 1.6                         | Inverse functions   |                  |             |           | 24              |
| 1.7                         | Cartesian and polar coordinates   |                  |             |           | 25              |
| 1.8                         | Factorials  |                  |             |           | - 26            |
| 1.9                         | Sophisticated counting: permutations,                                   | combinations, an | d probabili | ty        | 29              |
| 1.10                        | Modulo arithmetic   | ·                | • • •       | • • • • • | 43              |
| 1.11                        | Delta functions   |                  |             |           | 43              |
| 1.12                        | Series  |                  | ,           |           | 44              |
| 1.13                        | Estimation  |                  |             | •         | 45              |
| 1.14                        | Rounding numbers and units  |                  |             |           | 46              |
| 1.15                        | SI units and prefixes   | :                |             |           | 48              |
|                             | or anno and promote   |                  |             |           | ,0              |
|                             |   |                  |             |           |                 |
| 2                           | Complex Numbers   |                  |             |           |                 |
| 2.1                         | Motivation and concept  |                  | • •         |           | 53              |
| 2.2                         | Complex conjugate   |                  |             | •         | 54              |
| 2.3                         | Summary   |                  |             |           | <sup>`</sup> 56 |
| 2.4                         | Using Maple   | •                |             |           | 57              |
| 2.5                         | Questions   |                  | 10 m        | •         | 57              |
| 2.6                         | DeMoivre's theorem and powers of co                                     | mplex numbers    |             | ٠         | . 58            |
| 2.7                         | Questions   |                  |             |           | 60              |
| 2.8                         | Euler's theorem   |                  |             |           | 60              |
| 2.9                         | Questions   |                  | •           |           | 62              |
|                             |   |                  |             |           |                 |
|                             |   |                  | · ·         | ·         |                 |
| 3                           | Differentiation   | · ·              | · · · :     | ,         | ;;              |
| 50 3.1                      | Concepts  |                  | i           | •         | . 64            |
| 3.2                         | Differentiation   | · .              |             | •         | 65              |
| 3.3                         | Questions   |                  | •           |           | 66              |
| કું 3.4<br>કું 3.4          | The machinery of differentiation  |                  | ,           |           | 67              |
| % 3.5<br><sub>(∂S</sub> 3.5 | Going beyond simple functions   |                  |             | •         | . 77            |
| 3.6                         | Summary   |                  |             |           | . 83            |
| LET 1                       |   |                  |             |           | ,               |

| 3.7     | Questions  | 84  |
|---------|--|-----|
| 3.8     | Limits: l'Hôspital's rule  | 91  |
| 3.9     | Extrema: maxima, minima, and inflection points                               | 92  |
| 3.10    | The Newton-Raphson algorithm: Finding the roots of equations numerically     | 105 |
| 3.11    | Minimizing or maximizing with constraints: Lagrange undetermined multipliers | 112 |
| 3.12    | Partial differentiation  | 116 |
| 3.13    | Differentiation of vectors   | 128 |
|         |  |     |
| 4       | Integration  |     |
|         |  |     |
| 4.1     | Basic concepts   | 130 |
| 4.2     | Mechanics of integration   | 135 |
| 4.3     | Integration by substitution  | 145 |
| 4.4     | Three useful results with a function and its derivative                      | 147 |
| 4.5     | Integration by parts   | 148 |
| 4.6     | Integration using parametric equations                                       | 151 |
| 4.7     | Integration in plane polar coordinates                                       | 152 |
| 4.8     | Calculating the average value of an expression                               | 161 |
| 4.9     | The Variational Method in Quantum Mechanics                                  | 175 |
| 4.10    | Multiple integrals   | 180 |
| 4.11    | Change of variables in integrals: Jacobians                                  | 185 |
| 4.12    | Line integrals   | 199 |
| 4.13    | Definitions of some different forms of line integrals                        | 201 |
| ~4.14   | Path integrals in thermodynamics   | 204 |
|         |  |     |
|         | Summations, Series, and Expansion of Functions                               |     |
| 5       | Summations, Series, and Expansion of Functions                               |     |
| ··· 5.1 | Motivation   | 209 |
| 5.2     | Power series   | 209 |
| 5.3     | Average quantities   | 211 |
| 5.4     | Partition functions  | 213 |
| 5.5     | Questions  | 213 |
| 5.6     | Maclaurin and Taylor series expansions                                       | 217 |
| 5.7     | Euler-Maclaurin formula  | 223 |
| 5.8     | Perturbation theory  | 232 |
| 5.9     | Quantum superposition and wave packets                                       | 240 |
|         |  |     |
|         |  |     |
| 6       | Vectors  |     |
| 6.1     | Motivation and concept   | 248 |
| 6.2     | Vector multiplication: dot, cross, and triple products                       | 250 |
| 6.3     | The orthonormal i, j, k base vectors   | 255 |
| : 6.4   | Summary  | 256 |
| 6.5     | Questions  | 256 |
| 6.6     | Projections and components   | 264 |
| 6.7     | Questions  | 267 |
| 6.8     | Not all ayes are right-angled or of equal length                             | 270 |

| 6.9           | Conversion from one basis set to another                      | 273           |
|---------------|---|---------------|
| 6.10          | Transformation of basis vectors                               | 276           |
| 6.11          | Questions   | 279           |
| 6.12          | Basis sets with more than three dimensions                    | 279           |
| 6.13          | Large and infinite basis sets                                 | 281           |
| 6.14          | Basis sets in molecules                                       | 282           |
| 6.15          | Questions   | 284           |
| <b>6.16</b> . | Cross product or vector product:                              | 289           |
| 6.17          | Scalar triple products are numbers                            | 295           |
| 6.18          | Vector triple product •                                       | 296           |
| 6.19          | Questions   | 297           |
| 6.20          | Torsion or dihedral angles                                    | 298           |
| 6.21          | Torsion angles in sugars and DNA                              | 302           |
| 6.22          | Questions   | 304           |
| 6.23          | Torque and angular momentum                                   | 308           |
|               |   | •             |
|               |   | <del></del>   |
| 7             | Matrices  |               |
|               |   | ·. ·          |
| 7.1           | Motivation and concept  | 313           |
| 7.2           | Determinants  | 314           |
| 7.3           | Questions   | 318           |
| 7.4           | Matrices  | 320           |
| 7.5           | Matrix multiplication   | 325           |
| 7.6           | Molecular group theory  | 331           |
| 7.7           | Rotation matrices: moving molecules                           | 356           |
| 7.8           | Using Jacobians to calculate derivatives in polar coordinates | 361           |
| 7.9           | Questions   | 363           |
| 7.10          | Matrices in optics and lasers                                 | . 364         |
| 7.11          | Polarizing optics   | 373           |
| 7.12          | Solving equations using matrices                              | 379           |
| 7.13          | Rate equations and chemical kinetics                          | 389           |
| 7.14          | Molecular vibrations and pendulums                            | 400           |
| 7.15          | Moments of inertia  | 413           |
|               |   |               |
| 8             | Matrices in Quantum Mechanics                                 |               |
|               | Matrices in Quantum Mechanics                                 |               |
| 8.1           | Concept and motivation  | 424           |
| 8.2           | Expectation values  | 425           |
| 8.3           | NMR spectrum with two spins                                   | 433           |
| 8.4           | Basis sets and bra-ket algebra                                | 443           |
|               |   |               |
|               |   | <del></del> - |
| . 9           | Fourier Series and Transforms                                 |               |
|               |   | •             |
| 9.1           | Motivation and concept  | 452           |
| 9.2           | Some formal points about the Fourier series                   | 460           |
| 9.3           | Integrating series  | 461           |
| 9.4           | Generalized Fourier series with orthogonal polynomials        | 463           |
| 9.5           | Fourier transforms  | 468           |

| 9.6    | The Fourier transform equations  | 476              |
|--------|--|------------------|
| 9.7    | Convolution  | 485              |
| 9.8    | Autocorrelation and cross-correlation  | 490              |
| 9.9    | Discrete Fourier transforms (DFT) and fast Fourier transforms (FFT)                | 502              |
| 9.10   | Using Fourier transforms for filtering, smoothing, and noise reduction on data     | 511              |
| 9.11   | Hadamard transform: encoding and decoding  | 515              |
|        |  |                  |
| 10     | Differential Equations   |                  |
| 10.1   | Motivation and Concept   | 520              |
| 10.2   | Separable variables  | 521              |
| 10.3   | Phase planes and solving equations by separating variables                         | 524              |
| 10.4   | Integrating factors  | 539              |
| ^ 10.5 | Second-order differential equations  | 543              |
| 10.6   | The 'D' operator. Solving linear differential equations with constant coefficients | 551              |
| 10.7   | Simultaneous equations   | 565              |
| 10.8   | Linear equations with variable coefficients  | <sup>*</sup> 573 |
| 10.9   | Partial differential equations   | 580              |
|        |  |                  |
| 11     | Numerical Methods  |                  |
| 11.1   | Numerical accuracy   | 601              |
| · 11.2 | Numerical methods to find the roots of an equation                                 | 605              |
| 11.3   | Numerical integration  | 606              |
| 11.4   | Numerical solution of differential equations                                       | 618              |
| 11.5   | Coupled equations  | 629              |
| 11.6   | The phase plane, nullclines, and stable points                                     | 634              |
| 11.7   | SIR equations and the spread of diseases   | 638              |
| 11.8   | Reaction schemes with feedback   | 644              |
| ` 11.9 | Boundary value problems: shooting method   | 653              |
| 11.10  | Numerical integration of the Schrödinger equation                                  | 657              |
|        |  |                  |
| 12     | Monte Carlo Methods  |                  |
| 12.1   | Integration  | 666              |
| 12.2   | Solving rate equations   | 672              |
| , 12.3 | Monte Carlo simulations and calculations   | 681              |
| 12.4   | The Metropolis algorithm   | 686              |
| 12.5   | Forster or dipole-dipole energy transfer   | 693              |
| 12.6   | Autocatalytic reaction on a surface and the spreading of fires                     | 695              |
| 12.7   | Questions  | 699              |
| : .    |  | -                |
|        | Data Analysis  |                  |
|        |  |                  |
| -13.1  | Characterizing experimental data   | 703              |
| 13.2   | Central limit theorem  | 706              |

|      | dix 1 A Maple™ Language Crib  | <del></del> |     |
|------|---|-------------|-----|
|      |   | •           |     |
| 13.9 | Principal component analysis (PCA)  |             | 744 |
| 13.8 | Non-linear least squares, gradient expansion, and the<br>Levenberg-Marquardt Method |             | 739 |
| 13.7 | Photon and particle counting and the Poisson distribution                           |             | 736 |
| 13.6 | Modelling data with polynomials is simpler using matrices                           |             | 731 |
| 13.5 | Modelling data  |             | 719 |
| 13.4 | Propagation or combination of errors  |             | 716 |
| 13.3 | Confidence intervals  |             | 708 |

| A.1  | Finding your way around   | 749 |
|------|---|-----|
| A.2  | Some useful points  | 749 |
| A.3  | General syntax  | 750 |
| A.4  | Packages  | 750 |
| A.5  | Converting units  | 751 |
| A.6  | Defining your own function  | 751 |
| A.7  | Two examples of plotting  | 752 |
| A.8  | Examples using expand and factor                                  | 752 |
| A.9  | simplify, normal, rationalize, collect, combine                   | 753 |
| A.10 | Substitutions and evaluations: subs and algsubs, evalf            | 754 |
| A.11 | convert and evala   | 755 |
| A.12 | map   | 756 |
| A.13 | Numerical calculations  | 756 |
| A.14 | Sum (algebraic summation), add (numerical summation), and product | 757 |
| A.15 | Differentiation and integration                                   | 757 |
| A.16 | The D operator  | 758 |
| A.17 | Integration   | 759 |
| A.18 | solve, fsolve, and unapply  | 760 |
| A.19 | Solving differential equations, dsolve                            | 761 |
| A.20 | Plotting functions  | 762 |
| A.21 | Plotting data   | 764 |
| A.22 | Parametric plots ,  | 766 |
| A.23 | axes  | 766 |
| A.24 | Sequences   | 766 |
| A.25 | Arrays, vectors, and matrices                                     | 767 |
| A.26 | Sorting   | 768 |
| A.27 | Verify  | 768 |
| A.28 | Programming: for and while do loops, and if then statements       | 768 |
| A.29 | Procedures  | 769 |
| A.30 | Concatenation   | 770 |
| A.31 | Sets and lists  | 770 |
| A.32 | Example of integration and more complex plotting                  | 771 |
|      |   |     |

Maple and Mathematica Syntax Conversion.

References

Index

773

777

781