

James Sneyd · Rachel M. Fewster
Duncan McGillivray

Mathematics and Statistics for Science



 Springer

Mathematics and Statistics for Science

James Sneyd • Rachel M. Fewster
Duncan McGillivray

Mathematics and Statistics for Science

 Springer

James Sneyd
Department of Mathematics
University of Auckland
Auckland, New Zealand

Rachel M. Fewster
Department of Statistics
University of Auckland
Auckland, New Zealand

Duncan McGillivray
School of Chemical Sciences
University of Auckland
Auckland, New Zealand

ISBN 978-3-031-05317-7 ISBN 978-3-031-05318-4 (eBook)
<https://doi.org/10.1007/978-3-031-05318-4>

Mathematics Subject Classification (2020): 00-01, 00A06, 62-01

© The Editor(s) (if applicable) and The Author(s), under exclusive license to Springer Nature Switzerland AG 2022

This work is subject to copyright. All rights are solely and exclusively licensed by the Publisher, whether the whole or part of the material is concerned, specifically the rights of translation, reprinting, reuse of illustrations, recitation, broadcasting, reproduction on microfilms or in any other physical way, and transmission or information storage and retrieval, electronic adaptation, computer software, or by similar or dissimilar methodology now known or hereafter developed.

The use of general descriptive names, registered names, trademarks, service marks, etc. in this publication does not imply, even in the absence of a specific statement, that such names are exempt from the relevant protective laws and regulations and therefore free for general use.

The publisher, the authors, and the editors are safe to assume that the advice and information in this book are believed to be true and accurate at the date of publication. Neither the publisher nor the authors or the editors give a warranty, expressed or implied, with respect to the material contained herein or for any errors or omissions that may have been made. The publisher remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.

This Springer imprint is published by the registered company Springer Nature Switzerland AG

The registered company address is: Gewerbestrasse 11, 6330 Cham, Switzerland

Preface

This book is aimed at university students in the sciences who are not planning on continuing with a degree in mathematics, statistics, physics, or computer science, but who nevertheless need to learn some more mathematics and statistics for their science degrees. So, for example, if you're studying a discipline such as chemistry, molecular biology, biochemistry, physiology, geography, psychology, geology, or ecology, you will find this book useful for learning the mathematics and statistics you will need in your scientific career.

And you will need to know some mathematics and statistics, nothing more certain. You won't need to know a lot of theory – no theorems or proofs or corollaries or lemmas or things like that will be required – and you might not need to know a lot of advanced techniques, but nowadays science has become so quantitative that mathematics and statistics simply cannot be avoided.

Although this is certainly true, mathematics and statistics are not always taught in a way that is appropriate for students who want to learn useful techniques, but don't need to know any theory. Therefore, in this book we have taken what we think is a very different approach. Firstly, we have covered only those topics that we believe to be directly useful to a practising scientist. If it's something that we have never used ourselves in practice, then we simply leave it out. For example, the theory of Gaussian elimination is something we learned in detail ourselves, but have never used in practice. Ever. Not one of us has solved a large linear system in any way other than using a piece of software. Sure, the software uses Gaussian elimination. If you write the software you'll need to know how to do that. But if you just want to use the software, knowledge of the underlying theory is a step too far. Similarly, who now draws two-dimensional surfaces by hand? *We* don't. In fact, we probably can't, not any more; it's been too long since we learned how to do it, but never did it again. But then, why would we want to, when a computer can do that job so much more efficiently?

Secondly, each topic is approached in a way that focuses on how that topic is applied, how it can be used in practice. We don't prove theorems, or give results and propositions; we give no lemmas. Many times we simply state a result, without proving that it's actually correct. But that again is how scientists operate. They don't

need to know the detailed theoretical background of why it works. They just need to know that it *does* work, and how to use it.

Of course, there are dangers in an approach like this. It's not uncommon for scientists to study complex and difficult problems, for which basic mathematical and statistical techniques are insufficient. Sometimes, application of the basic methods can lead to errors and problems; often, an understanding of *why* the basic result is true is needed. However, these cases are the exception rather than the rule. When scientists meet problems of this nature they can learn the theory then, should they wish to do so. To present the theory too soon serves only to hinder rather than to help.

There is, unfortunately, a lot that a book of this type simply cannot cover. After all, we don't want to end up with a book so large that it could not possibly be carried around. So we assume that you're already familiar with the basic operations of arithmetic, algebra and trigonometry. We assume that you can add fractions, take square roots and cube roots, factor polynomials, sketch straight lines and parabolas, and so on.

If you have no idea of how to do these things, then we suggest a more foundational mathematics/statistics book would be a lot better for you. If you've already learned how to do these things, but aren't too confident about them – maybe you learned them at school a long time ago and you've forgotten – then, fortunately, there are many places on the internet that can help you.

One of our favourite places to brush up on mathematical and statistical stuff that you may have forgotten is the [Khan Academy](#). This site covers a huge amount of foundation material. It has problems, solutions and instructional videos. It explains things clearly. We recommend it highly.

Another excellent site is [mathsisfun.com](#). It's not as comprehensive as the Khan Academy site, but contains some lovely animated demonstrations that are definitely worth watching.

Not only does this book omit a lot of foundational material, it also omits some more advanced topics of great scientific importance. In particular, although we consider differential equations in Chapters 25 and 26, the presentation there is only brief and doesn't cover such important things as higher-order ordinary differential equations, systems of differential equations, or partial differential equations. Similarly, we omit practically all the theory of linear systems and matrices. These are all fundamentally important for all branches of science, but there simply isn't space to discuss everything in a single book. If you want to learn more about more advanced topics like this, we suggest one of the many books on Engineering Mathematics, such as the [book by Kreyszig](#) or the [book by Greenberg](#). There are many other possibilities, all quite similar.

How could this book be used? Well, we authors have used it to teach a course called "Mathematics for Science" at the University of Auckland, New Zealand. This course is designed for science majors (particularly chemistry and biology majors) who don't need to do more advanced mathematics courses. We have also used the statistics parts of this text to teach a statistics course in Auckland with the similar goal of teaching science majors rather than statistics or mathematics majors. This book could also be used as a supplementary text for providing more scientific context and explanation that is typically present in an undergraduate mathematics textbook. However, it would not be all that suitable as a stand-alone text to teach a course for continuing mathematics students, as the necessary theoretical development is mostly absent.

We authors are a bit of a mixed bag. One of us (James Sneyd) is an applied mathematician who specialises in the application of mathematics to cell physiology; one of us (Rachel Fewster) is a statistician who specialises in statistical ecology; one of us (Duncan McGillivray) is a chemist who specialises in the study of biological membranes using tools like neutron and X-ray scattering. However, despite our different backgrounds and research interests, there is one thing we all have in common. Each of us has used mathematics and statistics on a daily basis to solve scientific problems. We know what kind of methods are used. We know the kinds of things that scientists need to know. And we hope that we have managed to convey some of that knowledge to you, in such a way that this book will remain relevant throughout your scientific career.

Auckland,
February 2022

James Sneyd
Rachel Fewster
Duncan McGillivray

Acknowledgements

In writing this book we have had a lot of help from a lot of people. John Mitry, Julia Novak and Andrew Wang all contributed greatly, particularly to the exercises, while David Williams, Cather Simpson and Sheila Woodgate all had a significant effect on the overall direction and content. Joel Schiff and Brian Cox also made significant contributions with their comments and suggestions, as did Joe Mahaffy, who provided an extensive set of comments on an earlier draft.

In particular, we thank Remi Lodh, from Springer, for his help in determining the content and layout, and, more importantly, for his enormous patience.

Early versions of this book were based (very loosely) on the Maths 108, Stats 210 and Stats 20x lecture notes (at the University of Auckland).

Contents

I	Units and Measurement	1
1	Units	3
1.1	Numbers	3
1.2	Decimals	5
1.3	Orders of magnitude and scientific notation	5
1.4	Numbers and units	7
1.5	Units in equations	9
1.6	Unit conversion	12
1.7	Parts per million, parts per billion	15
2	Measurement, rounding and uncertainty	23
2.1	Precision and accuracy	24
2.2	Significant figures and rounding	24
2.3	Measurement uncertainty	27
2.4	Significant figures in equations	28
2.5	Uncertainty analysis	29
II	Functions and Complex Numbers	39
3	Functions	41
3.1	What is a function?	41
3.2	Domain of a function	42
3.3	Graphing functions	46
3.4	Functions represented by a table	46
3.5	Functions and units	47
3.6	Proportionality	50
3.7	Piecewise-defined functions	53
3.8	Operations on functions	56
3.9	Function composition	56
4	Exponential and log functions	67
4.1	Exponential functions	67
4.2	Log functions	73
5	Periodic functions	89
5.1	Trigonometric functions	91
5.2	Arcs and sectors	95
5.3	Trigonometric identities	95

5.4	Calculating period and frequency	97
5.5	Solving simple trigonometric equations	100
5.6	Polar coordinates	102
5.7	Periodic functions as models of the real world	104
6	Linearising functions	121
6.1	Revision: the equation of a line	122
6.2	Lineweaver–Burke plots	124
6.3	Linearising the Arrhenius equation	125
6.4	Power laws	127
7	Complex numbers	135
7.1	The number i and other complex numbers	136
7.2	Adding and subtracting complex numbers	137
7.3	Multiplying complex numbers	137
7.4	Dividing complex numbers; the conjugate	138
7.5	The complex plane	140
7.6	Complex roots of polynomials	145
7.7	Euler’s formula	148
III	Vectors, Matrices and Linear Systems	157
8	Vectors	159
8.1	Adding and subtracting vectors	161
8.2	Scalar multiplication	162
8.3	Parallel vectors	163
8.4	Length of a vector	163
8.5	Distance between two vectors	166
8.6	Unit vectors	166
8.7	The angle between two vectors	168
9	Matrices	181
9.1	Some basic matrix properties	182
9.2	Row and column vectors	185
9.3	Matrix multiplication	186
9.4	A matrix as a linear transformation	192
9.5	The inverse of a matrix	195
10	Systems of linear equations	203
10.1	Linear equations	205
10.2	Solutions in two dimensions	210
10.3	Solutions in three dimensions	211
11	Solving systems of linear equations using matrices	219
11.1	Writing linear systems as matrix equations	220
11.2	Computing matrix inverses	225
11.3	Warning: not all matrices have an inverse	229
11.4	Linear systems can be written in an alternative way	236

IV	Differentiation: Functions of One Variable	251
12	Limits	253
12.1	The simple cases	254
12.2	Limits of ratios of functions	258
12.3	Horizontal asymptotes	260
12.4	Vertical asymptotes	266
13	Differentiation as a limit	279
13.1	Motivating the definition	280
13.2	Distance and velocity	283
13.3	Rate of a chemical reaction	286
14	Differentiation in practice	291
14.1	Differentiating polynomials	292
14.2	Differentiating trig functions	295
14.3	Differentiating exponential and log functions	296
14.4	Higher derivatives	297
14.5	Product rule	298
14.6	Quotient rule	300
14.7	Chain rule	301
14.8	Using a computer	305
14.9	Positions and velocities	306
15	Numerical differentiation	315
15.1	Calculating approximate derivatives	316
15.2	Data with increased resolution	318
15.3	Problems with high resolution	319
16	Implicit differentiation	325
16.1	Using the chain rule	326
16.2	Relative rates of change	329
17	Maxima and minima	337
17.1	Local maxima and local minima	339
17.2	Critical points and stationary points	340
17.3	Concavity and points of inflection	341
17.4	Second derivative test	344
V	Differentiation: Functions of Multiple Variables	355
18	Functions of multiple variables	357
18.1	Graphing functions of two variables	359
18.2	Level curves	363
19	Partial derivatives	371
19.1	Slopes of a surface	372
19.2	Partial differentiation	373

19.3 The chain rule for multiple variables 377
 19.4 Partial derivatives and uncertainty analysis 380
 19.5 Higher order partial derivatives 382

20 Extrema of functions of two (or more) variables **391**
 20.1 Maximum and minimum points 392
 20.2 Saddle points 395

VI Integration 401

21 The area under a curve **403**
 21.1 Geometric intuition 405
 21.2 Notation: the integral sign 406
 21.3 Riemann sums 406
 21.4 The Fundamental Theorems of Calculus 409

22 Calculating antiderivatives and areas **413**
 22.1 Antiderivatives are not unique 415
 22.2 Indefinite integrals 415
 22.3 Basic formulas 415
 22.4 Calculating areas underneath graphs 419
 22.5 Integrating vectors 422
 22.6 Velocity and distance 423
 22.7 The average value of a function 426
 22.8 Work 430

23 Integration techniques **439**
 23.1 Integration by substitution 441
 23.2 Integration by parts 444
 23.3 The LATE rule 445
 23.4 Looking it up or using a computer 447

24 Numerical integration **453**
 24.1 Some pretend data 454
 24.2 The trapezoid method 456
 24.3 The special case of equal intervals 458

VII Differential Equations 467

25 First-order ordinary differential equations **469**
 25.1 Differential equations from the real world 471
 25.2 Initial conditions 474
 25.3 Separation of variables 475
 25.4 Using a computer 484
 25.5 Qualitative analysis 486

26 Numerical solutions of differential equations **505**
 26.1 Euler’s method 507

26.2 Using computer packages	511
--	-----

VIII Probability 523

27 Probability foundations	525
27.1 Sample space	527
27.2 Events	528
27.3 Probability	530
27.4 Probability distributions in pictures	534
27.5 Tables of counts	535
28 Random variables	543
28.1 Standard notation for random variables	545
28.2 Discrete and continuous	548
28.3 The probability function	549
28.4 Cumulative distribution function	550
29 Binomial distribution	561
29.1 Bernoulli trials	563
29.2 Binomial distribution	568
29.3 Shape of the binomial distribution	569
29.4 Binomial probability function	570
29.5 Binomial probabilities by computer	576
30 Conditional probability	583
30.1 Conditional probability: shrinking the sample space	587
30.2 Conditional probability in pictures	588
30.3 Conditionals and intersections	590
30.4 Bayes' theorem for inverting conditionals	593
30.5 Statistical independence	594
31 Total probability rule	605
31.1 Total probability of an event	607
31.2 The partition theorem in pictures	610
31.3 Some examples	611

IX Statistical Inference 621

32 Hypothesis tests	623
32.1 What is statistical inference?	623
32.2 A simple hypothesis test	626
32.3 Principles of hypothesis testing	633
33 Hypothesis testing in practice	651
33.1 Presidents	652
33.2 Deep-sea divers	656
33.3 Sports stars	657

33.4 Role of hypothesis testing in science 659

34 Estimation and likelihood 667

34.1 Estimation 669
34.2 Likelihood 670
34.3 Finding the maximum likelihood estimate 674
34.4 Estimators 677
34.5 Role of likelihood in scientific modelling 681

X Discrete Probability Distributions 687

35 Simulation and visualisation 689

35.1 Simulation 691
35.2 Histograms 693
35.3 Histograms as empirical probability functions 695

36 Mean 703

36.1 The distribution mean 706
36.2 Binomial distribution mean 712
36.3 Combining random variables with constants 714
36.4 Combining random variables 720
36.5 Expectation of X^2 and other transformations 722
36.6 Binomial mean explained 724
36.7 Mean of estimators 726

37 Variance 735

37.1 The distribution variance 737
37.2 Variance properties 741
37.3 Binomial distribution variance 743
37.4 Standard deviation 745
37.5 Variance of estimators 746

38 Discrete probability models 761

38.1 Binomial distribution 762
38.2 Poisson distribution 764
38.3 Inference with the Poisson distribution 770
38.4 Geometric distribution 778
38.5 Negative binomial distribution 782

XI Continuous Probability Distributions 797

39 Continuous random variables 799

39.1 What does it mean to be continuous? 801
39.2 Probability density function 804
39.3 Calculating probabilities 810
39.4 Inference with continuous random variables 815
39.5 Mean and variance 817

40	Common continuous probability models	829
40.1	Uniform distribution	831
40.2	Exponential distribution	836
40.3	Gamma distribution	847
40.4	Inference with the exponential distribution	851
41	Normal distribution and inference	867
41.1	Normal distribution	868
41.2	The central limit effect	877
41.3	One-size-fits-all statistical inference	882
XII	Linear Regression	897
42	Fitting linear functions: theory and practice	899
42.1	Finding relationships between variables	900
42.2	Key questions	902
42.3	The simple linear model	902
42.4	The method of least squares	907
42.5	Fitting a linear function to data; a simple example	910
42.6	Fitting a linear function to data; a more complex example	912
42.7	Fitting the simple linear model using R	913
43	Quantifying relationships	923
43.1	Finding P-values using R	927
43.2	False positives, or Type I errors	928
43.3	False negatives, or Type II errors	929
43.4	Confidence intervals	930
	References	945
	Index	955