

Cambridge University Press

978-0-521-11940-5 - A Student's Guide to Data and Error Analysis

Herman J. C. Berendsen

Frontmatter

[More information](#)

## *A Student's Guide to Data and Error Analysis*

All students taking laboratory courses within the physical sciences and engineering will benefit from this book, whilst researchers will find it an invaluable reference. This concise, practical guide brings the reader up to speed on the proper handling and presentation of scientific data and its inaccuracies. It covers all the vital topics with practical guidelines, computer programs (in Python), and recipes for handling experimental errors and reporting experimental data. In addition to the essentials, it also provides further background material for advanced readers who want to understand how the methods work. Plenty of examples, exercises, and solutions are provided to aid and test understanding, whilst useful data, tables, and formulas are compiled in a handy section for easy reference.

HERMAN J. C. BERENDSEN is Emeritus Professor of Physical Chemistry at the University of Groningen, the Netherlands. His research started in nuclear magnetic resonance, but focused later on molecular dynamics simulations on systems of biological interest. He is one of the pioneers in this field and, with over 37 000 citations, is one of the most quoted authors in physics and chemistry. He has taught courses in molecular modeling worldwide and authored the book *Simulating the Physical World* (Cambridge University Press, 2007).

Cambridge University Press

978-0-521-11940-5 - A Student's Guide to Data and Error Analysis

Herman J. C. Berendsen

Frontmatter

[More information](#)

---

Cambridge University Press  
978-0-521-11940-5 - A Student's Guide to Data and Error Analysis  
Herman J. C. Berendsen  
Frontmatter  
[More information](#)

---

# *A Student's Guide to Data and Error Analysis*

HERMAN J. C. BERENDSEN

*Emeritus Professor of Physical Chemistry,  
University of Groningen, the Netherlands*



CAMBRIDGE  
UNIVERSITY PRESS

Cambridge University Press  
 978-0-521-11940-5 - A Student's Guide to Data and Error Analysis  
 Herman J. C. Berendsen  
 Frontmatter  
[More information](#)

CAMBRIDGE UNIVERSITY PRESS  
 Cambridge, New York, Melbourne, Madrid, Cape Town,  
 Singapore, São Paulo, Delhi, Mexico City

Cambridge University Press  
 The Edinburgh Building, Cambridge CB2 8RU, UK

Published in the United States of America by Cambridge University Press, New York

[www.cambridge.org](http://www.cambridge.org)  
 Information on this title: [www.cambridge.org/9780521119405](http://www.cambridge.org/9780521119405)

© H. Berendsen 2011

This publication is in copyright. Subject to statutory exception  
 and to the provisions of relevant collective licensing agreements,  
 no reproduction of any part may take place without the written  
 permission of Cambridge University Press.

First published 2011

*A catalogue record for this publication is available from the British Library*

*Library of Congress Cataloguing in Publication Data*

Berendsen, Herman J.C.  
 A student's guide to data and error analysis / Herman J.C. Berendsen.  
 p. cm.  
 ISBN 978-0-521-11940-5 (Hardback) – ISBN 978-0-521-13492-7 (pbk.)  
 1. Error analysis (Mathematics) I. Title.  
 QA275.B43 2011  
 511'.43–dc22

2010048231

ISBN 978-0-521-11940-5 Hardback  
 ISBN 978-0-521-13492-7 Paperback

Cambridge University Press has no responsibility for the persistence or  
 accuracy of URLs for external or third-party internet websites referred to in  
 this publication, and does not guarantee that any content on such websites is,  
 or will remain, accurate or appropriate. Information regarding prices, travel  
 timetables, and other factual information given in this work is correct at  
 the time of first printing but Cambridge University Press does not guarantee  
 the accuracy of such information thereafter.

Cambridge University Press

978-0-521-11940-5 - A Student's Guide to Data and Error Analysis

Herman J. C. Berendsen

Frontmatter

[More information](#)

---

**To my wife and daughters**

Cambridge University Press

978-0-521-11940-5 - A Student's Guide to Data and Error Analysis

Herman J. C. Berendsen

Frontmatter

[More information](#)

---

Contents

Preface	<i>page xi</i>
<b>Part I Data and error analysis</b>	<b>1</b>
<b>1 Introduction</b>	<b>3</b>
<b>2 The presentation of physical quantities with their inaccuracies</b>	<b>5</b>
2.1 How to report a series of measurements	5
2.2 How to represent numbers	9
2.3 How to express inaccuracies	10
2.4 Reporting units	13
2.5 Graphical presentation of experimental data	14
<b>3 Errors: classification and propagation</b>	<b>18</b>
3.1 Classification of errors	18
3.2 Error propagation	19
<b>4 Probability distributions</b>	<b>27</b>
4.1 Introduction	27
4.2 Properties of probability distributions	29
4.3 The binomial distribution	32
4.4 The Poisson distribution	36
4.5 The normal distribution	37
4.6 The central limit theorem	41
4.7 Other distributions	42
<b>5 Processing of experimental data</b>	<b>53</b>
5.1 The distribution function of a data series	54
5.2 The average and the mean squared deviation of a data series	57
5.3 Estimates for mean and variance	58
5.4 Accuracy of mean and Student's t-distribution	59
	vii

viii	CONTENTS
5.5 Accuracy of variance	60
5.6 Handling data with unequal weights	61
5.7 Robust estimates	63
<b>6 Graphical handling of data with errors</b>	<b>71</b>
6.1 Introduction	71
6.2 Linearization of functions	73
6.3 Graphical estimates of the accuracy of parameters	77
6.4 Using calibration	78
<b>7 Fitting functions to data</b>	<b>84</b>
7.1 Introduction	84
7.2 Linear regression	87
7.3 General least-squares fit	92
7.4 The chi-squared test	95
7.5 Accuracy of the parameters	98
7.6 F-test on significance of the fit	106
<b>8 Back to Bayes: knowledge as a probability distribution</b>	<b>111</b>
8.1 Direct and inverse probabilities	111
8.2 Enter Bayes	112
8.3 Choosing the prior	114
8.4 Three examples of Bayesian inference	114
8.5 Conclusion	121
References	123
<b>Answers to exercises</b>	<b>125</b>
<b>Part II Appendices</b>	<b>133</b>
<b>A1 Combining uncertainties</b>	<b>135</b>
<b>A2 Systematic deviations due to random errors</b>	<b>138</b>
<b>A3 Characteristic function</b>	<b>141</b>
<b>A4 From binomial to normal distributions</b>	<b>143</b>
A4.1 The binomial distribution	143
A4.2 The multinomial distribution	144
A4.3 The Poisson distribution	145
A4.4 The normal distribution	146



CONTENTS	ix
<b>A5 Central limit theorem</b>	148
<b>A6 Estimation of the variance</b>	151
<b>A7 Standard deviation of the mean</b>	154
<b>A8 Weight factors when variances are not equal</b>	158
<b>A9 Least-squares fitting</b>	160
A9.1 How do you find the best parameters $a$ and $b$ in $y \approx ax + b$ ?	160
A9.2 General linear regression	161
A9.3 SSQ as a function of the parameters	162
A9.4 Covariances of the parameters	163
<b>Part III Python codes</b>	<b>167</b>
<b>Part IV Scientific data</b>	<b>197</b>
Chi-squared distribution	199
F-distribution	201
Least-squares fitting	203
Normal distribution	205
Physical constants	209
Probability distributions	211
Student's t-distribution	213
Units	215
 Index	 220

Cambridge University Press

978-0-521-11940-5 - A Student's Guide to Data and Error Analysis

Herman J. C. Berendsen

Frontmatter

[More information](#)

---

## *Preface*

This book is written as a guide for the presentation of experimental data including a consistent treatment of experimental errors and inaccuracies. It is meant for experimentalists in physics, astronomy, chemistry, life sciences and engineering. However, it can be equally useful for theoreticians who produce simulation data: they are often confronted with statistical data analysis for which the same methods apply as for the analysis of experimental data. The emphasis in this book is on the determination of best estimates for the values and inaccuracies of parameters in a theory, given experimental data. This is the problem area encountered by most physical scientists and engineers. The problem area of experimental design and hypothesis testing – excellently covered by many textbooks – is only touched on but not treated in this book.

The text can be used in education on error analysis, either in conjunction with experimental classes or in separate courses on data analysis and presentation. It is written in such a way – by including examples and exercises – that most students will be able to acquire the necessary knowledge from self study as well. The book is also meant to be kept for later reference in practical applications. For this purpose a set of “data sheets” and a number of useful computer programs are included.

This book consists of parts. Part I contains the main body of the text. It treats the most common statistical distributions for experimental errors and emphasizes the error processing needed to arrive at a correct evaluation of the accuracy of a reported result. It also pays attention to the correct reporting of physical data with their units. The last chapter considers the inference of knowledge from data from a Bayesian point of view, hopefully inducing the reader to sit back and think. The material in Part I is kept practical, without much discussion of the theoretical background on which the various types of analysis are based. This will not at all satisfy the eager student who has sufficient background in mathematics and who wishes to grasp a fuller understanding of the principles involved. Part II is to satisfy the curious: it contains several Appendices that explain various issues in more detail and provide derivations of the equations quoted in Part I. The Appendices in

Part II obviously require more mathematical skills (in particular in the field of linear algebra) than Part I. Part III contains Python code examples and Part IV provides answers to exercises. Finally, Part V contains practical information in the form of a number of “data sheets” which provide reference data in a compact form.

Throughout the book computer programs are included to facilitate the computations needed for applications. There are several professional software packages available for statistical data analysis. In the context of an educational effort, I strongly advise against the use of a specialized “black-box” software package that can be easily misused to produce ill-understood results. A “black-box” computer program should never be a magic substitute for a method that is not understood by the user! If a software package is to be used, it should provide general mathematical and graphical tools, preferably in an interactive way using an interpreter rather than a compiler. The commercial packages MATHEMATICA, MATLAB and MATHCAD are suitable for this purpose. However, most readers of this book will not have access to any or all of these packages, or – if they have temporary access through their institution – may not be able to continue access at a later point in time. Therefore for this book the choice was made to use the generally available, actively developing, open-source interpretative language PYTHON. With its array-handling and scientific extensions NUMPY and SCIPY the capabilities of this language come close to those of the commercial packages. Software related to this book, including a Python module `plotsvg.py` providing easy plotting routines, can be found on [www.hjcb.nl/](http://www.hjcb.nl/).

This book is the successor of the Dutch textbook *Goed meten met fouten* (Berendsen, 1997) that has been used in courses at the departments of physics and chemistry of the University of Groningen since 1997. The author is indebted to Emile Apol, A. van der Pol and Ruud Scheek for corrections and suggestions. Comments from readers are welcome to [author@hjcb.nl](mailto:author@hjcb.nl).