# APPLIED STATISTICS ALGORITHMS

P. GRIFFITHS and I.D. HILL





#### APPLIED STATISTICS ALGORITHMS





## ELLIS HORWOOD SERIES IN MATHEMATICS AND ITS APPLICATIONS

Series Editor: Professor G. M. BELL, Chelsea College, University of London

#### Statistics and Operational Research

Editor: B. W. CONOLLY, Professor of Operational Research, Queen Mary College, University of London

Introductory Applied Probability Beaumont, G. P. Beaumont, G. P. Basic Probability and Random Variables\* Conolly, B. W. Techniques in Operational Research: Vol. 1, Queueing Systems Conolly, B. W. Techniques in Operational Research: Vol. 2, Models, Search, Randomization French, S. Sequencing and Scheduling: Mathematics of the Job Shop French, S. **Decision Theory** Griffiths, P. & Hill, I. D. Applied Statistics Algorithms Hartley R. Linear Methods of Mathematical Programming Jones, A. J. Game Theory Kemp, K. W. Dice, Data and Decisions: Introductory Statistics Oliveira-Pinto, F. Simulation Concepts in Mathematical Modelling Oliveira-Pinto, F. & Conolly, B. W. Applicable Mathematics of Non-physical Phenomena Schendel, U. Introduction to Numerical Methods for Parallel Computers Stoodley, K. D. C. Applied and Computational Statistics A First Course Stoodley, K. D. C., Lewis, T. & Stainton, C. L. S. **Applied Statistical Techniques** Thomas, L. C. Games, Theory and Applications Whitehead, J. R. The Design and Analysis of Sequential Clinical Trials \*In preparation



# APPLIED STATISTICS ALGORITHMS

Editors:

P. GRIFFITHS, B.Sc., Ph.D. Oxford University Computing Service

and

I. D. HILL, D.Sc.

Division of Computing and Statistics Clinical Research Centre of the Medical Research Council Harrow, Middlesex





Published by ELLIS HORWOOD LIMITED Publishers • Chichester



THE ROYAL STATISTICAL SOCIETY London



First published in 1985 by

#### ELLIS HORWOOD LIMITED

Market Cross House, Cooper Street, Chichester, West Sussex, PO19 1EB, England

The publisher's colophon is reproduced from James Gillison's drawing of the ancient Market Cross, Chichester.

#### Distributors:

Australia, New Zealand, South-east Asia: Jacaranda-Wiley Ltd., Jacaranda Press, JOHN WILEY & SONS INC., G.P.O. Box 859, Brisbane, Queensland 40001, Australia

Canada

JOHN WILEY & SONS CANADA LIMITED 22 Worcester Road, Rexdale, Ontario, Canada.

Europe, Africa:
JOHN WILEY & SONS LIMITED
Baffins Lane, Chichester, West Sussex, England.

North and South America and the rest of the world: Halsted Press: a division of JOHN WILEY & SONS 605 Third Avenue, New York, N.Y. 10016, U.S.A.

#### © 1985 Royal Statistical Society/Ellis Horwood Limited

#### British Library Cataloguing in Publication Data

Griffiths, Paul
Applied statistics algorithms. –
(Ellis Horwood series in mathematics and its applications)
1. Mathematical statistics 2. Algorithms
1. Title II. Hill, I.D. (Ian David), 1926 –
001.4'22 QA276

#### Library of Congress Card No. 85-891

ISBN 0-85312-772-7 (Ellis Horwood Limited) ISBN 0-470-20184-3 (Halsted Press)

Typeset by Ellis Horwood Limited. Printed in Great Britain by Unwin Brothers of Woking.

#### COPYRIGHT NOTICE -

#### All Rights Reserved

No part of this book may be reproduced or transmitted by any means without the prior permission of the publisher. The only exceptions are for the purposes of review, or as provided for by the Copyright (Photocopying) Act or in order to enter the algorithms herein into a computer program for non-profit-making purposes.



# Table of Contents

Prefa	ice
Chap	eter 1 — Introduction
1.1	The Royal Statistical Society and its Journals
1.2	Statistical computing
1.3	The publication of algorithms
1.4	The Chilton meeting, and the Working Party on Statistical Computing 20
1.5	Algorithms in Applied Statistics
1.6	Languages and standards
1.7	Remarks and corrigenda
1.8	Planning this book
	References
	23
Chap	ter 2 — The construction and description of algorithms
	revised by P. Griffiths, I. D. Hill, J. P. Royston and J. B. Webb
2.0	Introduction
2.1	Submission
2.2	Refereeing
2.3	Languages
2.4	Introductory text
2.5	Layout
2.6	Comments
2.0	Comments

2.7	Input/output
2.8	Constants and variables
2.9	Precision
2.10	Machine-dependence
2.11	Error diagnostics
2.12	Parentheses
2.13	Labels, jumps and ifs
2.14	Construction of loops
	Parameters in Algol 60
	Common storage and global identifiers
2.17	Use of work-space
	Multidimensional arrays
2.19	Standard Fortran
2.20	Character handling
2.21	Copyright and disclaimer
	References
The A	Algorithms
Algor	ithm AS 3 — The integral of Student's t-distribution by B. E. Cooper 38
Algor	ithm AS 5 — The integral of the non-central t-distribution
	by B. E. Cooper
Algor	ithm AS 6 — Triangular decomposition of a symmetric matrix
	by M. J. R. Healy
Algor	ithm AS 7 — Inversion of a positive semi-definite symmetric matrix
	by M. J. R. Healy
Algor	ithm AS 13 — Minimum spanning tree by G. J. S. Ross
Algor	ithm AS 14 $-$ Printing the minimum spanning tree by G. J. S. Ross 53
Algor	ithm AS 15 — Single linkage cluster analysis by G. J. S. Ross
Algor	ithm AS 30 — Half-normal plotting by D. N. Sparks
Algori	thm AS 41 — Updating the sample mean and dispersion matrix
	by M. R. B. Clarke70
Algori	thm AS 45 – Histogram plotting by D. N. Sparks
Algori	thm AS 47 — Function minimization using a simplex procedure
	by R. O'Neill
Algori	thm AS 51 - Log-linear fit for contingency tables
	by S. J. Haberman
Algori	thm AS 52 - Calculation of power sums of deviations about the mean
	by C. C. Spicer
Algori	thm AS 57 — Printing multidimensional tables by S. J. Haberman 101
Algori	thm AS 60 — Latent roots and vectors of a symmetric matrix
	by D. N. Sparks and A. D. Todd110
Algori	thm AS 63 — The incomplete beta integral by K. L. Majumder and
A 1	G. P. Bhattacharjee
Algori	thm AS 64/AS 109 — Inverse of the incomplete beta function ratio
	by K. L. Majumder and G. P. Bhattachariee 121

Algorithm AS 66 — The normal integral by I. D. Hill 126
Algorithm AS 75 — Basic procedures for large, sparse or weighted linear
least squares problems by W. Morven Gentleman 130
Algorithm AS 76 — An integral useful in calculating non-central t and
bivariate normal probabilities by J. C. Young and
Ch. E. Minder
Algorithm AS 83 - Complex discrete fast Fourier transform
by Donald M. Monro
Algorithm AS 91 – The percentage points of the $\chi^2$ distribution
by D. J. Best and D. E. Roberts
Algorithm AS 97 – Real discrete fast Fourier transform
by Donald M. Monro
Algorithm AS 99 – Fitting Johnson curves by moments by I. D. Hill.
R. Hill and R. L. Holder
Algorithm AS 100 — Normal—Johnson and Johnson—normal transformations
by I. D. Hill
Algorithm AS 111 — The percentage points of the normal distribution
by J. D. Beasley and S. G. Springer
Algorithm AS 136 – A K-means clustering algorithm by J. A. Hartigan
and M. A. Wong
Algorithm AS 147 — A simple series for the incomplete gamma integral
by Chi-Leung (Andy) Lau
Algorithm AS 154 — An algorithm for exact maximum likelihood estimation
of autoregressive—moving average models by means of
Kalman filtering by G. Gardner, A. C. Harvey and
G. D. A. Phillips
Algorithm AS 168 – Scale selection and formatting
by W. Douglas Stirling
Algorithm AS 169 — An improved algorithm for scatter plots
by W. Douglas Stirling
Algorithm AS 183 – An efficient and portable pseudo-random number
generator by B. A. Wichmann and I. D. Hill 228
Algorithm ACM 291 – Logarithm of gamma function by M. C. Pike and
I. D. Hill
Index of statistical algorithms
List of routine names
Keyword index
Index to Chapters 1 and 2
and 2

To the memory of
Abu Ja'far Mohammed ben Musa
from whose description as
al-Khwarazmi (the native of Khwarazm)
the word Algorithm is derived

A'LGORISM, In. J. Arabick words, which are used to imply A'LGORITHM: In fix operations of arithmetick, or the science of numbers.

Diff.

Dr Samuel Johnson's definition of algorithm has been reproduced in facsimile from his Dictionary of the English Language, (1755)

### Foreword

It gives me great satisfaction to introduce this collection of algorithms from  $Applied\ Statistics$ . It comes with a scholarly introduction describing the history of algorithms, which stretches back to a time long before a group of us began the algorithm section of  $Applied\ Statistics$  in 1968. We began tentatively, and we made inevitable mistakes, some of which are tactfully alluded to in the book; what I suspect none of us realized at the beginning were the difficulties that beset the production of a good algorithm. It is hard to get the code right, to ensure that the algorithm is efficient and well structured, that it adheres to the language standard, that all kinds of potential misuse are trapped, and that the description is clear and accurate. The whole exercise is iterative and, as the editors show, not even the scrutiny of past editors and referees (to whom all of us, users and authors alike, owe so much) has avoided further scrutiny and amendment in preparing the algorithms for reproduction in book form. (Doubtless some energetic individuals will soon be doing their best to prove that all is still not yet perfect — I predict that they will have a hard job.)

Statisticians have become major users of packages, and packages depend heavily on reliable and tested algorithms. The writer of a one-off program for a particular analysis is equally in need of such modules as the algorithms represent; they may be black boxes but the contents must be of top quality. To the extent that increasing numbers of people are now learning statistics from running programs rather than from reading books, the executable algorithm has become part of a new and powerful form of literature, with its own style and perhaps eventually its own masterpieces. The editors have made their careful selection — can you see which may eventually become classics?

J. A. Nelder President (1985/86) The Royal Statistical Society London

The algorithms contained in this book are available in machine-readable form from the publisher. Please address all enquiries to:

Ellis Horwood Limited, Market Cross House, Cooper Street, Chichester, England, PO19 1EB

## Preface

A police electronics engineer admitted in the Johannesburg Magistrates' Court yesterday that, by applying unerring logic, a winning number could be determined in an electronic computerised card game played in a Hillbrow casino. . . . Col R.D. Hull said the electronic computerised machines have an algo rhythm, which is a series of rhythmic manipulations to determine the outcome of a game. The algo rhythm is a "mathematical recipe for numbers" which is the key to the game. The programmer knows the key.

Johannesburg Star

(Acknowledgement to Computer Weekly where we first saw this quoted.)

Applied Statistics, one of the journals published by the Royal Statistical Society, has included an Algorithms Section for the last 16 years, and the total number of algorithms published exceeds 200. The time has come for an anthology of them, which we now present.

Algorithms are the building blocks of computer programs, each designed to perform a specific purpose, and to be slotted into a program at will. At its best an algorithm should be so well tested, known to be efficient and always to give the correct results, that it can be used simply as a 'black box' whose inner workings can be ignored, and need not be understood, provided that one thoroughly understands its purpose, how to feed it with input and how to handle its output. But even the blackest of boxes needs its construction to be fully specified so that further copies of it can be made, and so that experts can suggest improvements. It is the aim of both the journal and this book that the algorithms presented should fulfil all such requirements.

14 Preface

As more fully described in Chapter 1, the book does not simply reproduce what has previously appeared in the journal. Corrections and improvements have been made, some previously published as separate entities but now fully incorporated, others new to the book, if further study has shown them to be desirable.

All who write computing instructions know the fascination of pitting one's wits against the pure logic of a machine that does what you told it, not what you meant to tell it. It is humbling as well as fascinating, and we have been humbled often enough to be aware that our aim, for which we have tried so hard, of a book that is free from 'bugs' has almost certainly not been achieved. We ask readers to let us know of any discovered.

#### ALGORISMS AND ALGORITHMS

Dr R A Griffiths and Mr W R Good (Radcliffe Infirmary, Oxford OX2 6HE) and Mr J G Griffith (Jesus College, University of Oxford) write: We note the use in a recent series of articles of the neologism 'algorithm'. The Oxford English Dictionary describes this as a 'recent pseudo-etymological perversion' in which 'algorism' is learnedly confused with ' $\alpha\rho \theta\mu \dot{\phi}\varsigma$ , 'number'. 'Algorism' is, of course, from the Arabic and without Greek derivation. 'Algorithm' could only be a fusion of ' $\dot{\alpha}\lambda\gamma o\varsigma$  (pain) and ' $\alpha\rho \theta\mu \dot{\phi}\varsigma$  (number) and would presumably denote 'measurement or counting of pain'. (British Medical Journal, 23 June 1984)

There are many words in the English language that started life as a 'recent pseudo-etymological perversion'. The exact point at which any such word passes the boundary, and becomes correct usage, is difficult to determine, but we have no doubt at all that *algorithm* did so many years ago, and it would be inexcusable affectation to refuse to use it.

Can any word still be a neologism if it appeared in Dr Johnson's dictionary, admittedly not with the current meaning, but with both spellings allowed? He knew only one spelling for 'arithmetick', but Boswell's hope that 'the authority of the great Master of our language will stop that curtailing innovation, by which we see *critic*, *public*, &c., frequently written instead of *critick*, *publick*, &c.' remained unsatisfied. Those who think 'algorithm' an incorrect spelling must therefore regard 'arithmetic' as even more so.

Since Dr Johnson's day 'algorithm' has come to mean a recipe for computing operations. Even if it is this meaning that is objected to as neologistic, it goes back nearly half a century at least, as the Supplement to the Oxford English Dictionary shows by quoting a reference to 'Euclid's algorithm' from 1938.

Algorism has never taken on this new meaning but remains defined as 'The Arabic, or decimal, system of numeration'. Why should anyone be expected to take an almost unknown word with the wrong meaning, when a better-known word with the right meaning is available?

#### UNSELECTED ALGORITHMS

To those algorithm authors whose contributions have not been selected for the book we should like to give assurance that lack of space is the reason. No-one should assume that the absence of a given algorithm implies in any way that it lacks merit.

Preface 15

#### **ACKNOWLEDGEMENTS**

We thank not only all who have helped in the preparation of this book, but also all whose labours have contributed to the Algorithms Section of the journal. In particular John Nelder as founder and first editor, Howard Simpson as a subsequent editor, and Patrick Royston and Janet Webb who have now taken on the task, deserve gratitude. Maria de la Hunty, as the Society's Executive Editor (for all its journals) has always been a tower of strength. None of them, nor ourselves when in the editorial chair, could have done much without the selfless efforts of all the anonymous referees who so carefully examine and test all the contributions. We are deeply grateful to all those algorithm authors (and their employers in some instances) who have so willingly agreed to let us reproduce their work, and also to the Association for Computing Machinery for permission to use one algorithm from their *Communications*.

Finally, we thank our good friends the computers, but for whom our subject matter would not exist other than as a speculative dream of science fiction.

P. Griffiths I. D. Hill

December 1984