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An Introduction to Generalized Linear Models

Fourth Edition



Annette J. Dobson Adrian G. Barnett





An Introduction to Generalized Linear Models

Fourth Edition

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Printed on acid-free paper Version Date: 20180306

International Standard Book Number-13: 978-1-138-74168-3 (Hardback) International Standard Book Number-13: 978-1-138-74151-5 (Paperback)

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Library of Congress Cataloging-in-Publication Data

Names: Dobson, Annette J., 1945- author. | Barnett, Adrian G., author. Title: An introduction to generalized linear models / by Annette J. Dobson, Adrian G. Barnett. Other titles: Generalized linear models Description: Fourth edition. | Boca Raton : CRC Press, 2018. | Includes bibliographical references and index. Identifiers: LCCN 2018002845| ISBN 9781138741683 (hardback : alk. paper) | ISBN 9781138741515 (pbk. : alk. paper) | ISBN 9781315182780 (e-book : alk. paper) Subjects: LCSH: Linear models (Statistics) Classification: LCC QA276.D589 2018 | DDC 519.5--dc23 LC record available at https://lccn.loc.gov/2018002845

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To Beth.



Contents

Pr	reface	ace					
1	Intr	oductio	n	1			
	1.1	Backg	round	1			
	1.2	Scope		1			
	1.3	Notati	on	6			
	1.4	Distrib	butions related to the Normal distribution	8			
		1.4.1	Normal distributions	8			
		1.4.2	Chi-squared distribution	9			
		1.4.3	t-distribution	10			
		1.4.4	F-distribution	10			
		1.4.5	Some relationships between distributions	11			
	1.5	Quadr	ratic forms	11			
	1.6	Estima	ation	13			
		1.6.1	Maximum likelihood estimation	13			
		1.6.2	Example: Poisson distribution	15			
		1.6.3	Least squares estimation	15			
		1.6.4	Comments on estimation	16			
		1.6.5	Example: Tropical cyclones	17			
	1.7	Exerci	rcises				
2	Moo	lel Fitti	ng	21			
	2.1	Introd	uction	21			
	2.2	Exam	ples	21			
		2.2.1	Chronic medical conditions	21			
		2.2.2	Example: Birthweight and gestational age	25			
	2.3	Some	principles of statistical modelling	35			
		2.3.1	Exploratory data analysis	35			
		2.3.2	Model formulation	36			
		2.3.3	Parameter estimation	36			

viii

		2.3.4 Residuals and model checking		36							
		2.3.5 Inference and interpretation		39							
		2.3.6 Further reading		40							
	2.4	Notation and coding for explanatory variable	es	40							
		2.4.1 Example: Means for two groups		41							
		2.4.2 Example: Simple linear regression for	.2 Example: Simple linear regression for two groups								
		2.4.3 Example: Alternative formulations for	or comparing the								
		means of two groups		42							
		2.4.4 Example: Ordinal explanatory variab	oles	43							
	2.5	Exercises		44							
3	Exp	ponential Family and Generalized Linear Mo	odels	49							
	3.1	Introduction		49							
	3.2	Exponential family of distributions		50							
		3.2.1 Poisson distribution		51							
		3.2.2 Normal distribution		52							
		3.2.3 Binomial distribution		52							
	3.3	Properties of distributions in the exponential	family	53							
	3.4	Generalized linear models		56							
	3.5	Examples		58							
		3.5.1 Normal linear model		58							
		3.5.2 Historical linguistics		58							
		3.5.3 Mortality rates		59							
	3.6	Exercises		61							
4	Esti	imation		65							
	4.1	Introduction		65							
	4.2	Example: Failure times for pressure vessels		65							
	4.3	Maximum likelihood estimation		70							
	4.4	Poisson regression example		73							
	4.5	Exercises		76							
5	Infe	erence		79							
	5.1	Introduction		79							
	5.2	Sampling distribution for score statistics		81							
		5.2.1 Example: Score statistic for the Norr	nal distribution	82							
		5.2.2 Example: Score statistic for the Binor	mial distribution	82							
	5.3	Taylor series approximations		83							
	5.4	Sampling distribution for maximum likelihood estimators 8									

				ix						
		5.4.1	Example: Maximum likelihood estimators for the							
			Normal linear model							
	5.5	Log-li	elihood ratio statistic							
	5.6	Sampl	ing distribution for the deviance	87						
		5.6.1	Example: Deviance for a Binomial model	88						
		5.6.2	Example: Deviance for a Normal linear model	89						
		5.6.3	Example: Deviance for a Poisson model	91						
	5.7	Hypot	hesis testing	92						
		5.7.1	Example: Hypothesis testing for a Normal linear							
			model	94						
	5.8	Exerci	ses	95						
6	Nor	mal Lir	near Models	97						
	6.1	Introd	uction	97						
	6.2	Basic	results	98						
		6.2.1	Maximum likelihood estimation	98						
		6.2.2	Least squares estimation	98						
		6.2.3	Deviance	99						
		6.2.4	Hypothesis testing	99						
		6.2.5	Orthogonality	100						
		6.2.6	Residuals	101						
		6.2.7	Other diagnostics	102						
	6.3	Multip	ble linear regression	104						
		6.3.1	Example: Carbohydrate diet	104						
		6.3.2	Coefficient of determination, R^2	108						
		6.3.3	Model selection	111						
		6.3.4	Collinearity							
	6.4	Analy	sis of variance	119						
		6.4.1	One-factor analysis of variance	119						
		6.4.2	Two-factor analysis of variance	126						
	6.5	Analy	sis of covariance	132						
	6.6	Gener	al linear models	135						
	6.7	Non-li	near associations	137						
		6.7.1	PLOS Medicine journal data	138						
	6.8	Fractio	onal polynomials	141						
	6.9	Exercises 1								

7	Bina	ry Var	iables and Logistic Regression	149						
	7.1	Probat	bility distributions	149						
	7.2	Genera	alized linear models	150						
	7.3	Dose r	esponse models	151						
		7.3.1	Example: Beetle mortality	154						
	7.4	Genera	eral logistic regression model							
		7.4.1	Example: Embryogenic anthers	159						
	7.5	Goodr	less of fit statistics	162						
	7.6	Residu	als	166						
	7.7	Other	diagnostics	167						
	7.8	Examp	ble: Senility and WAIS	168						
	7.9	Odds 1	atios and prevalence ratios	171						
	7.10	Exerci	ses	174						
8	Nom	inal an	d Ordinal Logistic Regression	179						
	8.1	Introd	uction	179						
	8.2	Multin	nomial distribution	180						
	8.3	Nomir	al logistic regression	181						
		8.3.1	Example: Car preferences	183						
	8.4	Ordina	al logistic regression	188						
		8.4.1	Cumulative logit model	189						
		8.4.2	Proportional odds model	189						
		8.4.3	Adjacent categories logit model	190						
		8.4.4	Continuation ratio logit model	191						
		8.4.5	Comments	192						
		8.4.6	.6 Example: Car preferences							
	8.5	General comments								
	8.6	Exercises								
9	Poiss	son Reg	gression and Log-Linear Models	197						
	9.1	Introdu	duction							
	9.2	Poisso	visson regression							
		9.2.1	Example of Poisson regression: British doctors'							
			smoking and coronary death	201						
	9.3	Examp	iples of contingency tables							
		9.3.1	Example: Cross-sectional study of malignant							
			melanoma	205						
		9.3.2	Example: Randomized controlled trial of influenza							
			vaccine	206						

х

9.3.3 Example: Case-control study of gastric and duodenal ulcers and aspirin use 20 9.4 Probability models for contingency tables 20 9.4.1 Poisson model 20 9.4.2 Multinomial model 20 9.4.3 Product multinomial models 21 9.5 Log-linear models 21 9.6 Inference for log-linear models 21 9.7 Numerical examples 21 9.7.1 Cross-sectional study of malignant melanoma 21 9.7.2 Case-control study of gastric and duodenal ulcer and aspirin use 21 9.8 Remarks 21 9.9 Exercises 21 10.1 Introduction 22 10.2 Survival Analysis 22 10.2.1 Exponential distribution 22 10.2.2 Proportional hazards models 22 10.3.1 Example: Remission times 23 10.4 Estimation 23 10.4.1 Example: Reponential model 23 10.5 Inference 23 10.6 Model checking <th></th> <th></th> <th></th> <th>xi</th>				xi					
ulcers and aspirin use 20 9.4 Probability models for contingency tables 20 9.4.1 Poisson model 20 9.4.2 Multinomial model 20 9.4.3 Product multinomial models 21 9.5 Log-linear models 21 9.6 Inference for log-linear models 21 9.7 Numerical examples 21 9.7.1 Cross-sectional study of malignant melanoma 21 9.7.2 Case-control study of gastric and duodenal ulcer and aspirin use 21 9.8 Remarks 21 9.9 Exercises 21 10.1 Introduction 22 10.2 Survival Analysis 22 10.2.1 Exponential distribution 22 10.2.2 Proportional hazards models 22 10.2.3 Weibull distribution 22 10.3 Empirical survivor function 23 10.4 Example: Remission times 23 10.4.1 Example: Keibull model 23 10.5 Inference 23 10.6<			9.3.3 Example: Case–control study of gastric and duodenal						
9.4 Probability models for contingency tables 20 9.4.1 Poisson model 20 9.4.2 Multinomial model 20 9.4.3 Product multinomial models 21 9.5 Log-linear models 21 9.6 Inference for log-linear models 21 9.7 Numerical examples 21 9.7.1 Cross-sectional study of malignant melanoma 21 9.7.2 Case-control study of gastric and duodenal ulcer and aspirin use 21 9.8 Remarks 21 9.9 Exercises 21 10.1 Introduction 22 10.2 Survival Analysis 22 10.1 Introduction 22 10.2 Survivor functions and hazard functions 22 10.2.1 Exponential distribution 22 10.2.2 Proportional hazards models 23 10.3 Empirical survivor function 23 10.4 Example: Remission times 23 10.4 Example: Weibull model 23 10.5 Inference 23			ulcers and aspirin use						
9.4.1 Poisson model 20 9.4.2 Multinomial model 20 9.4.3 Product multinomial models 21 9.5 Log-linear models 21 9.6 Inference for log-linear models 21 9.7 Numerical examples 21 9.7.1 Cross-sectional study of malignant melanoma 21 9.7.2 Case-control study of gastric and duodenal ulcer and aspirin use 21 9.8 Remarks 21 9.9 Exercises 21 10.1 Introduction 22 10.2 Survival Analysis 22 10.2.1 Exponential distribution 22 10.2.2 Proportional hazard functions 22 10.2.3 Weibull distribution 22 10.3 Empirical survivor function 23 10.4 Example: Remission times 23 10.4.1 Example: Weibull model 23 10.5 Inference 23 10.6 Model checking 23 10.7 Example: Remission times 23 10.8 <td></td> <td>9.4</td> <td>Probability models for contingency tables</td> <td>209</td>		9.4	Probability models for contingency tables	209					
9.4.2Multinomial model209.4.3Product multinomial models219.5Log-linear models219.6Inference for log-linear models219.7Numerical examples219.7.1Cross-sectional study of malignant melanoma219.7.2Case-control study of gastric and duodenal ulcer and aspirin use219.8Remarks219.9Exercises2110Survival Analysis2210.1Introduction2210.2Survivor functions and hazard functions2210.2.1Exponential distribution2210.2.2Proportional hazards models2210.3Empirical survivor function2310.4Estimation2310.4.1Example: Remission times2310.5Inference2310.6Model checking2310.7Example: Remission times2310.8Exercises24			9.4.1 Poisson model	209					
9.4.3 Product multinomial models 21 9.5 Log-linear models 21 9.6 Inference for log-linear models 21 9.7 Numerical examples 21 9.7 Case-control study of gastric and duodenal ulcer and aspirin use 21 9.8 Remarks 21 9.9 Exercises 21 10 Survival Analysis 22 10.1 Introduction 22 10.2 Survivor functions and hazard functions 22 10.2.1 Exponential distribution 22 10.2.2 Proportional hazards models 22 10.3.1 Example: Remission times 23 10.4 Example: Remission times 23 10.5 Infer			9.4.2 Multinomial model	209					
9.5Log-linear models219.6Inference for log-linear models219.7Numerical examples219.7.1Cross-sectional study of malignant melanoma219.7.2Case-control study of gastric and duodenal ulcer and aspirin use219.8Remarks219.9Exercises2110Survival Analysis2210.1Introduction2210.2Survivor functions and hazard functions2210.2.1Exponential distribution2210.2.2Proportional hazards models2210.3Empirical survivor function2310.4Estimation2310.5Inference2310.6Model checking2310.7Example: Remission times2310.8Exercises24			9.4.3 Product multinomial models	210					
9.6Inference for log-linear models219.7Numerical examples219.7.1Cross-sectional study of malignant melanoma219.7.2Case-control study of gastric and duodenal ulcer and aspirin use219.8Remarks219.9Exercises2110Survival Analysis2210.1Introduction2210.2Survivor functions and hazard functions2210.2.1Exponential distribution2210.2.2Proportional hazards models2210.3Empirical survivor function2310.4Estimation2310.5Inference2310.6Model checking2310.7Example: Remission times2310.8Exercises24		9.5	Log-linear models	210					
9.7Numerical examples219.7.1Cross-sectional study of malignant melanoma219.7.2Case-control study of gastric and duodenal ulcer and aspirin use219.8Remarks219.9Exercises2110Survival Analysis2210.1Introduction2210.2Survivor functions and hazard functions2210.2.1Exponential distribution2210.2.2Proportional hazards models2210.3Empirical survivor function2310.4Extimation2310.4.1Example: Remission times2310.5Inference2310.6Model checking2310.7Example: Remission times2310.8Exercises24		9.6	Inference for log-linear models	212					
9.7.1Cross-sectional study of malignant melanoma219.7.2Case-control study of gastric and duodenal ulcer and aspirin use219.8Remarks219.9Exercises2110Survival Analysis2210.1Introduction2210.2Survivor functions and hazard functions2210.2.1Exponential distribution2210.2.2Proportional hazards models2210.3Empirical survivor function2310.4Example: Remission times2310.4.1Example: Exponential model2310.5Inference2310.6Model checking2310.7Example: Remission times2310.8Exercises24		9.7	Numerical examples	212					
9.7.2Case-control study of gastric and duodenal ulcer and aspirin use219.8Remarks219.9Exercises2110Survival Analysis2210.1Introduction2210.2Survivor functions and hazard functions2210.2.1Exponential distribution2210.2.2Proportional hazards models2210.2.3Weibull distribution2210.3Empirical survivor function2310.4Estimation2310.4.1Example: Remission times2310.5Inference2310.6Model checking2310.7Example: Remission times2310.8Exercises24			9.7.1 Cross-sectional study of malignant melanoma	212					
aspirin use219.8Remarks219.9Exercises2110Survival Analysis2210.1Introduction2210.2Survivor functions and hazard functions2210.2.1Exponential distribution2210.2.2Proportional hazards models2210.2.3Weibull distribution2210.3Empirical survivor function2310.4Estimation2310.4.1Example: Remission times2310.5Inference2310.6Model checking2310.7Example: Remission times2310.8Exercises24			9.7.2 Case–control study of gastric and duodenal ulcer and						
9.8Remarks219.9Exercises2110Survival Analysis2210.1Introduction2210.2Survivor functions and hazard functions2210.2.1Exponential distribution2210.2.2Proportional hazards models2210.2.3Weibull distribution2210.3.1Example: Remission times2310.4Estimation2310.4.1Example: Exponential model2310.5Inference2310.6Model checking2310.7Example: Remission times2310.8Exercises24			aspirin use	215					
9.9 Exercises2110 Survival Analysis2210.1 Introduction2210.2 Survivor functions and hazard functions2210.2 Survivor functions and hazard functions2210.2.1 Exponential distribution2210.2.2 Proportional hazards models2210.2.3 Weibull distribution2210.3 Empirical survivor function2310.4 Estimation2310.4.1 Example: Remission times2310.5 Inference2310.6 Model checking2310.7 Example: Remission times2310.8 Exercises24		9.8	Remarks	216					
10Survival Analysis2210.1Introduction2210.2Survivor functions and hazard functions2210.2.1Exponential distribution2210.2.2Proportional hazards models2210.2.3Weibull distribution2210.3Empirical survivor function2310.3.1Example: Remission times2310.4Estimation2310.4.1Example: Exponential model2310.5Inference2310.6Model checking2310.7Example: Remission times2310.8Exercises24		9.9	Exercises	217					
10.1Introduction2210.2Survivor functions and hazard functions2210.2.1Exponential distribution2210.2.2Proportional hazards models2210.2.3Weibull distribution2210.3Empirical survivor function2310.4Estimation2310.4.1Example: Remission times2310.5Inference2310.6Model checking2310.7Example: Remission times2310.8Exercises24	10	Surv	ival Analysis	223					
10.2Survivor functions and hazard functions2210.2.1Exponential distribution2210.2.2Proportional hazards models2210.2.3Weibull distribution2210.3Empirical survivor function2310.3.1Example: Remission times2310.4Estimation2310.4.1Example: Exponential model2310.5Inference2310.6Model checking2310.7Example: Remission times2310.8Exercises24		10.1	Introduction	223					
10.2.1Exponential distribution2210.2.2Proportional hazards models2210.2.3Weibull distribution2210.3Empirical survivor function2310.3.1Example: Remission times2310.4Estimation2310.4.1Example: Exponential model2310.5Inference2310.6Model checking2310.7Example: Remission times2310.8Exercises24		10.2	Survivor functions and hazard functions	225					
10.2.2 Proportional hazards models2210.2.3 Weibull distribution2210.3 Empirical survivor function2310.3.1 Example: Remission times2310.4 Estimation2310.4.1 Example: Exponential model2310.4.2 Example: Weibull model2310.5 Inference2310.6 Model checking2310.7 Example: Remission times2310.8 Exercises24			10.2.1 Exponential distribution	226					
10.2.3 Weibull distribution2210.3 Empirical survivor function2310.3.1 Example: Remission times2310.4 Estimation2310.4.1 Example: Exponential model2310.4.2 Example: Weibull model2310.5 Inference2310.6 Model checking2310.7 Example: Remission times2310.8 Exercises24			10.2.2 Proportional hazards models	227					
10.3 Empirical survivor function2310.3.1 Example: Remission times2310.4 Estimation2310.4.1 Example: Exponential model2310.4.2 Example: Weibull model2310.5 Inference2310.6 Model checking2310.7 Example: Remission times2310.8 Exercises24			10.2.3 Weibull distribution	228					
10.3.1 Example: Remission times2310.4 Estimation2310.4.1 Example: Exponential model2310.4.2 Example: Weibull model2310.5 Inference2310.6 Model checking2310.7 Example: Remission times2310.8 Exercises24		10.3	Empirical survivor function						
10.4 Estimation2310.4.1 Example: Exponential model2310.4.2 Example: Weibull model2310.5 Inference2310.6 Model checking2310.7 Example: Remission times2310.8 Exercises24			10.3.1 Example: Remission times						
10.4.1 Example: Exponential model2310.4.2 Example: Weibull model2310.5 Inference2310.6 Model checking2310.7 Example: Remission times2310.8 Exercises24		10.4	Estimation						
10.4.2 Example: Weibull model2310.5 Inference2310.6 Model checking2310.7 Example: Remission times2310.8 Exercises24			10.4.1 Example: Exponential model						
10.5 Inference2310.6 Model checking2310.7 Example: Remission times2310.8 Exercises24			10.4.2 Example: Weibull model						
10.6 Model checking2310.7 Example: Remission times2310.8 Exercises24		10.5	Inference	236					
10.7 Example: Remission times2310.8 Exercises24		10.6	Model checking	236					
10.8 Exercises 24		10.7	Example: Remission times						
		10.8	Exercises	240					
11 Clustered and Longitudinal Data 24	11	Clus	tered and Longitudinal Data	245					
11.1 Introduction 24		11.1	Introduction	245					
11.2 Example: Recovery from stroke 24		11.2	Example: Recovery from stroke	247					
11.3 Repeated measures models for Normal data 25		11.3	Repeated measures models for Normal data 2:						
11.4 Repeated measures models for non-Normal data 25		11.4	Repeated measures models for non-Normal data	257					
11.5 Multilevel models 25		11.5	Multilevel models	259					
11.6 Stroke example continued 26		11.6	Stroke example continued	262					
11.7 Comments 26		11.7	Comments	265					
11.8 Exercises 26		11.8	Exercises	266					

12	Baye	esian Ar	nalysis	271			
	12.1	Freque	ntist and Bayesian paradigms	271			
		12.1.1	Alternative definitions of p-values and confidence				
			intervals	271			
		12.1.2	Bayes' equation	272			
		12.1.3	Parameter space	273			
		12.1.4	Example: Schistosoma japonicum	273			
	12.2	Priors		275			
		12.2.1	Informative priors	276			
		12.2.2	Example: Sceptical prior	276			
		12.2.3	Example: Overdoses amongst released prisoners	279			
	12.3	Distrib	utions and hierarchies in Bayesian analysis	281			
	12.4	WinBU	JGS software for Bayesian analysis	281			
	12.5	Exercis	ses	284			
13	Mar	kov Ch	ain Monte Carlo Methods	287			
	13.1	Why st	andard inference fails	287			
	13.2	Monte	Carlo integration	287			
	13.3	Marko	v chains	289			
		13.3.1	The Metropolis–Hastings sampler	291			
		13.3.2	The Gibbs sampler	293			
		13.3.3	Comparing a Markov chain to classical maximum				
			likelihood estimation	295			
		13.3.4	Importance of parameterization	299			
	13.4	- Bayesian inference					
	13.5	Diagnostics of chain convergence					
		13.5.1	Chain history	302			
		13.5.2	Chain autocorrelation	304			
		13.5.3	Multiple chains	305			
	13.6	Bayesi	an model fit: the deviance information criterion	306			
	13.7	Exercis	ses	308			
14	Exar	nple Ba	yesian Analyses	315			
	14.1	Introdu	iction	315			
	14.2	Binary	variables and logistic regression	316			
		14.2.1	Prevalence ratios for logistic regression	319			
	14.3	Nomin	al logistic regression	322			
	14.4	Latent	variable model	324			
	14.5	Surviva	al analysis	326			
	14.6	Rando	m effects	328			

xii

	xiii
14.7 Longitudinal data analysis	331
14.8 Bayesian model averaging	338
14.8.1 Example: Stroke recovery	340
14.8.2 Example: PLOS Medicine journal data	340
14.9 Some practical tips for WinBUGS	342
14.10 Exercises	344
Postface	347
Appendix	355
Software	357
References	359
Index	371



Preface

The original purpose of the book was to present a unified theoretical and conceptual framework for statistical modelling in a way that was accessible to undergraduate students and researchers in other fields.

The second edition was expanded to include nominal and ordinal logistic regression, survival analysis and analysis of longitudinal and clustered data. It relied more on numerical methods, visualizing numerical optimization and graphical methods for exploratory data analysis and checking model fit.

The third edition added three chapters on Bayesian analysis for generalized linear models. To help with the practical application of generalized linear models, Stata, R and WinBUGS code were added.

This fourth edition includes new sections on the common problems of model selection and non-linear associations. Non-linear associations have a long history in statistics as the first application of the least squares method was when Gauss correctly predicted the non-linear orbit of an asteroid in 1801.

Statistical methods are essential for many fields of research, but a widespread lack of knowledge of their correct application is creating inaccurate results. Untrustworthy results undermine the scientific process of using data to make inferences and inform decisions. There are established practices for creating reproducible results which are covered in a new Postface to this edition.

The data sets and outline solutions of the exercises are available on the publisher's website: http://www.crcpress.com/9781138741515. We also thank Thomas Haslwanter for providing a set of solutions using Python: https://github.com/thomas-haslwanter/dobson.

We are grateful to colleagues and students at the Universities of Queensland and Newcastle, Australia, and those taking postgraduate courses through the Biostatistics Collaboration of Australia for their helpful suggestions and comments about the material.

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Chapter 1

Introduction

1.1 Background

This book is designed to introduce the reader to generalized linear models, these provide a unifying framework for many commonly used statistical techniques. They also illustrate the ideas of statistical modelling.

The reader is assumed to have some familiarity with classical statistical principles and methods. In particular, understanding the concepts of estimation, sampling distributions and hypothesis testing is necessary. Experience in the use of t-tests, analysis of variance, simple linear regression and chi-squared tests of independence for two-dimensional contingency tables is assumed. In addition, some knowledge of matrix algebra and calculus is required.

The reader will find it necessary to have access to statistical computing facilities. Many statistical programs, languages or packages can now perform the analyses discussed in this book. Often, however, they do so with a different program or procedure for each type of analysis so that the unifying structure is not apparent.

Some programs or languages which have procedures consistent with the approach used in this book are **Stata**, **R**, **S-PLUS**, **SAS** and **Genstat**. For Chapters 13 to 14, programs to conduct Markov chain Monte Carlo methods are needed and **WinBUGS** has been used here. This list is not comprehensive as appropriate modules are continually being added to other programs.

In addition, anyone working through this book may find it helpful to be able to use mathematical software that can perform matrix algebra, differentiation and iterative calculations.

1.2 Scope

The statistical methods considered in this book all involve the analysis of relationships between measurements made on groups of subjects or objects.

For example, the measurements might be the heights or weights and the ages of boys and girls, or the yield of plants under various growing conditions. We use the terms **response**, **outcome** or **dependent variable** for measurements that are free to vary in response to other variables called **explanatory variables** or **predictor variables** or **independent variables**—although this last term can sometimes be misleading. Responses are regarded as random variables. Explanatory variables are usually treated as though they are nonrandom measurements or observations; for example, they may be fixed by the experimental design.

Responses and explanatory variables are measured on one of the following scales.

- 1. **Nominal** classifications: e.g., red, green, blue; yes, no, do not know, not applicable. In particular, for **binary**, **dichotomous** or **binomial** variables there are only two categories: male, female; dead, alive; smooth leaves, serrated leaves. If there are more than two categories the variable is called **polychotomous, polytomous** or **multinomial**.
- 2. Ordinal classifications in which there is some natural order or ranking between the categories: e.g., young, middle aged, old; diastolic blood pressures grouped as \leq 70, 71–90, 91–110, 111–130, \geq 131 mmHg.
- 3. **Continuous** measurements where observations may, at least in theory, fall anywhere on a continuum: e.g., weight, length or time. This scale includes both **interval scale** and **ratio scale** measurements—the latter have a well-defined zero. A particular example of a continuous measurement is the time until a specific event occurs, such as the failure of an electronic component; the length of time from a known starting point is called the **failure time**.

Nominal and ordinal data are sometimes called **categorical** or **discrete variables** and the numbers of observations, **counts** or **frequencies** in each category are usually recorded. For continuous data the individual measurements are recorded. The term **quantitative** is often used for a variable measured on a continuous scale and the term **qualitative** for nominal and sometimes for ordinal measurements. A qualitative, explanatory variable is called a **factor** and its categories are called the **levels** for the factor. A quantitative explanatory variable is sometimes called a **covariate**.

Methods of statistical analysis depend on the measurement scales of the response and explanatory variables.

This book is mainly concerned with those statistical methods which are relevant when there is just *one response variable* although there will usually be several explanatory variables. The responses measured on different subjects are usually assumed to be statistically independent random variables

SCOPE

although this requirement is dropped in Chapter 11, which is about correlated data, and in subsequent chapters. Table 1.1 shows the main methods of statistical analysis for various combinations of response and explanatory variables and the chapters in which these are described. The last three chapters are devoted to Bayesian methods which substantially extend these analyses.

The present chapter summarizes some of the statistical theory used throughout the book. Chapters 2 through 5 cover the theoretical framework that is common to the subsequent chapters. Later chapters focus on methods for analyzing particular kinds of data.

Chapter 2 develops the main ideas of classical or frequentist statistical modelling. The modelling process involves four steps:

- 1. Specifying models in two parts: equations linking the response and explanatory variables, and the probability distribution of the response variable.
- 2. Estimating fixed but unknown parameters used in the models.
- 3. Checking how well the models fit the actual data.
- 4. Making inferences; for example, calculating confidence intervals and testing hypotheses about the parameters.

The next three chapters provide the theoretical background. Chapter 3 is about the **exponential family of distributions**, which includes the Normal, Poisson and Binomial distributions. It also covers **generalized linear models** (as defined by Nelder and Wedderburn (1972)). Linear regression and many other models are special cases of generalized linear models. In Chapter 4 methods of classical estimation and model fitting are described.

Chapter 5 outlines frequentist methods of statistical inference for generalized linear models. Most of these methods are based on how well a model describes the set of data. For example, **hypothesis testing** is carried out by first specifying alternative models (one corresponding to the null hypothesis and the other to a more general hypothesis). Then test statistics are calculated which measure the "goodness of fit" of each model and these are compared. Typically the model corresponding to the null hypothesis is simpler, so if it fits the data about as well as a more complex model it is usually preferred on the grounds of parsimony (i.e., we retain the null hypothesis).

Chapter 6 is about **multiple linear regression** and **analysis of variance** (ANOVA). Regression is the standard method for relating a continuous response variable to several continuous explanatory (or predictor) variables. ANOVA is used for a continuous response variable and categorical or qualitative explanatory variables (factors). **Analysis of covariance** (ANCOVA) is used when at least one of the explanatory variables is continuous. Nowa-

INTRODUCTION

Table 1.1 Major methods of statistical analysis for response and explanatory variables measured on various scales and chapter references for this book. Extensions of these methods from a Bayesian perspective are illustrated in Chapters 12–14.

Response (chapter)	Explanatory variables	Methods
Continuous	Binary	t-test
(Chapter 6)		
	Nominal, >2 categories	Analysis of variance
	Ordinal	Analysis of variance
	Continuous	Multiple regression
	Nominal & some	Analysis of
	continuous	covariance
	Categorical & continuous	Multiple regression
Binary	Categorical	Contingency tables
(Chapter 7)		Logistic regression
	Continuous	Logistic, probit &
		other dose-response
		models
	Categorical & continuous	Logistic regression
Nominal with	Nominal	Contingency tables
>2 categories		
(Chapters 8 & 9)	Categorical & continuous	Nominal logistic
		regression
Ordinal	Categorical & continuous	Ordinal logistic
(Chapter 8)		regression
Counts	Categorical	Log-linear models
(Chapter 9)		
	Categorical & continuous	Poisson regression
Failure times	Categorical & continuous	Survival analysis
(Chapter 10)		(parametric)
Correlated	Categorical & continuous	Generalized
responses		estimating equations
(Chapter 11)		Multilevel models

SCOPE

days it is common to use the same computational tools for all such situations. The terms **multiple regression** or **general linear model** are used to cover the range of methods for analyzing one continuous response variable and multiple explanatory variables. This chapter also includes a section on **model selection** that is also applicable for other types of generalized linear models

Chapter 7 is about methods for analyzing binary response data. The most common one is **logistic regression** which is used to model associations between the response variable and several explanatory variables which may be categorical or continuous. Methods for relating the response to a single continuous variable, the dose, are also considered; these include **probit analysis** which was originally developed for analyzing dose-response data from bioassays. Logistic regression has been generalized to include responses with more than two nominal categories (**nominal**, **multinomial**, **polytomous** or **polychotomous logistic regression**) or ordinal categories (**ordinal logistic regression**). These methods are discussed in Chapter 8.

Chapter 9 concerns count data. The counts may be frequencies displayed in a contingency table or numbers of events, such as traffic accidents, which need to be analyzed in relation to some "exposure" variable such as the number of motor vehicles registered or the distances travelled by the drivers. Modelling methods are based on assuming that the distribution of counts can be described by the Poisson distribution, at least approximately. These methods include **Poisson regression** and **log-linear models**.

Survival analysis is the usual term for methods of analyzing failure time data. The parametric methods described in Chapter 10 fit into the framework of generalized linear models although the probability distribution assumed for the failure times may not belong to the exponential family.

Generalized linear models have been extended to situations where the responses are correlated rather than independent random variables. This may occur, for instance, if they are **repeated measurements** on the same subject or measurements on a group of related subjects obtained, for example, from **clustered sampling**. The method of **generalized estimating equations** (GEEs) has been developed for analyzing such data using techniques analogous to those for generalized linear models. This method is outlined in Chapter 11 together with a different approach to correlated data, namely **multilevel modelling** in which some parameters are treated as random variables rather than fixed but unknown constants. Multilevel modelling involves both fixed and random effects (mixed models) and relates more closely to the Bayesian approach to statistical analysis.

The main concepts and methods of Bayesian analysis are introduced in Chapter 12. In this chapter the relationships between classical or frequentist methods and Bayesian methods are outlined. In addition the software Win-BUGS which is used to fit Bayesian models is introduced.

Bayesian models are usually fitted using computer-intensive methods based on Markov chains simulated using techniques based on random numbers. These methods are described in Chapter 13. This chapter uses some examples from earlier chapters to illustrate the mechanics of Markov chain Monte Carlo (MCMC) calculations and to demonstrate how the results allow much richer statistical inferences than are possible using classical methods.

Chapter 14 comprises several examples, introduced in earlier chapters, which are reworked using Bayesian analysis. These examples are used to illustrate both conceptual issues and practical approaches to estimation, model fitting and model comparisons using WinBUGS.

Finally there is a Postscript that summarizes the principles of good statistical practice that should always be used in order to address the "**reproducibility crisis**" that plagues science with daily reports of "break-throughs" that turn out to be useless or untrue.

Further examples of generalized linear models are discussed in the books by McCullagh and Nelder (1989), Aitkin et al. (2005) and Myers et al. (2010). Also there are many books about specific generalized linear models such as Agresti (2007, 2013), Collett (2003, 2014), Diggle et al. (2002), Goldstein (2011), Hilbe (2015) and Hosmer et al. (2013).

1.3 Notation

Generally we follow the convention of denoting random variables by uppercase italic letters and observed values by the corresponding lowercase letters. For example, the observations $y_1, y_2, ..., y_n$ are regarded as realizations of the random variables $Y_1, Y_2, ..., Y_n$. Greek letters are used to denote parameters and the corresponding lowercase Roman letters are used to denote estimators and estimates; occasionally the symbol $\widehat{}$ is used for estimators or estimates. For example, the parameter β is estimated by $\widehat{\beta}$ or *b*. Sometimes these conventions are not strictly adhered to, either to avoid excessive notation in cases where the meaning should be apparent from the context, or when there is a strong tradition of alternative notation (e.g., *e* or ε for random error terms).

Vectors and matrices, whether random or not, are denoted by boldface lower- and uppercase letters, respectively. Thus, \mathbf{y} represents a vector of observations

$$\left[\begin{array}{c} y_1\\ \vdots\\ y_n \end{array}\right]$$

or a vector of random variables

$$\left[\begin{array}{c}Y_1\\\vdots\\Y_n\end{array}\right],$$

 $\boldsymbol{\beta}$ denotes a vector of parameters and \mathbf{X} is a matrix. The superscript T is used for a matrix transpose or when a column vector is written as a row, e.g., $y = [Y_1, \dots, Y_n]^{T}$.

The probability density function of a continuous random variable Y (or the probability mass function if Y is discrete) is referred to simply as a **probability distribution** and denoted by

$$f(y; \boldsymbol{\theta})$$

where $\boldsymbol{\theta}$ represents the parameters of the distribution.

We use dot (\cdot) subscripts for summation and bars ($^-$) for means; thus,

$$\overline{\mathbf{y}} = \frac{1}{N} \sum_{i=1}^{N} \mathbf{y}_i = \frac{1}{N} \mathbf{y} \cdot .$$

The expected value and variance of a random variable *Y* are denoted by E(Y) and var(Y), respectively. Suppose random variables Y_1, \ldots, Y_N are independent with $E(Y_i) = \mu_i$ and $var(Y_i) = \sigma_i^2$ for $i = 1, \ldots, n$. Let the random variable *W* be a **linear combination** of the Y_i 's

$$W = a_1 Y_1 + a_2 Y_2 + \ldots + a_n Y_n, \tag{1.1}$$

where the a_i 's are constants. Then the expected value of W is

$$E(W) = a_1 \mu_1 + a_2 \mu_2 + \ldots + a_n \mu_n$$
(1.2)

and its variance is

$$\operatorname{var}(W) = a_1^2 \sigma_1^2 + a_2^2 \sigma_2^2 + \ldots + a_n^2 \sigma_n^2.$$
(1.3)

1.4 Distributions related to the Normal distribution

The sampling distributions of many of the estimators and test statistics used in this book depend on the Normal distribution. They do so either directly because they are derived from Normally distributed random variables or asymptotically, via the Central Limit Theorem for large samples. In this section we give definitions and notation for these distributions and summarize the relationships between them. The exercises at the end of the chapter provide practice in using these results which are employed extensively in subsequent chapters.

1.4.1 Normal distributions

1. If the random variable *Y* has the Normal distribution with mean μ and variance σ^2 , its probability density function is

$$f(y; \mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{1}{2}\left(\frac{y-\mu}{\sigma}\right)^2\right].$$

We denote this by $Y \sim N(\mu, \sigma^2)$.

- 2. The Normal distribution with $\mu = 0$ and $\sigma^2 = 1$, $Y \sim N(0, 1)$, is called the standard Normal distribution.
- 3. Let Y_1, \ldots, Y_n denote Normally distributed random variables with $Y_i \sim N(\mu_i, \sigma_i^2)$ for $i = 1, \ldots, n$ and let the covariance of Y_i and Y_j be denoted by

$$\operatorname{cov}(Y_i, Y_j) = \rho_{ij}\sigma_i\sigma_j,$$

where ρ_{ij} is the correlation coefficient for Y_i and Y_j . Then the joint distribution of the Y_i 's is the **multivariate Normal distribution** with mean vector $\boldsymbol{\mu} = [\mu_1, \dots, \mu_n]^T$ and variance-covariance matrix \mathbf{V} with diagonal elements σ_i^2 and non-diagonal elements $\rho_{ij}\sigma_i\sigma_j$ for $i \neq j$. We write this as $\mathbf{y} \sim \text{MVN}(\boldsymbol{\mu}, \mathbf{V})$, where $\mathbf{y} = [Y_1, \dots, Y_n]^T$.

4. Suppose the random variables Y_1, \ldots, Y_n are independent and Normally distributed with the distributions $Y_i \sim N(\mu_i, \sigma_i^2)$ for $i = 1, \ldots, n$. If

$$W = a_1Y_1 + a_2Y_2 + \ldots + a_nY_n,$$

where the a_i 's are constants, then W is also Normally distributed, so that

$$W = \sum_{i=1}^{n} a_i Y_i \sim N\left(\sum_{i=1}^{n} a_i \mu_i, \sum_{i=1}^{n} a_i^2 \sigma_i^2\right)$$

by Equations (1.2) and (1.3).

1.4.2 Chi-squared distribution

1. The **central chi-squared distribution** with *n* degrees of freedom is defined as the sum of squares of *n* independent random variables Z_1, \ldots, Z_n each with the standard Normal distribution. It is denoted by

$$X^2 = \sum_{i=1}^n Z_i^2 \sim \chi^2(n).$$

In matrix notation, if $\mathbf{z} = [Z_1, \dots, Z_n]^T$, then $\mathbf{z}^T \mathbf{z} = \sum_{i=1}^n Z_i^2$ so that $X^2 = \mathbf{z}^T \mathbf{z} \sim \chi^2(n)$.

- 2. If X^2 has the distribution $\chi^2(n)$, then its expected value is $E(X^2) = n$ and its variance is $var(X^2) = 2n$.
- 3. If Y_1, \ldots, Y_n are independent, Normally distributed random variables, each with the distribution $Y_i \sim N(\mu_i, \sigma_i^2)$, then

$$X^{2} = \sum_{i=1}^{n} \left(\frac{Y_{i} - \mu_{i}}{\sigma_{i}}\right)^{2} \sim \chi^{2}(n)$$
(1.4)

because each of the variables $Z_i = (Y_i - \mu_i) / \sigma_i$ has the standard Normal distribution N(0,1).

4. Let $Z_1, ..., Z_n$ be independent random variables each with the distribution N(0, 1) and let $Y_i = Z_i + \mu_i$, where at least one of the μ_i 's is non-zero. Then the distribution of

$$\sum Y_{i}^{2} = \sum (Z_{i} + \mu_{i})^{2} = \sum Z_{i}^{2} + 2 \sum Z_{i} \mu_{i} + \sum \mu_{i}^{2}$$

has larger mean $n + \lambda$ and larger variance $2n + 4\lambda$ than $\chi^2(n)$ where $\lambda = \sum \mu_i^2$. This is called the **non-central chi-squared distribution** with *n* degrees of freedom and **non-centrality parameter** λ . It is denoted by $\chi^2(n, \lambda)$.

5. Suppose that the Y_i 's are not necessarily independent and the vector $\mathbf{y} = [Y_1, \dots, Y_n]^T$ has the multivariate Normal distribution $\mathbf{y} \sim \text{MVN}(\boldsymbol{\mu}, \mathbf{V})$ where the variance–covariance matrix \mathbf{V} is non-singular and its inverse is \mathbf{V}^{-1} . Then

$$X^{2} = (\mathbf{y} - \boldsymbol{\mu})^{T} \mathbf{V}^{-1} (\mathbf{y} - \boldsymbol{\mu}) \sim \chi^{2}(n).$$
(1.5)

- 6. More generally if $\mathbf{y} \sim \text{MVN}(\boldsymbol{\mu}, \mathbf{V})$, then the random variable $\mathbf{y}^T \mathbf{V}^{-1} \mathbf{y}$ has the non-central chi-squared distribution $\chi^2(n, \lambda)$ where $\lambda = \boldsymbol{\mu}^T \mathbf{V}^{-1} \boldsymbol{\mu}$.
- 7. If X_1^2, \ldots, X_m^2 are *m* independent random variables with the chi-squared distributions $X_i^2 \sim \chi^2(n_i, \lambda_i)$, which may or may not be central, then their sum

also has a chi-squared distribution with $\sum n_i$ degrees of freedom and noncentrality parameter $\sum \lambda_i$, that is,

$$\sum_{i=1}^m X_i^2 \sim \chi^2 \left(\sum_{i=1}^m n_i, \sum_{i=1}^m \lambda_i \right).$$

This is called the **reproductive property** of the chi-squared distribution.

Let y ~ MVN(μ, V), where y has n elements but the Y_i's are not independent so that the number k of linearly independent rows (or columns) of V (that is, the rank of V) is less than n and so V is singular and its inverse is not uniquely defined. Let V⁻ denote a generalized inverse of V (that is a matrix with the property that VV⁻V = V). Then the random variable y^TV⁻y has the non-central chi-squared distribution with k degrees of freedom and non-centrality parameter λ = μ^TV⁻μ.

For further details about properties of the chi-squared distribution see Forbes et al. (2010).

9. Let y₁,..., y_n be *n* independent random vectors each of length *p* and y_n ~ MVN(0, V). Then S = ∑_{i=i}ⁿ y_iy_i^T is a *p* × *p* random matrix which has the Wishart distribution W(V, *n*). This distribution can be used to make inferences about the covariance matrix V because S is proportional to V. In the case *p* = 1 the Y_i's are independent random variables with Y_i ~ N(0, σ²), so Z_i = Y_i/σ ~ N(0, 1). Hence, S = ∑_{i=1}ⁿ Y_i² = σ² ∑_{i=1}ⁿ Z_i² and therefore S/σ² ~ χ²(*n*). Thus, the Wishart distribution can be regarded as a generalisation of the chi-squared distribution.

1.4.3 t-distribution

The **t-distribution** with n degrees of freedom is defined as the ratio of two independent random variables. The numerator has the standard Normal distribution and the denominator is the square root of a central chi-squared random variable divided by its degrees of freedom; that is,

$$T = \frac{Z}{(X^2/n)^{1/2}} \tag{1.6}$$

where $Z \sim N(0,1)$, $X^2 \sim \chi^2(n)$ and Z and X^2 are independent. This is denoted by $T \sim t(n)$.

1.4.4 F-distribution

1. The **central F-distribution** with *n* and *m* degrees of freedom is defined as the ratio of two independent central chi-squared random variables, each

QUADRATIC FORMS

divided by its degrees of freedom,

$$F = \frac{X_1^2}{n} \left/ \frac{X_2^2}{m} \right.$$
(1.7)

where $X_1^2 \sim \chi^2(n), X_2^2 \sim \chi^2(m)$ and X_1^2 and X_2^2 are independent. This is denoted by $F \sim F(n,m)$.

2. The relationship between the t-distribution and the F-distribution can be derived by squaring the terms in Equation (1.6) and using definition (1.7) to obtain

$$T^{2} = \frac{Z^{2}}{1} \left/ \frac{X^{2}}{n} \sim \mathbf{F}(1, n) \right.$$
(1.8)

that is, the square of a random variable with the t-distribution, t(n), has the F-distribution, F(1,n).

3. The **non-central F-distribution** is defined as the ratio of two independent random variables, each divided by its degrees of freedom, where the numerator has a non-central chi-squared distribution and the denominator has a central chi-squared distribution, that is,

$$F = \frac{X_1^2}{n} \left/ \frac{X_2^2}{m} \right.$$

where $X_1^2 \sim \chi^2(n, \lambda)$ with $\lambda = \boldsymbol{\mu}^T \mathbf{V}^{-1} \boldsymbol{\mu}$, $X_2^2 \sim \chi^2(m)$, and X_1^2 and X_2^2 are independent. The mean of a non-central F-distribution is larger than the mean of central F-distribution with the same degrees of freedom.

1.4.5 Some relationships between distributions

We summarize the above relationships in Figure 1.1. In later chapters we add to this diagram and a more extensive diagram involving most of the distributions used in this book is given in the Appendix. Asymptotic relationships are shown using dotted lines and transformations using solid lines. For more details see Leemis (1986) from which this diagram was developed.

1.5 Quadratic forms

1. A quadratic form is a polynomial expression in which each term has degree 2. Thus, $y_1^2 + y_2^2$ and $2y_1^2 + y_2^2 + 3y_1y_2$ are quadratic forms in y_1 and y_2 , but $y_1^2 + y_2^2 + 2y_1$ or $y_1^2 + 3y_2^2 + 2$ are not.



Figure 1.1 Some relationships between common distributions related to the Normal distribution, adapted from Leemis (1986). Dotted line indicates an asymptotic relationship and solid lines a transformation.

2. Let A be a symmetric matrix

```
\begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix},
```

where $a_{ij} = a_{ji}$; then the expression $\mathbf{y}^T \mathbf{A} \mathbf{y} = \sum_i \sum_j a_{ij} y_i y_j$ is a quadratic form in the y_i 's. The expression $(\mathbf{y} - \boldsymbol{\mu})^T \mathbf{V}^{-1} (\mathbf{y} - \boldsymbol{\mu})$ is a quadratic form in the terms $(y_i - \mu_i)$ but not in the y_i 's.

3. The quadratic form $\mathbf{y}^T \mathbf{A} \mathbf{y}$ and the matrix \mathbf{A} are said to be **positive definite** if $\mathbf{y}^T \mathbf{A} \mathbf{y} > 0$ whenever the elements of \mathbf{y} are not all zero. A necessary and sufficient condition for positive definiteness is that all the determinants

$$|A_1| = a_{11}, |A_2| = \begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix}, |A_3| = \begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix}, \dots, \text{ and}$$

 $|A_n| = \det \mathbf{A}$ are positive. If a matrix is positive definite, then it can be inverted and also it has a square root matrix \mathbf{A}^* such that $\mathbf{A}^*\mathbf{A} = \mathbf{A}$. These

ESTIMATION

properties are useful for the derivation of several theoretical results related to estimation and the probability distributions of estimators.

- 4. The rank of the matrix A is also called the degrees of freedom of the quadratic form $Q = \mathbf{y}^T \mathbf{A} \mathbf{y}$.
- 5. Suppose Y_1, \ldots, Y_n are independent random variables each with the Normal distribution N(0, σ^2). Let $Q = \sum_{i=1}^n Y_i^2$ and let Q_1, \ldots, Q_k be quadratic forms in the Y_i 's such that

$$Q=Q_1+\ldots+Q_k,$$

where Q_i has m_i degrees of freedom (i = 1, ..., k). Then $Q_1, ..., Q_k$ are independent random variables and $Q_1/\sigma^2 \sim \chi^2(m_1), Q_2/\sigma^2 \sim \chi^2(m_2), ...,$ and $Q_k/\sigma^2 \sim \chi^2(m_k)$, if and only if

$$m_1+m_2+\ldots+m_k=n.$$

This is Cochran's theorem. A similar result also holds for non-central distributions. For more details see Forbes et al. (2010).

6. A consequence of Cochran's theorem is that the difference of two independent random variables, $X_1^2 \sim \chi^2(m)$ and $X_2^2 \sim \chi^2(k)$, also has a chi-squared distribution

$$X^2 = X_1^2 - X_2^2 \sim \chi^2(m-k)$$

provided that $X^2 \ge 0$ and m > k.

1.6 Estimation

1.6.1 Maximum likelihood estimation

Let $\mathbf{y} = [Y_1, \dots, Y_n]^T$ denote a random vector and let the joint probability density function of the Y_i 's be

$$f(\mathbf{y}; \boldsymbol{\theta})$$

which depends on the vector of parameters $\boldsymbol{\theta} = [\theta_1, \dots, \theta_p]^T$.

The likelihood function $L(\boldsymbol{\theta}; \mathbf{y})$ is algebraically the same as the joint probability density function $f(\mathbf{y}; \boldsymbol{\theta})$ but the change in notation reflects a shift of emphasis from the random variables \mathbf{y} , with $\boldsymbol{\theta}$ fixed, to the parameters $\boldsymbol{\theta}$, with \mathbf{y} fixed. Since L is defined in terms of the random vector \mathbf{y} , it is itself a random variable. Let Ω denote the set of all possible values of the parameter vector $\boldsymbol{\theta}$; Ω is called the **parameter space**. The **maximum likelihood** estimator of $\boldsymbol{\theta}$ is the value $\hat{\boldsymbol{\theta}}$ which maximizes the likelihood function, that is,

$$L(\boldsymbol{\theta}; \mathbf{y}) \ge L(\boldsymbol{\theta}; \mathbf{y})$$
 for all $\boldsymbol{\theta}$ in Ω .

Equivalently, $\hat{\boldsymbol{\theta}}$ is the value which maximizes the **log-likelihood function** $l(\boldsymbol{\theta}; \mathbf{y}) = \log L(\boldsymbol{\theta}; \mathbf{y})$ since the logarithmic function is monotonic. Thus,

$$l(\boldsymbol{\theta}; \mathbf{y}) \ge l(\boldsymbol{\theta}; \mathbf{y})$$
 for all $\boldsymbol{\theta}$ in Ω .

Often it is easier to work with the log-likelihood function than with the likelihood function itself.

Usually the estimator $\hat{\boldsymbol{\theta}}$ is obtained by differentiating the log-likelihood function with respect to each element θ_j of $\boldsymbol{\theta}$ and solving the simultaneous equations

$$\frac{\partial l(\boldsymbol{\theta}; \mathbf{y})}{\partial \boldsymbol{\theta}_j} = 0 \qquad \text{for } j = 1, \dots, p.$$
(1.9)

It is necessary to check that the solutions do correspond to maxima of $l(\boldsymbol{\theta}; \mathbf{y})$ by verifying that the matrix of second derivatives

$$\frac{\partial^2 l(\boldsymbol{\theta}; \mathbf{y})}{\partial \boldsymbol{\theta}_i \partial \boldsymbol{\theta}_k}$$

evaluated at $\boldsymbol{\theta} = \hat{\boldsymbol{\theta}}$ is negative definite. For example, if $\boldsymbol{\theta}$ has only one element $\boldsymbol{\theta}$, this means it is necessary to check that

$$\left[\frac{\partial^2 l(\theta, y)}{\partial \theta^2}\right]_{\theta=\widehat{\theta}} < 0.$$

It is also necessary to check if there are any values of $\boldsymbol{\theta}$ at the edges of the parameter space Ω that give local maxima of $l(\boldsymbol{\theta}; \mathbf{y})$. When all local maxima have been identified, the value of $\hat{\boldsymbol{\theta}}$ corresponding to the largest one is the maximum likelihood estimator. (For most of the models considered in this book there is only one maximum and it corresponds to the solution of the equations $\partial l/\partial \theta_i = 0, j = 1, ..., p$.)

An important property of maximum likelihood estimators is that if $g(\theta)$ is any function of the parameters θ , then the maximum likelihood estimator of $g(\theta)$ is $g(\hat{\theta})$. This follows from the definition of $\hat{\theta}$. It is sometimes called the **invariance property** of maximum likelihood estimators. A consequence is that we can work with a function of the parameters that is convenient for maximum likelihood estimation and then use the invariance property to obtain maximum likelihood estimates for the required parameters.

In principle, it is not necessary to be able to find the derivatives of the likelihood or log-likelihood functions or to solve Equation (1.9) if $\hat{\theta}$ can be found numerically. In practice, numerical approximations are very important for generalized linear models.

14

ESTIMATION

Other properties of maximum likelihood estimators include consistency, sufficiency, asymptotic efficiency and asymptotic normality. These are discussed in books such as Cox and Hinkley (1974) or Forbes et al. (2010).

1.6.2 Example: Poisson distribution

Let Y_1, \ldots, Y_n be independent random variables each with the Poisson distribution

$$f(y_i; \boldsymbol{\theta}) = \frac{\boldsymbol{\theta}^{y_i} e^{-\boldsymbol{\theta}}}{y_i!}, \qquad y_i = 0, 1, 2, \dots$$

with the same parameter θ . Their joint distribution is

$$f(y_1, \dots, y_n; \theta) = \prod_{i=1}^n f(y_i; \theta) = \frac{\theta^{y_1} e^{-\theta}}{y_1!} \times \frac{\theta^{y_2} e^{-\theta}}{y_2!} \times \dots \times \frac{\theta^{y_n} e^{-\theta}}{y_n!}$$
$$= \frac{\theta^{\sum y_i} e^{-n\theta}}{y_1! y_2! \dots y_n!}.$$

This is also the likelihood function $L(\theta; y_1, ..., y_n)$. It is easier to use the loglikelihood function

$$l(\theta; y_1, \dots, y_n) = \log L(\theta; y_1, \dots, y_n) = (\sum y_i) \log \theta - n\theta - \sum (\log y_i!).$$

To find the maximum likelihood estimate $\hat{\theta}$, use

$$\frac{dl}{d\theta} = \frac{1}{\theta} \sum y_i - n.$$

Equate this to zero to obtain the solution

$$\widehat{\theta} = \sum y_i / n = \overline{y}.$$

Since $d^2l/d\theta^2 = -\sum y_i/\theta^2 < 0$, *l* has its maximum value when $\theta = \hat{\theta}$, confirming that \overline{y} is the maximum likelihood estimate.

1.6.3 Least squares estimation

Let Y_1, \ldots, Y_n be independent random variables with expected values μ_1, \ldots, μ_n , respectively. Suppose that the μ_i 's are functions of the parameter vector that we want to estimate, $\boldsymbol{\beta} = [\beta_1, \ldots, \beta_p]^T$; p < n. Thus

$$E(Y_i) = \mu_i(\boldsymbol{\beta}).$$

The simplest form of the method of least squares consists of finding the

estimator $\hat{\beta}$ that minimizes the sum of squares of the differences between Y_i 's and their expected values

$$S = \sum \left[Y_i - \mu_i(\boldsymbol{\beta}) \right]^2.$$

Usually $\widehat{\boldsymbol{\beta}}$ is obtained by differentiating S with respect to each element β_j of $\boldsymbol{\beta}$ and solving the simultaneous equations

$$\frac{\partial S}{\partial \beta_j} = 0, \qquad j = 1, \dots, p.$$

Of course it is necessary to check that the solutions correspond to minima (i.e., the matrix of second derivatives is positive definite) and to identify the global minimum from among these solutions and any local minima at the boundary of the parameter space.

Now suppose that the Y_i 's have variances σ_i^2 that are not all equal. Then it may be desirable to minimize the weighted sum of squared differences

$$S = \sum w_i \left[Y_i - \mu_i \left(\boldsymbol{\beta} \right) \right]^2,$$

where the weights are $w_i = (\sigma_i^2)^{-1}$. In this way, the observations which are less reliable (i.e., the Y_i 's with the larger variances) will have less influence on the estimates.

More generally, let $\mathbf{y} = [Y_1, \dots, Y_n]^T$ denote a random vector with mean vector $\boldsymbol{\mu} = [\mu_1, \dots, \mu_n]^T$ and variance–covariance matrix **V**. Then the **weighted least squares estimator** is obtained by minimizing

$$S = (\mathbf{y} - \boldsymbol{\mu})^T \mathbf{V}^{-1} (\mathbf{y} - \boldsymbol{\mu}).$$

1.6.4 Comments on estimation

- 1. An important distinction between the methods of maximum likelihood and least squares is that the method of least squares can be used without making assumptions about the distributions of the response variables Y_i beyond specifying their expected values and possibly their variance–covariance structure. In contrast, to obtain maximum likelihood estimators we need to specify the joint probability distribution of the Y_i 's.
- 2. For many situations maximum likelihood and least squares estimators are identical.
- Often numerical methods rather than calculus may be needed to obtain parameter estimates that maximize the likelihood or log-likelihood function or minimize the sum of squares. The following example illustrates this approach.

EXERCISES

1.6.5 Example: Tropical cyclones

Table 1.2 shows the number of tropical cyclones in northeastern Australia for the seasons 1956–7 (season 1) through 1968–9 (season 13), a period of fairly consistent conditions for the definition and tracking of cyclones (Dobson and Stewart 1974).

Table 1.2	Num	bers	of tr	opic	al cy	vclor	ies in	13 s	иссе.	ssive s	seasor	ıs.	
Season	1	2	3	4	5	6	7	8	9	10	11	12	13
No. of cyclones	6	5	4	6	6	3	12	7	4	2	6	7	4

Let Y_i denote the number of cyclones in season *i*, where i = 1, ..., 13. Suppose the Y_i 's are independent random variables with the Poisson distribution with parameter θ . From Example 1.6.2, $\hat{\theta} = \overline{y} = 72/13 = 5.538$. An alternative approach would be to find numerically the value of θ that maximizes the log-likelihood function. The component of the log-likelihood function due to y_i is

$$l_i = y_i \log \theta - \theta - \log y_i!$$

The log-likelihood function is the sum of these terms

$$l = \sum_{i=1}^{13} l_i = \sum_{i=1}^{13} (y_i \log \theta - \theta - \log y_i!).$$

Only the first two terms in the brackets involve θ and so are relevant to the optimization calculation because the term $\sum_{i=1}^{13} \log y_i!$ is a constant. To plot the log-likelihood function (without the constant term) against θ , for various values of θ , calculate $(y_i \log \theta - \theta)$ for each y_i and add the results to obtain $l^* = \sum (y_i \log \theta - \theta)$. Figure 1.2 shows l^* plotted against θ .

Clearly the maximum value is between $\theta = 5$ and $\theta = 6$. This can provide a starting point for an iterative procedure for obtaining $\hat{\theta}$. The results of a simple bisection calculation are shown in Table 1.3. The function l^* is first calculated for approximations $\theta^{(1)} = 5$ and $\theta^{(2)} = 6$. Then subsequent approximations $\theta^{(k)}$ for k = 3, 4, ... are the average values of the two previous estimates of θ with the largest values of l^* (for example, $\theta^{(6)} = \frac{1}{2}(\theta^{(5)} + \theta^{(3)})$). After 7 steps, this process gives $\hat{\theta} \simeq 5.54$ which is correct to 2 decimal places.

1.7 Exercises

1.1 Let Y_1 and Y_2 be independent random variables with $Y_1 \sim N(1,3)$ and $Y_2 \sim N(2,5)$. If $W_1 = Y_1 + 2Y_2$ and $W_2 = 4Y_1$

 $Y_1 \sim N(1,3)$ and $Y_2 \sim N(2,5)$. If $W_1 = Y_1 + 2Y_2$ and $W_2 = 4Y_1 - Y_2$, what is the joint distribution of W_1 and W_2 ?

INTRODUCTION



Figure 1.2 Graph showing the location of the maximum likelihood estimate for the data in Table 1.2 on tropical cyclones.

Table 1.3 Successive approximations to the maximum likelihood estimate of the mean number of cyclones per season.

k	$oldsymbol{ heta}^{(k)}$	l^*
1	5	50.878
2	6	51.007
3	5.5	51.242
4	5.75	51.192
5	5.625	51.235
6	5.5625	51.243
7	5.5313	51.24354
8	5.5469	51.24352
9	5.5391	51.24360
10	5.5352	51.24359

1.2 Let Y_1 and Y_2 be independent random variables with $Y_1 \sim N(0, 1)$ and $Y_2 \sim N(3, 4)$.

- a. What is the distribution of Y_1^2 ?
- b. If $\mathbf{y} = \begin{bmatrix} Y_1 \\ (Y_2 3)/2 \end{bmatrix}$, obtain an expression for $\mathbf{y}^T \mathbf{y}$. What is its distribution?
- c. If $\mathbf{y} = \begin{pmatrix} Y_1 \\ Y_2 \end{pmatrix}$ and its distribution is $\mathbf{y} \sim \text{MVN}(\boldsymbol{\mu}, \mathbf{V})$, obtain an expression for $\mathbf{y}^T \mathbf{V}^{-1} \mathbf{y}$. What is its distribution?

EXERCISES

1.3 Let the joint distribution of Y_1 and Y_2 be MVN(μ , V) with

$$\boldsymbol{\mu} = \begin{pmatrix} 2\\ 3 \end{pmatrix}$$
 and $\mathbf{V} = \begin{pmatrix} 4 & 1\\ 1 & 9 \end{pmatrix}$.

- a. Obtain an expression for $(\mathbf{y} \boldsymbol{\mu})^T \mathbf{V}^{-1} (\mathbf{y} \boldsymbol{\mu})$. What is its distribution?
- b. Obtain an expression for $\mathbf{y}^T \mathbf{V}^{-1} \mathbf{y}$. What is its distribution?
- 1.4 Let Y_1, \ldots, Y_n be independent random variables each with the distribution $N(\mu, \sigma^2)$. Let

$$\overline{Y} = \frac{1}{n} \sum_{i=1}^{n} Y_i$$
 and $S^2 = \frac{1}{n-1} \sum_{i=1}^{n} (Y_i - \overline{Y})^2$.

- a. What is the distribution of \overline{Y} ?
- b. Show that $S^2 = \frac{1}{n-1} \left[\sum_{i=1}^n (Y_i \mu)^2 n(\overline{Y} \mu)^2 \right].$
- c. From (b) it follows that $\sum (Y_i \mu)^2 / \sigma^2 = (n-1)S^2 / \sigma^2 + [(\overline{Y} \mu)^2 n / \sigma^2]$. How does this allow you to deduce that \overline{Y} and S^2 are independent?
- d. What is the distribution of $(n-1)S^2/\sigma^2$?
- e. What is the distribution of $\frac{\overline{Y} \mu}{S/\sqrt{n}}$?
- 1.5 This exercise is a continuation of the example in Section 1.6.2 in which Y_1, \ldots, Y_n are independent Poisson random variables with the parameter θ .
 - a. Show that $E(Y_i) = \theta$ for i = 1, ..., n.
 - b. Suppose $\theta = e^{\beta}$. Find the maximum likelihood estimator of β .
 - c. Minimize $S = \sum (Y_i e^{\beta})^2$ to obtain a least squares estimator of β .
- 1.6 The data in Table 1.4 are the numbers of females and males in the progeny of 16 female light brown apple moths in Muswellbrook, New South Wales, Australia (from Lewis, 1987).
 - a. Calculate the proportion of females in each of the 16 groups of progeny.
 - b. Let Y_i denote the number of females and n_i the number of progeny in each group (i = 1, ..., 16). Suppose the Y_i 's are independent random variables each with the Binomial distribution

$$f(y_i; \boldsymbol{\theta}) = {n_i \choose y_i} \boldsymbol{\theta}^{y_i} (1 - \boldsymbol{\theta})^{n_i - y_i}.$$

Find the maximum likelihood estimator of θ using calculus and evaluate it for these data.

c. Use a numerical method to estimate $\hat{\theta}$ and compare the answer with the one from (b).

Progeny	Females	Males
group		
1	18	11
2	31	22
3	34	27
4	33	29
5	27	24
6	33	29
7	28	25
8	23	26
9	33	38
10	12	14
11	19	23
12	25	31
13	14	20
14	4	6
15	22	34
16	7	12

Table 1.4 Progeny of light brown apple moths.

Chapter 2

Model Fitting

2.1 Introduction

The model fitting process described in this book involves four steps:

- 1. Model specification—a model is specified in two parts: an equation linking the response and explanatory variables and the probability distribution of the response variable.
- 2. Estimation of the parameters of the model.
- 3. Checking the adequacy of the model—how well it fits or summarizes the data.
- 4. Inference—for classical or frequentist inference this involves calculating confidence intervals, testing hypotheses about the parameters in the model and interpreting the results.

In this chapter these steps are first illustrated using two small examples. Then some general principles are discussed. Finally there are sections about notation and coding of explanatory variables which are needed in subsequent chapters.

2.2 Examples

2.2.1 Chronic medical conditions

Data from the Australian Longitudinal Study on Women's Health (Lee et al. 2005) show that women who live in country areas tend to have fewer consultations with general practitioners (family physicians) than women who live near a wider range of health services. It is not clear whether this is because they are healthier or because structural factors, such as shortage of doctors, higher costs of visits and longer distances to travel, act as barriers to the use of general practitioner (GP) services. Table 2.1 shows the numbers of chronic medical conditions (for example, high blood pressure or arthritis) reported

Table 2.1 Number of chronic medical conditions of 26 town women and 23 country women with similar use of general practitioner services.

Town
0 1 1 0 2 3 0 1 1 1 1 2 0 1 3 0 1 2 1 3 3 4 1 3 2 0
n = 26, mean = 1.423, standard deviation = 1.172, variance = 1.374
Country
$2 \ 0 \ 3 \ 0 \ 0 \ 1 \ 1 \ 1 \ 0 \ 0 \ 2 \ 2 \ 0 \ 1 \ 2 \ 0 \ 0 \ 1 \ 1 \ 1 \ 0 \ 2$
n = 23, mean = 0.913, standard deviation = 0.900, variance = 0.810

by samples of women living in large country towns (town group) or in more rural areas (country group) in New South Wales, Australia. All the women were aged 70–75 years, had the same socio-economic status and had three or fewer GP visits during 1996. The question of interest is: Do women who have similar levels of use of GP services in the two groups have the same need as indicated by their number of chronic medical conditions?

The Poisson distribution provides a plausible way of modelling these data as they are count data and within each group the sample mean and variance are similar. Let Y_{jk} be a random variable representing the number of conditions for the *k*th woman in the *j*th group, where j = 1 for the town group and j = 2 for the country group and $k = 1, ..., K_j$ with $K_1 = 26$ and $K_2 = 23$. Suppose the Y_{jk} 's are all independent and have the Poisson distribution with parameter θ_j representing the expected number of conditions.

The question of interest can be formulated as a test of the null hypothesis $H_0: \theta_1 = \theta_2 = \theta$ against the alternative hypothesis $H_1: \theta_1 \neq \theta_2$. The model fitting approach to testing H_0 is to fit two models, one assuming H_0 is true, that is

$$\mathbf{E}(Y_{ik}) = \boldsymbol{\theta}; \quad Y_{ik} \sim \mathrm{Po}(\boldsymbol{\theta}), \tag{2.1}$$

and the other assuming it is not, so that

$$\mathbf{E}(Y_{jk}) = \boldsymbol{\theta}_j; \quad Y_{jk} \sim \operatorname{Po}(\boldsymbol{\theta}_j), \tag{2.2}$$

where j = 1 or 2. Testing H₀ against H₁ involves comparing how well Models (2.1) and (2.2) fit the data. If they are about equally good, then there is little reason for rejecting H₀. However, if Model (2.2) is clearly better, then H₀ would be rejected in favor of H₁.

If H_0 is true, then the log-likelihood function of the Y_{jk} 's is

$$l_0 = l(\boldsymbol{\theta}; \mathbf{y}) = \sum_{j=1}^J \sum_{k=1}^{K_j} (y_{jk} \log \boldsymbol{\theta} - \boldsymbol{\theta} - \log y_{jk}!), \qquad (2.3)$$

EXAMPLES

where J = 2 in this case. The maximum likelihood estimate, which can be obtained as shown in the example in Section 1.6.2, is

$$\widehat{\theta} = \sum \sum y_{jk} / N,$$

where $N = \sum_{j} K_{j}$. For these data the estimate is $\hat{\theta} = 1.184$ and the maximum value of the log-likelihood function, obtained by substituting this value of $\hat{\theta}$ and the data values y_{jk} into (2.3), is $\hat{l}_{0} = -68.3868$.

If H₁ is true, then the log-likelihood function is

$$l_{1} = l(\theta_{1}, \theta_{2}; \mathbf{y}) = \sum_{k=1}^{K_{1}} (y_{1k} \log \theta_{1} - \theta_{1} - \log y_{1k}!) + \sum_{k=1}^{K_{2}} (y_{2k} \log \theta_{2} - \theta_{2} - \log y_{2k}!).$$
(2.4)

(The subscripts on l_0 and l_1 in (2.3) and (2.4) are used to emphasize the connections with the hypotheses H₀ and H₁, respectively). From (2.4) the maximum likelihood estimates are $\hat{\theta}_j = \sum_k y_{jk}/K_j$ for j = 1 or 2. In this case $\hat{\theta}_1 = 1.423$, $\hat{\theta}_2 = 0.913$ and the maximum value of the log-likelihood function, obtained by substituting these values and the data into (2.4), is $\hat{l}_1 = -67.0230$.

The maximum value of the log-likelihood function l_1 will always be greater than or equal to that of l_0 because one more parameter has been fitted. To decide whether the difference is statistically significant, we need to know the sampling distribution of the log-likelihood function. This is discussed in Chapter 4.

If $Y \sim \text{Po}(\theta)$ then $\text{E}(Y) = \text{var}(Y) = \theta$. The estimate $\widehat{\theta}$ of E(Y) is called the **fitted value** of *Y*. The difference $Y - \widehat{\theta}$ is called a **residual** (other definitions of residuals are also possible, see Section 2.3.4). Residuals form the basis of many methods for examining the adequacy of a model. A residual is usually standardized by dividing by its standard error. For the Poisson distribution an approximate standardized residual is

$$r=\frac{Y-\widehat{\theta}}{\sqrt{\widehat{\theta}}}.$$

The standardized residuals for Models (2.1) and (2.2) are shown in Table 2.2 and Figure 2.1. Examination of individual residuals is useful for assessing certain features of a model such as the appropriateness of the probability distribution used for the responses or the inclusion of specific explanatory variables. For example, the residuals in Table 2.2 and Figure 2.1 exhibit some skewness, as might be expected for the Poisson distribution.