Use R!

Series Editors:

Robert Gentleman Kurt Hornik Giovanni Parmigiani

For other titles published in this series, go to http://www.springer.com/series/6991

J.O. Ramsay • Giles Hooker • Spencer Graves

Functional Data Analysis with R and MATLAB



J.O. Ramsay 2748. Howe Street Ottawa, ON K2B 6W9 Canada ramsay@psych.mcgill.ca Giles Hooker Department of Biological Statistics & Computational Biology Cornell University 1186, Comstock Hall Ithaca, NY 14853 USA gih27@cornell.edu

Spencer Graves Productive Systems Engineering 751. Emerson Ct. San Jose, CA 95126 USA spencer.graves@prodsyse.com

Series Editors:

Robert Gentleman Program in Computational Biology Division of Public Health Sciences Fred Hutchinson Cancer Research Center 1100, Fairview Avenue, N. M2-B876 A-1090 Wien Seattle, Washington 98109 USA

Kurt Hornik Department of Statistik and Mathematik Wirtschaftsuniversität Wien Augasse 2-6 Austria

Giovanni Parmigiani The Sidney Kimmel Comprehensive Cancer Center at Johns Hopkins University 550, North Broadway Baltimore, MD 21205-2011 USA

ISBN 978-0-387-98184-0 e-ISBN 978-0-387-98185-7 DOI 10.1007/978-0-387-98185-7 Springer Dordrecht Heidelberg London New York

Library of Congress Control Number: 2009928040

© Springer Science+Business Media, LLC 2009

All rights reserved. This work may not be translated or copied in whole or in part without the written permission of the publisher (Springer Science+Business Media, LLC, 233 Spring Street, New York, NY 10013, USA), except for brief excerpts in connection with reviews or scholarly analysis. Use in connection with any form of information storage and retrieval, electronic adaptation, computer software, or by similar or dissimilar methodology now known or hereafter developed is forbidden.

The use in this publication of trade names, trademarks, service marks, and similar terms, even if they are not identified as such, is not to be taken as an expression of opinion as to whether or not they are subject to proprietary rights.

Printed on acid-free paper

Springer is part of Springer Science+Business Media (www.springer.com)

Preface

This contribution to the useR! series by Springer is designed to show newcomers how to do functional data analysis in the two popular languages, Matlab and R. We hope that this book will substantially reduce the time and effort required to use these techniques to gain valuable insights in a wide variety of applications.

We also hope that the practical examples in this book will make this learning process fun, interesting and memorable. We have tried to choose rich, real-world problems where the optimal analysis has yet to be performed. We have found that applying a spectrum of methods provides more insight than any single approach by itself. Experimenting with graphics and other displays of results is essential.

To support the acquisition of expertise, the "scripts" subdirectory of the companion fda package for R includes files with names like "fdarm-ch01.R", which contain commands in R to reproduce virtually all of the examples (and figures) in the book. This can be found on any computer with R and fda installed using system.file('scripts', package='fda'). The Matlab code is provides as part of the fda package for R. From within R, it can be found using system.file('Matlab', package='fda'). It also can obtained by downloading the .tar.gz version of the fda package for R from the Comprehensive R Archive Network (CRAN, www.r-project.org), unzipping it and looking for the inst/Matlab subdirectory.

The contents of a book are fixed by schedules for editing and printing. These script files are not similarly constrained. Thus, in some cases, the script files may perform a particular analysis differently from how it is described in the book. Such differences will reflect improvements in our understanding of preferred ways of performing the analysis described in the book. The web site www.functionaldata.org is a resource for ongoing developments of software, new tools and current events.

The support for two languages is perhaps a bit unusual in this series, but there are good reasons for this. Matlab is expensive for most users, but its for capacity modeling dynamical systems and other engineering applications has been critical in the development of today's fda package, especially in areas such chemical engineering where functional data are the rule rather than the exception and where Matlab is widely used. On the other hand, the extendibility of R, the easy interface with lower-

vi Preface

level languages, and above all its cost explain its popularity in many fields served by statisticians, students and new researchers. We hope that we can help many of our readers to appreciate the strengths of each language, so as to invest wisely later on. Secondarily, we hope that any user of either language wanting to learn the other can benefit from seeing the same analyses done in both languages.

As with most books in this useR! series, this is not the place to gain enough technical knowledge to claim expertise in functional data analysis nor to develop new tools. But we do hope that some readers will find enough of value here to want to turn to monographs on functional data analysis already published, such as Ramsay and Silverman (2005), and to even newer works.

We wish to end this preface by thanking our families, friends, students, employers, clients and others who have helped make us what we are today and thereby contributed to this book and to our earlier efforts. In particular, we wish to thank John Kimmel of Springer for organizing this series and inviting us to create this book.

James Ramsay, McGill University Giles Hooker, Cornell University Spencer Graves, San Jose, CA

Contents

1	Intro	duction to Functional Data Analysis 1
	1.1	What Are Functional Data?
		1.1.1 Data on the Growth of Girls
		1.1.2 Data on US Manufacturing
		1.1.3 Input/Output Data for an Oil Refinery 4
	1.2	Multivariate Functional Data
		1.2.1 Data on How Children Walk 5
		1.2.2 Data on Handwriting
	1.3	Functional Models for Nonfunctional Data
	1.4	Some Functional Data Analyses
	1.5	First Steps in a Functional Data Analysis
		1.5.1 Data Representation: Smoothing and Interpolation
		1.5.2 Data Registration or Feature Alignment
		1.5.3 Graphing Functional Data
		1.5.4 Plotting Pairs of Derivatives: Phase-Plane Plots
	1.6	Exploring Variability in Functional Data
		1.6.1 Functional Descriptive Statistics
		1.6.2 Functional Principal Components Analysis
		1.6.3 Functional Canonical Correlation
	1.7	Functional Linear Models
	1.8	Using Derivatives in Functional Data Analysis
	1.9	Concluding Remarks
	1.10	Some Things to Try
2	Essen	itial Comparisons of the Matlab and R Languages 21
	2.1	A Quick Comparison of Matlab and R Syntax
		2.1.1 Minor Differences
		2.1.2 Using Functions in the Two Languages
	2.2	Singleton Index Issues
	2.3	Classes and Objects in R and Matlab
	2.4	More to Read

viii Contents

3	How	to Specify Basis Systems for Building Functions	29
	3.1	Basis Function Systems for Constructing Functions	29
	3.2	Fourier Series for Periodic Data and Functions	32
	3.3	Spline Series for Nonperiodic Data and Functions	33
		3.3.1 Break Points and Knots	33
		3.3.2 Order and Degree	34
		3.3.3 Examples	34
		3.3.4 B-Splines	35
		3.3.5 Computational Issues Concerning the Range of <i>t</i>	38
	3.4	Constant, Monomial and Other Bases	39
		3.4.1 The Constant Basis	39
		3.4.2 The Monomial Basis	39
		3.4.3 Other Basis Systems	40
	3.5	Methods for Functional Basis Objects	40
	3.6	The Structure of the basisfd or basis Class	42
	3.7	Some Things to Try	44
4	How	to Build Functional Data Objects	45
•	4.1	Adding Coefficients to Bases to Define Functions	45
	7.1	4.1.1 Coefficient Vectors, Matrices and Arrays	45
		4.1.2 Labels for Functional Data Objects	46
	4.2	Methods for Functional Data Objects	48
	7.2	4.2.1 Illustration: Sinusoidal Coefficients	50
	4.3	Smoothing Using Regression Analysis	51
	4.3	4.3.1 Plotting the January Thaw	52
	4.4	The Linear Differential Operator or Lfd Class	55
	4.5	Bivariate Functional Data Objects: Functions of Two Arguments .	56
	4.6	The Structure of the fd and Lfd Classes	57
	4.7	Some Things to Try	57
		•	
5		othing: Computing Curves from Noisy Data	59
	5.1	Regression Splines: Smoothing by Regression Analysis	59
	5.2	Data Smoothing with Roughness Penalties	62
		5.2.1 Choosing a Roughness Penalty	62
		5.2.2 The Roughness Penalty Matrix R	64
		5.2.3 The Smoothing or "Hat" Matrix and Degrees of Freedom.	65
		5.2.4 Defining Smoothing by Functional Parameter Objects	66
		5.2.5 Choosing Smoothing Parameter λ	66
	5.3	Case Study: The Log Precipitation Data	67
	5.4	Positive, Monotone, Density and Other Constrained Functions	70
		5.4.1 Positive Smoothing	70
		5.4.2 Monotone Smoothing	71
		5.4.3 Probability Density Functions	74
	5.5	Assessing the Fit to the Data	77
	5.6	Details for the fdPar Class and smooth basis Function	78

Contents ix

		5.6.1 The fdPar class	. 78	
		5.6.2 The smooth basis Function	. 80	
	5.7	Some Things to Try		
	5.8	More to Read		
6	Desc	riptions of Functional Data	. 83	
	6.1	Some Functional Descriptive Statistics	. 83	
		6.1.1 The Bivariate Covariance Function $v(s,t)$		
	6.2	The Residual Variance-Covariance Matrix Σ_e	. 87	
	6.3	Functional Probes ρ_{ξ}	. 87	
	6.4	Phase-Plane Plots of Periodic Effects	. 88	
		6.4.1 Phase-Plane Plots Show Energy Transfer	. 88	
		6.4.2 The Nondurable Goods Cycles	. 90	
		6.4.3 Phase-Plane Plotting the Growth of Girls	. 91	
	6.5	Confidence Intervals for Curves and Their Derivatives	. 92	
		6.5.1 Two Linear Mappings Defining a Probe Value	. 93	
		6.5.2 Computing Confidence Limits for Probe Values	. 95	
		6.5.3 Confidence Limits for Prince Rupert's Log Precipitation.	. 95	
	6.6	Some Things to Try	. 96	
7	Exploring Variation: Functional Principal and Canonical			
	Com	ponents Analysis		
	7.1	An Overview of Functional PCA		
	7.2	PCA with Function pca.fd		
		7.2.1 PCA of the Log Precipitation Data		
		7.2.2 PCA of Log Precipitation Residuals		
	7.3	More Functional PCA Features		
	7.4	PCA of Joint X-Y Variation in Handwriting	. 108	
	7.5	Exploring Functional Covariation with Canonical Correlation Analysis	110	
	7.6	Details for the pca.fd and cca.fd Functions		
	7.0	7.6.1 The pca.fd Function		
		7.6.2 The cca.fd Function		
	7.7	Some Things to Try		
	7.8	More to Read		
0	ъ.			
8		stration: Aligning Features for Samples of Curves		
	8.1	Amplitude and Phase Variation	. 11/	
	8.2	Time-Warping Functions and Registration		
	8.3	Landmark Registration with Function landmarkreg		
	8.4	Continuous Registration with Function register.fd		
	8.5	A Decomposition into Amplitude and Phase Sums of Squares		
	8.6	Registering the Chinese Handwriting Data		
	8.7	Details for Functions landmarkreg and register.fd		
		8.7.1 Function landmarkreg	. 127	

x Contents

		8.7.2 Function register.fd	
	8.8	Some Things to Try	129
	8.9	More to Read	130
9	Funct	ional Linear Models for Scalar Responses	131
	9.1	Functional Linear Regression with a Scalar Response	131
	9.2	A Scalar Response Model for Log Annual Precipitation	132
	9.3	Setting Up the Functional Linear Model	132
	9.4	Three Estimates of the Regression Coefficient Predicting	
		Annual Precipitation	
		9.4.1 Low-Dimensional Regression Coefficient Function β .	
		9.4.2 Coefficient β Estimate Using a Roughness Penalty	
		9.4.3 Choosing Smoothing Parameters	
		9.4.4 Confidence Intervals	140
		9.4.5 Scalar Response Models by Functional Principal	
		Components	
	9.5	Statistical Tests	
	9.6	Some Things to Try	
	9.7	More to Read	146
10		r Models for Functional Responses	
	10.1	Functional Responses and an Analysis of Variance Model	
		10.1.1 Climate Region Effects on Temperature	
		10.1.2 Trends in Seabird Populations on Kodiak Island	
		10.1.3 Choosing Smoothing Parameters	153
	10.2	Functional Responses with Functional Predictors: The	
		Concurrent Model	
		10.2.1 Estimation for the Concurrent Model	
		10.2.2 Confidence Intervals for Regression Functions	
		10.2.3 Knee Angle Predicted from Hip Angle	
	10.3	Beyond the Concurrent Model	
	10.4	A Functional Linear Model for Swedish Mortality	
	10.5	Permutation Tests of Functional Hypotheses	
		10.5.1 Functional <i>t</i> -Tests	
		10.5.2 Functional F-Tests	168
	10.6	Details for R Functions fRegress, fRegress.CV and	1.60
		fRegress.stderr	
		10.6.1 Function fRegress	
		10.6.2 Function fRegress.CV	
	10.5	10.6.3 Function fRegress.stderr	
	10.7	Details for Function plotbeta	
	10.8	Details for Function linmod	
	10.9	Details for Functions Fperm.fd and tperm.fd	
		10.9.1 Function Fperm.fd	
		10.9.2 Function tperm.fd	176

Contents xi

	10.10	Some Things to Try	. 177
		More to Read	
11	Functi	ional Models and Dynamics	. 179
	11.1	Introduction to Dynamics	. 179
		11.1.1 An Example of First-Order Dynamics	. 180
		11.1.2 Interpreting Second-Order Linear Dynamics	. 181
		11.1.3 Higher-Dimensional Linear Systems	
	11.2	Principal Differential Analysis for Linear Dynamics	
	11.3	Principal Differential Analysis of the Lip Data	
	11.4	PDA of the Handwriting Data	
	11.5	Registration and PDA	
	11.6	Details for pda.fd, eigen.pda, pda.overlay and	
		register.newfd	. 191
		11.6.1 Function pda.fd	
		11.6.2 Function eigen.pda	
		11.6.3 Function pda.overlay	
		11.6.4 Function register.newfd	
	11.7	Some Things to Try	
	11.8	More to Read	
Syn	ıbol Ta	ble	. 197
Ref	erences	5	. 199
Ind	ex		. 203