

Contents

Preface	xvii
List of Contributors	xix
Part I Introduction	1
1 A Short History of Compositional Data Analysis	3
<i>John Bacon-Shone</i>	
1.1 Introduction	3
1.2 Spurious Correlation	3
1.3 Log and Log-Ratio Transforms	4
1.4 Subcompositional Dependence	5
1.5 alr, clr, ilr: Which Transformation to Choose?	5
1.6 Principles, Perturbations and Back to the Simplex	6
1.7 Biplots and Singular Value Decompositions	7
1.8 Mixtures	7
1.9 Discrete Compositions	8
1.10 Compositional Processes	8
1.11 Structural, Counting and Rounded Zeros	8
1.12 Conclusion	9
Acknowledgement	9
References	9
2 Basic Concepts and Procedures	12
<i>Juan José Egozcue and Vera Pawłowsky-Glahn</i>	
2.1 Introduction	12
2.2 Election Data and Raw Analysis	13
2.3 The Compositional Alternative	15
2.3.1 Scale Invariance: Vectors with Proportional Positive Components Represent the Same Composition	15
2.3.2 Subcompositional Coherence: Analyses Concerning a Subset of Parts Must Not Depend on Other Non-Involved Parts	16

2.3.3	Permutation Invariance: The Conclusions of a Compositional Analysis Should Not Depend on the Order of the Parts	17
2.4	Geometric Settings	17
2.5	Centre and Variability	22
2.6	Conclusion	27
	Acknowledgements	27
	References	27
Part II	Theory – Statistical Modelling	29
3	The Principle of Working on Coordinates <i>Glòria Mateu-Figueras, Vera Pawłowsky-Glahn and Juan José Egozcue</i>	31
3.1	Introduction	31
3.2	The Role of Coordinates in Statistics	32
3.3	The Simplex	33
3.3.1	Basis of the Simplex	34
3.3.2	Working on Orthonormal Coordinates	35
3.4	<i>Move or Stay</i> in the Simplex	38
3.5	Conclusions	40
	Acknowledgements	41
	References	41
4	Dealing with Zeros <i>Josep Antoni Martín-Fernández, Javier Palarea-Albaladejo and Ricardo Antonio Olea</i>	43
4.1	Introduction	43
4.2	Rounded Zeros	44
4.2.1	Non-Parametric Replacement of Rounded Zeros	45
4.2.2	Parametric Modified EM Algorithm for Rounded Zeros	47
4.3	Count Zeros	50
4.4	Essential Zeros	53
4.5	Difficulties, Troubles and Challenges	55
	Acknowledgements	57
	References	57
5	Robust Statistical Analysis <i>Peter Filzmoser and Karel Hron</i>	59
5.1	Introduction	59
5.2	Elements of Robust Statistics from a Compositional Point of View	60
5.3	Robust Methods for Compositional Data	63
5.3.1	Multivariate Outlier Detection	64
5.3.2	Principal Component Analysis	64
5.3.3	Discriminant Analysis	65
5.4	Case Studies	66
5.4.1	Multivariate Outlier Detection	66
5.4.2	Principal Component Analysis	68
5.4.3	Discriminant Analysis	68
5.5	Summary	70

Acknowledgement	71
References	71
6 Geostatistics for Compositions	73
<i>Raimon Tolosana-Delgado, Karl Gerald van den Boogaart and Vera Pawłowsky-Glahn</i>	
6.1 Introduction	73
6.2 A Brief Summary of Geostatistics	74
6.3 Cokriging of Regionalised Compositions	76
6.4 Structural Analysis of Regionalised Composition	76
6.5 Dealing with Zeros: Replacement Strategies and Simplicial Indicator Cokriging	78
6.6 Application	79
6.6.1 Delimiting the Body: Simplicial Indicator Kriging	81
6.6.2 Interpolating the Oil–Brine–Solid Content	82
6.7 Conclusions	84
Acknowledgements	84
References	84
7 Compositional VARIMA Time Series	87
<i>Carles Barceló-Vidal, Lucía Aguilar and Josep Antoni Martín-Fernández</i>	
7.1 Introduction	87
7.2 The Simplex S^D as a Compositional Space	89
7.2.1 Basic Concepts and Notation	89
7.2.2 The Covariance Structure on the Simplex	90
7.3 Compositional Time Series Models	91
7.3.1 $\mathcal{C}$ -Stationary Processes	92
7.3.2 $\mathcal{C}$ -VARIMA Processes	93
7.4 CTS Modelling: An Example	94
7.4.1 Expenditure Shares in the UK	94
7.4.2 Model Selection	95
7.4.3 Estimation of Parameters	96
7.4.4 Interpretation and Comparison	96
7.5 Discussion	99
Acknowledgements	99
References	100
Appendix	102
8 Compositional Data and Correspondence Analysis	104
<i>Michael Greenacre</i>	
8.1 Introduction	104
8.2 Comparative Technical Definitions	105
8.3 Properties and Interpretation of LRA and CA	107
8.4 Application to Fatty Acid Compositional Data	107
8.5 Discussion and Conclusions	111
Acknowledgements	112
References	112

9	Use of Survey Weights for the Analysis of Compositional Data	114
	<i>Monique Graf</i>	
9.1	Introduction	114
9.2	Elements of Survey Design	115
9.2.1	Randomization	115
9.2.2	Design-Based Estimation	118
9.3	Application to Compositional Data	122
9.3.1	Weighted Arithmetic and Geometric Means	123
9.3.2	Closed Arithmetic Mean of Amounts	123
9.3.3	Centred Log-Ratio of the Geometric Mean Composition	124
9.3.4	Closed Geometric Mean Composition	124
9.3.5	Example: Swiss Earnings Structure Survey (SESS)	125
9.4	Discussion	126
	References	126
10	Notes on the Scaled Dirichlet Distribution	128
	<i>Gianna Serafina Monti, Glòria Mateu-Figueras and Vera Pawlowsky-Glahn</i>	
10.1	Introduction	128
10.2	Genesis of the Scaled Dirichlet Distribution	129
10.3	Properties of the Scaled Dirichlet Distribution	131
10.3.1	Graphical Comparison	131
10.3.2	Membership in the Exponential Family	133
10.3.3	Measures of Location and Variability	134
10.4	Conclusions	136
	Acknowledgements	137
	References	137
Part III	Theory – Algebra and Calculus	139
11	Elements of Simplicial Linear Algebra and Geometry	141
	<i>Juan José Egozcue, Carles Barceló-Vidal, Josep Antoni Martín-Fernández, Eusebi Jarauta-Bragulat, José Luis Díaz-Barrero and Glòria Mateu-Figueras</i>	
11.1	Introduction	141
11.2	Elements of Simplicial Geometry	142
11.2.1	n -Part Simplex	142
11.2.2	Vector Space	143
11.2.3	Centred Log-Ratio Representation	146
11.2.4	Metrics	147
11.2.5	Orthonormal Basis and Coordinates	149
11.3	Linear Functions	151
11.3.1	Linear Functions Defined on the Simplex	152
11.3.2	Simplicial Linear Function Defined on a Real Space	153
11.3.3	Simplicial Linear Function Defined on the Simplex	154
11.4	Conclusions	156
	Acknowledgements	156
	References	156

12	Calculus of Simplex-Valued Functions	158
	<i>Juan José Egozcue, Eusebi Jarauta-Bragulat and José Luis Díaz-Barrero</i>	
12.1	Introduction	158
12.2	Limits, Continuity and Differentiability	161
12.2.1	Limits and Continuity	161
12.2.2	Differentiability	163
12.2.3	Higher Order Derivatives	169
12.3	Integration	171
12.3.1	Antiderivatives, Indefinite Integral	171
12.3.2	Integration of Continuous SV Functions	172
12.4	Conclusions	174
	Acknowledgements	175
	References	175
13	Compositional Differential Calculus on the Simplex	176
	<i>Carles Barceló-Vidal, Josep Antoni Martín-Fernández and Glòria Mateu-Figueras</i>	
13.1	Introduction	176
13.2	Vector-Valued Functions on the Simplex	177
13.2.1	Scale-Invariant Vector-Valued Functions on $\mathbb{R}_+^n$	177
13.2.2	Vector-Valued Functions on $\mathcal{S}^n$	178
13.3	$\mathcal{C}$ -Derivatives on the Simplex	178
13.3.1	Derivative of a Scale-Invariant Vector-Valued Function on $\mathbb{R}_+^n$	178
13.3.2	Directional $\mathcal{C}$ -Derivatives	180
13.3.3	$\mathcal{C}$ -Derivative	182
13.3.4	$\mathcal{C}$ -Gradient	184
13.3.5	Critical Points of a $\mathcal{C}$ -Differentiable Real-Valued Function on $\mathcal{S}^n$	184
13.4	Example: Experiments with Mixtures	185
13.4.1	Polynomial of Degree One	185
13.4.2	Polynomial of Degree Two	186
13.4.3	Polynomial of Degree One in Logarithms	187
13.4.4	A numerical Example	188
13.5	Discussion	189
	Acknowledgements	190
	References	190
Part IV	Applications	191
14	Proportions, Percentages, PPM: Do the Molecular Biosciences Treat Compositional Data Right?	193
	<i>David Lovell, Warren Müller, Jen Taylor, Alec Zwart and Chris Helliwell</i>	
14.1	Introduction	193
14.2	The Omics Imp and Two Bioscience Experiment Paradigms	194
14.3	The Impact of Compositional Constraints in the Omics	197
14.3.1	Univariate Impact of Compositional Constraints	197
14.3.2	Impact of Compositional Constraints on Multivariate Distance Metrics	199

14.4	Impact of Compositional Constraints on Correlation and Covariance	201
14.4.1	Compositional Constraints, Covariance, Correlation and Log-Transformed Data	202
14.4.2	A Simulation Approach to Understanding the Impact of Closure	202
14.5	Implications	204
14.5.1	Gathering Information to Infer Absolute Abundance	204
14.5.2	Analysing Compositional Omics Data Appropriately	205
	Acknowledgements	206
	References	206
15	Hardy–Weinberg Equilibrium: A Nonparametric Compositional Approach <i>Jan Graffelman and Juan José Egozcue</i>	208
15.1	Introduction	208
15.2	Genetic Data Sets	209
15.3	Classical Tests for HWE	210
15.4	A Compositional Approach	210
15.5	Example	214
15.6	Conclusion and Discussion	215
	Acknowledgements	215
	References	215
16	Compositional Analysis in Behavioural and Evolutionary Ecology <i>Michele Edoardo Raffaele Pierotti and Josep Antoni Martín-Fernández</i>	218
16.1	Introduction	218
16.2	CODA in Population Genetics	219
16.3	CODA in Habitat Choice	222
16.4	Multiple Choice and Individual Variation in Preferences	224
16.5	Ecological Specialization	228
16.6	Time Budgets: More on Specialization	229
16.7	Conclusions	231
	Acknowledgements	231
	References	231
17	Flying in Compositional Morphospaces: Evolution of Limb Proportions in Flying Vertebrates <i>Luis Azevedo Rodrigues, Josep Daunis-i-Estadella, Glòria Mateu-Figueras and Santiago Thió-Henestrosa</i>	235
17.1	Introduction	235
17.2	Flying Vertebrates – General Anatomical and Functional Characteristics	236
17.3	Materials	236
17.4	Methods	238
17.5	Aitchison Distance Disparity Metrics	239
17.5.1	Intragroup Aitchison Distance	239
17.5.2	Intergroup Aitchison Distance	240
17.6	Statistical Tests	243

17.7	Biplots	244
17.7.1	Chiroptera	244
17.7.2	Pterosauria	245
17.8	Balances	246
17.9	Size Effect	249
17.10	Final Remarks	249
17.10.1	All Groups	250
17.10.2	Aves	250
17.10.3	Pterosauria	250
17.10.4	Chiroptera	251
	Acknowledgements	252
	References	252
18	Natural Laws Governing the Distribution of the Elements in Geochemistry: The Role of the Log-Ratio Approach <i>Antonella Buccianti</i>	255
18.1	Introduction	255
18.2	Geochemical Processes and Log-Ratio Approach	256
18.3	Log-Ratio Approach and Water Chemistry	258
18.4	Log-Ratio Approach and Volcanic Gas Chemistry	261
18.5	Log-Ratio Approach and Subducting Sediment Composition	263
18.6	Conclusions	265
	Acknowledgements	265
	References	265
19	Compositional Data Analysis in Planetology: The Surfaces of Mars and Mercury <i>Helmut Lammer, Peter Würz, Josep Antoni Martín-Fernández and Herbert Iwo Maria Lichtenegger</i>	267
19.1	Introduction	267
19.1.1	Mars	267
19.1.2	Mercury	269
19.1.3	Analysis of Surface Composition	270
19.2	Compositional Analysis of Mars' Surface	270
19.3	Compositional Analysis of Mercury's Surface	274
19.4	Conclusion	278
	Acknowledgement	278
	References	278
20	Spectral Analysis of Compositional Data in Cyclostratigraphy <i>Eulogio Pardo-Igúzquiza and Javier Heredia</i>	282
20.1	Introduction	282
20.2	The Method	283
20.3	Case Study	285
20.4	Discussion	287
20.5	Conclusions	288
	Acknowledgement	288
	References	288

21	Multivariate Geochemical Data Analysis in Physical Geography	290
	<i>Jennifer McKinley and Christopher David Lloyd</i>	
21.1	Introduction	290
21.2	Context	291
21.3	Data	293
21.4	Analysis	295
21.5	Discussion	299
21.6	Conclusion	300
	Acknowledgement	300
	References	300
22	Combining Isotopic and Compositional Data: A Discrimination of Regions Prone to Nitrate Pollution	302
	<i>Roger Puig, Raimon Tolosana-Delgado, Neus Otero and Albert Folch</i>	
22.1	Introduction	302
22.2	Study Area	303
22.2.1	Maresme	304
22.2.2	Osona	305
22.2.3	Lluçanès	305
22.2.4	Empordà	306
22.2.5	Selva	306
22.3	Analytical Methods	306
22.4	Statistical Treatment	307
22.4.1	Data Scaling	307
22.4.2	Linear Discriminant Analysis	309
22.4.3	Discriminant Biplots	310
22.5	Results and Discussion	311
22.6	Conclusions	314
	Acknowledgements	315
	References	315
23	Applications in Economics	318
	<i>Tim Fry</i>	
23.1	Introduction	318
23.2	Consumer Demand Systems	319
23.3	Miscellaneous Applications	322
23.4	Compositional Time Series	323
23.5	New Directions	323
23.6	Conclusion	325
	References	325
	Part V Software	327
24	Exploratory Analysis Using CoDaPack 3D	329
	<i>Santiago Thió-Henestrosa and Josep Daunis-i-Estadella</i>	
24.1	CoDaPack 3D Description	329
24.2	Data Set Description	331

24.3	Exploratory Analysis	333
24.3.1	Numerical Analysis	333
24.3.2	Biplot	334
24.3.3	The Ternary Diagram	335
24.3.4	Principal Component Analysis	336
24.3.5	Balance-Dendrogram	336
24.3.6	By Groups Description	338
24.4	Summary and Conclusions	339
	Acknowledgements	340
	References	340
25	robCompositions: An R-package for Robust Statistical Analysis of Compositional Data	341
	<i>Matthias Templ, Karel Hron and Peter Filzmoser</i>	
25.1	General Information on the R-package robCompositions	341
25.1.1	Data Sets Included in the Package	342
25.1.2	Design Principles	343
25.2	Expressing Compositional Data in Coordinates	343
25.3	Multivariate Statistical Methods for Compositional Data Containing Outliers	345
25.3.1	Multivariate Outlier Detection	345
25.3.2	Principal Component Analysis and the Robust Compositional Biplot	347
25.3.3	Discriminant Analysis	350
25.4	Robust Imputation of Missing Values	351
25.5	Summary	354
	References	354
26	Linear Models with Compositions in R	356
	<i>Raimon Tolosana-Delgado and Karl Gerald van den Boogaart</i>	
26.1	Introduction	356
26.2	The Illustration Data Set	357
26.2.1	The Data	357
26.2.2	Descriptive Analysis of Compositional Characteristics	358
26.3	Explanatory Binary Variable	360
26.4	Explanatory Categorical Variable	363
26.5	Explanatory Continuous Variable	365
26.6	Explanatory Composition	367
26.7	Conclusions	370
	Acknowledgement	371
	References	371
	Index	373