

Compositional Data Analysis in the Geosciences

From Theory to Practice

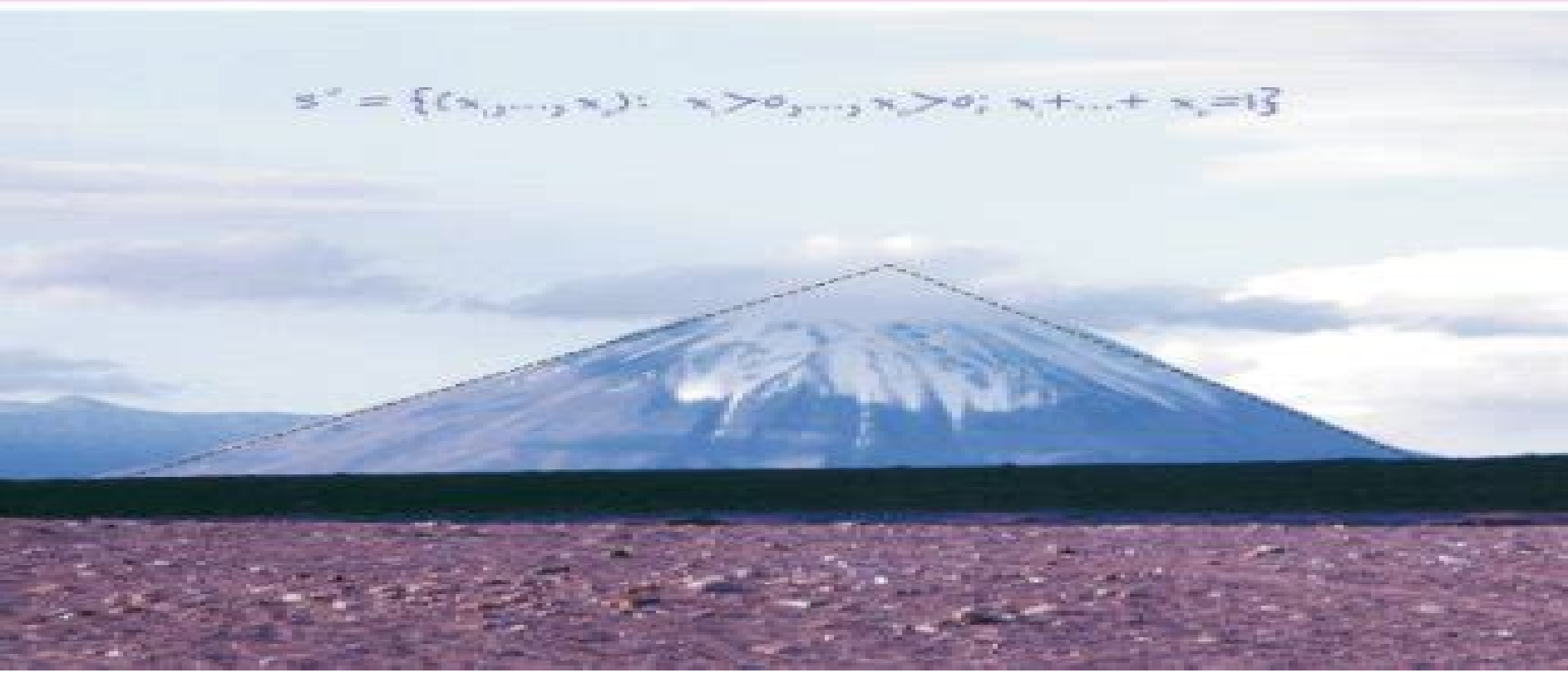
Edited by

A. Buccianti, G. Mateu-Figueras and V. Pawłowsky-Glahn



Geological Society
Special Publication 264

$$S^+ = \{(x_1, \dots, x_n) : x_1 > 0, \dots, x_n > 0; x_1 + \dots + x_n = 1\}$$



**Compositional Data Analysis In The Geosciences From
Theory To Practice Special Publication No 264
Geological Society Special Publication**

**Antonella Buccianti, G. Mateu-
Figueras, Vera Pawlowsky-Glahn**

Compositional Data Analysis In The Geosciences From Theory To Practice Special Publication No 264 Geological Society Special Publication:

Compositional Data Analysis in the Geosciences Antonella Buccianti, G. Mateu-Figueras, Vera Pawlowsky-Glahn, 2006 Since Karl Pearson wrote his paper on spurious correlation in 1897 a lot has been said about the statistical analysis of compositional data mainly by geologists such as Felix Chayes The solution appeared in the 1980s when John Aitchison proposed to use logratios Since then the approach has seen a great expansion mainly building on the idea of the natural geometry of the sample space Statistics is expected to give sense to our perception of the natural scale of the data and this is made possible for compositional data using logratios This publication will be a milestone in this process The Routledge Handbook of Census Resources, Methods and Applications John Stillwell, 2017-08-24 The collection of reliable and comprehensive data on the magnitude composition and distribution of a country's population is essential in order for governments to provide services administer effectively and guide a country's development The primary source of basic demographic statistics is frequently a population census which provides hugely important data sets for policy makers practitioners and researchers working in a wide range of different socio demographic contexts The Routledge Handbook of Census Resources Methods and Applications provides a comprehensive and authoritative guide to the collection processing quality assessment and delivery of the different data products that constitute the results of the population censuses conducted across the United Kingdom in 2011 It provides those interested in using census data with an introduction to the collection processing and quality assessment of the 2011 Census together with guidance on the various types of data resources that are available and how they can be accessed It demonstrates how new methods and technologies such as interactive infographics and web based mapping are now being used to visualise census data in new and exciting ways Perhaps most importantly it presents a collection of applications of census data in different social and health science research contexts that reveal key messages about the characteristics of the UK population and the ways in which society is changing The operation of the 2011 Census and the use of its results are set in the context of census taking around the world and its historical development in the UK over the last 200 years The results of the UK 2011 Census are a unique and reliable source of detailed information that are immensely important for users from a wide range of public and private sector organisations as well as those working in Population Studies Human Geography Migration Studies and the Social Sciences more generally Handbook of Mathematical Geosciences B.S. Daya Sagar, Qiuming Cheng, Frits Agterberg, 2018-06-25 This Open Access handbook published at the IAMG's 50th anniversary presents a compilation of invited path breaking research contributions by award winning geoscientists who have been instrumental in shaping the IAMG It contains 45 chapters that are categorized broadly into five parts i theory ii general applications iii exploration and resource estimation iv reviews and v reminiscences covering related topics like mathematical geosciences mathematical morphology geostatistics fractals and

multifractals spatial statistics multipoint geostatistics compositional data analysis informatics geocomputation numerical methods and chaos theory in the geosciences **Compositional Data Analysis** Josep Antoni Martín-Fernández, Santiago Thió-Henestrosa, 2016-11-19 The authoritative contributions gathered in this volume reflect the state of the art in compositional data analysis CoDa The respective chapters cover all aspects of CoDa ranging from mathematical theory statistical methods and techniques to its broad range of applications in geochemistry the life sciences and other disciplines The selected and peer reviewed papers were originally presented at the 6th International Workshop on Compositional Data Analysis CoDaWork 2015 held in L Escala Girona Spain Compositional data is defined as vectors of positive components and constant sum and more generally all those vectors representing parts of a whole which only carry relative information Examples of compositional data can be found in many different fields such as geology chemistry economics medicine ecology and sociology As most of the classical statistical techniques are incoherent on compositions in the 1980s John Aitchison proposed the log ratio approach to CoDa This became the foundation of modern CoDa which is now based on a specific geometric structure for the simplex an appropriate representation of the sample space of compositional data The International Workshops on Compositional Data Analysis offer a vital discussion forum for researchers and practitioners concerned with the statistical treatment and modelling of compositional data or other constrained data sets and the interpretation of models and their applications The goal of the workshops is to summarize and share recent developments and to identify important lines of future research **Robust Statistics Through the Monitoring Approach** Anthony C. Atkinson, Marco Riani, Aldo Corbellini, Domenico Perrotta, Valentin Todorov, 2025-07-26 This open access book presents robust statistical methods and procedures through the monitoring approach with an emphasis on applications to linear regression Illustrating the theory it explores both large and small sample properties The performance of the forward search and of the monitoring of static robust estimators for regression data are illuminated through numerous data analyses using MATLAB and R The book describes the results of many years work of the authors in the development of powerful methods of robust regression analysis Robust methods are designed to analyse contaminated data The well established static robust methods estimate model features such as parameter estimates assuming the amount of contamination in the data is known These methods are described in detail in Chapter 2 for estimation in a simple sample The extension to regression is presented in Chapter 3 with an emphasis on S estimation and related procedures as well as on least trimmed squares The monitoring methods of Chapter 4 including the forward search find the appropriate level of robustness for each data set and so avoid biased estimation from the inclusion of outliers and inefficiency due to the deletion of uncontaminated observations This analysis is followed by examples which illustrate the use of the interactive graphical analyses associated with the authors FSDA toolbox Numerical comparisons of the size and power of outlier tests appear in Chapter 5 Later chapters illustrate applications to response transformation in regression and to non parametric regression Extensions of the robust multiple

regression model include Bayesian heteroskedastic time series and compositional regression together with the clustering of regression models Finally several approaches to model selection are investigated and robust analyses of regression data are presented that illustrate the use of the techniques introduced earlier Exercises are given at the end of each chapter with solutions at the end of the book The MATLAB code can be reproduced using MATLAB Online without the need for a license or via the language agnostic Jupyter notebook environment after installing the MATLAB kernel Online computer code is available for all examples and exercises together with a series of YouTube videos Aimed at professional statisticians and researchers concerned with insightful data analysis as well as postgraduate students the book may also serve as a text for a modern interactive robust regression course

The British National Bibliography Arthur James Wells,2006

Forthcoming Books Rose Army,1992-10 *Geostatistical Analysis of Compositional Data* Vera Pawlowsky-Glahn,Ricardo A. Olea,2004-06-03 1 Introduction 2 Regionalized Compositions 3 Spatial Covariance Structure 4 Concepts of Null Correlation 5 Cokriging 6 Practical Aspects of Compositional Data Analysis 7 Application to Real Data Summary and Prospects References Index

Applied Statistical Modeling and Data Analytics Srikanta Mishra,Akhil

Datta-Gupta,2017-10-27 *Applied Statistical Modeling and Data Analytics A Practical Guide for the Petroleum Geosciences* provides a practical guide to many of the classical and modern statistical techniques that have become established for oil and gas professionals in recent years It serves as a how to reference volume for the practicing petroleum engineer or geoscientist interested in applying statistical methods in formation evaluation reservoir characterization reservoir modeling and management and uncertainty quantification Beginning with a foundational discussion of exploratory data analysis probability distributions and linear regression modeling the book focuses on fundamentals and practical examples of such key topics as multivariate analysis uncertainty quantification data driven modeling and experimental design and response surface analysis Data sets from the petroleum geosciences are extensively used to demonstrate the applicability of these techniques The book will also be useful for professionals dealing with subsurface flow problems in hydrogeology geologic carbon sequestration and nuclear waste disposal Authored by internationally renowned experts in developing and applying statistical methods for oil gas and other subsurface problem domains Written by practitioners for practitioners Presents an easy to follow narrative which progresses from simple concepts to more challenging ones Includes online resources with software applications and practical examples for the most relevant and popular statistical methods using data sets from the petroleum geosciences Addresses the theory and practice of statistical modeling and data analytics from the perspective of petroleum geoscience applications

Data Assimilation for the Geosciences Steven J. Fletcher,2022-11-16 *Data Assimilation for the Geosciences From Theory to Application* Second Edition brings together all of the mathematical and statistical background knowledge needed to formulate data assimilation systems into one place It includes practical exercises enabling readers to apply theory in both a theoretical formulation as well as teach them how to code the theory with toy problems to verify their

understanding It also demonstrates how data assimilation systems are implemented in larger scale fluid dynamical problems related to land surface the atmosphere ocean and other geophysical situations The second edition of Data Assimilation for the Geosciences has been revised with up to date research that is going on in data assimilation as well as how to apply the techniques The new edition features an introduction of how machine learning and artificial intelligence are interfacing and aiding data assimilation In addition to appealing to students and researchers across the geosciences this now also appeals to new students and scientists in the field of data assimilation as it will now have even more information on the techniques research and applications consolidated into one source Includes practical exercises and solutions enabling readers to apply theory in both a theoretical formulation as well as enabling them to code theory Provides the mathematical and statistical background knowledge needed to formulate data assimilation systems into one place New to this edition covers new topics such as Observing System Experiments OSE and Observing System Simulation Experiments and expanded approaches for machine learning and artificial intelligence

Statistics and Data Analysis in Geology John C. Davis, 2002-05-08

Thoroughly revised and updated this new edition of the text that helped define the field continues to present important methods in the quantitative analysis of geologic data while showing students how statistics and computing can be applied to commonly encountered problems in the earth sciences In addition to new and expanded coverage of key topics the Third Edition features new pedagogy end of chapter review exercises and an accompanying website that contains all of the data for every example and exercise found in the book

Aspects of Multivariate Statistical Analysis in Geology E. Savazzi, R.A. Reymont, 1999-11-24 The book presents multivariate statistical methods useful in geological analysis The essential distinction between multivariate analysis as applied to full space data measurements on lengths heights breadths etc and compositional data is emphasized with particular reference to geochemical data Each of the methods is accompanied by a practically oriented computer program and backed up by appropriate examples The computer programs are provided on a compact disk together with trial data sets and examples of the output An important feature of this book is the graphical system developed by Dr Savazzi which is entitled Graph Server Geological data often deviate from ideal statistical requirements For this reason close attention has been paid to the analysis of data that contain atypical observations

Geostatistics for Compositional Data with R Raimon Tolosana-Delgado, Ute Mueller, 2021-11-19 This book provides a guided approach to the geostatistical modelling of compositional spatial data These data are data in proportions percentages or concentrations distributed in space which exhibit spatial correlation The book can be divided into four blocks The first block sets the framework and provides some background on compositional data analysis Block two introduces compositional exploratory tools for both non spatial and spatial aspects Block three covers all necessary facets of multivariate spatial prediction for compositional data variogram modelling cokriging and validation Finally block four details strategies for simulation of compositional data including transformations to multivariate normality Gaussian cosimulation multipoint simulation of compositional data and common

postprocessing techniques valid for both Gaussian and multipoint methods All methods are illustrated via applications to two types of data sets one a large scale geochemical survey comprised of a full suite of geochemical variables and the other from a mining context where only the elements of greatest importance are considered R codes are included for all aspects of the methodology encapsulated in the R package gmGeostats available in CRAN

Principles and Practice of Analytical Techniques in Geosciences Kliti Grice, 2014-08-27 The pace of revolution in analytical chemistry in the field of Geosciences has been dramatic over recent decades and includes fundamental developments that have become common place in many related and unrelated disciplines The analytical tools nano to macro scale from stable to radioactive isotopes compound specific sulfur isotopes used have been applied to wide ranging applications from inorganic to organic geochemistry biodiversity and chronological tools to build an understanding of how the Earth system evolved to its present state This book will provide an essential guide to exploring the earth s natural resources and changing climate by detection science Individual chapters bring together expertise from across the globe to present a comprehensive outlook on the analytical technologies available to the geoscientist today Experienced researchers will appreciate the broad treatment of the subject as a valuable reference while students and those new to the field will quickly gain an appreciation of both the techniques at hand and the importance of constructing and analysing the complex data sets they can generate

Quantitative Geosciences: Data Analytics, Geostatistics, Reservoir Characterization and Modeling Y. Z. Ma, 2020-08-15 Earth science is becoming increasingly quantitative in the digital age Quantification of geoscience and engineering problems underpins many of the applications of big data and artificial intelligence This book presents quantitative geosciences in three parts Part 1 presents data analytics using probability statistical and machine learning methods Part 2 covers reservoir characterization using several geoscience disciplines including geology geophysics petrophysics and geostatistics Part 3 treats reservoir modeling resource evaluation and uncertainty analysis using integrated geoscience engineering and geostatistical methods As the petroleum industry is heading towards operating oil fields digitally a multidisciplinary skillset is a must for geoscientists who need to use data analytics to resolve inconsistencies in various sources of data model reservoir properties evaluate uncertainties and quantify risk for decision making This book intends to serve as a bridge for advancing the multidisciplinary integration for digital fields The goal is to move beyond using quantitative methods individually to an integrated descriptive quantitative analysis In big data everything tells us something but nothing tells us everything This book emphasizes the integrated multidisciplinary solutions for practical problems in resource evaluation and field development

Why and How Should Geologists Use Compositional Data Analysis. Ricardo A. Valls, 2016-06-23 Compositional data arise naturally in several branches of science including geology In geochemistry for example these constrained data seem to occur typically when one normalizes raw data or when one obtains the output from a constrained estimation procedure such as parts per one percentages ppm ppb molar concentrations etc Compositional data have proved

difficult to handle statistically because of the awkward constraint that the components of each vector must sum to unity The special property of compositional data the fact that the determinations on each specimen sum to a constant means that the variables involved in the study occur in constrained space defined by the simplex a restricted part of real space Pearson was the first to point out dangers that may befall the analyst who attempts to interpret correlations between Ratios whose numerators and denominators contain common parts More recently Aitchison Pawlowsky Glahn S Thio and other statisticians have developed the concept of Compositional Data Analysis pointing out the dangers of misinterpretation of closed data when treated with normal statistical methods It is important for geochemists and geologists in general to be aware that the usual multivariate statistical techniques are not applicable to constrained data It is also important for us to have access to appropriate techniques as they become available This is the principal aim of this book

Computational Geosciences with Mathematica William Haneberg, 2004-07-20 Computational Geosciences with Mathematica is the only book written by a geologist specifically to show geologists and geoscientists how to use Mathematica to formulate and solve problems It spans a broad range of geologic and mathematical topics which are drawn from the author's extensive experience in research consulting and teaching The reference and text leads readers step by step through geologic applications such as custom graphics programming data input and output linear and differential equations linear and nonlinear regression Monte Carlo simulation time series and image analysis and the visualization and analysis of geologic surfaces It is packed with actual Mathematica output and includes boxed Computer Notes with tips and exploration suggestions

Data Analysis for the Geosciences Michael W. Liemohn, 2023-10-31 An initial course in scientific data analysis and hypothesis testing designed for students in all science technology engineering and mathematics disciplines Data Analysis for the Geosciences Essentials of Uncertainty Comparison and Visualization is a textbook for upper level undergraduate STEM students designed to be their statistics course in a degree program This volume provides a comprehensive introduction to data analysis visualization and data model comparisons and metrics within the framework of the uncertainty around the values It offers a learning experience based on real data from the Earth ocean atmospheric space and planetary sciences About this volume Serves as an initial course in scientific data analysis and hypothesis testing Focuses on the methods of data processing Introduces a wide range of analysis techniques Describes the many ways to compare data with models Centers on applications rather than derivations Explains how to select appropriate statistics for meaningful decisions Explores the importance of the concept of uncertainty Uses examples from real geoscience observations Homework problems at the end of chapters The American Geophysical Union promotes discovery in Earth and space science for the benefit of humanity Its publications disseminate scientific knowledge and provide resources for researchers students and professionals

Wie Statistics and Data Analysis in Geology John C. Davis, Robert J. Sampson, 1973 About this book Geostatistics Measurement systems A false feeling of security Selected readings Computers and Programming Elementary statistics Matrix algebra Analysis of

sequences of data Map analysis Analysis of multivariate data

Geomathematics: Theoretical Foundations,

Applications and Future Developments Frits Agterberg, 2014-07-14 This book provides a wealth of geomathematical case history studies performed by the author during his career at the Ministry of Natural Resources Canada Geological Survey of Canada NRCan GSC Several of the techniques newly developed by the author and colleagues that are described in this book have become widely adopted not only for further research by geomathematical colleagues but by government organizations and industry worldwide These include Weights of Evidence modelling mineral resource estimation technology trend surface analysis automatic stratigraphic correlation and nonlinear geochemical exploration methods The author has developed maximum likelihood methodology and spline fitting techniques for the construction of the international numerical geologic timescale He has introduced the application of new theory of fractals and multi fractals in the geostatistical evaluation of regional mineral resources and ore reserves and to study the spatial distribution of metals in rocks The book also contains sections deemed important by the author but that have not been widely adopted because they require further research These include the geometry of preferred orientations of contours and edge effects on maps time series analysis of Quaternary retreating ice sheet related sedimentary data estimation of first and last appearances of fossil taxa from frequency distributions of their observed first and last occurrences tectonic reactivation along pre existing schistosity planes in fold belts use of the grouped jackknife method for bias reduction in geometrical extrapolations and new applications of the theory of permanent volume independent frequency distributions

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