

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

This volume contains a selection of papers presented at the Seventh Conference of the International Federation of Classification Societies (IFCS-2000), which was held in Namur, Belgium, July 11-14, 2000. From the originally submitted papers, a careful review process involving two reviewers per paper, led to the selection of 65 papers that were considered suitable for publication in this book. The present book contains original research contributions, innovative applications and overview papers in various fields within data analysis, classification, and related methods. Given the fast publication process, the research results are still up-to-date and coincide with their actual presentation at the IFCS-2000 conference. The topics captured are:

- Cluster analysis
- Comparison of clusterings
- Fuzzy clustering
- Discriminant analysis
- Mixture models
- Analysis of relationships data
- Symbolic data analysis
- Regression trees
- Data mining and neural networks
- Pattern recognition
- Multivariate data analysis
- Robust data analysis
- Data science and sampling

The IFCS (International Federation of Classification Societies) promotes the dissemination of technical and scientific information data analysis, classification, related methods, and their applications.

The earliest of the four Gospels, the book portrays Jesus as an enigmatic figure, struggling

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with enemies, his inner and external demons, and with his devoted but disconcerted disciples. Unlike other gospels, his parables are obscure, to be explained secretly to his followers. With an introduction by Nick Cave

Compositional Grading in Oil and Gas Reservoirs offers instruction, examples, and case studies on how to answer the challenges of modeling a compositional gradient subject. Starting with the basics on PVT analysis, applied thermodynamics, and full derivations of irreversible thermodynamic-based equations, this critical reference explains gravity-modified equations to be applied to reservoirs, enabling engineers to obtain fluid composition at any point of the reservoir from measured data to create a stronger model calibration. Once model-parameters are re-estimated, new sensibility can be acquired for more accurate modeling of composition, aiding engineers with stronger production curves, reserve estimations, and design of future development strategies. Multiple examples and case studies are included to show the application of the theory from very simple to more complex systems, such as actual reservoirs influenced by thermal diffusion and gravity simultaneously. Other example include a layer for which asphaltene precipitation takes place in the reservoir and three –phase flash algorithms for liquid-liquid-vapor equilibrium calculations, detailing the techniques necessary to ensure convergence. The book combines practical studies with the importance in modeling more complex phenomena, filling a gap for current and upcoming reservoir engineers to expand on solutions and make sense of their reservoir's output results. Presents a deeper level of detail on the heterogeneity composition and thermo-physical properties of petroleum fluids in the reservoir Includes tactics on how to Increase reliability of reservoir simulation initialization, with practice examples at the end of each chapter Helps readers make sense of compositional

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grading, with coverage on both theory and application that fulfill a gap in research on reservoir simulation

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.

Microcomputer Package for the Statistical Analysis of Compositional Data

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

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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.

Designed to serve as the first point of reference on the subject, Comprehensive Chemometrics presents an integrated summary of the present state of chemical and biochemical data analysis and manipulation. The work covers all major areas ranging from statistics to data acquisition, analysis, and applications. This major reference work provides broad-ranging, validated summaries of the major topics in chemometrics—with chapter introductions and advanced reviews for each area. The level of material is appropriate for graduate students as well as active researchers seeking a ready reference on obtaining and analyzing scientific data. Features the contributions of leading experts from 21 countries, under the guidance of the Editors-in-Chief and a team of specialist Section Editors: L. Buydens; D. Coomans; P. Van Espen; A. De Juan; J.H. Kalivas; B.K. Lavine; R. Leardi; R. Phan-Tan-Luu; L.A. Sarabia; and J. Trygg Examines the merits and limitations of each technique through practical examples and extensive visuals: 368 tables and more than 1,300 illustrations (750 in full color) Integrates coverage of chemical and biological methods, allowing readers to consider and test a range of techniques Consists of 2,200 pages and more than 90 review articles, making it the most comprehensive work of its kind Offers print and online purchase options, the latter of which

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delivers flexibility, accessibility, and usability through the search tools and other productivity-enhancing features of ScienceDirect

This book presents the statistical analysis of compositional data using the log-ratio approach. It includes a wide range of classical and robust statistical methods adapted for compositional data analysis, such as supervised and unsupervised methods like PCA, correlation analysis, classification and regression. In addition, it considers special data structures like high-dimensional compositions and compositional tables. The methodology introduced is also frequently compared to methods which ignore the specific nature of compositional data. It focuses on practical aspects of compositional data analysis rather than on detailed theoretical derivations, thus issues like graphical visualization and preprocessing (treatment of missing values, zeros, outliers and similar artifacts) form an important part of the book. Since it is primarily intended for researchers and students from applied fields like geochemistry, chemometrics, biology and natural sciences, economics, and social sciences, all the proposed methods are accompanied by worked-out examples in R using the package `robCompositions`.

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

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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. Compositional Data Analysis in Practice is a user-oriented practical guide to the analysis of data with the property of a constant sum, for example percentages adding up to 100%. Compositional data can give misleading results if regular statistical methods are applied, and are best analysed by first transforming them to logarithms of ratios. This book explains how this transformation affects the analysis, results and interpretation of this very special type of data. All aspects of compositional data analysis are considered: visualization, modelling, dimension-reduction, clustering and variable selection, with many examples in the fields of food science, archaeology, sociology and biochemistry, and a final chapter containing a complete case study using fatty acid compositions in ecology. The applicability of these methods extends to other

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fields such as linguistics, geochemistry, marketing, economics and finance. R Software
The following repository contains data files and R scripts from the book
<https://github.com/michaelgreenacre/CODAIinPractice>. The R package easyCODA, which accompanies this book, is available on CRAN -- note that you should have version 0.25 or higher. The latest version of the package will always be available on R-Forge and can be installed from R with this instruction: `install.packages("easyCODA", repos="http://R-Forge.R-project.org")`.

This book focuses on recent advances, approaches, theories and applications related to mixture models. In particular, it presents recent unsupervised and semi-supervised frameworks that consider mixture models as their main tool. The chapters considers mixture models involving several interesting and challenging problems such as parameters estimation, model selection, feature selection, etc. The goal of this book is to summarize the recent advances and modern approaches related to these problems. Each contributor presents novel research, a practical study, or novel applications based on mixture models, or a survey of the literature. Reports advances on classic problems in mixture modeling such as parameter estimation, model selection, and feature selection; Present theoretical and practical developments in mixture-based modeling and their importance in different applications; Discusses perspectives and challenging future works related to mixture modeling.

This book presents modern methods and real-world applications of compositional data

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analysis. It covers a wide variety of topics, ranging from an updated presentation of basic concepts and ideas in compositional data analysis to recent advances in the context of complex data structures. Further, it illustrates real-world applications in numerous scientific disciplines and includes references to the latest software solutions available for compositional data analysis, thus providing a valuable and up-to-date guide for researchers and practitioners working with compositional data. Featuring selected contributions by leading experts in the field, the book is dedicated to Vera Pawlowsky-Glahn on the occasion of her 70th birthday.

Compositional Data Analysis (CoDA) refers to the analysis of all those vectors representing parts of a whole which only carry relative information. This type of data is ubiquitous in most applications, especially in geology, chemistry, genetics, and environmental sciences. The last comprehensive treatment was written by John Aitchison in 1986, and this book represents an update of that classic book.

Reviews in Mineralogy & Geochemistry (RiMG) volumes contain concise advances in theoretical and/or applied mineralogy, crystallography, petrology, and geochemistry. 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

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will be a milestone in this process.

Compositional Data Analysis in Practice is a user-oriented practical guide to the analysis of data with the property of a constant sum, for example percentages adding up to 100%. Compositional data can give misleading results if regular statistical methods are applied, and are best analysed by first transforming them to logarithms of ratios. This book explains how this transformation affects the analysis, results and interpretation of this very special type of data. All aspects of compositional data analysis are considered: visualization, modelling, dimension-reduction, clustering and variable selection, with many examples in the fields of food science, archaeology, sociology and biochemistry, and a final chapter containing a complete case study using fatty acid compositions in ecology. The applicability of these methods extends to other fields such as linguistics, geochemistry, marketing, economics and finance. R Software The R package easyCODA, which accompanies this book, can be downloaded from R-Forge as follows: `install.packages("easyCODA", repos="")` and will be available on CRAN soon. Notice that the R packages `ca` and `vegan` also have to be installed (from CRAN in the usual way).

Applied Compositional Data Analysis With Worked Examples in R Springer

This unique book addresses the statistical modelling and analysis of microbiome data using cutting-edge R software. It includes real-world data from the authors' research and from the public domain, and discusses the implementation of R for data analysis step by step. The data and R computer programs are publicly available, allowing readers to replicate the model development and data analysis presented in each chapter, so that these new methods can be readily applied in their own research. The book also discusses recent developments in

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statistical modelling and data analysis in microbiome research, as well as the latest advances in next-generation sequencing and big data in methodological development and applications. This timely book will greatly benefit all readers involved in microbiome, ecology and microarray data analyses, as well as other fields of research.

A guide for constructing and using composite indicators for policy makers, academics, the media and other interested parties. In particular, this handbook is concerned with indicators which compare and rank country performance.

Based on a course taught by the author, this book combines the theoretical underpinnings of statistics with the practical analysis of Earth sciences data using MATLAB. The book is organized to introduce the underlying concepts, and then extends these to the data, covering methods that are most applicable to Earth sciences. Topics include classical parametric estimation and hypothesis testing, and more advanced least squares-based, nonparametric, and resampling estimators. Multivariate data analysis, not often encountered in introductory texts, is presented later in the book, and compositional data is treated at the end. Datasets and bespoke MATLAB scripts used in the book are available online, as well as additional datasets and suggested questions for use by instructors. Aimed at entering graduate students and practicing researchers in the Earth and ocean sciences, this book is ideal for those who want to learn how to analyse data using MATLAB in a statistically-rigorous manner.

Gen 14:18–20 is a brief episode depicting the encounter between Abram and Melchizedek. Taking this episode and its context in the Pentateuch as the starting point, Mathews sets out to analyze the text as it has been composed, in order to understand the biblical and theological significance of this priest-king Melchizedek. The thesis proposed and investigated is that

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Melchizedek's royal priestly portrayal in Genesis initiates a priesthood that is intentionally presented as an alternative to Aaron and his priesthood. The claim is that this distinct priestly order is evident in the biblical text as we have it, and it may be discerned by reading the text carefully, on its own terms, with close attention to its compositional features. Chapter 1 introduces the study and offers an overview of the history of interpretation related to Genesis 14 and Melchizedek. In ch. 2, various hermeneutical issues and approaches are examined in order to clarify methodology and identify some of the problems being addressed. In ch. 3, the heart of the book, Mathews considers Gen 14:18–20 in the context of the Pentateuch, focusing on Melchizedek in relation to the Abrahamic narrative and covenant, the royal message of the Pentateuch, and Aaron's priesthood. Beginning with Psalm 110, ch. 4 identifies echoes of Melchizedek and his priesthood in several texts in the Prophets and Writings. The book concludes in ch. 5 with a summary and synthesis of the preceding analysis as well as some implications and suggestions for further research.

Comprehensive overview of the spectroscopic, mineralogical, and geochemical techniques used in planetary remote sensing.

Modeling and Analysis of Compositional Data presents a practical and comprehensive introduction to the analysis of compositional data along with numerous examples to illustrate both theory and application of each method. Based upon short courses delivered by the authors, it provides a complete and current compendium of fundamental to advanced methodologies along with

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exercises at the end of each chapter to improve understanding, as well as data and a solutions manual which is available on an accompanying website.

Complementing Pawlowsky-Glahn's earlier collective text that provides an overview of the state-of-the-art in this field, *Modeling and Analysis of Compositional Data* fills a gap in the literature for a much-needed manual for teaching, self learning or consulting.

This book highlights major problems in the statistical analysis of compositions that have been known for over a century, as well as the corresponding solutions that have been put forward by specialists over the past 30 years. The basic assumptions of normality or multi-normality are pointed out and methods to test and achieve them are also covered. The conventional major and trace element geochemistry and modeling equations are discussed, and are followed by a more sophisticated multidimensional approach to data handling. The book's main focus is on the use of statistical techniques to facilitate data interpretation. It also highlights the classification (or nomenclature) and tectonic discrimination aspects for both igneous and sedimentary rocks. The book concludes by discussing computer programs that are helping pave the way from geochemistry to geochemometrics. Written by a leading expert in the area of geochemistry, it offers a valuable guide for students and professionals in the area.

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This book presents a unique collection of contributions on modern topics in statistics and econometrics, written by leading experts in the respective disciplines and their intersections. It addresses nonparametric statistics and econometrics, quantiles and expectiles, and advanced methods for complex data, including spatial and compositional data, as well as tools for empirical studies in economics and the social sciences. The book was written in honor of Christine Thomas-Agnan on the occasion of her 65th birthday. Given its scope, it will appeal to researchers and PhD students in statistics and econometrics alike who are interested in the latest developments in their field.

Compositional Data Analysis: Theory and Applications Edited by Vera Pawlowsky-Glahn, Department of Computer Science and Applied Mathematics, University of Girona, Spain. Antonella Buccianti, Department of Earth Sciences, University of Florence, Italy It is difficult to imagine that the statistical analysis of compositional data has been a major issue of concern for more than 100 years. It is even more difficult to realize that so many statisticians and users of statistics are unaware of the particular problems affecting compositional data, as well as their solutions. The issue of "spurious correlation", as the situation was phrased by Karl Pearson back in 1897, affects all data that measures parts of some whole, such as percentages, proportions, ppm and ppb. Such measurements are

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present in all fields of science, ranging from geology, biology, environmental sciences, forensic sciences, medicine and hydrology. This book presents the history and development of compositional data analysis along with Aitchison's log-ratio approach. "Compositional Data Analysis" describes the state of the art both in theoretical fields as well as applications in the different fields of science. Key Features: - Reflects the state-of-the-art in compositional data analysis. - Gives an overview of the historical development of compositional data analysis, as well as basic concepts and procedures. - Looks at advances in algebra and calculus on the simplex. - Presents applications in different fields of science, including, genomics, ecology, biology, geochemistry, planetology, chemistry and economics. - Explores connections to correspondence analysis and the Dirichlet distribution. - Presents a summary of three available software packages for compositional data analysis. - Supported by an accompanying website featuring R code. Applied scientists working on compositional data analysis in any field of science, both in academia and professionals will benefit from this book, along with graduate students in any field of science working with compositional data. Intended as a practical guide for polymer technologists, engineers and analysts in the plastics, composites and rubber fields, this title describes a range of techniques and strategies for compositional and failure analysis of polymeric

materials and products. Numerous examples illustrate the application of analytical methods for solving commonly encountered problems in the polymer industry. The reader is guided towards the most appropriate method of analysis and measurement and the most likely reasons for the failure. Areas covered include: * Migration and interaction of additives * Mechanical stress and stress cracking * Craze and fracture * Residual stress and weld lines * Contamination and discoloration Numerous pedagogical methods, illustrative flow diagrams, figures and tables are used throughout the text to make it an invaluable guide to all analysts and polymer engineers in industrial or academic laboratories. In this book we are concerned with Bayesian learning and forecasting in dynamic environments. We describe the structure and theory of classes of dynamic models, and their uses in Bayesian forecasting. The principles, models and methods of Bayesian forecasting have been developed extensively during the last twenty years. This development has involved thorough investigation of mathematical and statistical aspects of forecasting models and related techniques. With this has come experience with application in a variety of areas in commercial and industrial, scientific and socio-economic fields. Indeed much of the technical development has been driven by the needs of forecasting practitioners. As a result, there now exists a relatively complete statistical and

mathematical framework, although much of this is either not properly documented or not easily accessible. Our primary goals in writing this book have been to present our view of this approach to modelling and forecasting, and to provide a reasonably complete text for advanced university students and research workers. The text is primarily intended for advanced undergraduate and postgraduate students in statistics and mathematics. In line with this objective we present thorough discussion of mathematical and statistical features of Bayesian analyses of dynamic models, with illustrations, examples and exercises in each Chapter.

This book presents the statistical analysis of compositional data sets, i.e., data in percentages, proportions, concentrations, etc. The subject is covered from its grounding principles to the practical use in descriptive exploratory analysis, robust linear models and advanced multivariate statistical methods, including zeros and missing values, and paying special attention to data visualization and model display issues. Many illustrated examples and code chunks guide the reader into their modeling and interpretation. And, though the book primarily serves as a reference guide for the R package “compositions,” it is also a general introductory text on Compositional Data Analysis. Awareness of their special characteristics spread in the Geosciences in the early sixties, but a strategy for properly dealing with them was not available until the works of Aitchison in the eighties. Since then, research has expanded our understanding of their theoretical principles and the potentials and limitations of their

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interpretation. This is the first comprehensive textbook addressing these issues, as well as their practical implications with regard to software. The book is intended for scientists interested in statistically analyzing their compositional data. The subject enjoys relatively broad awareness in the geosciences and environmental sciences, but the spectrum of recent applications also covers areas like medicine, official statistics, and economics. Readers should be familiar with basic univariate and multivariate statistics. Knowledge of R is recommended but not required, as the book is self-contained.

BIG DATA, ARTIFICIAL INTELLIGENCE AND DATA ANALYSIS SET Coordinated by Jacques Janssen Data analysis is a scientific field that continues to grow enormously, most notably over the last few decades, following rapid growth within the tech industry, as well as the wide applicability of computational techniques alongside new advances in analytic tools. Modeling enables data analysts to identify relationships, make predictions, and to understand, interpret and visualize the extracted information more strategically. This book includes the most recent advances on this topic, meeting increasing demand from wide circles of the scientific community. **Applied Modeling Techniques and Data Analysis 2** is a collective work by a number of leading scientists, analysts, engineers, mathematicians and statisticians, working on the front end of data analysis and modeling applications. The chapters cover a cross section of current concerns and research interests in the above scientific areas. The collected material is divided into appropriate sections to provide the reader with both theoretical and applied information on data analysis methods, models and techniques, along with appropriate applications.

Originally published in 1986, this text contains a new Foreword, extensive postscript detailing

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developments in the field since its first publication, and a selection of more recent literature references. The work provides a clear and systematic account of statistical methods designed to meet the special needs of the compositional data analyst. (Mathematics)

As long ago as 1897 Karl Pearson, in a now classic paper on spurious correlation, first pointed out dangers that may befall the analyst who attempts to interpret correlations between ratios whose numerators and denominators contain common parts. He thus implied that the analysis of compositional data, with its concentration on relationships between proportions of some whole, is likely to be fraught with difficulty. History has proved him correct: over the succeeding years and indeed right up to the present day, there has been no other form of data analysis where more confusion has reigned and where more improper and inadequate statistical methods have been applied. The special and intrinsic feature of compositional data is that the proportions of a composition are naturally subject to a unit-sum constraint. For other forms of constrained data, in particular for directional data where there is a unit-length constraint on each direction vector, scientist and statistician alike have readily appreciated that new statistical methods, appropriate to the special nature of the data, are required; and there now exists an extensive literature on the successful statistical analysis of directional data. It is paradoxical that for compositional data, subject to an apparently simpler constraint, such an appreciation and development have been slower to emerge. In applications the unit-sum constraint has been widely ignored or wished away and inappropriate 'standard' statistical methods, devised for and successfully applied to unconstrained data, have been used with disastrous consequences.

This book is the outcome of contributions by many experts in the field from different disciplines,

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various backgrounds, and diverse expertise. This book provides information on biomass volume calculation methods and biomass valorization for energy production. The chapters presented in this book include original research and review articles. I hope the research presented in this book will help to advance the use of biomass for bioenergy production and valorization. The key features of the book are: Providing information on biomass volume estimation using direct, nondestructive and remote sensing methods Biomass valorization for energy using thermochemical (gasification and pyrolysis) and biochemical (fermentation) conversion processes.

Since the 1960s, testimony by representatives of the Federal Bureau of Investigation in thousands of criminal cases has relied on evidence from Compositional Analysis of Bullet Lead (CABL), a forensic technique that compares the elemental composition of bullets found at a crime scene to the elemental composition of bullets found in a suspect's possession. Different from ballistics techniques that compare striations on the barrel of a gun to those on a recovered bullet, CABL is used when no gun is recovered or when bullets are too small or mangled to observe striations. Forensic Analysis: Weighing Bullet Lead Evidence assesses the scientific validity of CABL, finding that the FBI should use a different statistical analysis for the technique and that, given variations in bullet manufacturing processes, expert witnesses should make clear the very limited conclusions that CABL results can support. The report also recommends that the FBI take additional measures to ensure the validity of CABL results, which include improving documentation, publishing details, and improving on training and oversight.

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