## Ansgar Steland Kwok-Leung Tsui *Editors*

Artificial Intelligence, Big Data and Data Science in Statistics

Challenges and Solutions in Environmetrics, the Natural Sciences and Technology



Artificial Intelligence, Big Data and Data Science in Statistics

Ansgar Steland • Kwok-Leung Tsui Editors

# Artificial Intelligence, Big Data and Data Science in Statistics

Challenges and Solutions in Environmetrics, the Natural Sciences and Technology



*Editors* Ansgar Steland Institute of Statistics and AI Center RWTH Aachen University Aachen, Germany

Kwok-Leung Tsui Grado Department of Industrial and Systems Engineering Virginia Polytechnic Institute and State University Blacksburg, VA, USA

ISBN 978-3-031-07154-6 ISBN 978-3-031-07155-3 (eBook) https://doi.org/10.1007/978-3-031-07155-3

© The Editor(s) (if applicable) and The Author(s), under exclusive licence to Springer Nature Switzerland AG 2022

This work is subject to copyright. All rights are solely and exclusively licensed by the Publisher, whether the whole or part of the material is concerned, specifically the rights of translation, reprinting, reuse of illustrations, recitation, broadcasting, reproduction on microfilms or in any other physical way, and transmission or information storage and retrieval, electronic adaptation, computer software, or by similar or dissimilar methodology now known or hereafter developed.

The use of general descriptive names, registered names, trademarks, service marks, etc. in this publication does not imply, even in the absence of a specific statement, that such names are exempt from the relevant protective laws and regulations and therefore free for general use.

The publisher, the authors, and the editors are safe to assume that the advice and information in this book are believed to be true and accurate at the date of publication. Neither the publisher nor the authors or the editors give a warranty, expressed or implied, with respect to the material contained herein or for any errors or omissions that may have been made. The publisher remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.

This Springer imprint is published by the registered company Springer Nature Switzerland AG The registered company address is: Gewerbestrasse 11, 6330 Cham, Switzerland

### Preface

The change to data-centrism in many fields, the need to extract information and knowledge from big data, and the increasing success of machine learning (ML) and artificial intelligence (AI) have created both opportunities and challenges to the field of statistics. These developments have, to some extent, led to the creation of data science, partially regarded as a new discipline, related to statistics and computer science. The intersections among ML/AI, data science, and statistics are much larger than people expect, particularly on theory, models, practical methods, and problems under investigation. All communities can learn a lot from each other.

The impressive successes of ML and AI methods, especially deep learners and convolutional networks, in many practical problems might seem to devalue statistical approaches. Quite a few researchers as well as practitioners regard machine learning as being more focused on problem solving and benchmark data sets than statistics. But, on the other hand, ML solutions are often tailored to a specific problem and thus can be difficult to generalize and implement for a wide range of applications.

Further, there is wide range of problems related to data for which statistics provides more appropriate or even optimal solutions and allows specific interpretable models. Stochastic models often provide mathematical descriptions of physical processes rather than relying on black boxes. Indeed, lack of model interpretability, potential bias, causality, and stability, and why and when deep learners may work are common questions for the ML approaches. Statistical thinking and approaches are good alternatives to rectify these problems, in terms of both theories, models, and practical methods. A further issue where statistics is indispensable is the question whether a given data set satisfies proper sampling designs, as studied by statistical sampling theory, and the sound statistical preprocessing, handling, and cleaning of data. Both topics are important to evaluate given data, to ensure high data quality, and to clarify what can be learnt from a certain data set. On the other hand, the flexibility of many ML and AI methods may yield superior results when reliable first-class data from well-selected variables are not available and one has to rely on noisy and surrogate data. Focusing on environmental science, natural science, and technology, this book contributes to the discussions of various issues and general interplay among statistics, data science, machine learning, and artificial intelligence. The chapters cover theoretical studies of machine learning methods, expositions of general methodologies for sound statistical analyses of data, as well as novel approaches for modeling and analyzing data in specific areas and problems. In terms of applications, the chapters deal with data as arising in industrial quality control, autonomous driving, transportation and traffic, chip manufacturing, photovoltaics, football, transmission of infectious diseases, Covid-19, and public health.

The idea for this volume came from the meetings of the Section on Environmetrics, Natural Science and Technology of Deutsche Statistische Gesellschaft of the last few years, and most authors have presented research at the annual conferences Statistische Woche. All chapters of this volume have been peer reviewed, and the editors are grateful to those colleagues who helped in the evaluation process as anonymous reviewers. Nevertheless, the authors of each chapters are solely responsible for their work.

Aachen, Germany Blacksburg, VA, USA November 2021 Ansgar Steland Kwok-Leung Tsui

### Contents

#### Part I Methodologies and Theoretical Studies

| <b>One-Round Cross-Validation and Uncertainty Determination for</b><br><b>Randomized Neural Networks with Applications to Mobile Sensors</b><br>Ansgar Steland and Bart E. Pieters  | 3   |
|---|-----|
| Scale Invariant and Robust Pattern Identification in Univariate<br>Time Series, with Application to Growth Trend Detection in<br>Music Streaming Data<br>Nermina Mumic, Oliver Leodolter, Alexander Schwaiger,<br>and Peter Filzmoser | 25  |
| <b>Fine-Tuned Parallel Piecewise Sequential Confidence Interval</b><br><b>and Point Estimation Strategies for the Mean of a Normal</b><br><b>Population: Big Data Context</b><br>Nitis Mukhopadhyay and Chen Zhang                    | 51  |
| Statistical Learning for Change Point and Anomaly Detection<br>in Graphs<br>Anna Malinovskaya, Philipp Otto, and Torben Peters  | 85  |
| On the Robustness of Kernel-Based Pairwise Learning<br>Patrick Gensler and Andreas Christmann   | 111 |
| Global Sensitivity Analysis for the Interpretation of Machine<br>Learning Algorithms<br>Sonja Kuhnt and Arkadius Kalka  | 155 |
| <b>Improving Gaussian Process Emulators with Boundary Information</b><br>Zhaohui Li and Matthias Hwai Yong Tan  | 171 |

| Part II Challenges and Solutions in Applications   |     |
|--|-----|
| An Overview and General Framework for Spatiotemporal<br>Modeling and Applications in Transportation and Public Health<br>Lishuai Li, Kwok-Leung Tsui, and Yang Zhao  | 195 |
| Introduction to Wafer Tomography: Likelihood-Based Prediction<br>of Integrated-Circuit Yield<br>Michael Baron, Emmanuel Yashchin, and Asya Takken  | 227 |
| Uncertainty Quantification Based on Bayesian Neural Networks<br>for Predictive Quality<br>Simon Cramer, Meike Huber, and Robert H. Schmitt   | 253 |
| Two Statistical Degradation Models of Batteries Under Different<br>Operating Conditions<br>Jin-Zhen Kong and Dong Wang   | 269 |
| Detecting Diamond Breakouts of Diamond Impregnated Tools<br>for Core Drilling of Concrete by Force Measurements<br>Christine H. Müller, Hendrik Dohme, Dennis Malcherczyk, Dirk<br>Biermann, and Wolfgang Tillmann | 283 |
| Visualising Complex Data Within a Data Science Loop: A<br>Spatio-Temporal Example from Football<br>Leo N. Geppert, Katja Ickstadt, Fabian Karl, Jonas Münch, and Michael<br>Steinbrecher                           | 301 |
| Application of the Singular Spectrum Analysis onElectroluminescence Images of Thin-Film PhotovoltaicModulesEvgenii Sovetkin and Bart E. Pieters  | 321 |
| The Impact of the Lockdown Restrictions on Air Quality DuringCOVID-19 Pandemic in Lombardy, ItalyPaolo Maranzano and Alessandro Fassó  | 343 |
| Author Index   | 375 |