

# Preface

This volume contains a substantial number of the papers presented at the MODA 10 workshop in Łagów Lubuski, Poland, in June 2013; MODA here stands for *Model Oriented Data Analysis and Optimal Design*. Design of experiments (DOE) constitutes a powerful statistics-based methodology playing a major role in the knowledge discovery process in science and engineering. Data collection issues, including DOE, are at least as important as data analysis since they determine how much information data contain. No statistical modelling or analysis methods can extract information which the data do not contain, whereas a poor analysis can always be corrected later. Thus, haphazard experimentation may be very wasteful of resources, lead to needless repetition, poor inference and, where human subjects are concerned, may be ethically unsound.

The subject began in an agricultural context, but the theory and practice of DOE have become important in many scientific and technological fields, ranging from optimal designs for dynamical models in pharmacological research, to designs for industrial experimentation, to designs of simulation experiments in environmental risk management, to name but a few. DOE has become even more important in recent years, because of the increased speed of scientific developments, the complexity of the systems currently under investigation and the continuously increasing pressure on businesses, industries and scientific researchers to reduce product and process development times. This increased competition requires ever increasing efficiency in experimentation, thus necessitating new statistical designs.

A model-oriented view on DOE, which is the pivot of the MODA meetings, assumes some knowledge of the form of the data-generating process. It naturally leads to the so-called optimum design of experiments. This approach has the potential to revolutionize experimental programs of drug development and testing. Standard methods of DOE are no longer adequate and research into new ways of planning clinical and non-clinical trials for dose-finding is receiving close attention. In turn, applications of DOE in engineering often deal with large scale and highly complex systems where time and/or space are inevitable components. These applications may involve models in the form of ordinary differential, differential algebraic or partial differential equations. The underlying design space can be a class of input sequences

(time-domain analysis), a range of frequencies (frequency domain), a range of sampling intervals (sampling strategies), or a set of spatial sensor locations. As a result, factors continuously changing in time and/or space (e.g., temperature, pressure) can be taken into account. Relevant application areas are as diverse as control engineering, analytical chemistry, air sampling, atmospheric science and geophysical surveys.

Surprisingly, for a long time, the resources devoted to research on DOE have been rather limited. Partly, this was because the developments in different application areas and in different branches of mathematics had led to a fragmentation of the theory and practice of DOE. Leading European experts on DOE therefore decided to form the MODA group to bring together the different approaches, primarily through organizing special workshops. The initiative was a success and the scope of MODA rapidly expanded to countries far beyond Europe, including the USA, South Africa and India. MODA meetings are known for their friendly atmosphere, leading to fruitful discussions and collaboration. Since the beginning, they have also been aimed at giving junior researchers the opportunity of establishing personal contacts and work together with leading researchers. In order to guarantee a high-scientific level, participation is only by invitation of the board and meetings take place every third year. The proceedings are always published before the date of the meeting, to allow detailed and intelligent discussion.

Here is the list of previous MODA conferences:

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| 1. Eisenach, former GDR, 1987          | 6. Puchberg/Schneeberg, Austria, 2001 |
| 2. St. Kyrik monastery, Bulgaria, 1990 | 7. Heeze, The Netherlands, 2004       |
| 3. Petrodvorets, Russia, 1992          | 8. Almagro, Spain, 2007               |
| 4. Spetses, Greece, 1995               | 9. Bertinoro, Italy, 2010             |
| 5. Marseilles, France, 1998            |                                       |

Organization of the 10-th anniversary edition of the workshop has been conferred to the University of Zielona Góra in Poland, which hosts an active group of researchers at the Institute of Control and Computation Engineering, who are concerned with optimum experimental design for spatiotemporal processes. The workshop itself takes place in Łagów Lubuski, a small, picturesque town with much charm and atmosphere attracting artists and intellectuals. It is a long tradition of MODA workshops that they are organized in such relatively isolated places, far from the hustle and bustle of big cities. As this book clearly demonstrates, the present meeting once more brings together researchers from all over the world. These papers have undergone a complete review to ensure that contributions were significant and the manuscripts remain of high quality and clarity.

The papers presented in this volume cover a large spectrum of topics that are all well aligned with the scope of the workshop. They have been arranged in alphabetical order of author, but some patterns of topics emerge. A breakdown is as follows:

1. The most common theme is that of clinical trials. This arises both in the papers by Biswas, Banerjee and Mandal and, in the form of dose finding studies, in

- the papers by Flournoy, Galbete, Moler and Plo, by Magnusdottir, by Gao and Rosenberger and by Dragalin, as well as that by Ghiglietti and Paganoni.
2. Designs for linear and non-linear mixed-effects models are developed in the papers by Prus and Schwabe, and by Mielke and Schwabe, while an approximation of the information matrix in a similar setting is advanced by Leonov.
  3. Lifetime experiments with exponential distribution and censoring feature in the contribution by Müller. Calibration designs for an extended Rasch-Poisson counts model are outlined by Graßhoff, Holling and Schwabe. Optimal designs for log-linear regression test models are refined by Wang, Pepelyshev and Flournoy.
  4. The papers by Ginsbourger, Durrande, and Roustant, as well as by Chevalier, Ginsbourger, Bect and Molchanov describe improved designs for computer experiments.
  5. The topic of the paper by Atkinson and Bogacka is discrimination between models. Designs for model selection are also considered by Skubalska-Rafajłowicz and Rafajłowicz.
  6. The paper by Pázman and Pronzato deals with regularized optimality criteria for experimental design. In turn, some new information criteria are proposed in the paper by Ferrari and Borrotti.
  7. Algorithmic issues are thoroughly treated in the context of the KL-optimality criterion by Aletti, May and Tommasi, or in the more general case of minimax criteria by Nyquist. A related problem of numerically constructing optimal designs using the functional approach is studied by Melas, Krylova and Uciński. A new technique of generating optimal designs by means of simulation tapping into approximate Bayesian computation is proposed by Hainy, Müller and Wynn.
  8. Finally, a number of papers are strongly application-driven. Thus, Bischoff focuses on checking linear regression models taking time into account. Fackle-Fornius and Wänström construct minimax designs for contingent valuation experiments. Choice experiments for measuring how the attributes of goods or services influence preference judgments are studied by Großmann. Coetzer and Haines put forward designs for response surface models involving multiple mixture and process variables. Rafajłowicz and Rafajłowicz determine optimum input signals for processes modelled by partial differential equations. Designs for correlated observations in spatial models are exposed by Pepelyshev.

In our personal opinion, the papers in this volume make notable contributions to the state of the art in the field of model-based optimum experimental design. We hope the reader will share our point of view and find this volume very useful. We would like to acknowledge all the authors for their efforts in submitting high-quality papers. Last, but not least, we are also very grateful to the reviewers for their thorough and critical reviews of the papers within the short stipulated time.

Zielona Góra, Poland

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