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# Process Optimization

## A Statistical Approach

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# PROCESS OPTIMIZATION

## A Statistical Approach

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Quique.*

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# Preface

This book is intended as a textbook for a second course in experimental optimization techniques for industrial production processes and other “noisy” systems where the main emphasis is process optimization. This includes courses in “Response Surface Methods” and related topics. The book has outgrown from class notes of a graduate course that I have given for the past 10 years to Industrial Engineering and Operations Research students at Penn State University and at the University of Texas at Arlington. Typically, students come to this course with some background in either Design of Experiments (DOE) or Linear Regression. Many students also come to the course with a background in optimization methods. After teaching this course for several years based on other DOE and Response Surface Methods (RSM) books, it became clear the need for a book more suited to graduate engineering students, who learn about a wide variety of optimization techniques in other courses yet are somewhat disenchanted because there is no apparent connection between those optimization techniques and DOE/RSM.

The point of view of the book is to provide in the form of a text a contemporary account not only of the classical techniques and tools used in DOE and RSM but also to present relatively more advanced process optimization techniques from the recent literature which, perhaps due to lack of exposure or due to their young age, have not been used that much in industrial practice. The book contains a mix of technical and practical sections, appropriate for a first year graduate text in the subject or useful for self-study or reference.

For a person with a more traditional Statistics or Quality Engineering background, the present book will serve as a reference to techniques that

complement and extend basic process optimization techniques from DOE and RSM, including statistical issues that arise in process optimization, Bayesian methods for process optimization, and an introduction to Stochastic Approximation, Kriging methods and “computer experiment” techniques. For a person with an Operations Research background which includes mathematical programming techniques, the present book will not only serve as a guide to DOE and RSM, but will show how important statistical considerations need to be taken into account while optimizing a noisy process.

The book contents are as follows. After an introduction presented in Chapter 1, classical DOE and RSM topics are covered in Part II (Chapters 2 to 5). This includes DOEs for first and 2nd order models (including the concepts of D and G-optimality and an introduction to mixture models), and optimization of these models using classical RSM tools such as steepest ascent, “canonical” analysis, and “Ridge” analysis.

Part III (Chapters 6 to 8) treats the very important issue of sampling variability in an optimization problem where experimental data can vary randomly. Although considerable work has appeared on this subject in the last 15 years in the Statistics literature, this has found very little impact in applications. The effect of sampling variability in the steepest ascent procedure, on the location of the optimal settings, and on the eigenvalues of a quadratic model is discussed. Recent computational techniques for finding confidence regions on the location of the optimal operating conditions of a process are presented here. A discussion of the debate that evolved among opposing schools in design of experiments is presented here (the “bias vs. variance” debate).

Part IV (Chapters 9 and 10) discusses optimization methods that achieve solutions that are insensitive, or robust, to variations in factors that are not controllable. This is the so-called Robust Parameter Design (RPD) problem. A discussion of Split Plot design problems, where there are hard to vary factors in an experiment is included here, as RPD problems often have hard to vary factors. The idea of finding solutions that are not sensitive to variations in the assumed model has become a popular topic in the area of mathematical programming. An approach that uses ideas from robust optimization to solve optimization problems based on models fitted from data is presented in Chapter 10. It is shown that robust optimization methods are closely related to methods

for finding a confidence region in the optimal settings discussed in Chapter 7. Relation of these methods with stochastic programming problems is noted.

Parts I-IV contain what could be described as frequentist statistical techniques for process optimization. In contrast, Part V (Chapters 11 and 12) present recently developed Bayesian methods for process optimization. This is an extremely useful and unfortunately not well-known method for process optimization that resolves many of the issues regarding optimization of a multiple response process based on models fitted from data. First, an overview of Bayesian inference is presented. Then, optimization of single and multiple response systems from a Bayesian perspective is discussed based on the Bayesian multivariate regression model. These approaches provide a means for handling not only the uncertainty in the parameters of the assumed model, but the uncertainty in the model form itself. A Bayesian technique due to Gilmour and Mead for stopping a sequence of experiments based on the gains that are expected from running further experiments is presented. Finally, Bayesian Mixture optimization problems are also discussed. Matlab programs that implement most of the techniques discussed in this chapter are presented.

Part VI deals with design, modeling, and optimization techniques that have received a great deal of interest in recent years but that lie outside the mainstream of techniques usually considered within DOE and RSM. This includes computer experiments, a field with assumptions usually in strong contrast with classic RSM. An introduction to space filling designs and Kriging methods for computer experiments is provided. This part of the book also discusses recently developed stochastic optimization techniques based on stochastic approximation, in particular, Spall's simultaneous perturbation methods. An approach for testing the Karush-Khun-Tucker (KKT) optimality conditions in a problem where models are fitted to noisy responses is presented. Although the methodology presented was developed for optimization of simulated processes, this problem also occurs when optimizing a real or physical (i.e., non-simulated) process.

The book concludes with four appendices on the basics of linear regression, analysis of variance, matrices and optimality results, and statistical results used in Part V. Sections that contain material at a relatively more advanced level are labeled with a \*\*. To facilitate reading, all examples and proofs of theorems end with a ■. MATLAB and MAPLE programs that implement some of the

techniques discussed in the book and solutions to end of chapter problems will be posted on the author's personal web page.

As the Mexican writer Carlos Monsivais has said, one only realizes what one thinks in a topic until it sees it written down. I think such writing activity is very healthy in particular for a university faculty member as myself. Therefore, I would like to thank first of all Professor Fred Hillier for inviting me writing this book. I thank my graduate students who have endured the classes and the preliminary version of the notes on which this book is based. I wish to thank my coauthors and Ph.D. students in RSM topics in recent years: Dr. John J. Peterson (Glaxo SmithKline Beecham), Dr. Ramkumar Rajagopal (formerly at Intel Corp.), Dr. Guillermo Miró-Quesada (Eli-Lilly Co.), Dr. Suntara Cahya (Eli Lilly), Dr. John Semple (Southern Methodist University), and Professors Bert Bentovil and Jack Kleijnen (Tilburg University, The Netherlands). Professor Kleijnen was very kind in reading the chapters on Bayesian optimization, written while he acted as host during my sabbatical visit to his department. I also wish to thank Dr. R. Jean Ruth and Ms. Sharon Zielinski (General Motors R&D), Dr. Mani Janakiram (Intel Corp.), and Dr. Arnon Hurwitz (formerly at SEMATECH) with whom I have had the privilege of working in research related to process modeling and optimization funded by their organizations. I am also indebted to the National Science Foundation, who has been a major source of funding in the last 10 years.

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