GLOBAL POLYNOMIAL OPTIMIZATION TO COMPUTE THE G-SCORE OF A CANDIDATE DESIGN MATRIX GENERATED BY THE COORDINATE EXCHANGE ALGORITHM.

by

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ABSTRACT

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PUBLIC ABSTRACT

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CHAPTER 1

REVIEW OF G OPTIMAL DESIGNS ON THE HYPERCUBE

1.1

Introduction

Optimal experimental designs are found by minimizing or maximizing a specific function of the model information matrix. Optimal designs can offer distinct advantages, especially when experimental constraints necessitate efficiency and when the researcher can predefine the response surface model. For example, situations characterized by budgetary constraints, which limit the number of experimental trials, are especially well-suited for optimal designs. In such cases, researchers might focus on tailoring their experiments to optimize objective measures of 'goodness' within the confines of limited trials, rather than attempting to conform the experiment to classical designs.

The terminology associated with optimal design literature will now be introduced. Keeping with standard procedure for identifying optimal designs, we will work with the second-order model under standard assumptions. Let N represent the number of design points and K represent the number of experimental factors. Use $\mathbf{x}'$ to denote a design point, a $1 \times K$ row vector where each $x \in \mathbf{x}'$ specifies a factor level. Standard practice is to scale the feasible domain to $[-1, 1]$ so the space of all $\mathbf{x}'$ design points is the $\chi = [-1, 1]^K$ hypercube. The collection of N design points as rows in a matrix engenders the design matrix $\mathbf{X}$, an NK-dimensional hypercube. We denote

$$\mathbf{X} \in \bigtimes_{j=1}^{N} \chi = \bigtimes_{j=1}^{N} [-1, 1]^K = [-1, 1]^{NK} = \chi^N.$$

The second-order linear model contains $\binom{K+2}{2}$ linear coefficient parameters and is written in scalar form

$$y = \beta_0 + \sum_{i=1}^{K} \beta_i x_i + \sum_{i=1}^{K-1} \sum_{j=i+1}^{K} \beta_{ij} x_i x_j + \sum_{i=1}^{K} \beta_{ii} x_{ii}^2 + \epsilon,$$

or as

$$\mathbf{y} = \mathbf{F}\boldsymbol{\beta} + \boldsymbol{\epsilon}$$

in matrix-vector form. The standard ordinary least squares assumptions are imposed; $\boldsymbol{\epsilon} \sim \mathcal{N}_N(\mathbf{0}, \sigma^2 \mathbf{I}_N)$ where $\mathcal{N}_N$ is the N-dimensional multivariate normal distribution. $\mathbf{F}$, the $N \times p$ model matrix, is obtained from $\mathbf{X}$ through $\mathbf{F}(\mathbf{X})$. Rows in $\mathbf{F}$ are given by the expansion vector

$$\mathbf{f}'(\mathbf{x}_i') = (1 \quad x_{i1} \quad \dots \quad x_{ik} \quad x_{i1}x_{i2} \quad \dots \quad x_{i(K-1)}x_{iK} \quad x_{i1}^2 \quad x_{iK}^2).$$

$\mathbf{F}(\mathbf{X})$ and $\mathbf{F}$ are used interchangeably in literature, but it should be clear that $\mathbf{F}$ is always a function of $\mathbf{X}$.

The ordinary least squares estimator of $\boldsymbol{\beta}$ is $\hat{\boldsymbol{\beta}} = (\mathbf{F}'\mathbf{F})^{-1}\mathbf{F}'\mathbf{y}$, which has variance $\text{Var}(\hat{\boldsymbol{\beta}}) = \sigma^2(\mathbf{F}'\mathbf{F})^{-1}$. Both $\hat{\boldsymbol{\beta}}$ and $\text{Var}(\hat{\boldsymbol{\beta}})$ are expressed as quantities of $\mathbf{F}'\mathbf{F}$, the total information matrix. Because of its ubiquitoutness, let $\mathbf{M}(\mathbf{X}) = \mathbf{F}'\mathbf{F}$. All optimal design objective criteria are dependent on total information matrix, so it is of considerable importance to the field [cite].

1.2

G-Optimality

CHAPTER 2

LITERATURE REVIEW: GUM, THE GUIDE TO UNCERTAINTY IN METROLOGY

Content

CHAPTER 3

UNCERTAINTY PROPAGATION FOR THE FREML MODEL VIA PARAMETRIC BOOTSTRAPPING FOR KNOWN AND REPORTED MEASUREMENT UNCERTAINTIES

Content

3.1

Section Title

Content

Theorem (Example)**.** *Very important theorem that is named and unnumbered*

Theorem 1. *Very important numbered theorem*

Proof. Very difficult proof.

Case 1. A part of the Proof.

Case 2. Another part of the proof.

□

3.1.1

Subsection Title

Lemma 1. *A numbered lemma*

Lemma. *An unnumbered lemma*

Definition (thing)**.** A definition of thing.

CHAPTER 4

EXTENSION OF THE FREML MODEL AND MAXIMUM-LIKELIHOOD ESTIMATION PROCEDURE WHEN MEASUREMENT UNCERTAINTIES ARE ESTIMATED AND REPORTED WITH A STATED DEGREES-OF-FREEDOM

CHAPTER 5

METHOD VALIDATION

CHAPTER 6

APPLICATION TO CASE STUDIES FROM THE CHEMISTRY AND METROLOGY LITERATURE

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APPENDICES

APPENDIX A

Appendix Subtitle.

Appendix content. (note that if you only have a single appendix it does not need to be label as Appendix A. You can just label it Appendix.)

APPENDIX B

Appendix Subtitle.

Content.