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Monotonic Metamodels for Deterministic Computer Experiments P. 1-10
Matthias Hwai Yong Tan

Abstract
In deterministic computer experiments, it is often known that the output is a monotonic function of some of the inputs. In these cases, a monotonic metamodel will tend to give more accurate and interpretable predictions with less prediction uncertainty than a nonmonotonic metamodel. The widely used Gaussian process (GP) models are not monotonic. A recent article in *Biometrika* offers a modification that projects GP sample paths onto the cone of monotonic functions. However, their approach does not account for the fact that the GP model is more informative about the true function at locations near design points than at locations far away. Moreover, a grid-based method is used, which is memory intensive and gives predictions only at grid points. This article proposes the weighted projection approach that more effectively uses information in the GP model together with two computational implementations. The first is isotonic regression on a grid while the second is projection onto a cone of monotone splines, which alleviates problems faced by a grid-based approach. Simulations show that the monotone B-spline metamodel gives particularly good results. Supplementary materials for this article are available online.

Sliced Full Factorial-Based Latin Hypercube Designs as a Framework for a Batch Sequential Design Algorithm P. 11-22
Weitao Duan, Bruce E. Ankenman, Susan M. Sanchez & Paul J. Sanchez

Abstract
When fitting complex models, such as finite element or discrete event simulations, the experiment design should exhibit desirable properties of both projectivity and orthogonality. To reduce experimental effort, sequential design strategies allow experimenters to collect data only until some measure of prediction precision is reached. In this article, we present a batch sequential experiment design method that uses sliced full factorial-based Latin hypercube designs (sFFLHDs), which are an extension to the concept of sliced orthogonal array-based Latin hypercube designs (OALHDs). At all stages of the sequential design, good univariate stratification is achieved. The structure of the FFLHDs also tends to produce uniformity in higher dimensions, especially at certain stages of the design. We show that our batch sequential design approach has good sampling and fitting qualities through both empirical studies and theoretical arguments. Supplementary materials are available online.

Joint Identification of Location and Dispersion Effects in Unreplicated Two-Level Factorials P. 23-35
Andrew J. Henrey & Thomas M. Loughin

Abstract
Most procedures that have been proposed to identify dispersion effects in unreplicated factorial designs assume that location effects have been identified correctly. Incorrect identification of location effects may impair subsequent identification of dispersion effects. We develop a method for joint identification of location and dispersion effects that

can reliably identify active effects of both types. A normal-based model containing parameters for effects in both the mean and variance is used. Parameters are estimated using maximum likelihood, and subsequent effect selection is done using a specially derived information criterion. An exhaustive search through a limited version of the space of possible models is conducted. Both a single-model output and model averaging are considered. The method is shown to be capable of identifying sensible location-dispersion models that are missed by methods that rely on sequential estimation of location and dispersion effects. Supplementary materials for this article are available online.

Design and Analysis of Experiments on Nonconvex Regions P. 36-47

Matthew T. Pratola, Ofir Harari, Derek Bingham & Gwenn E. Flowers

Abstract

Modeling a response over a nonconvex design region is a common problem in diverse areas such as engineering and geophysics. The tools available to model and design for such responses are limited and have received little attention. We propose a new method for selecting design points over nonconvex regions that is based on the application of multidimensional scaling to the geodesic distance. Optimal designs for prediction are described, with special emphasis on Gaussian process models, followed by a simulation study and an application in glaciology. Supplementary materials for this article are available online.

Benefits and Fast Construction of Efficient Two-Level Foldover Designs P. 48-57

Anna Errore, Bradley Jones, William Li & Christopher J. Nachtsheim

Abstract

Recent work in two-level screening experiments has demonstrated the advantages of using small foldover designs, even when such designs are not orthogonal for the estimation of main effects (MEs). In this article, we provide further support for this argument and develop a fast algorithm for constructing efficient two-level foldover (EFD) designs. We show that these designs have equal or greater efficiency for estimating the ME model versus competitive designs in the literature and that our algorithmic approach allows the fast construction of designs with many more factors and/or runs. Our compromise algorithm allows the practitioner to choose among many designs making a trade-off between efficiency of the main effect estimates and correlation of the two-factor interactions (2FIs). Using our compromise approach, practitioners can decide just how much efficiency they are willing to sacrifice to avoid confounded 2FIs as well as lowering an omnibus measure of correlation among the 2FIs.

Optimization of Multi-Fidelity Computer Experiments via the EQIE Criterion P. 58-68

Xu He, Rui Tuo & C. F. Jeff Wu

Abstract

Computer experiments based on mathematical models are powerful tools for understanding physical processes. This article addresses the problem of kriging-based optimization for deterministic computer experiments with tunable accuracy. Our approach is to use multi-fidelity computer experiments with increasing accuracy levels and a nonstationary Gaussian process model. We propose an optimization scheme that sequentially adds new computer runs by following two criteria. The first criterion, called EQI, scores candidate inputs with given level of accuracy, and the second criterion, called EQIE, scores candidate combinations of inputs and accuracy. From simulation results and a real example using finite element analysis, our method outperforms the expected improvement (EI) criterion that works for single-accuracy experiments. Supplementary materials for this article are available online.

Two-Level Designs to Estimate All Main Effects and Two-Factor Interactions P. 69-79

Pieter T. Eendebak & Eric D. Schoen

Abstract

We study the design of two-level experiments with N runs and n factors large enough to estimate the interaction model, which contains all the main effects and all the two-factor interactions. Yet, an effect hierarchy assumption suggests that main effect estimation should be given more prominence than the estimation of two-factor interactions. Orthogonal arrays (OAs) favor main effect estimation. However, complete enumeration becomes infeasible for cases relevant for practitioners. We develop a partial enumeration procedure for these cases and we establish upper bounds on the D-efficiency for the interaction model based on arrays that have not been generated by the partial enumeration. We also propose an optimal design procedure that favors main effect estimation. Designs created with this procedure have smaller D-efficiencies for the interaction model than D-optimal designs, but standard errors for the main effects in this model are improved. Generated OAs for 7–10 factors and 32–72 runs are smaller or have a higher D-efficiency than the smallest OAs from the literature. Designs obtained with the new optimal design procedure or strength-3 OAs (which have main effects that are not correlated with two-factor interactions) are recommended if main effects unbiased by possible two-factor interactions are of primary interest. D-optimal designs are recommended if interactions are of primary interest. Supplementary materials for this article are available online.

Calibration of Stochastic Computer Simulators Using Likelihood Emulation P. 80-92

Jeremy E. Oakley & Benjamin D. Youngman

Abstract

We calibrate a stochastic computer simulation model of “moderate” computational expense. The simulator is an imperfect representation of reality, and we recognize this discrepancy to ensure a reliable calibration. The calibration model combines a Gaussian process emulator of the likelihood surface with importance sampling. Changing the discrepancy specification changes only the importance weights, which lets us investigate sensitivity to different discrepancy specifications at little computational cost. We present a case study of a natural history model that has been used to characterize UK bowel cancer incidence. Datasets and computer code are provided as supplementary material.

Nonstationary Gaussian Process Models Using Spatial Hierarchical Clustering from Finite Differences P. 93-101

Matthew J. Heaton, William F. Christensen & Maria A. Terres

Abstract

Modern digital data production methods, such as computer simulation and remote sensing, have vastly increased the size and complexity of data collected over spatial domains. Analysis of these large spatial datasets for scientific inquiry is typically carried out using the Gaussian process. However, nonstationary behavior and computational requirements for large spatial datasets can prohibit efficient implementation of Gaussian process models. To perform computationally feasible inference for large spatial data, we consider partitioning a spatial region into disjoint sets using hierarchical clustering of observations and finite differences as a measure of dissimilarity. Intuitively, directions with large finite differences indicate directions of rapid increase or decrease and are, therefore, appropriate for partitioning the spatial region. Spatial contiguity of the resulting clusters is enforced by only clustering Voronoi neighbors. Following spatial clustering, we propose a nonstationary Gaussian process model across the clusters, which allows the computational burden of model fitting to be distributed across multiple cores and nodes. The methodology is primarily motivated and illustrated by an application to the validation of digital temperature data over the city of Houston as well as simulated datasets. Supplementary materials for this article are available online.

Anomaly Detection in Images With Smooth Background via Smooth-Sparse Decomposition P. 102-114

Hao Yan, Kamran Paynabar & Jianjun Shi

Abstract

In various manufacturing applications such as steel, composites, and textile production, anomaly detection in noisy images is of special importance. Although there are several methods for image denoising and anomaly detection, most of these perform denoising and detection sequentially, which affects detection accuracy and efficiency. Additionally, the low computational speed of some of these methods is a limitation for real-time inspection. In this article, we develop a novel methodology for anomaly detection in noisy images with smooth backgrounds. The proposed method, named smooth-sparse decomposition, exploits regularized high-dimensional regression to decompose an image and separate anomalous regions by solving a large-scale optimization problem. To enable the proposed method for real-time implementation, a fast algorithm for solving the optimization model is proposed. Using simulations and a case study, we evaluate the performance of the proposed method and compare it with existing methods. Numerical results demonstrate the superiority of the proposed method in terms of the detection accuracy as well as computation time. This article has supplementary materials that includes all the technical details, proofs, MATLAB codes, and simulated images used in the article.

Estimation of Field Reliability Based on Aggregate Lifetime Data P. 115-125

Piao Chen & Zhi-Sheng Ye

Abstract

Because of the exponential distribution assumption, many reliability databases recorded data in an aggregate way. Instead of individual failure times, each aggregate data point is a summation of a series of collective failures representing the cumulative operating time of one component position from system commencement to the last component replacement. The data format is different from traditional lifetime data and the statistical inference is challenging. We first model the individual component lifetime by a gamma distribution. Confidence intervals for the gamma shape parameter can be constructed using a scaled χ^2 approximation to a modified ratio of the geometric mean to the arithmetic mean, while confidence intervals for the gamma rate and mean parameters, as well as quantiles, are obtained using the generalized pivotal quantity method. We then fit the data using the inverse Gaussian (IG) distribution, a useful lifetime model for failures caused by degradation. Procedures for point estimation and interval estimation of parameters are developed. We also propose an interval estimation method for the quantiles of an IG distribution based on the generalized pivotal quantity method. An illustrative example demonstrates the proposed inference methods. Supplementary materials for this article are available online.