# DAE 2017 INVITED TALKS

— Day 1: Thursday, October 12, 2017 —

#### Session 1. INTERNET EXPERIMENTS

Organizer and Chair: David Steinberg, Tel Aviv University, Israel

## **Thompson Sampling for Infinite Armed Bandits**

Steven Scott, Google

Abstract: Thompson sampling is a heuristic for managing the explore-exploit tradeoff in multi-armed bandit problems. The algorithm works by serving arms at random according to their Bayesian posterior probability of having the largest mean reward. If the catalog of available arms is very large then direct Thompson sampling is infeasible. However, the algorithm can be modified by embedding the reward distributions for individual arms into a Bayesian hierarchical model. At time t the choice is to play one of the current arms or sample a new arm. The optimal arm probabilities for previously observed arms are determined as with ordinary Thompson sampling, while the probability of playing a new arm is given by the probability that a randomly chosen element from the prior distribution in the hierarchical model is superior to the the largest of the previously observed arms. The new algorithm is just as flexible as ordinary Thompson sampling in the sense that it can be used with regression based reward distributions. I will present simulations illustrating its performance.

Keywords: Multi-armed bandit, sequential experimental design

## Sliced Designs for Multi-Platform Online Experiments

Soheil (Sol) Sadeghi, Microsoft Corporation

Coauthor(s): Peter Qian, Neeraj Arora

Abstract: Multivariate testing is a popular method to improve websites, mobile apps, and email campaigns. A unique aspect of testing in the online space is that it needs to be conducted across multiple platforms such as a desktop and a smartphone. The existing experimental design literature does not offer precise guidance for such a multi-platform context. In this paper, we introduce a multi-platform design framework that allows us to measure the effect of the design factors for each platform and the interaction effect of the design factors with platforms. Substantively, the resulting designs are of great importance for testing digital campaigns across platforms. We illustrate this in an empirical email application to maximize engagement for a digital magazine. We introduce a novel "sliced effect hierarchy principle" and develop design criteria to generate factorial designs for multi-platform experiments. To help construct such designs, we prove two theorems that connect the proposed designs to the well-known minimum aberration designs. We find that experimental versions made for one platform should be similar to other platforms. From the standpoint of real world application, such homogeneous sub-designs are cheaper to implement. To assist practitioners, we provide two algorithms to construct the designs that we propose. We also tabulate sliced factorial designs with 16, 32, and 64 runs for four-platform experiments.

Keywords: A/B testing; design of experiments; blocking; digital marketing; email testing; web experiments

## Trustworthy analysis of online A/B tests: Pitfalls, challenges and solutions

### Jiannan Lu, Microsoft Corporation

## Coauthor(s): Alex Deng, Jonathan Litz

*Abstract*: A/B testing plays an integral role in the research and development cycles at Microsoft. In this talk, we'll first provide a high-level picture of the experimentation pipeline at Microsoft, focusing on challenges from treatment assignment, log instrumentation, and data analytics. We will next discuss two case studies where statistical science can be employed to ensure trustworthy analysis and interpretation of online A/B tests. The first case shows how classic survey sampling can help solve a challenging engineering problem, where the treatment assignment is, although random, complicated or even unknown. The second case highlights how we can leverage our rich historical experimental results to conduct Bayesian analyses of future experiments. Simulated and empirical examples will be provided to demonstrate our methodologies.

Keywords: Causal inference; randomization unit; random effect; delta method; asymptotic variance

#### Session 2. Computational methods in design of experiments

Organizer and Chair: Dave Woods, University of Southampton, UK

## New methods for approximating the expected utility in Bayesian design for nonlinear models Yiolanda Englezou, University of Southampton, UK

Coauthor(s): David Woods, Tim Waite

*Abstract*: The estimation of empirical and physical models is often performed using data collected via experimentation. Hence, the design of the experiment is crucial in determining the quality of the results. For complex models, an optimal design often depends on features, particularly model parameters, which are uncertain prior to experimentation. This dependence leads naturally to a Bayesian approach which can (a) make use of any prior information on these features, and (b) be tailored to the reduction of posterior uncertainty.

Optimal Bayesian design for most realistic models is complicated by the need to approximate an analytically intractable expected utility; for example, the expected gain in Shannon information from the prior to posterior distribution. For models which are nonlinear in the uncertain parameters, this expected gain must be approximated numerically. The standard approach employs "double-loop" Monte Carlo integration using nested sampling from the prior distribution. Although this method is easy to implement, it produces biased approximations and is computationally expensive.

In this talk, we will describe, assess and compare some recent alternatives to simple Monte Carlo sampling from the prior for the approximation of expected utilities. The presented methods include combinations of features from importance sampling and Laplace approximations. Assessments will include both computational cost and the statistical qualities of the resulting approximations.

Keywords: Shannon information gain, Importance sampling, Laplace approximation

# The Construction of Missing-Robust Experimental Designs and their Comparison to Classical and Optimal Designs

Byran Smucker, Miami University (Oxford, OH)

*Coauthor(s)*: Willis Jensen, Zichen Wu, and Bo Wang

Abstract: Missing observations are not uncommon in real-world experiments. Consequently, the robustness of an experimental design to one or more missing runs is an important characteristic of the design. In contrast to most of the literature in this area, we generate designs based on a missing-robustness criterion. This criterion is related to the expected value of the D-criterion, under the assumption that a run will be unusable with some probability. The connection to the D-criterion allows some computational advantages as we adapt the coordinate exchange algorithm to this setting. We examine two-level designs as well as response surface experiments, and compare the missing-robust designs to classical and optimal designs in terms of several robustness measures, including their D- and/or I-efficiencies when up to three runs are missing. *Keywords*: missing observations; robustness; optimal design

## Computation of Optimal Experimental Design for Estimating Conditional Effects

# Bradley Jones, JMP Division/SAS

Coauthor(s): Peter Goos

Abstract: A common occurrence in practical design of experiments is that one factor can only be varied for some but not all the levels of another factor. It is preferable to perform one experiment that allows for assessing the effects of both factors. Clearly, the effect of one factor then is conditional on the levels of the other factor for which it can be varied. This presentation provides several examples of this kind of problem and an algorithm for generating an optimal design for a sensible model for each case. *Keywords*: conditional effect, contingent factor, coordinate exchange algorithm

Session 3. New Applications of Factorial Experiments

Organizer and Chair: Jessica Jaynes, California State University, Fullerton

## **Order of Addition Modeling**

Robert Mee, University of Tennessee

*Abstract*: The literature on order of addition experiments has relied on first-order models constructed from pair-wise ordering factors. This article defines second-order and higher-order terms based on interactions of the pairwise factors. Order-of-addition orthogonal arrays, as defined by Voelkel (2017), are optimal for fitting the first order model, but they differ in terms of their susceptibility to bias due to model misspecification. A measure computed from the alias matrix is proposed to identify better designs, and illustrated for cases with four and five components.

Keywords: Alias matrix, mixture experiment, model misspecification, orthogonal array, second-order model

## Application of Kriging Models for a Drug Combination Experiment on Lung Cancer

Qian Xiao, University of Georgia

## Coauthor(s): Lin Wang, Hongquan Xu

*Abstract*: The study of combinatorial drugs requires efficient experimental designs and proper follow-up statistical modelling techniques. Linear and non-linear models are often used in analyzing such biological experiments. We propose the use of Kriging models to better depict the response surfaces of combinatorial drugs. We further study how proper experimental designs can reduce the required number of runs. We illustrate our method via a combinatorial drug experiment on lung cancer. We demonstrate that only 27 runs are needed to predict all 512 runs in the original experiment and achieve better precision than existing methods.

Keywords: Kriging models, Experimental designs, Combinatorial drugs, response surface.

## Using blocked fractional factorial designs to construct discrete choice experiments

## Jessica Jaynes, California State University, Fullerton

*Coauthor(s)*: Pimbucha Rusmevichientong; Weng Kee Wong; Hongquan Xu

Abstract: A discrete choice experiment (DCE) is a survey method that gives insight into individual preferences for particular attributes. They provide a rich source of data to assess real-life decision-making processes, which involve trade-offs between desirable characteristics. Traditionally, methods for constructing DCEs focus on identifying the individual effect of each attribute. However, an interaction effect between two attributes better represents real-life trade-offs, and provides us a better understanding of subjects' competing preferences. The choice of the design for a DCE is critical because it determines which attributes' effects and their interactions are identifiable. We propose the use of blocked fractional factorial designs to construct DCEs and address some identification issues by utilizing the known structure of blocked fractional factorial designs. These designs are easy to construct and for many practical scenarios are readily available in the literature. Further, we discuss the implementation of our design methodology with an application in health sciences pertaining to college students' snack selection and nutritional ingredient attributes.

*Keywords*: Blocked fractional factorial design; Discrete choice experiments; Health Sciences; Nutritional ingredients

## Session 4. DESIGNS FOR NON-NORMAL DATA

Organizer and Chair: Abhyuday Mandal, University of Georgia

#### **Robust Dose-level Designs for Binary Responses**

Wanchunzi Yu, Arizona State University

## Coauthor(s): John Stufken

*Abstract*: The estimation of a benchmark dose (BMD) is a common objective in environmental risk analysis. In a BMD estimation study, measurements are taken at different dose levels for a pollutant of interest. These dose levels need to be selected in a controlled experiment, which is a design problem. However, few design strategies have been developed for BMD estimation, especially with consideration of model uncertainty and misspecification. We propose a weighted c-efficiency criterion to obtain a design, which is robust with respect to various risk functions simultaneously for BMD estimation. In simulation studies using particle swarm optimization (PSO) and 8 weighted possible models, efficient designs are found. The proposed method for identifying robust designs is also demonstrated through the mammalian carcinogenicity of cumene  $(C_9H_{12})$ example.

Keywords: Robust designs; Locally optimal designs; Generalized linear models; Benchmark analysis

#### Constructing Efficient Designs for a Ballooned Beta-Logistic Model in Toxicology

Seung Won Hyun, North Dakota State University

Coauthor(s): Weng Kee Wong

Abstract: We study the dose response relationship of sea urchin treated by different doses of trimethoprim and show that the sigmoid response curve exhibits inhomogeneous variances on the responses. The Ballooned Beta-Logistic (BBL) model was recently proposed by Yi, Flournoy, and Kpamegan (2017) and we show it provides a much better fit than several of its competitors. The BBL model is flexible yet relatively understudied, especially on its design issues. In this paper, we construct various types of efficient designs for the BBL model using optimal design theory. In particular, we note that for some nominal values, the optimal designs do not exist unless restrictions are placed on the parameter values. We also investigate robustness properties of optimal designs to the nominal parameter values and evaluate the efficiency of the actual experimental design used in the sea urchin study.

Keywords: Approximate Design, D-optimality, Heteroscedasticity, Locally Optimal, Nominal Value

## D-optimal Designs for Multinomial Logistic Models

Jie Yang, University of Illinois at Chicago

Coauthor(s): Xianwei Bu, Dibyen Majumdar

Abstract: We consider optimal designs for fairly general multinomial logistic models, which covers baselinecategory, cumulative, adjacent-categories, and continuation-ratio logit models, with proportional odds, nonproportional odds, or partial proportional odds assumption. We derive the corresponding Fisher information matrices in three different forms to facilitate their calculation, the determination of their positive definiteness, and the search for optimal designs, respectively. We conclude that unlike the designs for binary responses, a feasible design for a multinomial logistic model may contain much less experimental settings than parameters, which is of practical significance. We also conclude that even for a minimally supported design, a uniform allocation, which is typically used in practice, is not optimal for a multinomial logistic model in general. We develop efficient algorithms for searching D-optimal designs. We show by real experiments that the efficiency of an experiment can be significantly improved if our designs are adopted.

*Keywords*: Approximate design, exact design, Fisher information matrix, multinomial response, minimally supported design, lift-one algorithm

# DAE 2017 INVITED TALKS

— Day 2: Friday, October 13, 2017 —

Session 5. DESIGN AND ANALYSIS OF COMPUTER EXPERIMENTS Organizer and Chair: Peter Qian, University of Wisconsin-Madison

# Data farming research: opportunities for the design and analysis of large-scale simulation experiments

# Susan Sanchez, The Naval Postgraduate School

*Abstract*: The ready availability of computing power has fundamentally changed the way simulation and other computational models can be used to provide insights to decision makers. Nonetheless, there are many opportunities for research methods that could further enhance this process. I will provide an overview of the current state-of-the-art in data farming, which has already yielded great benefits for a variety of applications in defense and national security. I will then describe several key areas where additional research could lead to substantive near-term improvements on the large-scale simulation experiments are designed and analyzed. My goal is to convince simulation practitioners to apply data farming techniques to their upcoming simulation studies, and to stimulate methodological research in this area.

# A Stochastic Process Approach to Generating Designs

# Matthew Pratola, The Ohio State University

Abstract: Statistical design of experiments is a fundamental topic in applied statistics with a long history. Yet its application is often limited by the complexity and costliness of constructing experimental designs in the first place. For example, in optimal design, constructing the designed experiment involves searching the high-dimensional input space - a computationally expensive procedure that only guarantees a locally optimal solution. This is a hard problem that, typically, can only be "simplified" by changing the optimality criterion to be based on a simpler model. Such approximations are sometimes justifiable but rarely broadly desirable. In this work, we introduce a novel approach to the challenging design problem. We will take a probabilistic view of the problem by representing the optimal design as being one element (or a subset of elements) of a probability space. Given a suitable distribution on this space, a generative process can be specified from which stochastic design realizations can be drawn. We describe two scenarios where the classical (point estimate) optimal design solution coincides with the mode of the generative process we specify. We conclude with outlining an algorithm for drawing such design realizations and applying it to a few simple examples.

# Predictive Distribution for Gaussian Process Models with Design-Based Subagging

## Linglin He, Rutgers University

#### *Coauthor(s)*: Ying Hung

*Abstract*: Gaussian process (GP) models are widely used in the analysis of computer experiments. Based on an efficient design-based GP model developed by Hung and Zhao (2017), we construct a bootstrap predictive distribution. The new bootstrap procedure borrows the strength of space-filling designs to reduce computational complexity and the predictive distribution can be used to capture the prediction uncertainty. Theoretical properties of the bootstrap predictors will be discussed.

Keywords: Gaussian process, Predictive distribution, Space-filling design

## Session 6. RECENT ADVANCES IN ORTHOGONAL ARRAYS AND COVERING ARRAYS

Organizer and Chair: Frederick Phoa, Academia Sinica, Taiwan

## Strong Orthogonal Arrays of Strength Two Plus

Boxin Tang, Simon Fraser University, Canada

*Coauthor(s)*: Yuanzhen He and Ching-Shui Cheng

Abstract: Strong orthogonal arrays were recently introduced and studied in He and Tang (2013) as a class of space-filling designs for computer experiments. To enjoy the benefits of better space-filling properties, when

compared to ordinary orthogonal arrays, strong orthogonal arrays need to have strength three or higher, which may require run sizes that are too large for experimenters to afford. To address this problem, we introduce a new class of arrays, called strong orthogonal arrays of strength two plus. These arrays, while being more economical than strong orthogonal arrays of strength three, still enjoy the better two-dimensional space-filling property of the latter. Among the many results we have obtained on the characterizations and construction of strong orthogonal arrays of strength two plus, worth special mention is their intimate connection with second order saturated designs.

Keywords: complementary design; computer experiment; Latin hypercube; second order saturated design; space-filling design

# Geometric Orthogonal Array (GOA): A new class of space-filling designs with good uniformities in multiple dimensions

Frederick Kin Hing Phoa, Academia Sinica, Taiwan

Coauthor(s): Cheng-Yu Sun, Shaowei Cheng

Abstract: This paper introduces a new class of space-filling designs optimized under a new multi-dimensional space-filling property called *geometric strength*. We propose a systematic construction method via techniques in Galois field for this new class of designs. In specific, the factor levels in a regular design are collapsed and the strength of the collapsed design is enhanced. The reversed process to relabel factor levels of the regular design improves its space-filling property. This method is more efficient than the existing methods via level permutations, especially when the number of factor levels is large. When two collapsers are indistinguishable in terms of the strength of the collapsed designs, we propose a new criterion called maximal strength efficiency. It not only maximizes the strength of the collapsed design, but also maximizes the proportion of the projected sub-designs that are full factorials.

Keywords: Space-Filling Designs, Factor Subgroup Collapse, Galois Field, Geometric Strength, Maximal Strength Efficiency

# High Index Covering Array: A Useful Class of Cost-Efficient and Outlier-Resistant Designs With Repeated Tuple Observations

Yasmeen Akhtar, Academia Sinica, Taiwan

Coauthor(s): Frederick Kin Hing Phoa

Abstract: Orthogonal array has been well-known for its applications in designing factorial experiments. Its existence is restricted as all tuples appear in equal number of times, and it guarantees a standardized estimation on the response variations associated with all tuples. On the other hands, covering array of  $\lambda = 1$  is an important class of designs in hardware and software testings. Its existence is less restrictive as all tuples only need to appear at least once, but the responses associated to tuples with only one observation lack the measure on variations and the ability to resist outliers. To bridge the wide spectrum from two extreme settings (orthogonal arrays and covering arrays of  $\lambda = 1$ ) in terms of the number of repeated measures of tuples, we construct a useful class of experimental designs, namely the covering arrays of  $\lambda$  (CA<sub> $\lambda$ </sub>), where  $\lambda > 1$ . It allows experimenters to adjust their required  $\lambda$  parameter so that all tuples in the resulting  $CA_{\lambda}$ appear at least  $\lambda$  times. Given the number of factors of interest,  $CA_{\lambda}$  utilizes less resources than an orthogonal array and gains the ability to resist outliers that a traditional  $CA_1$  fails to achieve. We theoretically study the properties of  $CA_{\lambda}$ , and develop a systematic method to construct families of  $CA_{\lambda}$  with small run sizes under different number of factors, number of levels, strength and  $\lambda$ .

*Keywords*: Orthogonal arrays, Covering arrays

# Session 7. INFERENCE FOR ADAPTIVE DESIGNS

Organizer and Chair: Nancy Flournoy, University of Missouri

# Blinded and Unblinded Sample Size Recalculation for generalized linear models

Sergev Tarima, Medical College of Wisconsin

Abstract: We introduce a design re-sampling framework for approximating distributions of quantities of

interest in the presence of nuisance parameters in pre-planned adaptive designs. We apply design resampling for sample size re-estimation (SSR) for likelihood ratio tests in Linear, Logistic and Poisson multiple regression models in blinded and unblinded manner. At the interim analysis, the sample size recalculation procedure resamples the whole study design to find a total sample size and a new critical value. As shown in our Monte-Carlo simulation studies this re-sampling method shows more accurate control of type I error and power when compared with naive sample size recalculation. The naive sample size recalculation uses Z-test based sample size formula relying on asymptotic normality of maximum likelihood estimators. This resampling procedure for SSR allows researchers to spend less resources than the naive SSR while it asymptotically secures the pre-determined type I error and power against a local alternative. *Keywords*: sample size recalculation; adaptive designs; nuisance parameters

## Adaptive Procedures for Optimum Observed Fisher Information

Adam Lane, Cincinnati Children's Hospital Medical Center

Abstract: Expected Fisher information can be found a priori and as a result its inverse is the primary variance approximation used in the design of experiments. This is in contrast to the common claim that the inverse of observed Fisher information is a better estimate of the variance of the maximum likelihood estimator (MLE). Observed Fisher information cannot be known a priori, however, if an experiment is conducted sequentially (in a series of runs) the observed Fisher information from previous runs is available. In the current work adaptive procedures are proposed that use the observed Fisher information from previous runs to inform the design of the current run. Designing experiments using observed Fisher information instead of expected Fisher information provides a better connection between the design and analysis of the experiment. In order to evaluate designs with respect to observed Fisher information an upper bound is developed. The error bound on observed efficiency related to this upper bound is investigated. Conditions are given in order for adaptive procedure to achieve second order observed efficiency. This is compared to the optimal design which has only first order observed efficiency. If the model is in translation family conditions are given such that the conditional variance of the MLE following the proposed procedures have second order efficiency. Once again compared to first order efficiency of the conditional variance of MLE for the optimal design. *Keywords*: Adaptive Design, Observed Information, efficiency,

# Optimal Adaptive Subsampling under the A-optimality Criterion for Logistic Regression

#### Haiying Wang, University of Connecticut

Abstract: For massive data, the family of subsampling algorithms is popular to downsize the data volume and reduce computational burden. Existing studies focus on approximating the ordinary least squares estimate in linear regression, where statistical leverage scores are often used to define subsampling probabilities. In this paper, we propose fast subsampling algorithms to efficiently approximate the maximum likelihood estimate in logistic regression. We first establish consistency and asymptotic normality of the estimator from a general subsampling algorithm, and then derive optimal subsampling probabilities that minimize the asymptotic variance of the resultant estimator under the A-optimality criterion. An alternative minimization criterion is also proposed to further reduce the computational cost. The optimal subsampling probabilities depend on the full data estimate, so we develop a two-step adaptive algorithm to approximate the optimal subsampling procedure. This algorithm is computationally efficient and has a significant reduction in computing time compared to the full data approach. Consistency and asymptotic normality of the estimator from the adaptive algorithm are also established. Synthetic and real data sets are used to evaluate the practical performance of the proposed method.

Keywords: A-optimality; Logistic Regression; Massive Data; Optimal Subsampling; Rare Event

## Session 8. COMPUTER EXPERIMENTS AND UNCERTAINTY QUANTIFICATION

*Organizer:* Ying Hung, Rutgers University *Chair:* C. Devon Lin, Queen's University, Canada

Exact Knowledge Gradient-Based Sequential Data collection for Optimal Decision Making

Qiong Zhang, Virginia Commonwealth University

## *Coauthor(s)*: Youngdeok Hwang

Abstract: Optimization using stochastic computer experiments is commonplace in engineering and industry. This article addresses the problem of optimization, in which the input space of stochastic computer model is continuous, whereas the decision space in real problems is restricted to be finite. We propose a new Bayesian sequential data collection method based on exact knowledge gradient for optimal decision making. We demonstrate the benefit of our proposed methodology, comparing with the existing model-based optimization methods.

Keywords: Sequential design; Fixed-rank kriging; Gaussian process; Model-based optimization

# Invariance-Preserving Emulation for Computer Models, with Application to Structural Energy Prediction

## Peter Qian, University of Wisconsin-Madison

Abstract: Computer models with invariance properties appear frequently in materials science, physics, biology and other fields. These properties are consequences of dependency on structural geometry, and cannot be accommodated by standard emulation methods. We propose a new statistical framework for building emulators to preserve invariance. This framework uses a weighted complete graph to represent the geometry and introduces a new class of function, called the relabeling symmetric functions, associated with the graph. We establish a characterization theorem of the relabeling symmetric functions, and propose a nonparametric kernel method for estimating such functions. The effectiveness of the proposed method is illustrated by several examples from materials science.

Keywords: Computer Experiments; Design of Experiments; Uncertainty Quantification

# Local Gaussian Process Model for Large-scale Dynamic Computer Experiments

# C. Devon Lin, Queen's University, Canada

## *Coauthor(s)*: Ru Zhang and Pritam Ranjan

*Abstract*: The recent accelerated growth in the computing power has generated popularization of experimentation with dynamic computer models in various physical and engineering applications. We propose a computationally efficient statistical emulator for a large-scale dynamic computer simulator (i.e., simulator which gives time series outputs). The main idea is to first find a good local neighbourhood for every input location, and then emulate the simulator output via a singular value decomposition (SVD) based Gaussian process (GP) model. We develop a new design criterion for sequentially finding this local neighbourhood set of training points. Several test functions and a real-life application have been used to demonstrate the performance of the proposed approach over a naive method of choosing local neighbourhood set using the Euclidean distance among design points.

*Keywords*: Nearest neighbour; Sequential design; Singular value decomposition; Statistical emulator; Time series output

# DAE 2017 INVITED TALKS

— Day 3: Saturday, October 14, 2017 —

Session 9. ADVANCES IN OPTIMAL DESIGN OF DOSE RANGING STUDIES Organizer and Chair: Valerii Fedorov, ICONplc, USA

# Operational tuning optimal design of clinical trials "time-to-event" endpoints to increase operational probability of success

Xiaoqiang Xue, *QuintilesIMS* 

Coauthor(s): Valerii V. Fedorov

*Abstract*: In the typical clinical trials the subject arrival times can be modeled as the outcomes of a point process. Subsequently the follow-up times can be viewed as random variables and they become known only after trial completion. Thus the information that is gained depends on the sample size (number of subjects), enrollment process and random follow up times (specific for each subject). We present results for proportional hazard model that follows from optimal design theory and illuminate them with numerical examples.

# Optimal model-based design, dose ranging, and population pharmacokinetic measures

Sergei Leonov, ICON Clinical Research

*Abstract*: In this presentation, we discuss a link between optimal design problems arising in dose-ranging studies and pharmacokinetic (PK) studies, in which various population PK measures are estimated, such as area under the curve (AUC), maximal concentration (Cmax) and time to maximal concentration (Tmax). In order to select doses which are efficacious and have an acceptable safety profile, it is critical to provide accurate estimates of the PK measures. We compare parametric (model-based) and nonparametric approaches for the estimation of population PK measures, using the model-based approach as a benchmark.

 $\mathit{Keywords}:$  Optimal model-based design, Population pharmacokinetic measures, Area under the curve, Tmax, Cmax

# A universal approach to optimal design of experiments based on the use of elemental information matrices

## Valerii Fedorov, ICONplc, USA

Abstract: In most approaches, the construction of optimal experimental designs requires knowledge of the information matrix of a single observation. The latter can be found if the elemental information matrix corresponding to the distribution of the response is known. In fact, the knowledge of elemental matrices makes the design problem a rather routine task and allows us to develop the universal numerical methods and respective software tools. I present underlying results from optimal experimental design theory and illustrate the approach with several examples, including bivariate binary responses and beta distributed responses. *Keywords*: Elemental Fisher information matrix, generalized regression model, optimal for convex criteria

## Session 10. INFORMATION-BASED OPTIMAL SUBDATA SELECTION FOR BIG DATA

Organizer and Chair: Min Yang, University of Illinois at Chicago

# Optimal design of sampling survey for efficient parameter estimation

Wei Zheng, University of Tennessee

Coauthor(s): Xueqin Wang

Abstract: For many tasks of data analysis, we may only have the information of the explanatory variable and the evaluation of the response values are quite expensive. While it is impractical or too costly to obtain the responses of all units, a natural remedy is to judiciously select a good sample of units, for which the responses are to be evaluated. In this paper, we adopt the classical criteria in design of experiments to quantify the information of a given sample regarding parameter estimation. Then, we provide a theoretical justification for approximating the optimal sample problem by a continuous problem, for which fast algorithms can be further developed with the guarantee of global convergence. Our results have the following novelties: (i) The

statistical efficiency of any candidate sample can be evaluated without knowing the exact optimal sample; (ii) It can be applied to a very wide class of statistical models; (iii) It can be integrated with a broad class of information criteria; (iv) It is much faster than existing algorithms. (v) A geometric interpretation is adopted to theoretically justify the relaxation of the original combinatorial problem to continuous optimization problem.

Keywords: Optimal design; active learning; sample; equivalence theorem; precision medicine.

# **On Data Reduction of Big Data**

## Min Yang, University of Illinois at Chicago

Abstract: Extraordinary amounts of data are being produced in many branches of science. Proven statistical methods are no longer applicable with extraordinary large data sets due to computational limitations. A critical step in Big Data analysis is data reduction. In this presentation, I will review some existing approaches in data reduction and introduce a new strategy called information-based optimal subdata selection (IBOSS). Under linear and nonlinear models set up, theoretical results and extensive simulations demonstrate that the IBOSS approach is superior to other approaches in term of parameter estimation and predictive performance. The tradeoff between accuracy and computation cost is also investigated. When models are mis-specified, the performance of different data reduction methods are compared through simulation studies. Some ongoing research work as well as some open questions will also be discussed. *Keywords*: Big data, data reduction, IBOSS Strategy

# Information-Based Optimal Subdata Selection for Big Data Lasso Regression

# Xin Wang, University of Illinois at Chicago

# Coauthor(s): Min Yang

*Abstract*: Extraordinary amounts of data are being produced in many branches of science as well as people's daily activity. Such data are usually huge in both rows and columns. Modeling such data with limited computation resource has been a challenging problem. We propose an approach to select an informative subset of the data based on optimal design theory, using LASSO regression to perform variable selection and estimation. Compare to existing methods like balanced or weighted sampling, our approach avoids involving sampling error and thus provides more accurate estimation/prediction, also takes much less time. *Keywords*: Big data, optimal design, lasso, subdata selection

# DAE 2017 INVITED POSTERS

— Day 1: Thursday, October 12, 2017 —

## Optimal design involving profile factors

Maria Adamou, University of Southampton, UK

Coauthor(s): Dave Woods

*Abstract*: Increasing numbers of experiments in science and engineering involve profile factors, whose values can be varied (e.g. as a function of time) within a single run of the experiment. A typical example of a profile factor is temperature which can perhaps be varied monotonically or as a step function. The design problem then becomes choosing suitable functions for the profile factor for each run of the experiment.

Motivated by biopharmaceutical studies, we present some initial results on optimal design for factorial experiments with profile factors. Both frequentist and Bayesian designs are considered, and some connections are made between smoothness of functional parameters and sparsity inducing prior distributions. *Keywords*: Functional linear model, basis expansion, roughness penalty

## A Bayesian-inspired minimum aberration criterion for two-level multi-stratum factorial designs

Ming-Chung Chang, Academia Sinica, Taiwan

Coauthor(s): Ching-Shui Cheng

Abstract: In a multi-stratum factorial experiment, there are multiple error terms (strata) with different variances that arise from complicated structures of the experimental units. For unstructured experimental units, (generalized) minimum aberration is a popular criterion for choosing fractional factorial designs. One difficulty in extending this criterion to multi-stratum factorial designs is that the formulation of a wordlength pattern based on which minimum aberration is defined requires an order of desirability among the relevant words, but a natural order is often lacking. Furthermore, a criterion based only on wordlength patterns does not account for the different stratum variances. Mitchell, Morris, and Ylvisaker (1995) proposed a framework for two-level Bayesian factorial designs. We adopt this approach to study optimal and efficient multi-stratum factorial designs. A Bayesian-inspired minimum aberration criterion, which depends on wordlength patterns and stratum variances, is proposed. A tool is developed for eliminating inferior designs and reducing the designs that need to be considered without requiring any knowledge of stratum variances. Some numerical examples are used to illustrate the theory.

Keywords: block structure, Gaussian process, wordlength pattern, Bayesian optimality

## Hybrid numerical optimization algorithms for generating optimal discrimination designs

Ping-Yang Chen, National Cheng Kung University, Taiwan

Coauthor(s): Ray-Bing Chen, Cheng-Lin Hsu, Weng Kee Wong

Abstract: Finding discrimination designs based on the T- and KL-optimal criteria is generally a difficult task because the corresponding design search problems involve nested optimization problems. We propose to tackle the problem using hybrid optimization algorithms which are based on particle swarm optimization (PSO). We consider two types of discrimination design scenarios that are dependent on the numbers of competing models. When there are only two competing models, a hybrid algorithm combining PSO and Newton-type algorithm is used to search the optimal designs. When we consider more than 2 competing models, a multi-layer algorithm is proposed based on max-min T- and KL-optimal criteria. Several classical examples are used to illustrate the performances of the proposed hybrid optimization algorithms and a real application on finding optimal design for discriminating among five nonlinear dose-response models in toxicology is also studied.

*Keywords*: *KL*-optimal designs; max-min *KL*-optimal designs; max-min *T*-optimal designs; particle swarm optimization; *T*-optimal designs.

# Algorithms for searching saturated D-Optimal designs for two level factorial designs

Kouakou Francois Domagni, University of Illinois, Chicago

### Coauthor(s): Samad Hedayat

Abstract: We solve analytically the problem of finding saturated D-optimal designs for two level fractional factorial designs when the number of missing effects is relatively small. Keywords: D-optimal designs, Main effects, interaction effects

# CV, ECV, and Robust CV designs for replications under a class of linear models in factorial experiments

## Subir Ghosh, University of California, Riverside

Abstract: A class of linear models is considered for describing the data collected from an experiment. Any two models have some common as well as uncommon parameters. To discriminate between any two models, the uncommon parameters play a major role. A common variance (CV) design is proposed for collecting the data so that all the uncommon parameters are estimated with as similar variances as possible in all models. The variance equality for a CV design is attained exactly when there is one uncommon parameter for any two models within the class. A new concept "Robust CV designs for replications" having the possibility of replicated observations is introduced. The conditions are presented for a CV design having no replicated observations to be robust for general replicated observations. A CV design having no replicated observations is always robust for any equally replicated observations. In the class of linear models considered for factorial experiments, the common parameters for all models correspond to the general mean and main effects, and the other parameters correspond to two factor interactions. Two general CV designs are presented for three level factorial experiments. Examples of Efficient CV (ECV) designs as well as Robust CV designs for general replicated observations are also presented. A simple illustrative example of the complete  $2 \times 3$  factorial design is demonstrated to be not a CV design and then the condition on replications of each run is obtained to turn it into a CV design. (Joint work with Dr. Shrabanti Chowdhury)

Keywords: Factorial Experiments, Model Uncertainty, Variance Balanced, Interaction Effects

# Simulation-Based Optimal Bayesian Design for Sequential Experiments

Xun Huan, Sandia National Laboratories

Coauthor(s): Youssef M. Marzouk

Abstract: The optimal design of a sequence of experiments needs to account for both (1) feedback between experiments and (2) future effects and consequences of design decisions. Common practices such as non-sequential batch design (no feedback) and greedy/myopic design (not forward-looking) are mathematically suboptimal under a sequential setting, and can be particularly disadvantageous for dynamically-evolving environments and systems.

We formulate the optimal sequential design problem using dynamic programming (DP), and employ a Bayesian framework that seeks to maximize expected information gain in continuous parameters given continuous design variables and observations. We find near-optimal policies via approximate value iteration. To make this iteration tractable, transport maps are employed to represent non-Gaussian posteriors and to enable fast approximate Bayesian inference. We construct a Knothe-Rosenblatt map that couples a standard Gaussian to the joint distribution of designs, observations, and parameters, where posteriors can be obtained easily by conditioning. Maps are built using trajectories from exploration and exploitation in an adaptive manner, iteratively discovering and increasing accuracy over state regions that are more likely to be visited. The overall method is demonstrated on a problem of optimal sequential sensing: inferring contaminant source location from a mobile sensor in a time-dependent convection-diffusion system.

*Keywords*: sequential design, optimal experimental design, Bayesian, simulation-based design, information gain

## Power and Practicality of Large Supersaturated Designs

Varun Khemani, University of Maryland

Coauthor(s): Jon Stallings

Abstract: Supersaturated designs (SSDs) are used for factor screening in experiments where the number of factors, m, is greater than the number of runs, N. The goal with such designs is to identify, at minimum cost,

the few factors having large effects. Although catered towards situations having an un-manageable number of factors, much of the research literature on the analysis of SSDs has focused on designs where m is not much larger than N. For example, the most frequently studied supersaturated design in the literature is the 23 factor, 14 run supersaturated design on the Williams (1968) dataset. This design is certainly useful as it identifies the significant factors in 14 runs instead of the 24 runs it would have taken in a saturated design. Analysis techniques for supersaturated designs are known to perform well when the number of significant factors is no more than half the number of runs, which has been established through extensive simulation studies. Little attention though has been given to the performance of different analysis methods of large supersaturated design analysis, where m is much greater than N. This paper summarizes and compares the performance of existing techniques to a 125 factor, 24 run balanced SSD. Bayesian Regression using a Horseshoe Prior, which to the best of the authors' knowledge has not been demonstrated on supersaturated designs, is also introduced and shown to perform better than well- established methods. Extensive simulations and a dataset collected from the Additive Manufacturing domain are used to study the performance. *Keywords*: Large Supersaturated designs, Horseshoe prior

## **Robust Design of Generalized Linear Model**

Yiou Li, DePaul University

# Coauthor(s): Xinwei Deng

Abstract: Generalized linear regression model is a flexible generalization of classical linear regression model and is used widely for approximation and classification problems in different areas, e.g., business, computer science, medical science, etc. Choosing a high quality design can improve the efficiency of the regression model. In this article, a theoretical upper bound is derived on the scaled integrated mean squared error in terms of the discrepancy of the design, and this bound can be used to choose designs that are both efficient and robust under model uncertainty. Numerical examples are conducted to support the theoretical result. *Keywords*: Generalized linear model; Efficiency; Robustness; Integrated mean squared error; Low discrepancy.

## Augmenting Definitive Screening Designs for Estimating Quadratic Models

Abigael Nachtsheim, Arizona State University

# Coauthor(s): Bradley Jones; Douglas C. Montgomery; John Stufken

Abstract: Jones and Nachtsheim (2011) introduced a class of three-level screening designs called definitive screening designs (DSDs). The structure of these designs results in the statistical independence of main effects and two-factor interactions; the absence of complete confounding among two-factor interactions; and the ability to estimate all quadratic effects. Because quadratic effects can be estimated, DSDs can allow for the screening and optimization of a system to be performed in one step, but only when the number of terms found to be active during the screening phase of analysis is less than about half the number of runs required by the DSD (Errore, et al., 2016). Otherwise, estimation of second-order models requires augmentation of the DSD. In this paper we explore the construction of series of augmented designs, moving from the starting DSD to designs capable of estimating the full second-order model. We use power calculations, model-robustness criteria, and model-discrimination criteria to determine the number of runs by which to augment in order to identify the active second-order effects with high probability.

Keywords: Model discrimination; Foldover; Model robustness; Model selection; Simulation

## On A-efficient treatment-control designs constructed by generalized cyclic designs

#### Kazuhiro Ozawa, Gifu College of Nursing, Japan

## Coauthor(s): Shinji Kuriki

*Abstract*: We consider an experiment to compare test treatments with a standard treatment (control) using blocks. Such a design is called a treatment-control design. Das, Dey, Kageyama and Sinha (2005) have given a list of A-efficient balanced treatment incomplete block (BTIB) designs in the practically useful ranges of the parameters. In this poster we give a list of A-efficient treatment-control (not always BTIB) designs constructed by generalized cyclic designs and we compare the efficiencies of our designs with the efficiencies

of the designs given by Das, Dey, Kageyama and Sinha (2005) as treatment-control designs. *Keywords*: A-optimality, efficiency, generalized cyclic design, treatment-control design.

### **Design of Order-of-Addition Experiments**

Jiayu Peng, Penn State University

Coauthor(s): Rahul Mukerjee, Dennis K.J. Lin

Abstract: In an order-of-addition experiment, each treatment is a permutation of m components. It is often unaffordable to test all the m! treatments, and the design problem arises. We consider the model in which the response of a treatment depends on the pairwise orders of the components. We establish the optimal design theory under this model, and derive the optimal values of the D-, A-, E-, and M.S-efficiency. We identify a special constraint on the correlation structure of such designs. The closed-form construction of a class of optimal designs is provided.

Keywords: Design equivalence; Optimal design; Order of addition; Pairwise order

# An algebra for conditional main effects

Arman Sabbaghi, Purdue University

*Abstract*: Indicator functions are applied to establish an algebra for the conditional main effects parameterization system in two-level designs. Aliasing relations, and the implications of the maximum clear two-factor interactions, minimum aberration, and maximum estimation capacity design criteria for conditional main effects analysis are illuminated by consideration of this algebra. Calculations of D-efficiency for models composed of specified traditional and conditional effects are simplified as a consequence.

Keywords: Complex aliasing; D-optimality; Fractional factorial design; Partial aliasing; Regular design

## **Differential Evolution for Optimal Design Creation**

Zack Stokes, UCLA

*Coauthor(s)*: Abhyuday Mandal and Weng Kee Wong

Abstract: Differential Evolution (DE) is a metaheuristic algorithm that has found great success in recent applications from many fields. However, one area where DEÕs abilities have not been properly tested is experimental design. In this paper a review of the DE literature as well as a discussion of parameter tuning is given. Following this, preliminary results of using DE to find optimal designs under a variety of settings are detailed and comparisons are drawn between DE and a competitor algorithm from the same class, Particle Swarm Optimization (PSO). Through this testing it appears that DE is capable of quickly locating optimal designs that have already been established in the literature.

Keywords: Differential Evolution, Metaheuristics, Evolutionary Algorithms, Mixture Designs

# Finding D-Optimal Designs for High Dimensional Logistic Models via Two-Layer Tournament Swarm Optimization

Zizhao Zhang, UCLA

# *Coauthor(s)*: Weng Kee Wong

Abstract: Solving optimal design problems is always a challenging topic across research disciplines. Optimal designs can result in huge savings in cost without sacrificing statistical efficiency. However, finding them for high dimensional models, which invariably do not have closed form solutions, are fraught with difficulties. In particular, conventional algorithms for searching optimal designs do not work well at all. We propose a new optimizer based on swarm optimization techniques and call it Two-Layer Tournament Swarm Optimization (TLTSO). The basic idea behind TLTSO is to construct a two-layer swarm structure and let winners generated from lower layer swarm competition constitute upper layer competition league. Some losers might be replaced by more promising players to avoid premature convergence. TLTSO is quite simple to implement and we show it outperforms several of its competitors for a variety of design problems. As an illustration, we construct both local and Bayesian D-optimal designs for logistic models with several factors with and without interactions for different types of prior distributions. We also apply our methodology to a real problem where we show designs generated by TLTSO outperform many designs used in practice. Keywords: Optimal Design, D-Optimal Design, Two-Layer Tournament Swarm Optimization, Logistic Model, Design Efficiency

### Individual Factor Word Length Pattern For Nonregular Fractional Factorial Designs

Qi Zhou, Tianjin University of Finance and Economics, China

Coauthor(s): William Li, Robert Mee.

Abstract: Literature on constructing efficient experimental designs has been plentiful, but how best to incorporate prior information when assigning factors to the columns on a nonregular design has received little attention. Following Li et al. (2015), we propose a new criterion called the individual generalized word length pattern (iGWLP) for ranking columns of a nonregular design. A theorem is given to relate the iGWLP to the expected bias caused by model mis-specifications. We also show that the proposed criterion may lead to designs having better projection properties in the factors considered most likely to be important. Taking examples from the literature of recommended orthogonal arrays, we illustrate how iGWLP helps identify important differences in the aliasing that is likely otherwise missed. Given the complexity of characterizing partial aliasing for nonregular designs, iGWLP will help practitioners make more informed assignment of factors to columns when utilizing nonregular fractions. Furthermore, we introduce a factor-wise plot of generalized alias lengths to help practitioners visualize differences in aliasing among terms in the two-factor interaction model.

Keywords: Effect hierarchy principle, Generalized alias length plot, Generalized resolution, Generalized word length pattern, Minimum  $G_2$ -aberration, Projection.

# DAE 2017 INVITED POSTERS

# — Day 2: Friday, October 13, 2017 —

## Purely sequential estimation of a negative binomial mean with applications in ecology

Sudeep R. Bapat, University of California, Santa Barbara

*Coauthor(s)*: Nitis Mukhopadhyay

Abstract: We discuss a set of purely sequential strategies to estimate an unknown negative binomial mean  $\mu$  under different forms of loss functions. We develop point estimation techniques where the thatch parameter  $\tau$  may be known or unknown. Both asymptotic first-order efficiency and risk efficiency properties will be elaborated. The results will be supported by an extensive set of data analysis carried out via computer simulations for a wide variety of sample sizes. We observe that all of our purely sequential estimation strategies perform remarkably well under different situations. We also illustrate the implementation of these methodologies using real data-sets from ecology, namely, weed count data and data on migrating woodlark. *Keywords*: Negative Binomial, Sequential, Agriculture, Ecology

## Information-Based Optimal Subdata Selection for Big Data Logistic Regression

Qianshun Cheng, University of Illinois at Chicago

Coauthor(s): Min Yang

*Abstract:* Technological advances have enabled an exponential growth in data collection and the size of data sets. For the extraordinary large data sets, proven statistical methods are no longer applicable due to computational limitations. A critical step in Big Data analysis is data reduction. In this manuscript, we investigate the sampling approach of selecting subsets under logistic regression model. For random sampling approaches, it is shown that the information contained in the subdata is limited by the size of the subset. A novel framework of selecting subsets is proposed. The information contained in the subdata based on the new framework increases as size of full data increases. Performances of the proposed approaches, along with some of the widely-applied existing methods, are compared under various criteria based on extensive simulation studies.

*Keywords*: IBOSS Strategy, D-Optimality, DDOSS Strategy

## Comparison of Gaussian process modeling software

Collin Erickson, Northwestern University

Coauthor(s): Bruce Ankenman and Susan Sanchez

Abstract: Gaussian process fitting, or kriging, is often used to create a model from a set of data. Many available software packages do this, but we show that very different results can be obtained from different packages even when using the same data and model. Eight different fitting packages that run on four different platforms are compared using various data functions and data sets that reveal there are stark differences between the packages. In addition to comparing the prediction accuracy, the predictive variance — which is important for evaluating precision of predictions and is often used in stopping criteria — is also evaluated. Keywords: Simulation, Gaussian processes, kriging, metamodels, computer experiments

## Replication or exploration? Sequential design for stochastic simulation experiments

Jiangeng Huang, Virginia Tech

Coauthor(s): Mickael Binois, and Robert B. Gramacy

*Abstract*: Historically, design and analysis of computer experiments focuses on deterministic solvers from the physical sciences. But nowadays computer modeling is common in the social and biological sciences, where stochastic simulations abound. As the simulations become noisier the experiments need to be bigger, in order to identify signal from noise. Replication offers a pure look at noise, not obfuscated by signal, but ultimately it is the signal which is of primary interest. So how much replication should be performed in the context of simulation experiments? We develop a sequential design scheme that can actively determine if new runs should be at new input locations, or rather should instead be replications (at existing input locations). Our heteroskedastic Gaussian process (hetGP) model learns the signal-to-noise ratio throughout the input space, in a way that is computationally favorable when replication is present. Based on those estimates, hetGP can dynamically determine the balance of replicates in the design, differentially throughout the input space. We show designs so-developed for two challenging real-data simulation experiments, from inventory management and epidemiology.

*Keywords*: Sequential learning; Computer experiments; Stochastic kriging; Replication; Input dependent noise; Integrated mean-square error; Latent variable.

## The application of design of experiments to precision medicine clinical trial

Kim May Lee, University of Cambridge, UK

Coauthor(s): Stefanie Biedermann, James Wason

Abstract: Precision/ personalized medicine uses genomic information to refine cancer treatments such that different treatments may provide maximum benefit to the heterogeneous patients who suffer from a common disease. Considering a linear model with first order interaction terms, we propose the use of a weighted L-optimality to find the treatment allocation scheme for a confirmatory trial based on data from previous stage. We consider the relative importance of the linear combinations of model parameters in the design framework, and study the characteristics of the designs using simulation. We explore the efficiency loss of using other standard designs such as a randomized controlled trial with equal randomization probability when instead the optimal design should have been used.

Keywords: weighted L-optimality

### Hellinger information and optimal designs for nonregular models

Yi Lin, University of Illinois at Chicago

# Coauthor(s): Ryan Martin, Min Yang

Abstract: Fisher information is the object of interest in optimal experimental design. However, for nonregular models, where certain regularity conditions do not apply, Fisher information does not exist. This project proposes to use Hellinger information in optimal experimental design under nonregular conditions. We provided a definition for Hellinger information for non-regular multi-dimensional parameters and have shown that Hellinger information is a generalization of Fisher information; furthermore, this project has presented Hellinger information inequality, which shows that Hellinger information controls a local minimax risk bound for estimators. These results provide theoretical justification to use Hellinger information in optimal design problems. Finally, optimal designs for some non-regular regression models are derived. *Keywords*: Fisher information; Hellinger information; information inequality; nonregular model

# Experimental Design with Circulant Property and its Application to fMRI Experiment

Yuan-Lung Lin, Academia Sinica, Taiwan

Coauthor(s): Frederick Kin Hing Phoa and Ming-Hung Kao

Abstract: Cost-efficient experimental designs have been widely used nowadays. Orthogonal arrays are commonly used to study the effects of many factors simultaneously, but they do not exist in any sizes. Recently, orthogonal arrays with circulant property receive great attention and are applied to experiments in many fields, such as functional magnetic resonance imaging (fMRI), which is a pioneering technology for studying brain activity in response to mental stimuli. Efficient fMRI experimental designs are important for rendering precise statistical inference on brain functions, but a systematic construction method for this important class of designs does not exist. In this work, we propose an innovative and unified construction method for efficient, if not optimal, fMRI designs via circulant almost orthogonal arrays (CAOAs). Since circulant Hadamard matrices, that can also be viewed as circulant orthogonal arrays of symbols two and strength two, have been conjectured nonexistence, CAOAs are considered.

We characterize this new class of efficient designs and propose a systematic construction via a newly invented algebraic tool called complete difference system (CDS). We not only prove the equivalence relation of CDS and CAOA, but also construct many classes of CAOAs with very high efficiency. Finally, we apply these efficient CAOAs to fMRI experiments, showing that our constructed designs have better properties than the traditional designs in terms of cost-efficiency and effect independency.

*Keywords*: Optimal Designs; Circulant Orthogonal Arrays; Complete Difference System; functional Magnetic Resonance Imaging (fMRI).

# *d*-QPSO: A Quantum-Behaved Particle Swarm Technique for Finding *D*-Optimal Designs for Models with Mixed Factors and a Binary Response

Abhyuday Mandal, University of Georgia

Coauthor(s): Joshua Lukemire, Weng Kee Wong

Abstract: Identifying optimal designs for generalized linear models with a binary response can be a challenging task, especially when there are both continuous and discrete independent factors in the model. Theoretical results rarely exist for such models, and for the handful that do, they usually come with restrictive assumptions. In this paper, we propose a modified version of quantum-behaved particle swarm optimization and call it the d-QPSO algorithm to find a variety of locally D-optimal designs for experiments with mixed factors and a binary response. They include approximate and exact designs, designs for experiments on irregular design spaces, designs when factors are all discrete or all continuous, designs for many factors and designs that are more realistic in practice. We also show the d-QPSO algorithm can find robust pseudo-Bayesian designs when nominal values for the model parameters are not available. Additionally, we investigate robustness properties of the d-QPSO algorithm-generated designs to various model assumptions and provide real applications to design a bio-plastics odor removing experiment, an electrostatic discharge experiment and a ten-factor car refueling experiment.

*Keywords*: Approximate design, Design efficiency, Equivalence theorem, Exact design, Pseudo- Bayesian design

## Construction of Covering Arrays Using Parallel Strength Two Covering Arrays

Kevin Quinlan, Penn State University

# Coauthor(s): Dennis Lin

Abstract: Covering Arrays are commonly used in computer software and product testing. Rather than test all possible combinations of factor levels we ensure that any t-way projection of factors is tested for all factor level combinations. This work presents a new method for constructing binary strength three covering arrays using a sequence of strength two covering arrays. We additionally define criteria to efficiently select strength two covering arrays, as well as examine properties of arrays built using common construction methods. *Keywords*: Covering Arrays

# Geometric Orthogonal Array (GOA): A new class of space-filling designs with good uniformities in multiple dimensions

# Cheng-Yu Sun, Simon Fraser University, Canada

Coauthor(s): Shao-Wei Cheng, Frederick Kin Hing Phoa

Abstract: This paper introduces a new class of space-filling designs optimized under a new multi-dimensional space-filling property called *geometric strength*. We propose a systematic construction method via techniques in Galois field for this new class of designs. In specific, the factor levels in a regular design are collapsed and the strength of the collapsed design is enhanced. The reversed process to relabel factor levels of the regular design improves its space-filling property. This method is more efficient than the existing methods via level permutations, especially when the number of factor levels is large. When two collapsers are indistinguishable in terms of the strength of the collapsed designs, we propose a new criterion called maximal strength efficiency. It not only maximizes the strength of the collapsed design, but also maximizes the proportion of the projected sub-designs that are full factorials.

*Keywords*: Space-Filling Designs, Factor Subgroup Collapse, Galois Field, Geometric Strength, Maximal Strength Efficiency

## Super-simple bipartite orthogonal array

Yu Tang, Soochow University, China Coauthor(s): Jianxing Yin and Wenjie Zhong *Abstract*: Orthogonal array has been proved essential in both theoretical and practical sense. It has many connections with other combinatorial designs and is applied in statistical design of experiments, coding theory, cryptography and various types of software testing. In this paper, we define a special type of orthogonal array, called super-simple bipartite orthogonal array, and show that such an array can be useful for detecting faults in a jamming and anti-jamming experiment. We further discuss some properties of such super-simple bipartite orthogonal arrays of constructing saturated ones, which allow to assign maximal number of factors.

Keywords: bipartite orthogonal array, detecting array, difference matrix, saturated, super-simple

# Two-Level Designs Constructed by Concatenating Orthogonal Arrays of Strength Three

# Alan Vazquez-Alcocer, University of Antwerp, Belgium

Coauthor(s): Peter Goos and Eric D. Schoen

Abstract: Two-level orthogonal arrays of N runs, k factors and a strength of 3 provide suitable fractional factorial designs in situations where many of the main effects are expected to be active, as well as some two-factor interactions. If constructed using the fold-over technique, these designs are called even and allow at most N/2 - 1 interactions to be estimated. For k < N/3 factors, there exist strength-3 designs that are not fold-over designs. These are called even-odd designs can be extracted from complete catalogs of strength-3 orthogonal arrays. However, for larger run sizes, no complete catalogs exist. In order to construct even-odd designs with N > 48, we develop an algorithm for an optimal concatenation of strength-3 designs involving N/2 runs. Our approach involves column permutations of one of the concatenated designs, as well as sign switches of the elements of one or more columns of that design. We illustrate the potential of the algorithm by generating two-level even-odd designs. With a few exceptions, our even-odd designs outperform or are competitive with the literature designs in terms of the aliasing of two-factor interactions and in terms of the number of estimable two-factor interactions.

Keywords: Even-odd design, generalized aberration, local search, two-factor interaction, variable neighborhood search

# Optimal maximin $L_1$ -distance Latin hypercube designs based on good lattice point designs Lin Wang, UCLA

# Coauthor(s): Qian Xiao, Hongquan Xu

Abstract: Maximin distance Latin hypercube designs are commonly used for computer experiments, but the construction of such designs is challenging. We construct a series of maximin Latin hypercube designs via Williams transformations of good lattice point designs. Some constructed designs are optimal under the maximin  $L_1$ -distance criterion, while others are asymptotically optimal. Moreover, these designs are also shown to have small pairwise correlations between columns.

Keywords: computer experiment, correlation, space-filling design, Williams transformation

# Locally D-optimal Designs for Multiple-covariate Generalized Linear Models

## Zhongshen Wang, Arizona State University

Coauthor(s): John Stufken

*Abstract*: Optimal design results for multiple-covariate GLMs are relatively rare. Yang, Zhang and Huang (2011, Statistica Sinica, 21, p.1415-1430) considered a situation where all but one covariates are bounded and provided an explicit formula for locally D-optimal designs for main-effect models. We extend their results to more general models where interactions among bounded covariates can also exist. Additional insights will be discussed based on orthogonal arrays.

Keywords: equivalence theorem, D-optimality, orthogonal arrays

## Local Variable Selection in Experimental Design

Munir Winkel, North Carolina State University

## Coauthor(s): Brian Reich, Jonathan Stallings

Abstract: Experimenters are often faced with the challenge of finding a global maximum in an unexplored design space with a large number of input variables. Expected improvement algorithms, which aim to balance exploration of the design space with exploitation to find the global maximum, struggle in higher dimensions. Reducing the dimension of the design space will lead to faster identification of the maximum. However, current variable selection techniques are global; they include more variables than may be locally active in a specific region. In this paper, we construct a measure of local importance, and then use the (sparse) gradient of expected improvement to efficiently search the design space for a global maximum. We will present simulation studies involving high dimensional data and evaluate competing methods by comparing the number of steps needed to reach the global maximum as well as largest maximum identified. Initial results from a simulation study show that the local variable selection method takes fewer steps to arrive at a global maximum.

Keywords: variable selection, experimental design, expected information gain, optimization

#### Functional F tests for orthogonal designs

Bairu Zhang, Queen Mary, University of London

Coauthor(s): Heiko Grossmann

*Abstract*: Functional data analysis concerns the analysis of responses which are functions of time, space or other domains. We present a new method to analyse functional data that are collected from orthogonal designs by using a split-plot design as an example. The functional mixed-effects analysis of variance model is applied and the design matrices in the model reflect the structure of the design. Although the responses are more complicated, the structure of the design is supposed to be time-independent. To test treatment effects, we propose a functional F test which is derived by using the projection approach and the Karhunen-Loeve expansion of the stratum-based covariance function. The null distribution of the functional F test can be approximated by an F distribution with adjusted degrees of freedom that are calculated from the eigenvalues of the estimated covariance function. We apply the proposed approach to time-dense gait data and functional F tests are used to examine the effects of ankle-foot orthoses, which are commonly prescribed to patients with abnormal gait patterns.

Keywords: Functional data analysis; Split-plot design; Gait data