

# International Conference on Design of Experiments ICODOE 2019

May 18—21



THE UNIVERSITY OF  
**MEMPHIS**®

Department of Mathematical Sciences  
University of Memphis  
Memphis, TN 38152, USA

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Academic Session Organizers	Title of Session
David Woods, University of Southampton, UK	Opening
Nancy Flournoy, University of Missouri	Inference and information with adaptive designs
Min Yang, University of Illinois at Chicago	Subset selection for big data
Doug Wiens, University of Alberta, Canada	Robust design
Radoslav Harman, Comenius University in Bratislava	Computational aspects of optimal experimental design
Brad Jones, JMP	Generating designs for multiple objectives
John Stufken, Arizona State University	Design for discrete data
Hongquan Xu, UCLA	New developments in factorial design
Xinwei Deng, Virginia Tech	Experimental design thinking for large-scale statistical analyses
Deborah Street, University of Technology Sydney	Discrete choice experiments
Sergei Leonov, CSL Behring	Optimal design of dose-finding studies
Youssef Marzouk, MIT	Bayesian optimal design with physical models
Angela Dean, The Ohio State University	Multi-stage designs and blocking
Peter Chien, University of Wisconsin-Madison & Qiong Zhang, Clemson University	Computer Experiments
Timothy Waite, University of Manchester, UK & Tirthankar Dasgupta, Rutgers University	Randomization and causal inference
Susan Sanchez, Naval Postgraduate School	Agent-based simulation experiments: insights and examples
Will Welch, University of British Columbia, Canada	Computer experiments with big n
Maria Weese, University of Miami, Ohio	Design-based analysis of experiments
David Steinberg, Tel Aviv University, Israel	Designs for online experiments

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# International Conference on Design of Experiments (ICODOE-2019)

May 18—21

Department of Mathematical Sciences, University of Memphis

FedEx Institute of Technology, University of Memphis

TZ: The Zone conference room, first floor

MPT: Methodist Presentation Theater, first floor

## **Saturday, May 18**

6—7 PM Registration (Holiday Inn)

7—9 PM Reception Dinner (Holiday Inn, Tennessee Ballroom)

## **Sunday, May 19**

7—8 AM Breakfast (Holiday Inn, Tennessee Ballroom)

8 AM Registration (FedEx Institute Lobby)

8:15 AM Inauguration (TZ)

### **8:30—10 AM Session 1 (TZ): Opening**

Organizer: David Woods, University of Southampton, UK

Chair: David Woods

8:30—9 AM Timothy Waite, University of Manchester, UK.

Minimax efficient random experimental design strategies

9—9:30 AM Erin Leatherman, Kenyon College.

Designing combined physical and computer experiments to maximize global prediction accuracy

9:30—10 AM Matthew Plumlee, Northwestern University.

Composite grid designs for large scale computer model emulation

### **10—10:30 AM Coffee Break (FedEx Institute Lobby)**

### **10:30 AM—12:30 PM Session 2a (TZ): Inference and Information with Adaptive Designs**

Organizer: Nancy Flournoy, University of Missouri

Chair: Nancy Flournoy

10:30—11 AM Nancy Flournoy, University of Missouri

Some interesting results on inference and information with adaptive designs

11—11:30 AM Zhantao Lin, George Mason University

Random Norming Aids Analysis of Non-linear Regression Models with Sequential Informative Dose Selection

11:30 AM—NOON Adam Lane, Cincinnati Children's Hospital Medical Center

Adaptive designs for optimal observed Fisher information

NOON—12:30 PM Sergey Tarima, Medical College of Wisconsin  
Asymptotic properties of maximum likelihood estimators with sample size recalculation

**10:30AM—12:30 PM Session 2b (MPT): Subset Selection for Big Data**

Organizer: Min Yang, University of Illinois at Chicago

Chair: Min Yang

10:30—11 AM Chenlu Shi, Simon Fraser University, Canada  
Model-robust subdata selection for big data

11—11:30 AM Hongquan Xu, UCLA  
Orthogonal array based big data subsampling

11:30 AM—NOON Abigail Nachtsheim, Arizona State University  
Strategic subdata selection for linear regression modeling with big data

NOON—12:30 PM HaiYing Wang, University of Connecticut  
Optimal subsampling: sampling with replacement vs Poisson sampling

**12:30—2 PM Lunch (Holiday Inn, Tennessee Ballroom)**

**2—3:30 PM Session 3a (TZ): Computational Aspects of Optimal Experimental Design**

Organizer: Radoslav Harman, Comenius University in Bratislava, Slovakia

Chair: Radoslav Harman

2—2:30 PM Elisa Perrone, MIT  
Recent advances and new challenges in optimal designs for copula models

2:30—3 PM Wei Zheng, University of Tennessee  
Incomplete U-statistics

3—3:30 PM Radoslav Harman, Comenius University in Bratislava, Slovakia  
Ascent with quadratic assistance for the construction of exact experimental designs

**2—3:30 PM Session 3b (MPT): Robust Design**

Organizer: Doug Wiens, University of Alberta, Canada

Chair: John Stufken

2—2:30 PM Julie Zhou, University of Victoria, Canada  
Computing R-optimal designs for multi-response regression models via interior point method

2:30—3 PM Rui Hu, MacEwan University, Canada  
Robust designs for model discrimination

3—3:30 PM Xiaojian Xu, Brock University, Canada  
Optimal active learning for approximately specified linear regression

**3:30—4 PM Coffee Break (FedEx Institute lobby)**

**4—6 PM Session 4a (TZ): New Developments in Factorial Design I**

Organizer: Hongquan Xu, UCLA

Chair: Hongquan Xu

4—4:30 PM Frederick K.H. Phoa, Academia Sinica, Taiwan  
A systematic construction of cost-efficient designs for order-of-addition experiments

4:30—5 PM Qian Xiao, University of Georgia

Applications of universal Kriging models for drugs' order-of-addition problems with blocking

5—5:30 PM. William Li, Shanghai Jiao Tong University, China

Recent progress on using individual column information for design selections

5:30—6 PM Jose Nunez Ares, KU Leuven University, Belgium

OMARS designs: a new family of response surface designs

#### **4—6 PM Session 4b (MPT): Developments in Optimal Design of Experiments**

Organizers: Bradley Jones, JMP; John Stufken, Arizona State University

Chair: Bradley Jones

4—4:30 PM Olga Egorova, University of Southampton, UK

Compound optimality criteria accounting for potential model uncertainty

4:30—5 PM Anna Errore, University of Minnesota

Minimal aliasing optimal designs for non-linear models

5—5:30 PM Ming-Hung (Jason) Kao, Arizona State University

Optimal designs for mixed responses with quantitative and qualitative factors

5:30—6 PM Abhyuday Mandal, University of Georgia

d-QPSO: A quantum-behaved particle swarm technique for finding D-optimal designs with discrete and continuous factors and a binary response

#### **7—8:30 PM Dinner (Holiday Inn, Tennessee Ballroom)**

### **Monday, May 20**

#### **7:15—8:15 AM Breakfast (Holiday Inn, Tennessee Ballroom)**

#### **8:30—10 AM Session 5a (TZ): Experimental Design Thinking for Large-Scale Statistical Analyses**

Organizer: Xinwei Deng, Virginia Tech

Chair: JP Morgan

8:30—9 AM Youngdeok Hwang, Sungkyunkwan University, South Korea

Estimation of healthcare accessibility using an online experiment

9—9:30 AM Shifeng Xiong, Chinese Academy of Science, China

Linear screening for high-dimensional computer experiments

9:30—10 AM Yiou Li, DePaul University

$I_c$ -optimal design with a large candidate pool of generalized linear models

#### **8:30—10 AM Session 5b (MPT): Discrete Choice Experiments**

Organizer: Deborah Street, University of Technology Sydney, Australia

Chair: Deborah Street

8:30—9 AM Martina Vandebroek, KU Leuven University, Belgium

The choice set size: to be fixed or not to be fixed

9—9:30 AM Brendan Mulhern, University of Technology Sydney, Australia  
Comparing DCEs in the field: Does design construction method matter?

9:30—10 AM Ben White, SurveyEngine, Germany  
Discrete choice experiments in practice

### **10—10:30 AM Coffee Break (FedEx Institute Lobby)**

#### **10:30 AM—12:30 PM Session 6a (TZ): Bayesian Optimal Design with Physical Models**

Organizer: Youssef Marzouk, MIT

Chair: Youssef Marzouk

10:30—11 AM Omar Ghattas, University of Texas at Austin  
Large-scale optimal experimental design for Bayesian inverse problems

11—11:30 AM Wanggang Shen, University of Michigan  
Optimal Bayesian design of sequential experiments via reinforcement learning

11:30 AM—NOON Markus Hainy, Johannes Kepler University Linz, Austria  
Optimal Bayesian design for models with intractable likelihoods via supervised learning methods

NOON—12:30 PM Antony Overstall, University of Southampton, UK  
Bayesian design for physical models using computer experiments

#### **10:30 AM—12:30 PM Session 6b (MPT): Optimal Design of Dose-Finding Studies**

Organizer: Sergei Leonov, CSL Behring

Chair: Adam Lane

10:30—11 AM Vlad Dragalin, Janssen Pharmaceuticals  
Optimal designs for drug combination informed by longitudinal model for the response

11—11:30 AM Valerii Fedorov, Innovation Center, ICON, North Wales, USA  
Dose ranging studies for mixed populations

11:30 AM—NOON Mike Fries, CSL Behring  
Incorporating historical data into dose ranging design utilizing Bayesian methods.

NOON—12:30 PM Suman Sen, Novartis  
Adaptive dose escalation approaches for oncology combinations – theory and practice.

### **12:30—2 PM Lunch (Holiday Inn, Tennessee Ballroom)**

#### **2—3:30 PM Session 7a (TZ): Computer Experiments**

Organizer: Peter Chien, University of Wisconsin-Madison and Qiong Zhang, Clemson University

Chair: Qiong Zhang,

2—2:30 PM Qiong Zhang, Clemson University  
Bayesian sequential data collection for stochastic simulation calibration

2:30—3 PM Ryan Lekivetz, JMP  
Design and analysis of covering arrays using prior information

3—3:30 PM Tzu-Hsiang Hung, University of Wisconsin-Madison  
A random Fourier feature method for modeling computer experiments with gradient information

### **2—3:30 PM Session 7b (MPT): Multi-Stage Designs and Blocking**

Organizer: Angela Dean, The Ohio State University

Chair: Angela Dean

2—2:30 PM Rosemary Bailey, University of St Andrews, UK

Blocking in multi-stage experiments

2:30—3 PM Ming-Chung Chang, National Central University, Taiwan

A Bayesian approach to the selection of two-level multi-stratum factorial designs

3—3:30 PM Rakhi Singh, University of Dortmund, Germany

Pseudo generalized Youden designs

### **3:30—4 PM Coffee Break (FedEx Institute Lobby)**

### **4—5:30 PM Session 8a (TZ): Agent-Based Simulation Experiments: Insights and Examples**

Organizer: Susan Sanchez, Naval Postgraduate School

Chair: Susan Sanchez

4—4:30 PM Susan Sanchez, Naval Postgraduate School

Simulation experiments: designs for decision making

4:30—5 PM Eric Applegate, Purdue University

Multi-objective ranking and selection: Optimal sampling laws and tractable approximations via SCORE

5—5:30 PM Jeffrey Parker, Naval Postgraduate School

Agent-based simulation experiments: An innovative approach for the development of future marine corps amphibious capability

### **4—5:30 PM Session 8b (MPT): Randomization and Causal Inference**

Organizer: Timothy Waite, University of Manchester, UK; Tirthankar Dasgupta, Rutgers University

Chair: Timothy Waite,

4—4:30 PM Xinran Li, University of Pennsylvania

Rerandomization in  $2^K$  Factorial Experiments

4:30—5 PM Zach Branson, Harvard University

Sampling-based randomized designs for causal inference under the potential outcomes framework

5—5:30 PM David Puelz, University of Chicago

Randomization tests of causal effects under general interference

### **7—8:30 PM Conference Banquet (Holiday Inn, Tennessee Ballroom)**

## **Tuesday 21 May 2019**

### **7:15—8:15 AM Breakfast (Holiday Inn, Tennessee Ballroom)**

**8:30—10 AM Session 9 (TZ): Computer Experiments with Big n**

Organizer: Will Welch, University of British Columbia, Canada

Chair: Will Welch

8:30—9 AM Robert Gramacy, Virginia Tech

Replication or exploration? Sequential design for stochastic simulation experiments

9—9:30 AM Sonja Surjanovic, University of British Columbia, Canada

Gaussian process regression with large datasets

9:30—10 AM Samuel Jackson, University of Southampton, UK

Design of physical experiments using history matching methodology

**8:30—10 AM Session 9b (MPT): Design-Based Analysis of Experiments**

Organizer: Maria Weese, University of Miami, Ohio

Chair: Maria Weese

8:30—9 AM Jon Stallrich, North Carolina State University

Sign-informative design and analysis of SSDs

9—9:30 AM David Edwards, Virginia Commonwealth University

Utilizing the block diagonal covariance structure of nonregular two-level designs

9:30—10 AM Bradley Jones, JMP

Construction, properties, and analysis of group-orthogonal supersaturated designs

**10—10:30 AM Coffee Break (FedEx Institute Lobby)**

**10:30 AM—12:30 PM Session 10a (TZ): Designs for Online Experiments**

Organizer: David Steinberg, Tel Aviv University, Israel

Chair: David Steinberg,

10:30—11 AM Jiannan Lu, Microsoft Corporation

Heavy user effect in A/B testing: Identification and estimation

11—11:30 AM Sol Sadeghi, Microsoft Corporation

Novelty and Learning Effects in Online Experiments

11:30 AM—NOON Nathaniel Stevens, University of Waterloo

The analysis of A/B tests with comparative probability metrics

NOON—12:30 PM Paul Li, Microsoft Corporation

Experimentation in the operating system: The windows experimentation platform

**10:30 AM—12:30 PM Session 10b (MPT): New Developments in Factorial Design II**

Organizer: Hongquan Xu, UCLA

Chair: JP Morgan

10:30—11 AM Lin Wang, UCLA

A class of multilevel nonregular fractional factorial designs for studying quantitative factors

11—11:30 AM Alan Vazquez, KU Leuven University, Belgium

Construction of large two-level nonregular designs of strength three

11:30 AM—NOON Jay Beder, University of Wisconsin - Milwaukee

Aliasing in Hadamard arrays of size 12 and 16

NOON—12:30 PM R Vincent Paris, Iowa State University

Generalizing the foldover technique to  $3^{f-s}$  regular fractional factorial designs

**12:30—1:30 PM Lunch (Holiday Inn, Tennessee Ballroom)**

**1:30—3:20 PM Session 11a (TZ): Blocked Designs, Computer Experiments and Subsampling**  
(Contributed session)

Chair: Manohar Aggarwal

1:30—2 PM Nha Vo-Thanh, University of Hohenheim, Stuttgart, Germany

Construction of two-phase designs for experiments with a single block factor in each phase

2—2:20 PM Bushra Husain, Aligarh Muslim University, India

D- and A- optimal orthogonally blocked mixture component-amount designs via projections

2:20—2:40 PM Xu He, Chinese Academy of Sciences

Interleaved lattice-based minimax distance designs and maximin distance designs

2:40—3 PM Yaqiong Yao, University of Connecticut

Optimal two-stage adaptive subsampling design for softmax regression

3—3:20 PM Hyungmin Rha, Arizona State University

A probabilistic subset search (PSS) algorithm for optimizing functional data sampling designs

**1:30—3:20 PM Session 11b (MPT): Designs for Chemical, Medical and Industrial Experiments**

(Contributed session)

Chair: Jay Beder

1:30—2 PM Fabio D'Ottaviano, Dow Chemical

Challenges in experimental designs for the chemical industry

2—2:20 PM Cheng-Yu Sun, Simon Fraser University

Equivalence of 2-level designs between baseline and orthogonal parameterization

2:20—2:40 PM Timothy J. Keaton, Purdue University

Design and dismemberment for controlling the risk of regret for the multi-armed bandit

2:40—3 PM Reem Alghamdi, Arizona State University.

Experimental design issues in functional brain imaging with high temporal resolution

3—3:20 PM Anqing Zhang, University of Missouri

Adaptive Bayesian c-optimal design for estimating multiple EDps under the 4-parameter logistic model

**End of Conference**

**ABSTRACTS**  
(Alphabetically by Speaker)

**Experimental Design Issues in Functional Brain Imaging with High Temporal Resolution**

**Reem Alghamdi**, Arizona State University

**Coauthors:** Ming-Hung Kao

Functional brain imaging experiments are widely conducted in many fields, and an important design issue in such experiment is the selection of an optimal sequence of mental stimuli for making precise and valid statistical inferences at minimum cost. This work focuses on finding such optimal designs for brain mapping technology with an ultra-high temporal resolution. A major challenge is that the dimension of the information matrix becomes large, making it computationally difficult, if not infeasible, to evaluate the efficiencies of competing designs. Here, we propose an efficient approach to tackle this issue, and demonstrate that our approach outperforms existing methods.

**Multi-objective Ranking and Selection: Optimal Sampling Laws and Tractable Approximations via SCORE**

**Eric Applegate**, Purdue University

**Coauthors:** Guy Feldman, Susan Hunter, Raghu Pasupathy

Consider the context of selecting a set of Pareto-optimal systems from a finite set of systems based on three or more stochastic objectives. We characterize the exact asymptotically optimal sample allocation that maximizes the rate of decay of the probability of a misclassification event, and we provide a multi-objective Sampling Criteria for Optimization using Rate Estimators (SCORE) allocation for use when the number of non-Pareto systems is large relative to the number of Pareto systems. The SCORE allocation has three salient features: (a)~it simultaneously controls the probabilities of misclassification by exclusion and inclusion; (b)~it exploits phantom Pareto systems for computational efficiency, which we find using a dimension-sweep algorithm; and (c)~it models dependence between the objectives. The SCORE allocation is fast and accurate for problems with three objectives or a small number of systems. For problems with four or more objectives and a large number of systems, where modeling dependence has diminishing returns relative to computational speed, we propose independent SCORE (iSCORE). Our numerical experience is promising: SCORE and iSCOREi successfully solve MORS problems involving several thousand systems in three and four objectives.

**OMARS designs: a new family of response surface designs**

**Jose Nunez Ares**, KU Leuven, Belgium

**Coauthors:** Jeffrey Linderoth, Peter Goos

We define a new family of orthogonal RSDs, for which there is no aliasing between the main effects and the second-order effects. This family includes not only the classical RSDs, such as the Central Composite Designs or Box-Behnken Designs, but also the more modern Definitive Screening Designs. We name these designs orthogonal minimally aliased RSDs (or OMARS designs). Using integer programming techniques, we constructed a database of OMARS designs for 3 to 8 factors. Each design in the catalog is extensively characterized in terms of efficiency, power, fourth-order correlations, FDS plots, projection capabilities, etc. We identify interesting designs and investigate trade-offs between different quality criteria. Finally, we present a multi-attribute decision algorithm to select designs from the catalog. An important result of our study is that we discovered some novel and interesting designs that challenge standard RSDs in terms of the number of runs, projection capabilities and other criteria.

**Blocking in multi-stage experiments**

**R. A. Bailey**, University of St Andrews, UK

In a multi-stage experiment, the same experimental units are used in each stage but different treatment factors are applied at different stages. Experimental constraints imply that these units must be partitioned into blocks (such as batches or lots) at each stage. However, unlike in the classical situation, the blocks are not inherent, and

the designer of the experiment can choose the partition into blocks at each stage. Is it better to align the Stage 2 blocks with the Stage 1 blocks as far as possible or to make them as orthogonal to each other as possible? In either case, how should treatments be assigned?

In the simplest case, the treatment factors applied at each stage can be orthogonal to the blocks in that stage. In other cases, there may be one or more stages in which the treatment factor(s) applied in that stage must have each level applied to whole blocks.

Both of these are comparatively straightforward compared to the case where there is one (or more) stage(s) in which the allocation of the treatments to experimental units must be that of an incomplete-block design. I will develop some general principles for good design, along with methods for evaluating competing designs.

#### **Aliasing in Hadamard arrays of size 12 and 16**

**Jay H. Beder**, University of Wisconsin - Milwaukee

**Coauthors:** Jessica Savoie, Ezra Coutré,

We investigate the aliasing patterns in  $OA(12, 11, 2, 2)$  and  $OA(16, 15, 2, 2)$  designs. These include the Plackett-Burman designs of orders 12 and 16. Our main tool is a complete survey of the J-characteristics (Deng and Tang 1999) of each design, which affords a more detailed description than the generalized wordlength pattern. We pay special attention to effects for which  $|J| = 12$  and 16, respectively.

#### **Sampling-based randomized designs for causal inference under the potential outcomes framework**

**Zach Branson** Harvard University

**Coauthors:** Tirthankar Dasgupta

We establish the inferential properties of the mean-difference estimator for the average treatment effect in randomized experiments where each unit in a population is randomized to one of two treatments and then units within treatment groups are randomly sampled. The properties of this estimator are well-understood in the experimental design scenario where first units are randomly sampled and then treatment is randomly assigned, but not for the aforementioned scenario where the sampling and treatment assignment stages are reversed. We find that the inferential properties of the mean-difference estimator under this experimental design scenario are identical to those under the more common sample-first-randomize-second design. This finding will bring some clarifications about sampling-based randomized designs for causal inference, particularly for settings where there is a finite super-population. Finally, we explore to what extent pre-treatment measurements can be used to improve upon the mean-difference estimator for this randomize-first-sample-second design. Unfortunately, we find that pre-treatment measurements are often unhelpful in improving the precision of average treatment effect estimators under this design, unless a large number of pre-treatment measurements that are highly associative with the post-treatment measurements can be obtained. We confirm these results using a simulation study based on a real experiment in nanomaterials.

#### **A Bayesian Approach to the Selection of Two-level Multi-stratum Factorial Designs**

**Ming-Chung Chang**, National Central University, Taiwan

**Coauthors:** Ching-Shui Cheng

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, minimum aberration is a popular criterion for choosing regular fractional factorial designs. One difficulty in extending this criterion to multi-stratum factorial designs is that the formulation of a word length 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 word length patterns do not account for the different stratum variances. Mitchell, Morris and Ylvisaker [Statist. Sinica 5 (1995) 559–573] proposed a framework for Bayesian factorial designs. A Gaussian process is used as the prior for the treatment effects, from which a prior distribution

of the factorial effects is induced. This approach is applied to study optimal and efficient multi-stratum factorial designs. Good surrogates for the Bayesian criteria that can be related to word length and generalized word length patterns for regular and nonregular designs, respectively, are derived. A tool is developed for eliminating inferior designs and reducing the designs that need to be considered without requiring any knowledge of stratum variances. Numerical examples are used to illustrate the theory in several settings.

### **Challenges in Experimental Designs for the Chemical Industry**

**Fabio D'Ottaviano**, Dow Chemical

The Core R&D function of the Dow Chemical Company encompasses an array of pull services in the form of expertise in STEM disciplines to all businesses across the company. The Statistics Group of Core R&D provides statistical consultancy to researchers by assisting them in designing & analyzing the experiments that they need in an optimal manner. As such, design of experiments is the workhorse used by this group to meet the demands from researchers.

This presentation intends to demonstrate the challenges faced by the Statistics Group while designing experiments across the chemical industry. Given the diversified portfolio of businesses supported by the company, this group has to deal with multiple experimental design techniques which leads to challenges just as diverse. Specifically, the presentation covers issues in nonlinear, high throughput screening, and interrupted time series experimental designs.

### **Optimal designs for drug combination informed by longitudinal model for the response**

**Vladimir Dragalin**, Janssen Pharmaceuticals Companies of Johnson & Johnson

**Coauthors:** Tobias Mielke

The objective is to estimate the efficacy response surface in the safety-tolerated two-dimensional dose space of the two drugs that has been established in previous phases and to select the most efficient dose-combination for the final Phase III clinical trial. In contrast with the dose escalation designs for Phase I trials, in Phase II studies subjects can be allocated upfront to all dose-combinations in the acceptable dose-combination region. The problem is then to find the optimal design that allocates subjects to these dose-combinations in order to maximize the efficacy information obtained in the trial. We are using a binary endpoint as a measure of efficacy but consider the practical situation when the timing of the endpoint assessment period on the subject level is considerably longer relative to the inter-arrival time of subjects. This poses some implementation challenges and we propose a solution by using time-to-event as a particular type of longitudinal response models that helps to draw information from partial follow-up on subjects at the interim analysis.

### **Utilizing the Block Diagonal Covariance Structure of Nonregular Two-Level Designs**

**David J. Edwards**, Virginia Commonwealth University

**Coauthors:** Robert W. Mee

Two-level fractional factorial designs are often used in screening scenarios to identify active factors. This presentation investigates the block diagonal structure of the information matrix of certain nonregular two-level designs. This structure is appealing since estimates of parameters belonging to different diagonal submatrices are uncorrelated. As such, the covariance matrix of the least squares estimates is simplified, and the number of linear dependencies is reduced. We connect the block diagonal information matrix to the parallel flats design literature and gain insights into the structure of what is estimable and/or aliased using the concept of minimal dependent sets. Three parallel flat designs represent one common example, but we show how the block diagonal structure arises in other contexts. Recognizing this structure helps with understanding the advantages of alternative designs as well as analysis.

### **Compound optimality criteria accounting for potential model uncertainty**

**Dr. Olga Egorova**, University of Southampton

**Coauthors:** Steven Gilmour

The focus of the presented work is on developing composite optimality criteria for factorial experiments, concentrated on statistical inference objectives in the case of potential presence of a pre-specified polynomial model contamination. We discuss the basics of pure error based inference approach, and use it as a foundation for the construction of criteria components that correspond to various (and likely contradicting) objectives: obtaining reliable estimates of the fitted model parameters and minimising the impact of model misspecification.

The criteria are derived in the determinant- and trace-based forms, and are also adapted for designing blocked and multistratum experiments. The developed methodology is illustrated with examples of experimental layouts and constraints, the resulting designs and computational aspects are presented and explored as well.

### **Minimal Aliasing Optimal Designs for Non-Linear Models**

**Anna Errore**, University of Minnesota

**Coauthors:** R. D. Cook, C. J. Nachtsheim

For standard optimal design problems in linear models it is well established that foldover designs induce statistical independence between first order linear effects and two-factor interaction effects. When designs possess this feature, main linear effects are not biased by the presence of two-factor interactions. For example, definitive screening designs (Jones and Nachtsheim, 2011), and efficient foldover designs (Errore et al., 2017) leverage this property. In this paper, we ask the question: can designs for non-linear models be constructed such a way that main effects estimates are similarly independent of estimates of two-factor interactions? We use constrained optimization to explore this question. In particular, we construct optimal designs for nonlinear models with the primary objective to maximize the design efficiency for a first order logistic regression model, subject to a constraint on the amount of bias induced by the omission of two-factor interaction terms. To operationalize this optimization, we attempt to construct designs that lead to parameter orthogonality --- in the sense of Cox and Ried, 1987 --- between the parameters associated with the first and second order model terms.

### **Dose ranging studies for mixed populations**

**Valerii Fedorov**, Innovation Center, ICON, North Wales, USA

The models that include mixed distributions gained a notable popularity with the advent of precision medicine. In this presentation the respective extension of the traditional dose-response models is considered in the optimal design theory setting. The latter allows building optimal designs that either can be applied directly or can be used to generate benchmarks for various optimality criteria related to numerous empirical dose finding procedures.

### **Some interesting results on inference and information with adaptive designs**

**Nancy Flournoy**, University of Missouri

Adaptive procedures are increasingly popular in many fields, for example, using accruing information to change treatment allocation probabilities, increase estimation efficiency, decrease adverse outcomes, stop sampling and drop treatment arms. This talk discusses the effects of adaptation on established inference procedures and the opportunities adaptation provides for new approaches. In this discussion, we identify some similarities in the effects of adaption among procedures with disparate goals and provide an introduction to the other talks in this session.

### **Incorporating Historical Data into Dose Ranging Design Utilizing Bayesian Methods**

**Michael Fries**, CSL Behring

**Coauthors:** Jonathan French, Jonathan Sidi, Michael Tortorici, Jinesh Shah

Ideally, a dose ranging study would incorporate a wide range of doses, including placebo. However, it may be the case that placebo is not acceptable due to ethical reasons. We will describe a trial design that incorporated historical placebo through a minimally informative prior that increased the performance of the design while was still sufficiently flexible to perform well under misspecification of the placebo prior.

### **Large-Scale Optimal Experimental Design for Bayesian Inverse Problems**

**Omar Ghattas**, The University of Texas at Austin

**Coauthors:** Umberto Villa

We address optimal experimental design (OED) problems for Bayesian inverse problems governed by PDE forward models. Specifically, we consider the OED objective of maximizing the expected information gain (EIG), i.e. the expectation (wrt data) of the Kullback-Leibler divergence from prior to posterior. Naive evaluation of EIG is intractable due to double loop Monte Carlo sampling of the KL divergence and its expectation. Here we invoke an EIG approximation based on Laplace approximation of the posterior, which permits the KL divergence to be expressed in terms of the log-determinant and trace of the Hessian of the log posterior. Rapid spectral decay and a randomized eigensolver permit estimation of these invariants at a cost (measured in number of PDE solves) that is independent of the number of uncertain parameters and design variables, resulting in scalable evaluation of the OED objective and its gradient, and leading to scalable solution of the OED problem.

### **Replication or Exploration? Sequential Design for Stochastic Simulation Experiments**

**Robert B. Gramacy**, Virginia Tech

**Coauthors:** Mickael Binois, Jiangeng Huang, Chris Franck, Mike Ludkovski

We investigate the merits of replication, and provide methods that search for optimal designs (including replicates), in the context of noisy computer simulation experiments. We first show that replication offers the potential to be beneficial from both design and computational perspectives, in the context of Gaussian process surrogate modeling. We then develop a lookahead based sequential design scheme that can determine if a new run should be at an existing input location (i.e., replicate) or at a new one (explore). When paired with a newly developed heteroskedastic Gaussian process model, our dynamic design scheme facilitates learning of signal and noise relationships which can vary throughout the input space. We show that it does so efficiently, on both computational and statistical grounds. In addition to illustrative synthetic examples, we demonstrate performance on two challenging real-data simulation experiments, from inventory management and epidemiology.

### **Optimal Bayesian Design for Models with Intractable Likelihoods via Supervised Learning Methods**

**Markus Hainy**, Johannes Kepler University Linz, Austria

**Coauthors:** David J. Price, Olivier Restif, Christopher Drovandi

Optimal Bayesian experimental design is often computationally intensive due to the need to approximate many posterior distributions for datasets simulated from the prior predictive distribution. The issues are compounded further when the statistical models of interest do not possess tractable likelihood functions and only simulation is feasible. We employ supervised learning methods to facilitate the computation of utility values in optimal Bayesian design. This approach requires considerably fewer simulations from the candidate models than previous approaches using approximate Bayesian computation. The approach is particularly useful in the presence of models with intractable likelihoods but can also provide computational advantages when the likelihoods are manageable. We consider the two experimental goals of model discrimination and parameter estimation. The methods are applied to find optimal designs for models in epidemiology and cell biology.

### **Ascent with Quadratic Assistance for the Construction of Exact Experimental Designs**

**Radoslav Harman**, Comenius University, Bratislava, Slovakia

**Coauthors:** Lenka Filová

In the area of experimental design, there is a large body of theoretical knowledge and computational experience concerning so-called optimal approximate designs. However, for an approximate design to be executed in a practical setting, it must be converted into an exact design, which is usually done via rounding procedures. In this talk, we build on an alternative principle of utilizing optimal approximate designs for the computation of optimal, or nearly-optimal, exact designs. The principle, which we call ascent with quadratic assistance (AQuA), is an integer programming method based on the quadratic approximation of the design criterion in the neighborhood of the optimal approximate information matrix.

To this end, we present efficient quadratic approximations of all Kiefer's criteria with an integer parameter, including D-, and A-optimality and, by a suitable model transformation, I-optimality. Importantly, we also prove a low-rank property of the associated quadratic forms, which enables us to apply AQuA to large design spaces, for example via mixed integer second-order cone solvers. We numerically demonstrate the robustness and performance of the proposed method.

### **Interleaved Lattice-Based Minimax Distance Designs and Maximin Distance Designs**

**Xu He**, Chinese Academy of Sciences

Minimax and maximin distance designs are useful for computer experiments. Existing constructions use global optimization techniques to optimize the fill or separation distance. Such algorithms are suboptimal unless the number of variables or runs are small. We propose new methods which yield best minimax distance designs for moderate-to-large sample sizes or best maximin distance designs uniformly across moderate dimensions. These designs are constructed from interleaved lattices, which are lattices that have repeated or alternated layers based on any single dimension. The idea is to circumvent computational difficulties by restricting to designs with certain geometry structure and use distance properties of interleaved lattices in computation. Theoretical and numerical results are provided.

### **Robust Designs for Model Discrimination**

**Rui Hu**, MacEwan University

**Coauthors:** Doug Wiens

To aid in the discrimination between two, possibly nonlinear, regression models, we study the construction of experimental designs. Considering that each of these two models might be only approximately specified, robust "maximin" designs are proposed. The rough idea is as follows. We impose neighbourhood structures on each regression response, to describe the uncertainty in the specifications of the true underlying models. We determine the least favourable-in terms of Kullback-Leibler divergence-members of these neighbourhoods. Optimal designs are those maximizing this minimum divergence. Sequential, adaptive approaches to this maximization are studied. Asymptotic optimality is established.

### **A Random Fourier Feature Method for Modeling Computer Experiments with Gradient Information**

**Tzu-Hsiang Hung**, University of Wisconsin–Madison

**Coauthors:** Peter Chien

Computer experiments with gradient information are increasingly conducted in many fields in engineering and science. The gradient-enhanced Gaussian process emulator is often used to model data from such experiments. We propose a random Fourier feature method to mitigate potential numerical issues of this type of emulator. The proposed method employs random Fourier features to obtain an easily computable, low-dimensional feature representation for shift-invariant kernels involving gradients. The effectiveness of the proposed method is illustrated by several examples.

## **D- and A- Optimal Orthogonally Blocked Mixture Component -Amount Designs via Projections**

**Bushra Husain, Aligarh Muslim University, India**

**Coauthors:** Afrah Hafeez

Mixture experiments are usually designed to study the effects on the response by changing the relative proportions of the mixture ingredients. This is usually achieved by keeping the total amount fixed but in many practical applications such as medicine or biology, not only are the proportions of mixture ingredients involved but also their total amount is of particular interest. Such experiments are called mixture-amount experiments. In such experiments, the usual constraint on the mixture proportions that they should sum to unity is relaxed. The optimality of the design strictly depends on the nature of the underlying model. In this paper, we have obtained D- and A- optimal orthogonally blocked mixture component-amount designs in two and three ingredients via projections based on the reduced cubic canonical model presented by Husain and Sharma (2017) and the additive quadratic mixture model proposed by Husain and Parveen (2016), respectively.

## **Estimation of Healthcare Accessibility using an Online Experiment**

**Youngdeok Hwang, Sungkyunkwan University, South Korea**

**Coauthors:** Jae-Kwang Kim

Automated data collection using various sources becomes an important part of statistical practice. In this talk, we present a statistical approach to study the accessibility and coverage of the urgent health care that determines the patient outcomes. I will discuss an online experiment to estimate the nation-wide statistics for first medical contact to door time using a large scale automated map queries, combined with national patient statistics. The proposed approach utilizes the design of experiment to plan the data collection process, while taking into account the survey sampling perspective.

## **Design of Physical Experiments Using History Matching Methodology**

**Samuel Jackson, University of Southampton, UK**

**Coauthors:** Ian Vernon

Computer models are essential for aiding the understanding of real-world processes of interest. History matching aims to find the set of all possible combinations of computer model input rate parameters which are not inconsistent with observed data, gathered from a collection of physical experiments, given all the sources of uncertainty involved with the model and the measurements. Identification of such regions of input space is informative about the real-world quantities associated with the input parameters and the links between them. We therefore quantify the expected information gain resulting from performing possible individual, or sets of, future physical experiments in terms of history matching criteria related to scientific questions of interest. We can then make the decision to perform those experiments expected to be most informative. We demonstrate our techniques on an important systems biology model of hormonal crosstalk in the roots of an Arabidopsis plant.

## **Construction, Properties, and Analysis of Group-Orthogonal Supersaturated Design**

**Brad Jones, JMP**

This talk introduces a new method for constructing supersaturated designs that is based on the Kronecker product of two carefully-chosen matrices. The construction method leads to a partitioning of the columns of the design such that the columns within a group are correlated to the others within the same group, but are orthogonal to any factor in any other group. We refer to the resulting designs as group orthogonal supersaturated designs (GO-SSDs). We leverage this group structure to obtain an unbiased estimate of the error variance and to develop an effective, design-based model selection procedure. Simulation results show that the use of these designs, in conjunction with our model selection procedure enables the identification of larger numbers of active main effects than have previously been reported for supersaturated designs. The designs can also be used in group screening; however, unlike previous group-screening procedures, with our designs, main effects in a group are not confounded.

### **Optimal designs for mixed responses with quantitative and qualitative factors**

**Ming-Hung Kao**, Arizona State University

**Coauthors:** Hazar Khoogeer

We are concerned with optimal designs for experiments where bivariate responses of mixed variable types (binary and continuous) are collected from each experimental subject. Mixed response regression models involving both quantitative and qualitative factors are considered to jointly model the bivariate responses and results on locally optimal designs for such models are derived. We also utilize efficient algorithms to obtain these designs.

### **Design and Dismemberment for Controlling the Risk of Regret for the Multi-Armed Bandit**

**Timothy J. Keaton**, Purdue University

**Coauthors:** Arman Sabbaghi

The multi-armed bandit (MAB) problem refers to the task of sequentially assigning different treatments to experimental units so as to identify the best treatment(s) while controlling the regret, or opportunity cost, of exploration. The traditional criterion of interest for the design of an MAB algorithm has been control of the expected regret over the course of the algorithm's implementation. However, an additional criterion that must be considered for many practical, real-life problems is control of the variance, or risk, of regret. We develop a framework to address both of these criteria by means of two elementary concepts that can be incorporated into any existing MAB algorithm: design of a learning phase and dismemberment of interventions after the learning phase. The utility of our framework is demonstrated in the construction of new Thompson samplers that involve a small number of simple and interpretable tuning parameters.

### **Adaptive Designs for Optimal Observed Fisher Information**

**Adam Lane**, Cincinnati Children's Hospital Medical Center

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 approximation of the variance of the maximum likelihood estimator. 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 known. In the current work, two adaptive designs are proposed that use the observed Fisher information from previous runs to inform the design of future runs.

### **Designing combined physical and computer experiments to maximize global prediction accuracy**

**Erin Leatherman**, Kenyon College

**Coauthors:** Angela Dean and Thomas Santner

Computer experiments use (deterministic) simulators based on mathematical models of physical processes as experimental platforms to determine "responses" at user-specified "inputs." When a computer experiment is used to augment observations from a physical experiment, the latter may be used to calibrate the simulator. Compared with an uncalibrated simulator, calibration can lead to more accurate predictions of the mean physical response. This talk describes several classes of combined designs for physical/simulator experiments to maximize the global prediction accuracy of the mean physical response. The designs compared are (1) locally optimal for the combined experiment under the minimum integrated mean squared prediction error criterion; (2) locally optimal for either the physical or simulator experiment with a fixed design for the second; and (3) maximin augmented nested Latin Hypercube designs. The empirical prediction accuracies of the designs are compared over a test bed of examples and design recommendations are given.

### **Design and analysis of covering arrays using prior information**

**Ryan Lekivetz**, SAS Institute

**Coauthors:** Joseph Morgan

Covering arrays are increasingly being used by test engineers to derive test cases to test complex engineered systems. This approach to testing is known as combinatorial testing and has proven to be a cost-efficient way to determine test cases that are highly effective at identifying faults in the system due to the combination of several inputs. However, when such faults are encountered, and failures occur, the test engineer is tasked with determining the inputs and associated values that triggered the failures. This talk addresses this issue by considering the prior knowledge about the system under test (SUT) that is often held by test engineers. We discuss how this prior knowledge can be used to construct covering arrays and how it can also be used to evaluate the effectiveness of covering arrays before any test cases are executed. We then discuss how this prior knowledge can be used to analyze the outcomes of a set of test cases executed on the SUT when failures occur.

### **Experimentation in the Operating System: The Windows Experimentation Platform**

**Paul Li**, Microsoft

**Coauthors:** Pavel Dmitriev, Huibin Mary Hu, Xiaoyu Chai, Zoran Dimov, Brandon Paddock, Ying Li, Alex Kirshenbaum, Irina Niculescu, Taj Thoresen

Online controlled experiments are the gold standard for evaluating improvements and accelerating innovations in online and app worlds. However, little is known about applicability, implementation, and efficacy of experimentation for operating systems (OS), where many features are non-user-facing. In this paper, we present the Windows Experimentation platform (WExp), and insights from implementation and execution of real-world experiments in the OS. We start by discussing the need for experimentation in OS, using real experiments to illustrate the benefits. We then describe the architecture of WExp, focusing on unique considerations in its engineering. Finally, we discuss learnings and challenges from conducting real-world experiments. Our experiences and insights can motivate practitioners to start experimenting as well as to help them to successfully build their experimentation platforms. The learnings can also guide experimenters with best-practices and highlight promising avenues for future research

### **Recent Progress on Using Individual Column Information for Design Selections**

**William Li**, Shanghai Jiao Tong University, China

While literature on constructing efficient experimental designs has been plentiful, how best to incorporate prior information when assigning factors to the columns has received little attention. This talk summarizes a series of recent studies that focus on information of individual columns. For regular designs, we propose the individual word length pattern (iWLP) that can be used to rank columns. With prior information on how likely a factor is important, iWLP can be used to intelligently assign factors to columns, and select the best designs to accommodate such prior information. This criterion is then extended to study nonregular designs, which we denote as the individual generalized word length pattern (iGWLP). We illustrate how iGWLP helps to identify important differences in the aliasing that is likely otherwise missed. The theoretical justifications of the proposed iGWLP are provided in terms of statistical model and projection properties. In the third part, we consider clear effects involving an individual column (iCE). Motivated by a real application, we introduce the clear effects pattern, derived from iCE and propose a class of designs called maximized clear effects pattern (MCEP) designs. We compare MCEP designs with commonly used minimum aberration designs and MaxC2 designs that maximize the number of clear two-factor interaction. In the last part, we briefly introduce some recent progress on linking information on individual column with some previous criteria for choosing among factorial designs. Composite grid designs for large scale computer model emulation

### **I<sub>c</sub>-Optimal design with a large candidate pool of generalized linear models**

**Yiou Li**, DePaul University

**Coauthors:** Xinwei Deng

The generalized linear models are widely used in statistical analysis and the related design issues are undoubtedly challenging. The state-of-the-art works mostly apply to design criteria on the estimates of regression coefficients. It is of importance to study optimal designs for generalized linear models, especially on the prediction aspects. In this work, we consider the constrained I-optimality as a prediction-oriented design criterion for generalized linear models and develop efficient algorithms for such I<sub>c</sub>-optimal designs. The proposed efficient algorithm adequately combines the Fedorov-Wynn algorithm and multiplicative algorithm. It achieves great computational efficiency with guaranteed convergence property. The theoretical results and the proposed efficient algorithm also provide some inspiration on the subset selection of big data.

### **Random Norming Aids Analysis of Non-linear Regression Models with Sequential Informative Dose Selection**

**Zhantao Lin**, George Mason University

**Coauthors:** Nancy Flournoy, William F Rosenberger

A two-stage adaptive optimal design is an attractive option for increasing the efficiency of an experiment. In these designs, the locally optimal dose is chosen for further exploration based on interim data, which induces dependencies between data from the two stages. In a pilot study where the first stage sample size is fixed and the second stage sample size is large, under nonlinear regression models with independent normal errors, normalizing the maximum likelihood estimate (MLE) with the Fisher information fails to provide asymptotic normality. We present three alternative random information measures and show that using them to norm the MLE provides asymptotic normality. The performance of random information measures is investigated in simulation studies and the results suggest that the observed information performs best when the sample size is small.

### **Heavy user effect in A/B testing: Identification and estimation**

**Jiannan Lu**, Microsoft Corporation

**Coauthors:** Yu Wang, Somit Gupta, Ali Mahmoudzadeh, Sophia Liu

On-line experimentation (also known as A/B testing) has become an integral part of software development. To timely incorporate user feedback and continuously improve products, many software companies have adopted the culture of agile deployment, requiring online experiments to be conducted and concluded on limited sets of users for a short period. While conceptually efficient, the result observed during the experiment duration can deviate from what is seen after the feature deployment, which makes the A/B test result highly biased. While such bias can have multiple sources, we provide theoretical analysis as well as empirical evidence to show that the heavy user effect can contribute significantly to it. To address this issue, we propose to use a jackknife-resampling estimator. Simulated and real-life examples show that the jackknife estimator can reduce the bias and make A/B testing results closer to our long term estimate.

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

**Abhyuday Mandal**, University of Georgia

**Coauthors:** Joshua Lukemire, Weng-Kee Wong, Jie Yang

Identifying optimal designs for generalized linear models with a binary response can be a challenging task, especially when there are both discrete and continuous independent factors in the model. Theoretical results rarely exist for such models, and for the handful that do, they usually come with restrictive assumptions. We propose the d-QPSO algorithm, a modified version of quantum-behaved particle swarm optimization, to find a variety of D-optimal approximate and exact designs for experiments with discrete and continuous factors and a binary response. We show that the d-QPSO algorithm can efficiently find locally D-optimal designs even for experiments with a large number of factors and 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 removal experiment, an electronic static experiment, and a ten-factor car refueling experiment.

### **Comparing DCEs in the field: Does Design Construction Method Matter?**

**Brendan Mulhern** University of Technology Sydney, Australia

**Coauthors:** Richard Norman, Rosalie Viney, Mark Oppe, Deborah J Street

The accuracy of the parameter estimates obtained from a Discrete Choice Experiment depends on the set of choice sets used in the valuation. The aim of this study was to compare a range of different design construction methods using primary data collection in Australia. The DCE presented pairs of health states described by EQ-5D-5L (a widely used health measure). Nineteen designs were developed using different criteria focused on prior information (informative or non-informative), level of severity overlap (no overlap or overlap on two attributes), choice set selection strategy (generator developed, modified Fedorov, Bayesian efficient or swapping algorithms), and software used (NGene, Stata or SAS). More than 3,000 people completed 21 tasks each. The designs show apparent differences in performance in terms of a range of indicators including coefficient ordering, predictive ability, and identification of heterogeneity. The design construction method does not appear to be systematically associated with the results.

### **Strategic Subdata Selection for Linear Regression Modeling with Big Data**

**Abigael Nachtsheim**, Arizona State University

**Coauthors:** John Stufken

The need to handle datasets with millions or tens of millions of observations is not uncommon today. However, when datasets contain a very large number of observations, standard statistical methods can become infeasible due to computational limitations. A solution is to select a subset of the full data and conduct the statistical analysis using this subdata alone. One approach is to select the subdata to optimize a specified criterion, with the goal of improving properties of the resulting model estimators. Several related methods have been proposed in the context of linear regression, including leverage-based subsampling methods and the Information-Based Optimal Subdata Selection method (IBOSS) (Ma and Sun, 2015; Ma, Mahoney, and Yu, 2015; Wang, Yang, and Stufken, 2018). IBOSS borrows from the field of experimental design, selecting subdata to maximize the determinant of the information matrix for the model parameters, given a fixed subdata size. This strategy provides several advantages over both simple random sampling and leverage-based subsampling methods. We outline these advantages, providing selected results and comparisons from Wang, Yang, and Stufken (2018). Finally, we conclude with a discussion of remaining challenges in this area of research, and extensions to existing subdata selection methods.

### **Bayesian design for physical models using computer experiments**

**Antony Overstall**, University of Southampton, UK

Design of experiments is an "a-priori" activity making the Bayesian approach particularly attractive. Bayesian inference allows any available prior information to be included in both design and analysis, yielding posterior distributions for quantities of interest that are more interpretable by researchers. Furthermore, the design process allows the precise aim of the experiment to be incorporated. Mathematically, a Bayesian design is given by the maximisation of an expected utility function over all unknown quantities. While straightforward in principle, finding a Bayesian design in practice is difficult. The utility and expected utility functions are rarely available in closed form and require approximation, and the space of all designs can be high dimensional. These problems are compounded when the data-generating process is thought to depend on an analytically intractable physical model, i.e. an intractable likelihood model. This talk will review a recent research programme that has developed methodology to find practically-relevant Bayesian designs for a range of physical models. The methodology uses several layers of computer experiments to both approximate quantities of interest (utilities and expected utilities) and to use these approximations to find Bayesian designs.

### **On Generalizing the Foldover Technique to $3^{f-s}$ Regular Fractional Factorial Designs**

**R. Vincent Paris**, Iowa State University

**Coauthors:** Max D. Morris

The foldover technique allows for an expansion of a fractional factorial experiment with two level factors to achieve a resolution IV design from a resolution III design. Resolution IV designs allow for unbiased estimation of main effects if third order interactions and higher are 0. This presentation lays out a scheme that generalizes the foldover technique to regular fractional factorial experiments with three level factors by augmenting the design matrix by a rotation vector. The criterion for choosing an optimal rotation vector is discussed. While there is no perfect analog for always achieving resolution IV designs, minimum aberration can be gained in all situations where resolution IV designs are not available.

### **Agent-based simulation experiments: An Innovative Approach for the Development of Future Marine Corps Amphibious Capability**

**Jeffrey D. Parker**, Naval Postgraduate School

**Coauthors:** Susan M. Sanchez

Agent-based simulations are models where multiple entities sense and stochastically respond to conditions in their local environments, mimicking complex large-scale system behavior. We illustrate the use of designed experiments in challenging application to glean insights from agent-based models for a complex military operation: an opposed amphibious operation. Robust design approaches are particularly well-suited for these endeavors.

### **Recent advances and new challenges in optimal designs for copula models**

**Elisa Perrone**, Massachusetts Institute of Technology

The growing availability of data makes it challenging yet crucial to model complex dependence traits. For example, hydrological and financial data typically display tail dependences, non-exchangeability or stochastic monotonicity. Copulas serve as tools for capturing these complex traits and constructing accurate dependence models which resemble the underlying distributions of data.

This talk explores the many advantages of copula models in the optimal experimental design framework. In particular, we present an equivalence theory for copula models, which provides theoretical guarantees for a design to be optimal under popular optimality criteria, such as D-optimality and  $D_s$ -optimality. In addition, we discuss new challenges and research directions to further increase the popularity of copulas models in the optimal design practice.

### **A systematic construction of cost-efficient designs for order-of-addition experiments**

**Frederick Kin Hing Phoa**, Academia Sinica, Taiwan

**Coauthors:** Jin-Wen Huang, Yuan-Lung Lin

An order-of-addition (OofA) experiment aims at investigating how the order of factor inputs affects the experimental response, which is recently of great interest among practitioners in clinical trials and industrial processes. Although the initial framework was established for more than 70 years, recent studies in the design construction of OofA experiments focused on their properties of algebraic optimality rather than cost-efficiency. The latter is more practical in the sense that some experiments, like cancer treatments, may not easily have adequate number of observations. In this work, we propose a systematic construction method for designs in OofA experiments from a cost-efficient perspective. In specific, our designs take the effect of two successive treatments into consideration. To be cost-efficient, each pair of level settings from two different factors in our design matrix appears exactly once. Compared to recent studies in OofA experiments, our designs not only handle experiments of one-level factors (i.e. all factors are mandatorily considered), but also factors of two or more levels, so

practitioners may insert placebo or choose different dose when our designs are used in an OofA experiment in clinical trials for example.

### **Composite grid designs for large scale computer model emulation**

**Matthew Plumlee**, Northwestern University

Computer models with high dimensional inputs require many samples to get accurate emulators. After many (say 10000) samples from a computer model, classical computer model emulation techniques either break down or become completely infeasible. The common solution is to start approximating the emulation technique, which can completely eliminate the benefit of having many samples. This talk will discuss how one can deploy adaptive but structured computer experiments that can easily scale to the 10K or 100K samples regime with minimal computational overhead. The inference is exact; meaning there is no degradation your emulator caused by sloppy approximations.

### **Randomization Tests of Causal Effects Under General Interference**

**David Puelz**, University of Chicago

**Coauthors:** Guillaume Basse , Avi Feller, Panos Toulis

We develop randomization tests for estimating causal effects under general interference between interacting experimental units. In this setting, null hypotheses on causal effects are usually not sharp, and thus randomization tests, such as the Fisher randomization test, cannot be used. To resolve this, we rely on the fact that many of these null hypotheses can be viewed as implying a bipartite graphical structure between units and assignments, which helps to determine the appropriate conditioning for the randomization test. Specifically, bicliques in the graph include units and assignments for which all potential outcomes can be imputed under the null hypothesis and thus enable exact randomization tests. We illustrate our method in a large-scale policing experiment in Colombia.

### **A probabilistic subset search (PSS) algorithm for optimizing functional data sampling designs**

**Hyungmin Rha**, Arizona State University

**Coauthors:** Ming-Hung Kao, Rong Pan

We study optimal sampling times for functional data. Our main objective is to find the best sampling schedule on the predictor time axis to precisely recover the trajectory of predictor function and predict the scalar/functional response through a functional linear regression model. Three optimal designs are considered, namely, the schedule that maximizes the precision of recovering predictor function, the schedule that is the best for predicting response (function), and the schedule that optimizes a user-defined mixture of the relative efficiencies of the two objectives. We propose an algorithm that can efficiently generate nearly optimal designs, and demonstrate that our approach outperforms the previously proposed methods.

### **Novelty and Learning Effects in Online Experiments**

**Sol Sadeghi**, Microsoft

**Coauthors:** Stefan Gramatovici, Mohammed Helal, Shawn Chai, Sophia Peng, Mary Hu, Paul Li

Many organizations use A/B testing to assess the causal impacts of their features. However, since experiments are typically limited in duration (e.g. few weeks), this often leaves experimenters wondering about the long-term impact of their features: are the observed behavioral changes permanently stable, or are they increasing or decreasing over time? Novelty effect describes the desire to use new technology which diminishes over time. On the contrary, learning effect describes the growing engagement with technology as a result of adoption of the innovation. First, it is important to determine whether these long-term effects exist. Second, we need to measure and understand to what degree do these effects exist. Detection and quantification are important for experimenters seeking to make decisions about their features and setting proper expectations for management. To address this issue, we provide a model, based on difference-in-differences concept, that detects, estimates, and

corrects for long-term effects in the case that novelty or learning exist. This model reduces the experimental bias and contributes to trustworthiness of experimentation.

### **Simulation experiments: designs for decision making**

**Susan M. Sanchez**, Naval Postgraduate School

Data farming captures the notion of purposeful data generation from simulation models. 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. Large-scale designed experiments let us grow the simulation output efficiently and effectively. We can explore massive input spaces, uncover interesting features of complex response surfaces and explicitly identify cause-and-effect relationships. Nonetheless, there are many opportunities for research methods that could further enhance this process. I will begin with a brief overview of key differences between physical and simulation experiments, as well as current data farming capabilities and their relationship to emerging techniques in data science and analytics. I will then share some thoughts about opportunities and challenges for further improving the state of the art, and transforming the state of the practice, in this domain.

### **Adaptive dose escalation approaches for oncology combinations – theory and practice.**

**Suman K Sen**, Novartis Pharmaceuticals Corp.

**Coauthors:** Stuart Bailey

Since the introduction of the continual reassessment method<sup>1</sup> in 1990, model-based adaptive dose-escalation approaches have evolved to address many challenges of modern drug development. Many extensions have been proposed to address initial challenges with this approach including Bayesian Logistic Regression Model (BLRM) and alternative algorithmic designs, such as the modified toxicity probability interval (MTPI) have been introduced. With drug development being heavily focused on combination dose-finding, these approaches continue to be broadened into the combination setting<sup>4</sup> allowing the study of multi-drug therapies to incorporate data from historical single agent studies. While models or algorithms have advanced, the endpoint on which these designs are applied remains focused on dose-limiting toxicity (DLT) within a defined time window (usually one or two cycles of treatment) with a goal to establish a maximum tolerated dose (MTD). In the setting of many new cancer treatments, the observation of DLT may not occur and “dose-finding” will rely on more than the primary “dose escalation” design. We reflect on the learnings from ten years of adaptive Bayesian combination dose-finding in oncology and provide areas to consider when integrating historical single agent data and examples of decisions using non-DLT data.

### **Optimal Bayesian Design of Sequential Experiments via Reinforcement Learning**

**Wanggang Shen**, University of Michigan

**Coauthors:** Xun Huan

Experiments are indispensable for understanding physical systems and developing predictive models. When experiments are expensive, a careful design of these limited data-acquisition opportunities can be immensely beneficial. Optimal experimental design, while leveraging the predictive capabilities of a simulation model, provides a rigorous framework to systematically quantify and maximize the value of an experiment. We focus on sequential experimental design, seeking good design policies (strategies) that can adapt to newly collected data (feedback) and anticipated future changes (lookahead). We cast this sequential learning problem in a Bayesian setting with information-based rewards, and solve it numerically via reinforcement learning techniques. In particular, we enable policy gradient methods that directly parameterize the policies and improve them via gradient estimates. The overall method is demonstrated on an algebraic benchmark and a sensor placement application for source inversion. The results suggest substantial computational advantages compared to previous approaches using approximate dynamical programming.

### **Model-Robust Subdata Selection for Big Data**

**Chenlu Shi**, Simon Fraser University, Canada

**Coauthors:** Boxin Tang

Due to the challenge of analyzing big data using current computing resources, data reduction is desired. The existing work on subdata selections heavily relies on the specific model. This calls for an approach that is robust to model misspecifications. We propose the use of the maximin distance criterion for subdata selection and examine a fast algorithm for its implementation. To assess the performance of our approach in terms of model misspecifications, the comparison between our approach and a recent model-dependent method is made through simulations. Numerical results show that our approach gives both smaller variance and bias for the estimates of slope parameters, and this advantage becomes increasingly significant when the correlation in the simulated data gradually increases.

### **Pseudo generalized Youden designs**

**Rakhi Singh**, TU Dortmund, Germany

**Coauthors:** Ashish Das; Daniel Horsley

Youden square designs, or Youden rectangles, are classical objects in design theory. Extensions of these were introduced in 1958 by Kiefer and in 1981 by Cheng, in the form of generalized Youden designs (GYDs) and pseudo Youden designs (PYDs), respectively. In this talk, we introduce a common generalization of both these objects, which we call a pseudo generalized Youden design (PGYD). PGYDs share the statistically-desirable optimality properties of GYDs and PYDs, and we show that they exist in situations where neither GYDs nor PYDs do. We determine some numerical necessary conditions for the existence of PGYDs, classify their existence for small parameter sets, and provide constructions for families of PGYDs using patchwork methods based on affine planes. I will also talk about how GYDs or PGYDs are useful in crossover designs with slight modifications in their construction methods.

### **Sign-Informative Design and Analysis of SSDs**

**Jonathan Stallrich**, North Carolina State University

**Coauthors:** David Edwards, Byran Smucker, Maria Weese

Much of the literature on the design and analysis of supersaturated designs (SSDs) rests on design principles assuming a least-squares analysis. More recently, researchers have discovered the potential of analyzing SSDs with penalized regression methods like the LASSO and Dantzig selector estimators. There exists much theoretical work for these methods that establish connections between their variable selection performance and properties of a fixed design matrix. Surprisingly, there has been little research on design criteria motivated by these connections and insights. In this talk, we discuss new approaches to both the design and analysis of SSDs that incorporates prior knowledge about the effect signs (positive/negative coefficients). Examples are given to show how these new designs compare to those found under established SSD criteria. A new Bayesian analysis is discussed that incorporates sign information and a simulation study is performed to show its ability to improve power over current methods.

### **The Analysis of A/B Tests with Comparative Probability Metrics**

**Nathaniel Stevens**, University of Waterloo, Canada

A/B testing and online experimentation has become commonplace in the field of data science. Such experimentation is typically used to formally determine whether one product variant performs at least as well as one or more alternatives. Traditionally, such comparisons have been made via various data-dependent hypothesis tests which all require the correct interpretation of a p-value. However, the widespread misunderstanding and misuse of p-values often hinders the efficacy of such tests. In this talk I propose the use of comparative probability metrics (CPMs) as an estimation-based alternative to traditional hypothesis testing as a means to determine which among a collection of variants is optimal. CPMs provide a flexible and intuitive means of drawing such conclusions

by directly calculating, for example, the probability that one variant is superior to another or the probability that two variants are practically equivalent. The methodology will be illustrated on a real example, and its good properties will be demonstrated with simulated data.

### **Equivalence of 2-level Designs Between Baseline and Orthogonal Parameterization**

**Cheng-Yu Sun**, Simon Fraser University, Canada

**Coauthors:** Boxin Tang

2-level designs under baseline parameterization (BP) have received less attention in comparison with that under orthogonal parameterization (OP). With abundant results for OP, it is desired to establish some equivalence between OP and BP, finding good designs under BP. Based on the simple fact that an effect under BP is a linear combination of the effects under OP, and vice versa, it can be shown that the D-efficiencies under BP and OP are the same design criterion if one only takes nested models into account. This also implies that estimable nested models are the same under any design no matter one uses BP or OP. On the other hand, we found that for any model, nested or not, it is always estimable under the Rechtschaffner design and BP. If further the model is nested, then Rechtschaffner design can unbiasedly estimates every parameter without assuming negligible effect.

### **Gaussian Process Regression with Large Datasets**

**Sonja Surjanovic**, The University of British Columbia, Canada

**Coauthors:** William J. Welch

Computer models are used as surrogates for physical computer experiments in a large variety of applications. Nevertheless, the number of evaluations of the computer model is often limited due to the complexity and cost of the model. Historically, Gaussian process regression has proven to be the almost ubiquitous choice of statistical surrogate for such a computer model, due to its flexible form and analytical expressions for measures of predictive uncertainty. However, even this statistical surrogate can be computationally intractable for large designs, due to computing time increasing with the cube of the design size. Multiple methods have been proposed for addressing this problem. We discuss several of them, and compare their predictive and computational performance in several scenarios. We then propose a new method for solving this problem using a sequential approach.

### **Asymptotic Properties of Maximum Likelihood Estimators with Sample Size Recalculation**

**Sergey Tarima**, Medical College of Wisconsin

**Coauthors:** Nancy Flournoy

Consider an experiment in which the primary objective is to test a treatment effect at a predetermined type I error and statistical power. Assume that the sample size required to maintain these type I error and power will be re-estimated at an interim analysis. Our main finding is that the asymptotic distributions of standardized statistics are random mixtures of distributions, which are non-normal except under certain model choices for sample size re-estimation (SSR). Monte-Carlo simulation studies and an illustrative example highlight the fact that asymptotic distributions of estimators with SSR may differ from the asymptotic distribution of the same estimators without SSR.

### **The Choice Set Size: To Be Fixed Or Not To Be Fixed**

**Martina Vandebroek**, KU Leuven, Belgium

**Coauthors:** Deniz Akinc

Two-alternative choice tasks have long been preferred in choice experiments because they are simple to analyze. However, the increase in computer power has made it possible to design and analyze discrete choice experiments with more alternatives. Researchers have to select an appropriate number of alternatives that will yield enough information about the respondents' preferences without overloading the choice set. It is common to keep the choice set size fixed because it is hoped that it helps in keeping the error variance in each choice task more or less

constant. However, as the complexity of the choice set also influences the error variance, the relationship between the information in the experiment, the error variance and the size of the choice sets is much more complicated and small choice sets can be quite complex while large choice sets can be relatively simple.

In this paper, we investigate whether a design can be improved by allowing for different choice set sizes. We look for efficient designs with varying choice set sizes for the conditional logit (CL) model as well as for the heteroscedastic conditional logit (HCL) model introduced by Ben-Akiva and Lerman (1985) which parameterizes the error variance as a function of the complexity of the choice set.

While investigating efficient designs for the CL model, we showed once more that the overall efficiency increases with increasing fixed choice set size but, to our surprise, we also found designs with varying choice set sizes that outperform designs with fixed choice set size, given the same number of choice sets and total number of alternatives.

When the complexity is reflected in the error variance and modelled by the HCL, we show that designs with constant choice set size are far from optimal. We found many choice designs with varying choice set sizes that are much more efficient to estimate the preference parameters than designs with the same number of alternatives in each choice set. We show that these designs have smaller average complexity and larger efficiency than efficient designs with fixed choice set size.

### **Construction of Large Two-Level Nonregular Designs of Strength Three**

**Alan Vazquez**, University of Leuven, Belgium

**Coauthors:** Hongquan Xu

Two-level orthogonal designs of strength 3 permit the study of the main effects and the two-factor interactions of the experimental factors. These designs are classified into regular and nonregular. Good regular designs are available in the literature for large run sizes that are a power of 2. In contrast, good nonregular designs, which have run sizes that are multiples of 8 and are more flexible alternatives to regular designs, are not available for large run sizes because their construction is challenging. In this presentation, we introduce an effective method to construct large strength-3 nonregular designs. Our construction method concatenates several smaller regular designs and uses theoretical results and algorithmic approaches to improve the concatenated design in terms of the aliasing among the two-factor interactions. Using practical experiments, we illustrate the potential of our method to generate attractive large strength-3 nonregular designs, which fill the gaps between the available strength-3 designs.

### **Construction of Two-Phase Designs for Experiments with a Single Block Factor in Each Phase**

**Nha Vo-Tham**, University of Hohenheim, Stuttgart, Germany

**Coauthors:** Rosemary Bailey and Hans-Peter Piepho

Design of experiments is widely used in many areas (i.e. industrial engineering, agriculture, medical research, etc.). Often, experiments involve two different phases. For example, in plant breeding the first phase of the experiment is performed in a field involving a number of treatments (i.e. varieties) and a single blocking factor (i.e. field blocks), whereas the second phase is performed in a laboratory to measure the response using the samples from the first phase, taking into account the presence of another blocking factor (i.e. days or lab machines). Such experiments are referred as to two-phase experiments. Currently, in the literature, construction approaches for such experiments are mostly focused on the case when treatments are orthogonal to blocks and design construction using A-optimality as the optimality criterion can be conveniently based on the 'design key' proposed by Bailey (2016). However, there is as yet no general strategy to design generation, when treatments are not orthogonal to blocks, which is often the case, e.g., when constructing designs in plant breeding. In this article, we therefore propose three different approaches to generate such designs, which utilize a metaheuristics search method, namely, iterated Tabu search. The first one is a sequential approach in which we first obtain an optimal arrangement of treatments with respect to the first blocking factor (i.e. blocks in Phase 1). Given the resulting first-

phase design, we find an optimal arrangement of this design with respect to the second blocking factor (i.e. blocks in Phase 2). The second approach is a simultaneous approach, which allows to find an optimal arrangement of treatments in the first-phase and second-phase block factors simultaneously. The third approach arranges treatments in a nested row-column structure, where rows and columns correspond to the two blocking factors. To avoid a computational burden for all approaches, we use an efficient update formula for computing the A-optimality criterion. We demonstrate the capacity of our algorithms with various examples, along with discussion.

### **Minimax Efficient Random Experimental Design Strategies**

**Tim Waite**, University of Manchester, UK

**Coauthors:** Dave Woods

In game theory and statistical decision theory, it is well known that a random (i.e. 'mixed') decision strategy often outperforms a deterministic one in minimax expected loss. Experimental design can be viewed as a game pitting the statistician against nature, and so the use of a random strategy to choose a design should often be beneficial. Despite this simple observation, the topic of minimax-efficient random design strategies is mostly unexplored in the literature, with consideration limited primarily to Fisherian randomization of the allocation of a predetermined set of treatments to experimental units. In this talk we show that novel flexible random design strategies often outperform deterministic designs in various problems where the goal is estimation of, or prediction from, a linear model. The advantage of a random design strategy is particularly dramatic in the problem of model-robust design, in which an L2-neighbourhood of possible model departures is considered. Here, use of an appropriate random design strategy gives a finite maximum expected loss, in contrast to the infinite maximum expected loss of a deterministic design.

### **Optimal Subsampling: Sampling with Replacement vs Poisson Sampling**

**HaiYing Wang**, University of Connecticut

**Coauthors:** Jiahui Zou

Faced with massive data, subsampling is a commonly used technique to improve computational efficiency and using nonuniform subsampling probabilities is an effective approach to improve estimation efficiency. In the context of maximizing a general target function, this paper derives optimal subsampling probabilities for both subsampling with replacement and Poisson subsampling. The optimal subsampling probabilities minimize functions of the subsampling approximation variances in order to improve the estimation efficiency. Furthermore, they provide deep insights on the theoretical similarities and differences between subsampling with replacement and Poisson subsampling. Practically implementable algorithms are proposed based on the optimal structural results, which are evaluated by both theoretical and empirical analysis.

### **A Class of Multilevel Nonregular Fractional Factorial Designs for Studying Quantitative Factors**

**Lin Wang**, University of California, Los Angeles

**Coauthors:** Hongquan Xu

Nonregular fractional factorial designs can have better properties than regular designs, but their construction is challenging. Current research on the construction of nonregular designs focuses on two-level designs. We construct a novel class of multilevel nonregular designs by permuting levels of regular designs via the Williams transformation. The constructed designs can reduce aliasing among effects without increasing the run size. They are more efficient than regular designs for studying quantitative factors.

### **Discrete Choice Experiments in Practice**

**Ben White**, Survey Engine GmbH, Germany

In the past, options in choice experiments have usually been presented in a tabular format. It has been recognised that this format can implicitly bias the choices made. Ideally, we would like the presentation format to be as close

as possible to the actual choice context. Element format, positioning and framing can affect choices in critical policy areas such as food or drug labelling. In this talk we will present choice experiments of increasing layout complexity, ending with a set of highly realistic e-commerce sites as the choice options. We will discuss tools, methods and pitfalls of moving from a standard table layout to complex and realistic presentation formats.

### **Applications of Universal Kriging Models for Drugs' Order-of-Addition Problems with Blocking**

**Qian Xiao**, University of Georgia

**Coauthors:** Hongquan Xu

In modern pharmaceutical studies, treatments may include several drug components added sequentially, and the drugs' order-of-addition may have significant impacts on the responses. In many situations, performing the full design with all possible orders of addition is unaffordable. Thus, accurate statistical models are needed when only small subsets of the full design are applied. In this paper, we propose to use universal Kriging (UK) models for analyzing data from such experiments involving both order-of-addition and blocking factors. Furthermore, we propose an informative universal Kriging model (IUK) which can enhance the robustness and interpretability of UK models via incorporating the domain knowledge of medicine. We illustrate our models via two real drug experiments on lung cancer, and show that our methods outperform existing popular methods.

### **Linear Screening for High-Dimensional Computer Experiments**

**Shifeng Xiong**, Chinese Academy of Sciences, China

**Coauthors:** Chunya Li, Daijun Chen

In this paper we propose a linear variable screening method for computer experiments when the number of input variables is larger than the number of runs. This method uses a linear model to model the nonlinear data, and screens the important variables by existing screening methods for linear models. We prove that the linear screening method is asymptotically valid under mild conditions. To improve the screening accuracy, we also provide a two-stage procedure that uses different basis functions in the underlying linear model. The proposed methods are very simple and easy to implement. Numerical results indicate that our methods outperform existing model-free screening methods.

### **Orthogonal Array Based Big Data Subsampling**

**Hongquan Xu**, UCLA

**Coauthors:** Lin Wang, Jake Kramer and Weng Kee Wong

Data reduction is critical for big data. We propose a novel sampling method to select a subset from a large data set. The subset is selected based on orthogonal arrays and therefore inherit the optimality from orthogonal arrays for models with or without interactions. Theoretical results guarantee that the selected subsets are optimal for parameter estimations and minimize the mean squared error for fixed sample size under some mild conditions. Simulations confirm the effectiveness of the proposed method.

### **Optimal Active Learning for Approximately Specified Linear Regression**

**Xiaojian Xu**, Brock University, Canada

**Coauthors:** Anthony Greco

In this paper, we discuss the relation between active learning and optimal experimental designs. The techniques used in optimal regression design development can be employed with modification in an optimal active learning process. We consider approximate linear regression models and weighted least squares estimation. Both optimal weighting schemes and optimal design densities for selecting the training data utilized in active learning are investigated for a number of typical situations. Analytical forms of optimal design densities for active learning are given for general linear regression. Both simulation results and comparison studies have shown that the optimal designs newly obtained are more efficient than their competitors.

### **Optimal Two-Stage Adaptive Subsampling Design for SoftMax Regression**

**Yaqiong Yao**, University of Connecticut

**Coauthors:** Haiying Wang, Jiahui Zou

For massive datasets, statistical analysis using the full data can be extremely time demanding and subsamples are often taken and analyzed according to available computing power. For this purpose, Wang et al. (2018) developed a novel two-stage subsampling design for logistic regression. We generalize this method to include the SoftMax regression, which has multiple categories for the responses. We derive the asymptotic distribution of the estimator obtained from subsamples that are drawn according to arbitrary subsampling probabilities, and then derive the optimal subsampling probabilities that minimize the asymptotic variance-covariance matrix under the A-optimality and the L-optimality criteria. The optimal subsampling probabilities involve unknown parameters, so we adopt the idea of optimal adaptive design and use a small subsample to obtain pilot estimators. In addition to subsampling with replacement, we also consider Poisson subsampling for its higher computational and estimation efficiency. We provide both simulation and real data examples to demonstrate the performance of our algorithm.

### **Adaptive Bayesian c-optimal Design for Estimating Multiple EDps under the 4-parameter Logistic Model**

**Anqing Zhang**, University of Missouri

**Coauthors:** Seung Won Hyun

Under nonlinear models, optimal design truly depends on the pre-specified values of model parameter. If the nominal values of the parameter are not close to the true values, optimal designs become far from optimum. In this study, we focus on constructing an optimal design that works well for estimating multiple EDps taking into account the parameter uncertainty. To address the parameter dependency, an adaptive design technique is applied by incorporating Bayesian paradigm. One challenging task for the Bayesian approach is that it requires heavy computation when search for the Bayesian optimal design. To overcome this problem, a clustering method can be employed.

We propose an adaptive Bayesian c-optimal design that works fairly well for estimating multiple values of EDp simultaneously, whilst accounting for the parameter uncertainty. We use the flexible 4-parameter logistic model to illustrate the methodology but our approach can be extended to other types of nonlinear models. We also examine the performance of our proposed design by comparing with other traditional designs through different scenarios of simulations given a wide range of mis-specified model parameters.

### **Bayesian Sequential Data Collection for Stochastic Simulation Calibration**

**Qiong Zhang**, Clemson University

**Coauthors:** Bo Wang; Wei Xie

Simulation is often used to guide the decision making for real complex stochastic systems. To faithfully assess the mean performance of the real system, it is necessary to efficiently calibrate the simulation model. Existing calibration approaches are typically built on the summary statistics of simulation outputs and ignore the serial dependence of detailed output sample paths. Given a tight simulation budget, we develop a Bayesian sequential data collection approach for simulation calibration via exploring the detailed simulation outputs. Then, the calibrated simulation model can be used to guide decision making. Both theoretical and empirical studies demonstrate that we can efficiently use the simulation resources and achieve better calibration accuracy by exploring the first two moment dynamic information of simulation output sample paths.

### **Incomplete U-statistics**

**Wei Zheng**, University of Tennessee

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U-statistic is an important class of statistics widely used in the fields of economy, machine learning and statistical inference. Unfortunately, its computation easily becomes impractical as the data size  $n$  increases. Particularly, the number of combinations, say  $m$ , that a U-statistic of order  $d$  has to evaluate is in the order of  $O(n^d)$ . Many efforts have been made to approximate the original U-statistic by a small subset of the combinations in history since Blom (1976), who has coined such an approximation as an incomplete U-statistic. To the best of our knowledge, all existing methods require  $m$  to grow at least faster than  $n$ , albeit much slower than  $n^d$ , in order for the corresponding incomplete U-statistic to be asymptotically efficient in the sense of mean squared error. In this paper, we introduce a new type of incomplete U-statistics, which can be asymptotically efficient even when  $m$  grows slower than  $n$ . In some cases,  $m$  is only required to grow faster than  $\sqrt{n}$ . The results are also extended to the degenerate case and the multi-sample case.

### **Computing R-optimal Designs for Multi-Response Regression Models via Interior Point Method**

**Julie Zhou**, University of Victoria

We study R-optimal designs for multi-response regression designs with several factors. The R-optimal design problems on discrete design spaces are constrained convex optimization problems. There are effective and efficient algorithms to solve convex optimization problems, such as CVX and SeDuMi algorithms in MATLAB, and they are successfully applied to find A-, c-, D- and E-optimal designs. However, for R-optimal design problems we cannot write them in a form so that CVX and SeDuMi algorithms can be applied. In this talk we discuss an interior point method for computing R-optimal designs. In addition, we derive several properties of R-optimal designs which are useful for numerical algorithms.

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