International Conference on Design of Experiments
ICODOE 2022

May 8-11,2023

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

https://www.memphis.edu/msci/icodoe22/index.php

Supported by the National Science Foundation, and Fedex Institute of Technology

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Academic session organizers	Title of session
The Scientific Program Committee	Opening Session
Nancy Flournoy, University of Missouri	Adaptive Designs
Angela Dean, The Ohio State University	Screening Experiments
Sergei Leonov, CSL Behring	DOE in the Pharmaceutical Industry
Xun Huan, University Michigan	Variational Methods for Optimal Experimental Design
Ming-Hung Kao, Arizona State University	Design of Experiments for Functional Data Analysis
Weitao Duan & Shan Ba, LinkedIn, and Xinwei Deng, Virginia Tech,	Design in Business Decision Making Processes
Dennis K.J. Lin, Purdue University	Recent Advances in Order-of-Addition Experiments
Youssef Marzouk, MIT	Computational Methods for Bayesian Optimal Experimental Design
Max Morris, Iowa State University	Computer Experiments
Wei Zheng, University of Tennessee	Reinforcement Learning
Robert Mee, University of Tennessee	Factorial Experiments
Arman Sabbaghi, Unlearn.AI.	Advances in the Design and Analysis of Modern Experiments and Observational Studies
William Myers, Miami University	Design of Experiments in Industry: Still Solving Important Business Problems
Xinran Li, University of Illinois Urbana-Champaign	Design and Causal Inference
Deborah Street, University of Technology Sydney, Australia	Discrete Choice Experiments
Luc Pronzato, CNRS, France	Kernel and Sampling Methods for Design
HaiYing Wang, University of Connecticut	Recent Developments on Subsampling Methods
Jesús Lopez Fidalgo, University of Navarra, Spain	Optimal Design of Experiments

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International Conference on
Design of Experiments (ICODOE-2022)
May 8-11, 2023
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;
FB: Fishbowl (Room 203/205), second floor

Monday, May 8

6—7 PM Registration (Holiday Inn)

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

Tuesday, May 9

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

8 AM Registration (FedEx Institute Lobby)

8:15 AM Inauguration (TZ)

8:30—10.00 AM Session 1 (TZ): Opening Session
Organizer: The Scientific Program Committee
Chair: John Stufken, George Mason University

8:30—9 AM Qing Liu, University of Wisconsin-Madison
A Representative Sampling Method for Peer Encouragement Designs in Network Experiments

9—9:30 AM Jonathan Stallrich, North Carolina State University
Optimal Supersaturated Designs for Lasso Sign Recovery

9:30—10 AM Torsten Reuter, Otto von Guericke University, Magdeburg, Germany.
D-Optimal Subsampling Design for Big Data Regression

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

10:30 AM—12:30 PM Session 2a (TZ): Adaptive Designs.
Organizer: Nancy Flournoy, University of Missouri
Chair: Sergei Leonov, CSL Behring

10:30—11 AM Zhantao Lin, Eli Lilly
Inference for a Two-Stage Enrichment Design

11—11:30 AM Adam Lane, University of Cincinnati
Optimal Relevant Subset Designs in Nonlinear Models

11:30 AM—NOON Nancy Flournoy, University of Missouri
Optimality of Sequential Likelihood Ratio Tests Given an α-Spending Function and Interim Sample Sizes

NOON—12:30 PM Sergey Tarima, Medical College of Wisconsin
Cost of Sequential Adaptations

10:30AM—12:30 PM Session 2b (MPT): Screening Experiments.
Organizer: Angela Dean, The Ohio State University.
Chair: Angela Dean, The Ohio State University

10:30—11 AM Yasmeen Akhtar, Birla Institute of Technology and Science, Goa, India
Locating Arrays for Design Selection and Analysis of Screening Experiments

11—11:30 AM Hongquan Xu, UCLA
Designs for Order-of-Addition Screening Experiments

11:30 AM—NOON Rakhi Singh, Binghamton University
Design Selection for Multi- and Mixed-Level Supersaturated Designs

NOON—12:30 PM Eric Schoen, KU Leuven, Belgium
Systematic Enumeration of Two-Level Even-Odd Designs of Strength 3

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

2—3:30 PM Session 3a (TZ): DOE in the Pharmaceutical Industry.
Organizer: Sergei Leonov, CSL Behring
Chair: Nancy Flournoy, University of Missouri

2—2:30 PM Inna Perevozskaya, GSK
Applying Quantitative Decision-Making to Prediction of Clinical Trial Recruitment

2:30—3 PM Jinesh Shah, CSL Behring
Framework to design a Bayesian Group Sequential Clinical Study

3—3:30 PM Sergei Leonov, CSL Behring
On a Longitudinal Mixed Effects Model for a Dose-Finding Study

2—3:30 PM Session 3b (MPT): Variational Methods for Optimal Experimental Design
Organizer: Xun Huan, University Michigan
Chair: Xun Huan, University Michigan

2—2:30 PM Fengyi Li, Massachusetts Institute of Technology
Transport Map-Based Bayesian Optimal Experimental Design

2:30—3 PM Jiayuan Dong, University of Michigan
Variational Bayesian Optimal Experimental Design with Normalizing Flows

3—3:30 PM Ahmed Attia, Argonne National Laboratory
Robust Optimal Experimental Design for Bayesian Inverse Problems

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

4—5 PM Session 4a (TZ): Design of Experiments for Functional Data Analysis
Organizer: Ming-Hung (Jason) Kao, Arizona State University
Chair: Russell Barton, The Pennsylvania State University

4—4:30 PM Cai Li, St. Jude Children's Research Hospital.
Optimal design for Functional Data

4:30—5 PM Ming-Hung (Jason) Kao, Arizona State University
Optimal Designs for Functional Principal and Empirical Component Scores

5—6 PM Session 4b (TZ): Design in Business Decision Making Processes
Organizers: Weitao Duan & Shan Ba, LinkedIn, and Xinwei Deng, Virginia Tech
Chair: Russell Barton, The Pennsylvania State University

5—5:30 Ying Jin, Stanford University
Selection by Prediction: Machine-assisted Candidate Screening with Conformal p-Values

5:30—6 PM Yixin Tang, DoorDash
Business Policy Experiments using Factorial Designs

4—6 PM Session 4c (MPT): Contributed Session
Chair: David Edwards, Virginia Commonwealth University

4—4:30 PM Jay Beder, University of Wisconsin – Milwaukee
The Story of a Wikipedia Article

4:30—5 PM Olga Egorova, King's College London, UK.
Sequential Multi-Objective Design of Multistratum Experiments

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5—5:30 Kade Young, North Carolina State University
Comparing Supersaturated Screening Designs using Exact Screening Probabilities

5:30—6PM Alexandre Bohyn, KULeuven, Belgium.
Design And Analysis of a Microplate Assay in the Presence of Multiple Restrictions on the Randomization

7.00-8.30 PM Conference Banquet (Holiday Inn, Shelby Ballroom)

Wednesday, May 10

7:15—8:15 AM Breakfast (Holiday Inn, Shelby Ballroom)

8:30—10 AM Session 5a (TZ): Recent Advances in Order-of-Addition Experiments
Organizer: Dennis K.J. Lin, Purdue University.
Chair: Ching-Chi Yang, University of Memphis

8:30—9 AM Frederick Phoa, Academia Sinica, Taiwan
A Systematic Design Construction and Analysis for Cost-Efficient Order-of-addition Experiment

9—9:30 AM Xueru Zhang, Purdue University
Analysis of Order-of-addition Experiments

9:30—10 AM Dennis K.J. Lin, Purdue University,
Order-of-addition Experiments: Design and Analysis

8:30—10 AM Session 5b (MPT): Computational Methods for Bayesian Optimal Experimental Design
Organizer: Youssef Marzouk, MIT
Chair: Luc Pronzato, CNRS, France

8:30—9 AM Alen Alexanderian, North Carolina State University
Optimal Design of Large-Scale Bayesian Inverse Problems under Model Uncertainty

9—9:30 AM Desi R. Ivanova, University of Oxford, UK
Deep Adaptive Design

9:30—10 AM Jayanth Jagalur-Mohan, Lawrence Livermore National Laboratory
Randomized Algorithms for Design of Experiments in High-Dimensions

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

10.30 AM—12:30 PM Session 6a (TZ): Computer Experiments.
Organizer: Max Morris, Iowa State University
Chair: Max Morris, Iowa State University

10:30—11 AM Roshan Joseph, Georgia Institute of Technology
Maximum One-Factor-At-A-Time Designs for Screening in Computer Experiments

11—11:30 AM Russell Barton, The Pennsylvania State University
Experiment Designs for Inverse Approximations

11:30 AM—NOON Isaac Michaud, Los Alamos National Laboratory
Designing Integral Experiments to Eliminate Compensating Nuclear Data Errors

NOON—12:30 PM Alan Vazquez, University of Arkansas
An Integer Programming Algorithm for Constructing Maximin Distance Designs from Good
Lattice Point Sets

10.30 AM—12:30 PM Session 6b (MPT): Reinforcement Learning.
Organizer: Wei Zheng, University of Tennessee.
Chair: Jonathan Stallrich, NC State University.

10:30—11 AM Linglong Kong, University of Alberta, Canada
Damped Anderson Mixing for Deep Reinforcement Learning: Acceleration, Convergence,
and Stabilization

11—11:30 AM. Xun Huan, University of Michigan.
Variational Bayesian Sequential Optimal Experimental Design via Policy Gradient

11:30 AM—NOON Haoda Fu, Eli Lilly.
Multi-arm Single Step Reinforcement Learning Through a Direct Learning Algorithm.

NOON—12:30 PM   Wei Zheng, University of Tennessee.
Thompson Sampling with Discrete Prior

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

2—3:30 PM Session 7a (TZ): Factorial Experiments
Organizer: Robert Mee, University of Tennessee
Chair: Hongquan Xu, UCLA

2—2:30 PM Lin Wang, Purdue University
Group-Orthogonal Subsampling for Non-independent Data Based on Linear Mixed Models

2:30—3 PM David Edwards, Virginia Commonwealth University
Structure of Nonregular Two-Level Designs

3—3:30 PM Robert Mee, University of Tennessee
Split Plot Parallel Flats Designs

2—3:30 PM Session 7b (MPT): Advances in the Design and Analysis of Modern Experiments and Observational Studies.
Organizer: Arman Sabbaghi, Unlearn.AI.
Chair: HaiYing Wang, University of Connecticut

2—2:30 PM Iavor Bojinov, Harvard University
Design of Panel Experiments with Spatial and Temporal Interference

2:30—3 PM Nicole Pashley, Rutgers University
Estimating Heterogeneous Treatment Effects in Conjoint Analysis

3—3:30 PM Yuki Ohnishi, Purdue University
A Bayesian Analysis of Two-Stage Randomized Experiments in the Presence of Interference, Treatment Nonadherence, and Missing Outcomes

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

4—6:00 PM Session 8a (TZ) Design of Experiments in Industry: Still Solving Important Business Problems .
Organizer: William Myers, Miami University
Chair: Qing Liu, University of Wisconsin-Madison

4—4:30 PM Yanran Wei and Xinwei Deng, Virginia Tech.
An Efficient Filtering Approach for Model Estimation in Sparse Regression'.

4:30—5 PM Nathaniel Stevens, University of Waterloo, Canada.
An Overview of Statistical Challenges in Online Controlled Experiments

5—5:30 PM William Fisher, Clemson University
Non-Myopic Methods in Bayesian Sequential Preference Learning with Application to Tradespace Exploration for Vehicle Concept Design

5:30—6 PM Caroline Kerfonta, Clemson University
Sequential Selection for Minimizing the Variance with Application to Crystal Formation Experiments

4—5:30 PM Session 8b (MPT): Design and Causal Inference.
Organizer: Xinran Li, University of Illinois Urbana-Champaign
Chair: Xinran Li, University of Illinois Urbana-Champaign

4—4:30 PM Fredrik Sävje, Yale University.
Balancing Covariates in Randomized Experiments with the Gram-Schmidt Walk Design

4:30—5 PM Yuhao Wang, Tsinghua University, China
Rerandomization with Diminishing Covariate Imbalance and Diverging Number of Covariates

5—5:30 PM Adam Kapelner, Queens College, City University of New York
The Role of Pairwise Matching in Experimental Design for an Incidence Outcome

Thursday 11 May 2023

7:15—8:15 AM Breakfast (Holiday Inn, Shelby Ballroom)

8:30—10 AM Session 9a (TZ): Discrete Choice Experiments
Organizer: Deborah Street, University of Technology Sydney, Australia
Chair: Deborah Street, University of Technology Sydney, Australia

8:30—9 AM Peiwen Jiang, University of Technology Sydney, Australia
How Much Overlap is Just Right? Comparing Stated Preference with Model Consistency

9:30—10 AM Juan Marcos Gonzalez, Duke University School of Medicine
Patient Preferences in Regulatory Decision-making

9—9:30 AM Martina Vandebroek, KU Leuven, Belgium
New Sample Size Selection Methods for Discrete Choice Experiments

8:30—10 AM Session 9b (MPT): Kernel and Sampling Methods for Design
Organizer: Luc Pronzato, CNRS, France
Chair: Jayanth Jagalur-Mohan, Lawrence Livermore National Laboratory

8:30—9 AM Simon Mak and Yi (Irene) Ji, Duke University
Stacking Designs: Designing Multi-Fidelity Computer Experiments with Confidence

9—9:30 AM Luc Pronzato, CNRS, France
Incremental Space-filling Design

9:30—10 AM Ayoub Belhadji, ENS de Lyon, France
Function Reconstruction using Determinantal Sampling

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

10:30 AM—12:30 PM Session 10a (TZ): Recent Developments on Subsampling Methods
Organizer: HaiYing Wang, University of Connecticut
Chair: Lin Wang, Purdue University

10:30—11 AM JooChul Lee, University of Pennsylvania
Model Calibration and Evaluation via Optimal Sampling Using Electronic Health Record Data

11—11:30 AM Jing Wang, University of Connecticut
Scale-Invariant Optimal Sampling and Variable Selection with Rare-Events Data

11:30 AM—NOON HaiYing Wang, University of Connecticut
A Note on Centering in Subsample Selection for Linear Regression

NOON—12:30 PM Amalan Mahendran, Queensland University of Technology, Australia
A Model Robust Subsampling Approach for Generalised Linear Models in Big Data Settings

10:30 AM—12:30 PM Session 10b (MPT): Optimal Design of Experiments
Organizer: Jesús Lopez Fidalgo, University of Navarra, Spain
Chair: Jesús Lopez Fidalgo, University of Navarra, Spain

10:30—11 AM Carlos De-La-Calle-Arroyo, University of Navarra, Spain
Augmenting Designs with Controlled Efficiency

11—11:30 AM Sergio Pozuelo-Campos, University of Castilla-La Mancha, Spain
Optimal Designs for Detecting and Characterizing Hormesis in Toxicological Tests

11:30 AM—NOON Alvaro Cia-Mina, University of Navarra, Spain
Optimal Subdata Selection for Random-X Linear Regression

NOON—12:30 PM Irene Mariñas-Collado, University of Oviedo, Spain
Optimal Designs for Non-Standard Alcohol Clearance Models

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

1:30PM —3:10 PM Session 11a (TZ):   Contributed Session.
Chair: Alan Vazquez, University of Arkansas

1:30—1.50 PM   Adetola Adediran, University of Southampton, UK.
Designing Follow-up Samples; a Comprehensive Approach to Detect MNAR Missingness Efficiently

1.50—2:10 PM Thomas Coons, University of Michigan
A Multi-Fidelity Approach to Bayesian Optimal Experimental Design

2:10—2.30 PM Samuel Onyambu, University of California, Los Angeles.
Kriging Based Sequential Region Perturbation and Shrinkage with EGO For Hyper-parameter Optimization

2.30—2.50PM Jose Toledo, University of California, Los Angeles.
Enhancing Efficient Global Optimization through a Kriging Based Space Reduction

2.50—3:10 PM Yezhuo Li, Clemson University.
Uncertainty Quantification for Computer Experiments with Transformed Additive Gaussian Process

1:30PM —2.50 PM Session 11b (MPT):   Contributed Session.
Chair: Adam Lane, University of Cincinnati.

1:30—1.50 PM   Marco Arndt, University of Stuttgart, Germany
Power and Accuracy Characterization of Regression Models in The Presence of Orthogonality Deviations in CCDs:

1.50—2:10 PM Miguel Fudolig, University of Nevada Las Vegas
Incomplete and Confounded Block Designs in Visual Inference Experiments

2:10—2:30 PM Mohammed Saif Ismail Hameed, KU Leuven, Belgium
D- and A- optimal Screening Designs. What if n is Not a Multiple of 4?

2:30—2.50 PM Aisaku Nakamura, Cincinnati Children's Hospital
Simultaneous Tolerance Intervals for Response Surface and Mixture Designs Using the Adjusted Product Set Method

1:30PM —3:10 PM Session 11c (FB):   Contributed Session.
Chair: Rakhi Singh, Binghamton University

1:30—1.50 PM Kouakou Francois Domagni, California State University Northridge
One-pan D-Optimal Weighing Designs For 9 Objects via $E(s^2)$-optimal Supersaturated Designs for 10 Runs

1.50—2:10 PM Yao Shi, Qingdao University, China
Optimal Design for Generalized Linear Mixed Models Based on the Penalized Quasi-Likelihood Method

2:10—2:30 PM Yi Zhang, George Washington University
Independence-Encouraging Subsampling for Nonparametric Additive Models

2:30—2.50 PM Desi Ivanova, University of Oxford, UK
Are Tighter Mutual Information Bounds Necessarily Better?

2.50—3.10 PM Joseph Ayodele Kupolusi, Federal University of Technology Akure, Nigeria
Design Optimality in the Presence of Non-Normal Overdispersion Responses Model

End of Conference

Abstracts of Invited and Contributed Talks

Designing follow up samples – A comprehensive approach to detect MNAR missingness efficiently
Adetola Adediran, University of Southampton, UK

The presence of missing data may lead to bias and inefficiencies in analyses. The missing not at random (MNAR) mechanism is the most complex type of missingness. Understanding if it is present is of utmost importance as suitable adjustments must be made to correct for bias. However, it is not possible to detect MNAR based on the incomplete data and a follow up sample of some of the missing observations must be made. In this work, we explore how different designs of the follow up sample impact the power of a test for MNAR. We provide an algorithm for designing the follow up sample that significantly improves the power of this test compared with random sampling. We also explore the efficiency and robustness of our designs through simulations studies.

Locating arrays for design selection and analysis of screening experiments
Yasmeen Akhtar, Birla Institute of Technology and Science - Pilani, Goa, India

A (d,t)-locating array is a covering array of strength t with an additional property of distinguishing any set of d number of t-tuples from any other such set through the collection of rows covering them. In combinatorial testing, the locating array identifies the location of faults triggered by level combinations. The number of rows in a locating array grows logarithmically in the number of columns, making the consideration of a large number of factors in experimentation practical. This talk will discuss a design selection and analysis method based on the locating array for screening experiments. Under the assumption of effect sparsity, our analysis method focuses on t-tuples $(t \leq 2)$ in identifying important factors. We demonstrate the validity of our screening method on well-studied data sets available in the literature. This talk is based on joint work with Fan Zhang, Prof. Charles J. Colbourn, Prof. John Stufken, and Prof. Violet R. Syrotiuk.

Optimal design of large-scale Bayesian inverse problems under model uncertainty
Alen Alexanderian, North Carolina State University

We consider optimal experimental design (OED) under uncertainty for Bayesian nonlinear inverse problems governed by PDEs with infinite-dimensional inversion parameters. Typically, the governing PDEs contain several parameters that are not being estimated but are still not known exactly. These secondary uncertainties need to be accounted for in Bayesian inversion and OED. In this talk we consider methods for OED in such inverse problems. Our approach builds on the Bayesian Approximation Error (BAE) framework. BAE facilitates incorporating modeling uncertainties in the inverse problem and the OED problem. This is coupled with structure exploiting algorithms that enable fast computations. In particular, we can compute optimal designs at a cost, in terms of the required number of PDE solves, that does not grow with the dimension of the discretized inversion and secondary parameters.

Power and accuracy characterization of regression models in the presence of orthogonality deviations in CCDs
Marco Arndt, University of Stuttgart, Germany

For lifetime-testing in engineering, DoE is gaining an indispensable status as a cornerstone for evaluation of relevant factors and effects on reliability of machine components. Especially on a time scale, factors influencing lifetime may encounter two concerns: large variance in setting and result-measurement or loss of component functionality in extreme ranges of parameter combinations. In this paper, an evaluation of the extent is presented, to which coefficients of reliability-models are affected by arising phenomena in factor-level setting within machine-component testing. Therefore, an investigation model (response-surface-model) and test design (CCD) are predefined and performance indicators such as power and quality of model-coefficients are used as observables. Significant influencing factors like variance, omission of test-runs, the spread of test points in the parameter range for axial runs and the significance level are investigated on their basis. Eventually influences on power and quality per model-coefficient are evaluated and again described using regression equations.

Robust Optimal Experimental Design for Bayesian Inverse Problems
Ahmed Attia, Sven Leyffer, and Todd Munson, Argonne National Laboratory, U.S.,

An optimal design is defined as the one that maximizes a predefined utility function which is formulated in terms of the elements of an inverse problem. An example being optimal sensor placement for parameter identification. This formulation generally overlooks misspecification of the elements of the inverse problem such as the prior or the measurement uncertainties. In this talk, we present efficient recipes for designing optimal experimental design schemes, for Bayesian inverse problems, such that the optimal design is robust with respect to misspecification of elements of the inverse problem.

Experiment designs for inverse approximations
Russell Barton, Penn State University

Many simulation-based design optimization scenarios are driven by an underlying inverse problem. Rather than iteratively exercise the (computationally expensive) simulation to find a suitable design (i.e., match a target performance vector), one might instead iteratively exercise the simulation to fit an inverse approximation, and use the approximation to indicate designs meeting multivariate performance targets. This talk examines issues in defining optimal designs for fitting inverse approximations. This is joint work with Max Morris, Iowa State.

The story of a Wikipedia article.
Jay Beder, University of Wisconsin – Milwaukee

This talk is a somewhat personal discussion of the creation of a Wikipedia article to fill a gap in its coverage of factorial experiments. I will describe the need for the article and the goals I had in mind in writing it. This project carries implications for articles on adjacent topics. I will also touch on the challenges that face the statistical community in Wikipedia's coverage of statistics.

Design and analysis of a microplate assay in the presence of multiple restrictions on the randomization
Alexandre Bohyn, KULeuven, Belgium

Experiments using multi-step protocols often involve several restrictions on the randomization. For a specific application to in vitro testing on microplates, a design was required with both a split-plot and a strip-plot structure. On top of two-level treatment factors and the factors that define the randomization restrictions, a multi-level fixed blocking factor not involving further restrictions on the randomization had to be added. We develop a step-by-step approach to construct a design for the microplate experiment and analyze a response. To consolidate the approach, we study various alternative scenarios for the experiment.

Function reconstruction using determinantal sampling
Ayoub Belhadji, ENS de Lyon, France

The problem of reconstructing a continuous function based on discrete samples stimulated considerably rich literature. We propose a universal approach for function reconstruction based on repulsive nodes that comes with strong theoretical guarantees and empirical performances. More precisely, we study reconstructions based on nodes that follow the distributions of determinantal point processes adapted to a given reproducing kernel Hilbert space. We prove fast convergence rates that depend on the eigenvalues of the kernel. This unified analysis provides new insights into approximation problems based on determinantal point processes.

Design of panel experiments with spatial and temporal interference
Iavor Bojinov, Harvard Business School

One of the main challenges companies face when running experiments is interference, the setting where one experimental unit's treatment assignment at one time period impacts another's outcomes, possibly at the following time period. Existing literature has identified aggregating units into clusters as the gold standard to handle interference, yet the degree of aggregation remains an open question. In this work, we present a new randomized design of panel experiments and answer this question when all experimental units are modeled as vertices on a two-dimensional grid. Our proposed design has two features: the first is a notion of randomized spatial clustering that randomly partitions units into equal-size clusters; the second is a notion of balanced temporal randomization that extends the classical completely randomized designs to the temporal interference setting. We prove the theoretical performance of our design, develop its inferential techniques, and verify its superior performance by conducting a simulation study.

Augmenting designs with controlled efficiency
Carlos de la Calle-Arroyo, University of Navarra, Spain

Optimal experimental designs usually have too few points and often very extremal. In most models with a single independent variable the number of different points is simply the number of parameters to be estimated. This leads to them being impractical to use directly by an experimenter. Optimal designs; therefore, are used as a reference to measure how efficient are the designs used in practice.
In this work, the equivalence theorem is used to control the efficiency when adding points to a given design. The experimenter can then, starting from the optimal design, or a regulated experimental plan, add points controlling the efficiency in order to enhance the initial design to its liking. A software application has been built to allow to easily compute the augmented designs.

Optimal subdata selection for random-X linear regression
Alvaro Cia-Mina and Jesús Lopez-Fidalgo, University of Navarra, Spain

The subsampling procedure is widely used to downsize the data volume and allows computing estimators in regression models. The subsample can be chosen at random (Passive Learning), but in order to obtain better estimators, the optimal experimental design theory can be used to search for an influential sub-sample (Active Learning). This has been developed in the literature for several models, such as linear and logistic regression. To the authors knowledge, the distribution of the explanatory variables has never been considered in the criteria for obtaining the subsample. We study the effect of the explanatory variables distribution on the estimation as well as the optimal design. We propose a novel subdata selection method for Random-X linear regression.

A multi-fidelity approach to Bayesian optimal experimental design
Thomas Coons, University of Michigan

In many engineering applications, experiments are vital but costly. It is therefore important to find experimental design conditions that maximize the value of these experiments. Bayesian optimal experimental design (OED) provides a framework for identifying the ideal design by leveraging a mathematical model that simulates the experimental outcomes. The value of an experiment is quantified using the expected information gain (EIG). This quantity is typically evaluated numerically using double-nested Monte Carlo (DNMC). However, DNMC can be prohibitively expensive for computationally intensive models. We propose a multi-fidelity approach to accelerate the OED process, where an ensemble of EIG estimators of varying accuracy and cost (e.g. from simplified physics or coarsened meshes) are combined into a single estimator via approximate control variates. The multi-fidelity estimator achieves lower variance in estimating the EIG criterion. We demonstrate this approach by designing turbulent flow experiments for inferring the Reynolds-averaged Navier–Stokes closure model parameters.

One-pan D-optimal weighing designs for 9 objects via $E(s^2)$-optimal supersaturated designs for 10 runs
Kouakou Francois Domagni, California State University Northridge
We show that D-optimal one-pan weighing designs for 9 objects and m weighings for large m can be constructed via E(s2)-optimal supersaturated designs with 10 runs and m factors and explicitly describe D-optimal designs for 9 objects and a large number of weighings.

Variational Bayesian Optimal Experimental Design with Normalizing Flows
Jiayuan Dong, Christian Jacobsen, Karthik Duraisamy, Xun Huan, University of Michigan

Optimal experimental design (OED) seeks experimental design conditions that lead to the greatest expected information gain (EIG). The EIG is typically approximated through a double-nested Monte Carlo estimators, requiring $O(N^2)$ forward model evaluations. This becomes prohibitive when working with computationally intensive models commonly encountered in studies of complex and physical systems. Recently, Foster et al. proposed a variational EIG approximation technique that requires only $O(N)$ forward model evaluations, by maximizing a stochastic lower bound of the EIG that emerges from replacing the true posterior with a Gaussian variational distribution. However, Gaussian distributions are unable to capture non-Gaussian posterior behavior such as multi-modality and skewness, and it can lead to large bias (loose bound) in estimating the EIG. We improve the variational OED by deploying normalizing flows that transform standard normal latent variables to general non-Gaussian distributions through expressive neural networks, leading to lower bias estimators as well as an ability to produce accurate non-Gaussian posteriors. We illustrate this method on benchmark problems as well an application to design optimal observing times for inferring parameters of an aphid population model.

Structure of nonregular two-level designs
David Edwards, Virginia Commonwealth University

Two-level fractional factorial designs are often used in screening scenarios to identify active factors. This talk 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 this structure to the parallel flats design (PFD) literature. We show how to determine the number of parallel flats for any given design, and how to construct a design with a specified number of parallel flats. The usefulness of our construction method is illustrated by producing designs for estimation of the two-factor interaction model with three or more flats. We also provide a fuller understanding of recently proposed group orthogonal supersaturated designs. Benefits of PFDs for analysis, including bias containment, will be emphasized.

Sequential multi-objective design of multistratum experiments
Olga Egorova, King's College London, UK

While considering the response surface modelling approach, corresponding optimal design strategies usually rely on the goodness of the fitted model. In current work we consider relaxing this assumption and incorporate previously developed optimality criteria that account for such uncertainty regarding the fitted model by assigning a distribution on the potentially missed polynomial terms. Such an approach makes it more sensible to construct optimal designs in stages, allowing for the incoming data to influence the next stage decisions: updating the distributions as well as the sets of fitted and potential model terms and the individual criteria. The methodology is built for a general case of multistratum experiments, adopting a stratum-by-stratum approach; and constructing Pareto fronts of designs provides a set of alternatives for the experimenters. We discuss some particularities of the approach as well as potential challenges and future developments.

Non-myopic methods in Bayesian sequential preference learning with application to tradespace exploration for vehicle concept design

William Fisher, Qiong Zhang, Yongjia Song,   Clemson University

Engineering design is a complex decision making process that often involves communication between engineers and a decision maker, where the engineering team is attempting to iteratively figure out design requirements from the decision maker. One way to efficiently elicit these design requirements is through the use of an adaptive questionnaire, which is based on the framework of Bayesian sequential preference learning. This framework relies on dynamic programming to adaptively select queries to achieve Bayesian D-optimality of the preference model's parameter estimates. Previous work has focused on using greedy or myopic methods to solve the underlying dynamic programming problem, which may lead to suboptimal queries. In this work, we develop and investigate non-myopic methods based off of the rollout algorithm and two-step lookahead. We show that in many cases, non-myopic methods offer a statistically significant improvement in Bayesian D-error reduction without significantly biasing the corresponding preference estimate.
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Optimality of sequential likelihood ratio tests given an α-spending function and interim sample sizes

Nancy Flournoy, University of Missouri – Columbia

For Group Sequential Designs, Tsiatis (1982) assumes statistics to be independent and identically distributed; Proschan et al. (2006) assumes Brownian motion; asymptotic large deviation theory is employed by Chan and Lai (2000) and Lai and Shih (2004); Slud (1984), Gu and Lai (1991) and Lai and Shih (2004) rely on the Martingale central limit theorem. We show that components in the likelihood conditional on reaching a stage are the sub-densities of interim test statistics first described by Armitage (1969) and now commonly used to create stopping boundaries. We work directly with the natural convolutions induced by multiple testing on adapted support, with fewer-than-usual assumptions. This permits useful tractable characterizations of adapted events. Using this framework, we show that sequential likelihood ratio tests derived from one-parameter exponential family random variables are uniformly most powerful for a given alpha-spending function with pre-determined stage-specific sample sizes (no asymptotics or normality assumptions required).

Multi-arm single step reinforcement learning through a direct learning algorithm.

Haoda Fu, Eli Lilly

Estimating an optimal individualized treatment rule (ITR) based on patient information is a crucial problem in precision medicine. An optimal ITR is a decision function that maximizes patients' expected clinical outcomes. Most of the existing methods in the literature are designed for binary treatment settings with the focus on continuous outcomes. Little work has been done to estimate optimal ITRs in multiple treatment settings with good interpretations. In this article, we propose Angle-Based Direct Learning (AD-learning) to efficiently estimate optimal ITRs with multiple treatments. Our proposed method can be applied to various types of outcomes, including continuous, survival, or binary outcomes. Furthermore, it has an interesting geometric interpretation of the effect of different treatments for each patient, which can assist doctors and patients in making better decisions. Finite sample error bounds have been established to provide theoretical guarantees for AD-learning. Finally, we demonstrate the superior performance of our method through an extensive simulation study and real-data applications.

Incomplete and confounded block designs in visual inference experiments

Miguel Fudolig, University of Nevada Las Vegas

Visual statistical inference utilizes human visual perception to perform statistical inference. One method used to perform visual inference is the lineup protocol, where individuals are asked to identify the plot of the real data (or signal plot) among a panel of 20 plots. Evaluating multiple lineups in a short period of time could prove to be exhausting for study participants, therefore the number of lineups administered to each participant must be

controlled. We demonstrated the use of incomplete and confounded block designs in visual inference experiments to control the number of lineups to be evaluated by each participant. These block designs were compared to those used in prior experiments that utilized lineup protocols. Results show that incomplete and confounded block designs have clear advantages in randomization, block allocation, and block size but would encounter challenges in a digital implementation of the experiment.

Patient preferences in regulatory decision-making
Juan Marcos Gonzalez Sepulveda, Duke University School of Medicine

Patient preferences are increasingly considered in the regulatory review of new medical technologies. While the United States Food and Drug Administration has long had a process to collect patient input, recent guidance formalized the acceptance of quantitative patient preferences for this purpose. The guidance specifically addresses the use of stated-preference methods as a way to quantify patient risk tolerance for new medical technologies. Evidence on patient risk tolerance, and variations in the tolerance of various patient subgroups, offer an opportunity to contextualize clinical trial results from the patient perspective. This evidence also can be used to inform judgments about the acceptability of treatment benefits and risks. The presentation will: 1) describe some of the methods that are being used to collect patient-preference information, 2) how this information is transformed into evidence of risk tolerance, and 3) discuss how patient preferences are influencing trial design and the development of new technologies.

Variational Bayesian sequential optimal experimental design via policy gradient
Xun Huan, University of Michigan

We formulate the optimal design problem for a finite sequence of experiments using a Markov decision process, where the resulting design policy can adapt to newly collected data (feedback) and anticipate future consequences (lookahead). Adopting a Bayesian approach with information-based utilities, we derive a lower bound estimator for the objective function via a variational approximation to the parameter posterior distribution. We solve this problem numerically by applying policy gradient and variational optimization simultaneously. This is achieved by directly parameterizing the policy, value function, and variational posteriors using neural networks and improving them via gradient estimates produced from simulated design sequences. We demonstrate our method on an algebraic benchmark and a sensor movement application for source inversion. Our results provide insights into the benefits of feedback and lookahead and show substantial computational advantages compared to previous techniques of approximate dynamic programming. This is joint work with Wanggang Shen.

D- and A- optimal screening designs. What if n is not a multiple of 4?
Mohammed Saif Ismail Hameed, KU Leuven, Belgium

The literature on the construction of two-level D- and A- optimal main effects designs primarily concerns designs with run sizes that are multiples of four. It is fair to say that the construction of D- and A- optimal designs for run sizes that are not multiples of four has largely been ignored. It is known, however, that such D- and A- optimal designs for run sizes that are not multiples of four have unique aliasing structures between the main effects. This knowledge can be exploited to construct enumeration algorithms for D- and A-optimal designs with these run sizes. In this talk, we focus on the enumeration of D- and A- optimal designs for run sizes that are one more than a multiple of four. We present an overview of the standard approach in the literature to construct these designs, and our own results from a complete enumeration.

Deep adaptive design
Desi Ivanova, University of Oxford, UK

Bayesian experimental design (BED) provides a powerful framework for optimizing the design of adaptive experiments. However, its deployment often constitutes considerable computational challenges that hinder its

practical application. In this talk, we discuss some of the recent advances that have greatly enhanced our ability to overcome these challenges. Specifically, we present Deep Adaptive Design (DAD), a novel framework that amortizes the cost of adaptive BED by optimizing a design policy rather than individual designs. The policy is parametrized by a neural network, which takes past data as input and returns the design for the next experiment iteration. This enables quick and adaptive design decisions with a single pass through the network. We demonstrate empirically that DAD successfully amortizes the experimental design process, outperforming alternative strategies. Our results suggest that DAD can facilitate the widespread adoption of adaptive BED and enhance the efficiency of information gathering across scientific and engineering domains.

Are tighter mutual information bounds necessarily better?
Desi Ivanova, University of Oxford, UK

In Bayesian experimental design (BED), optimal designs are determined by maximizing the expected information gain (EIG), equivalently the mutual information (MI). Variational estimators, specifically variational lower bounds on MI, have become increasingly popular in the field, as they are computationally tractable and enable simultaneous estimation of the MI and optimization of the designs. In this talk, we explore various factors that can influence our choice of an estimator, such as its bias-variance trade-off, as well as the analytical availability of the model's likelihood and/or prior. Our empirical analysis investigates whether tighter bounds necessarily lead to better designs and more accurate parameter inference. By comparing different approaches, we hope to provide insights into their relative strengths and weaknesses that can ultimately assist researchers in selecting the most appropriate MI bound for their experimental design problem.

Randomized algorithms for design of experiments in high-dimensions
Jayanth Jagalur-Mohan, Lawrence Livermore National Laboratory

We explore new approaches for experimental design by leveraging connections to Determinantal point processes (DPPs). Determinantal point processes (DPPs) are probabilistic models originally used to study particle distributions. Our proposed ideas involve probabilistic modeling of the design space and
the use of sampling algorithms to query designs as MAP estimates or high-probability samples.
We characterize the relationship between DPP kernels and information theoretic OED criteria by relating the sampling probabilities of a suitably designed kernel to approximate information decomposition. By relating OED and DPP in the proposed manner our goal is to provide a general and flexible framework for experimental design with applicability in non-Gaussian and nonlinear settings. DPPs can circumvent the need for estimating expensive high dimensional (and perhaps intractable) design objectives, and aid the development of novel strategies for challenging problems.

How much overlap is just right? Comparing stated preference with model consistency
Peiwen Jiang, Deborah Street, Brendan Mulhern, Rosalie Viney, University of Technology Sydney, Australia

Engaged respondents who fully complete all the questions in a discrete choice experiment are the most informative. Instruments that assess aspects of quality of life are usually complicated and valuations of health states are often obtained by using a DCE in which the options are health states described by such an instrument. To make the tasks less complex, attribute level overlap is often used. We investigated the optimal number of attributes to overlap when using an 8-dimensional social care instrument.
Respondents answered 16 tasks divided into 4 subsets, with each subset having a different number of overlapped attributes. Respondents were randomly assigned to one of 3 arms which differed in the order of presentation of these subsets. We will discuss the stated number of overlapped and non-overlapped attributes that were considered and preferred, and the impact of attribute overlap and presentation order on the perceived difficulty when making a choice.

Selection by prediction: Machine-assisted candidate screening with conformal p-values
Ying Jin, Stanford University

Decision making or scientific discovery pipelines such as job hiring and drug discovery often involve multiple stages: before any resource-intensive step, there is often an initial screening that uses predictions from a machine learning model to shortlist a few candidates from a large pool. We study screening procedures that aim to select candidates whose unobserved outcomes exceed user-specified values. When some `experimental' data are available, we develop a method that wraps around any prediction model to produce a subset of candidates while controlling the proportion of falsely selected units. Building upon the conformal inference framework, our method first constructs p-values that quantify the statistical evidence for large outcomes; it then determines the shortlist by thresholding the p-values using multiple testing ideas. In many cases, the procedure selects candidates whose predictions are above a data-dependent threshold. We demonstrate the empirical performance of our method via simulations and real datasets.

Maximum one-factor-at-a-time designs for screening in computer experiments
V. Roshan Joseph, Georgia Institute of Technology

Identifying important factors from a large number of potentially important factors of a highly nonlinear and computationally expensive black box model is a difficult problem. Morris screening and Sobol' design are two commonly used model-free methods for doing this. In this work, we establish a connection between these two seemingly different methods in terms of their underlying experimental design structure and further exploit this connection to develop an improved design for screening called Maximum One-Factor-At-A-Time (MOFAT) design. We also develop efficient methods for constructing MOFAT designs with large number of factors. Several examples are presented to demonstrate the advantages of MOFAT designs compared to Morris screening and Sobol' design methods.
This is joint work with Qian Xiao, University of Georgia, Douglas Ray, US Army DEVCOM Armaments Center.

Optimal designs for functional principal and empirical component scores
Ming-Hung Kao, Arizona State University

Sparse functional data analysis (FDA) is powerful for making inference on the underlying random function when noisy observations are collected at sparse time points. To have a precise inference, knowledge on optimal designs that allow the experimenters to collect informative functional data is crucial. Here, we propose a framework for selecting optimal designs to precisely predict functional principal and empirical component scores. Our work gives a relevant generalization of previous results on the design for predicting individual response curves. We obtain optimal designs, and evaluate the performance of commonly used designs. We demonstrate that without a judiciously selected design, there can be a great loss in statistical efficiency.

The role of pairwise matching in experimental design for an incidence outcome
Adam Kapelner, Queens College, CUNY

We consider the problem of evaluating designs for a two-arm randomized experiment with an incidence (binary) outcome under a nonparametric general response model. Our two main results are that the priori pair matching design of Greevy et al. (2004) is (1) the optimal design as measured by mean squared error among all block designs which includes complete randomization. And (2), this pair-matching design is minimax, i.e. it provides the lowest mean squared error under an adversarial response model. Theoretical results are supported by simulations and clinical trial data.

Sequential selection for minimizing the variance with application to crystal formation experiments
Caroline Kerfonta, Clemson University

It is often the goal of sequential experiments to find the experimental setting with the minimum variance. This paper proposes a method using Bayesian Optimization techniques to sequentially find the experimental setting that minimizes the variance of a batch of experimental units. We developed a Bayesian model for the variances of a batch of measurements. The proposed method sequentially updates the prior distributions using experimental data and selects new experimental settings with knowledge gradient developed to minimize the variance. A numerical simulation will show that the proposed sequential selection for minimizing the variance approach will decrease the opportunity cost and increase the probability of correct selection. A case study illustrates the proposed method using data from slug flow crystallization experiments. These crystals are used in active pharmaceutical ingredients (APIs) and it is important for them to ensure a uniform size.

Damped Anderson mixing for deep reinforcement learning: acceleration, convergence, and stabilization
Linglong Kong, University of Alberta, Canada
Anderson mixing has been heuristically applied to reinforcement learning (RL) algorithms for accelerating convergence and improving the sampling efficiency of deep RL. In this paper, we provide deeper insights into a class of acceleration schemes built on Anderson mixing that improve the convergence of deep RL algorithms. Our main results establish a connection between Anderson mixing and quasi-Newton methods and prove that Anderson mixing increases the convergence radius of policy iteration schemes by an extra contraction factor. The key focus of the analysis roots in the fixed-point iteration nature of RL. We further propose a stabilization strategy by introducing a stable regularization term in Anderson mixing and a differentiable, non-expansive MellowMax operator that can allow both faster convergence and more stable behavior. Extensive experiments demonstrate that our proposed method enhances the convergence, stability, and performance of RL algorithms.

Design optimality in the presence of non-normal overdispersion responses model
Joseph Ayodele Kupolusi, Federal University of Technology Akure, Nigeria

This research specifically considered count data in optimal design setting over-dispersion data in Optimal Design. Two distributions from a family of generalized linear model (glm) considered are quasi-poisson family and negative binomial distribution. The estimation of over-dispersed models was obtained in optimal design settings using poisson-gamma model, poisson log normal model and negative binomial model. A dispersion index was built into the model to estimate the mean and variance of the model considered. The result of the analysis showed that both posterior mean of the group and posterior variance for the groups considered are close to the observed mean and variance respectively. 95% Highest Posterior Density intervals for the dispersion indices was calculated for dispersion parameter estimated by glm with quasi-Poisson likelihood.

Optimal relevant subset designs in nonlinear models
Adam Lane, University of Cincinnati

Fisher (1934) argued that certain ancillary statistics form a relevant subset, a subset of the sample space on which inference should be restricted and showed that conditioning on such ancillary statistics reduces the dimension of the data without a loss of information. The use of ancillary statistics in post-data inference has received significant attention; however, their role in the design of experiments has not been well characterized. Ancillary statistics are unknown prior to data collection and as a result, cannot be incorporated into the design a priori. Conversely, in sequential experiments, the ancillary statistics based on the data from the preceding observations are known and can be used to determine the design assignment of the current observation. The main results of this work describe the benefits of incorporating ancillary statistics, specifically, the ancillary statistic that constitutes a relevant subset, into adaptive designs.

Model calibration and evaluation via optimal sampling using electronic health record data
JooChul Lee, University of Pennsylvania

For validating a risk assessment tool using electronic health record (EHR) data, a common challenge is that labels for the predicted outcome are not directly observed. It is usually practical to label a small number of patients, but the power for evaluating model performance is low. Towards efficient and unbiased model validation, here we study optimal sampling designs for efficiently labeling an informative subsample of patients in an EHR cohort. Given a pre-specified number of outcome labels, our design aims to minimize the asymptotic variance of an improved inverse probability weighted ("I-IPW") estimator for predictive accuracy metrics. The optimal sampling requires accurate risk estimation and knowledge of the predictive accuracy metrics of interest. We therefore propose to implement sampling in two steps. First a portion of the target number of labels is acquired by applying an available informative sampling method, e.g., entropy sampling, to a random subset of the cohort. The model is then calibrated with the labeled data to reduce possible bias in risk estimation, and an estimate of the predictive accuracy metrics is obtained using the I-IPW estimator. The optimal sampling probabilities are then calculated based on the calibrated model and estimated metrics, which are used to acquire the remaining target number of labels from the remaining cohort. The final estimate of the predictive accuracy metrics is obtained by applying the I-IPW estimator to the full cohort and all acquired labels pooled together. Results from extensive simulation studies and application to a real EHR dataset indicate superior efficiency of the proposed sampling design and IPW estimator.

On a longitudinal mixed effects model for a dose-finding study
Sergei Leonov, CSL Behring

Dose-finding studies in rare diseases are faced with unique challenges including low patient numbers and limited understanding of the dose-exposure-response relationship. In addition, patient exposure to placebo is often not feasible. To describe the disease progression, we introduce a longitudinal model for the change from baseline for a clinical endpoint. We build a nonlinear mixed effects model using the techniques which have become popular over the past two decades in the design and analysis of population pharmacokinetic/pharmacodynamics studies. To evaluate operating characteristics of the
proposed design, we derive the Fisher information matrix and validate analytical results via simulations

Optimal design for functional data
Cai Li, St. Jude Children's Research Hospital

We study the design problem for the optimal prediction and classification of functional data. The goal is to select sampling time points so that functional data observed at these time points can be predicted accurately. We propose optimal designs that are applicable to either dense or sparse functional data. Using various functional predictive models, we formulate our design objectives as explicit functions of the sampling points. We study the theoretical properties of the proposed design objectives and provide practical implementations. The performance of the proposed design is evaluated through simulations and real data applications.

Transport map-based Bayesian optimal experimental design
Fengyi Li, Massachusetts Institute of Technology

The Bayesian optimal experimental design is essential in many fields of science and engineering. Given a prior and a design-dependent likelihood function, we would like to choose the design that maximizes the expected information gain (EIG) in the posterior. We introduce a flexible transport-map based framework that enables fast estimation of EIG by solving only convex optimization problems. This framework is also compatible with implicit models, where one can simulate from the likelihood but the conditional probability density function of the data is unknown. Several estimators naturally appear within our framework---in particular, positively and negatively biased estimators that provide bounds for the true EIG. We explore the bias and variance of our estimators and

study the optimal allocation between the training and the evaluation samples given a fixed number of samples. We then demonstrate the performance of our approach using both linear and nonlinear examples.

Uncertainty quantification for computer experiments with transformed additive gaussian process
Yezhuo Li, Clemson University

Transformed additive Gaussian process (Lin and Joseph, 2020) is proposed to surrogate a transformed output of a computer model with additive functions of inputs. The additive structure of the surrogate model can potentially improve the computational efficiency in quantifying the uncertainty contributions of each input to the output uncertainty. We develop an algorithm for uncertainty quantification of computer experiments with transformed additive Gaussian process, and compare the accuracy of the proposed approach with uncertainty measures given by brute-force simulations via a set of numerical examples.

Order-of-addition experiments: design and analysis
Dennis K.J. Lin, Purdue University

In Fisher (1971), a lady was able to distinguish (by tasting) from whether the tea or the milk was first added to the cup. This is probably the first popular Order of Addition (OofA) experiment. In general, there are m required components and we hope to determine the optimal sequence for adding these m components one after another. It is often unaffordable to test all the m! treatments (for example, m!=10! is about 3.5 millions), and the design problem arises. We consider the model in which the response of a treatment depends on the pairwise orders of the components. The optimal design theory under this model is established, and the optimal values of the D-, A-, E-, and M/S-criteria are derived. For Model-Free approach, an efficient sequential methodology is proposed, building upon the basic concept of quick-sort algorithm, to explore the optimal order without any model specification. The proposed method is capable to obtain the optimal order for large m ($\geq$ 20). This work can be regarded as an early work of OofA experiment for large number of components. Some theoretical supports are also discussed. One case study for job scheduling will be discussed in detail.

Inference for a two-stage enrichment design
Zhantao Lin, Eli Lilly

Two-stage enrichment designs can be used to target the benefiting population in clinical trials based on patients' biomarkers. In the case of continuous biomarkers, we show that using a bivariate model that treats biomarkers as random variables more accurately identifies a treatment-benefiting enriched population than assuming biomarkers are fixed. In our proposed design, the mean outcome for the whole population and the prediction strength of the biomarker is evaluated first, and the threshold is estimated if a benefiting subpopulation exists and is desired. Additionally, we show that under the bivariate model, the maximum likelihood estimators (MLEs) follow a randomly scaled mixture of normal distributions. Using random normings, we obtain asymptotically standard normal MLEs and construct hypothesis tests. Finally, in a simulation study, we demonstrate that our proposed design is more powerful than a single stage design when outcomes and biomarkers are correlated; the model-based estimators have smaller bias and mean square error (MSE) than weighted average estimators.
This is joint work with Nancy Flournoy and William Rosenberger.

A representative sampling method for peer encouragement designs in network experiments
Qing Liu, University of Wisconsin-Madison

Targeted marketing interventions are prevalent on social networks, ranging from referral campaigns to social advertising. Firms are increasingly interested in conducting network experiments through peer encouragement designs to causally quantify the potentially heterogeneous direct effect of a marketing program on focal individuals (egos) and the indirect effect on those connected to the focal ones (alters). A widely adopted practice to obtain clean estimates of the direct and indirect treatment effects is to draw random samples from the population network and then exclude contaminated egos and alters. However, this may lead to

underrepresentation and undersupply of the resulting treatment/control samples, which have been documented in the literature as two major technical challenges in conducting network experiments with peer encouragement designs. We propose a Bayesian representative sampling algorithm to improve the peer encourage designs and the related causal inference. The resulted samples from our proposed method not only better represent the population on individual network properties and personal characteristics that may drive heterogeneous responses to treatment, but also have a larger sample size to assist proper statistical inference and testing. Moreover, it is computationally efficient and can be conveniently adapted and incorporated into many applications for evaluating social influences. This is joint work with Yanyan Li and Sha Yang, University of Southern California.

A model robust subsampling approach for Generalised Linear Models in big data settings
Amalan Mahendran, Queensland University of Technology, Australia

Subsampling is a computationally efficient and scalable method to support timely insights and informed decision making in big data settings. An integral component of subsampling is determining what subsample should be extracted from the big data for analysis. Recent subsampling approaches propose determining subsampling probabilities for each data point based on optimality criteria from experimental design but we suggest this is of limited use in practice as these probabilities rely on an assumed model for the big data. To overcome this limitation, we propose a model robust approach where a set of models is considered, and the subsampling probabilities are evaluated based on the weighted average of probabilities that would be obtained if each model was considered singularly. Theoretical support for such an approach is provided and the results from considering a simulation study and two real world applications show that our model robust approach outperforms current subsampling practices

Stacking designs: designing multi-fidelity computer experiments with confidence
Simon Mak and Yi (Irene) Ji, Duke University

In an era where scientific experiments can be very costly, multi-fidelity emulators provide a useful tool for cost-efficient predictive scientific computing. For scientific applications, the experimenter is often limited by a tight computational budget, and thus wishes to (i) maximize predictive power of the multi-fidelity emulator via a careful design of experiments, and (ii) ensure this model achieves a desired error tolerance with confidence. Existing design methods, however, do not jointly tackle objectives (i) and (ii). We propose a novel stacking design approach which addresses both goals. Using a recently proposed multi-level Gaussian process emulator model, our stacking design provides a sequential approach for designing multi-fidelity runs such that a desired prediction error of $\epsilon > 0$ is met under regularity conditions. We then prove a novel cost complexity theorem which, under this multi-level Gaussian process emulator, establishes a bound on the computation cost (for training data simulation) needed to ensure a prediction bound of ϵ. This result provides novel insights on conditions under which the proposed multi-fidelity approach improves upon a standard Gaussian process emulator which relies on a single fidelity level. Finally, we demonstrate the effectiveness of stacking designs in a suite of simulation experiments and an application to finite element analysis.

Optimal designs for non-standard alcohol clearance models
Irene Mariñas-Collado, University of Oviedo, Spain

The equation most commonly used to estimate a person's blood alcohol concentration after consuming alcoholic drinks assumes the elimination process occurs in the body at a uniform rate and, very often, does not consider the phase of increasing concentration (absorption). In this work, optimal designs are proposed for a non-linear model that fits the different phases (absorption, distribution, and elimination) in order to compute the most informative observation times for the estimation of the parameters of the non-linear model. Because the parameters of the non-linear model depend on the characteristics of the subject in which the observations are taken, a covariance structure between responses is required in the design calculation.

Split plot parallel flats designs
Robert Mee, University of Tennessee

Nonregular fractional factorial designs for split plot experiments have been proposed by several authors. We review this literature and highlight complications for the analysis that may arise due to partial confounding of split-plot factor interactions. We then present a class of nonregular fractional factorial designs that avoid these complications. (This is joint work with Chunyan Wang and David Edwards).

Designing integral experiments to eliminate compensating nuclear data errors
Isaac J. Michaud, Los Alamos National Laboratory

Nuclear data are fundamental inputs to radiation transport codes used for reactor design and criticality safety. Designing integral experiments to reduce uncertainty and eliminate compensating in nuclear data pose numerous challenges not emphasized in classical optimal design, in particular: constrained design spaces (in both a statistical and engineering sense), severely underdetermined systems, and optimality criterion uncertainty. We will present a pipeline to optimize integral experiments that uses constrained Bayesian optimization within an iterative expert-in-the-loop framework capable of exploring richer design spaces and targeting regions of nuclear data important for reactor design and industrial applications. We will present some preliminary results from a successful experiment campaign designed with this framework that involved two critical configurations and multiple measurement modalities that targeted compensating errors in 239Pu nuclear data.

Simultaneous tolerance intervals for response surface and mixture designs using the adjusted product set method
Aisaku Nakamura, Cincinnati Children's Hospital

Response surface methodology (RSM) and mixture designs are heavily used in experimental designs. Calculating simultaneous confidence or prediction intervals using the corresponding estimated linear model can be accomplished with traditional methods, such as the Working–Hotelling or Scheffe's method. However, there is no gold-standard for fitting simultaneous tolerance intervals in this scenario. Recently, Nakamura and Young (2023) conducted an extensive empirical investigation of simultaneous tolerance interval methods and proposed an adjusted product set (APS) method, which demonstrated superior performance. In this presentation, the APS method is introduced in the context of models used in RSM and mixture experiments. Simulation results are presented which show that the APS method works well for these designs. Our method will be demonstrated on two real datasets.

A Bayesian analysis of two-stage randomized experiments in the presence of interference, treatment nonadherence, and missing outcomes
Yuki Ohnishi, Purdue University

Three critical issues for causal inference that often occur in modern, complicated experiments are interference, treatment nonadherence, and missing outcomes. A great deal of research efforts has been dedicated to developing causal inferential methodologies that address these issues separately. However, methodologies that can address these issues simultaneously are lacking. We propose a Bayesian causal inference methodology to address this gap. Our methodology extends existing causal frameworks and methods, specifically, two-staged randomized experiments and the principal stratification framework. In contrast to existing methods that invoke strong structural assumptions to identify principal causal effects, our Bayesian approach uses flexible distributional models that can accommodate the complexities of interference and missing outcomes, and that ensure that principal causal effects are weakly identifiable. We illustrate our methodology via simulation studies and a re-analysis of real-life data from an evaluation of India's National Health Insurance Program.

Kriging based sequential region perturbation and shrinkage with EGO for hyper-parameter optimization
Samuel Onyambu, University of California, Los Angeles

We propose a Kriging based sequential region shrinking method, that uses EGO for optimization while sequentially perturbing and reducing the region of interest based on the top n data points. The method does traverse both the high and low entropy areas and thus ensures that the optimization converges to the global or near global optimum. This method is applicable even if there is no feasible point in the initial samples. The efficiency of the proposed method is demonstrated on various physical well known test functions. We compare the method to well known gradient based optimization methods and show that the proposed method, although a derivative free-method, does match the expected results. Experimental results on datasets currently indicates that the method uses fewer resources and has a slight edge to the commonly used hyperparameter

Estimating heterogeneous treatment effects in conjoint analysis
Nicole Pashley, Rutgers University

Estimation of heterogeneous treatment effects is an active area of research in causal inference. Most of the existing methods, however, focus on estimating the conditional average treatment effects of a single, binary treatment given a set of pre-treatment covariates. In this paper, we propose a method to estimate the heterogeneous causal effects of high-dimensional treatments, which poses unique challenges in terms of estimation and interpretation. The proposed approach is based on a Bayesian mixture of regularized regressions to identify groups of units who exhibit similar patterns of treatment effects. By directly modeling cluster membership with covariates, the proposed methodology allows one to explore the unit characteristics that are associated with different patterns of treatment effects. Our motivating application is conjoint analysis, which is a popular survey experiment in social science and marketing research and is based on a high-dimensional factorial design. We apply the proposed methodology to the conjoint data, where survey respondents are asked to select one of two immigrant profiles with randomly selected attributes. We find that a group of respondents with a relatively high degree of prejudice appears to discriminate against immigrants from non-European countries like Iraq. An open-source software package is available for implementing the proposed methodology.

Applying quantitative decision-making to prediction of clinical trial recruitment
Inna Perevozskaya, GSK

Contemporary clinical trials often have complex logistics: they are run across multiple centers/countries and involve a lot of uncertainties about disease prevalence rates, patient characteristics and regulatory requirements, all of which can vary across countries and centers within a country. As a result, planning and delivering such studies on-time has long been recognized as a challenge in the pharmaceutical industry. The key to the accurate prediction is properly accounting for all the sources of uncertainty mentioned above. One well-known approach to modeling recruitment in complex trials which has been gaining traction steadily is Poisson-Gamma stochastic model. It's one of the applications of co-called predictive modelling approaches -the term that has been firmly embedded into the field of statistical innovation over the course of the past few years.
While the methodology based on Poi-Gamma stochastic process is complex on its own, it's represents only a tip of the "iceberg" of challenges posed by contemporary clinical trial recruitment planning . The more formidable challenge is getting the right data and organizing it into a form suitable for building prior distributions for the parameters the Poi-gamma model (e.g. predicting individual site performance from past performance data) . In this talk we will describe how we tackled this challenge by building a data pipeline from scratch and combining it with sophisticated Bayesian hierarchical modelling to create an internal decision-making platform that enabled users (ClinOps professionals) to calculate probability of successfully recruiting their study on time). This innovative project clearly demonstrated increased need for collaboration across different quantitative spaces (Statistics, Data science , ML , Tech) and resulting need for statisticians to acquire new skills essential for success of such collaboration.

A systematic design construction and analysis for cost-efficient order-of-addition experiment
Frederick Kin Hing Phoa, Institute of Statistical Science, Academia Sinica, Taipei, Taiwan

In this work, we propose a systematic design construction method for cost-efficient order-of-addition (OofA) experiments, and its corresponding statistical models for analyzing experimental results. In specific, our designs take the effects of two successive treatments into consideration. Each pair of level settings from two different factors in our design matrix appears exactly once to achieve cost-efficiency. Compared to designs in recent studies of OofA experiments, our design is capable of conducting experiments of one or more factors, so practitioners can insert a placebo, or choose different doses as level settings when our design is used as their experimental plans. We show an experimental analysis based on our design results in better performance than those based on the minimal-point design and Bayesian D-optimal design with the pairwise-order modeling in terms of identifying the optimal order. This is joint work with Jing-Wen Huang, Institute of Statistics, National Tsing Hua University.

Optimal designs for detecting and characterizing hormesis in toxicological tests
Sergio Pozuelo-Campos, Víctor Casero-Alonso, Mariano Amo-Salas
University of Castilla-La Mancha

Toxicological tests are experiments that show the effects of a toxic on organisms, ecosystems, etc. This study focuses on tests in the aquatic environment, in which the test involving *Ceriodaphnia Dubia* organism stands out. The literature indicates that in two out of every three experiments carried out with this organism, there is hormesis. This study applies optimal experimental design theory to a linear quadratic model with a Poisson distribution for the response, in order to obtain designs that allow efficient detection and characterization of hormesis. To this end, a variety of utility functions are used, including the dose for the zero equivalent point, the area under the curve, the dose at which maximum response is reached or the dose at which there is a given relative inhibition with respect to the control or the maximum. A study of cross efficiencies of the calculated designs shows the importance of correctly defining the goal of the experiment, in order to obtain the most appropriate design.

Incremental space-filling design
Luc Pronzato, Université Côte d'Azur, CNRS, France

The covering radius and L_r-quantization error (r>1) of a sampling design are key factors for the derivation of error bounds for function approximation or integration. Constructions of designs with small covering radii or small quantization error have received a lot of attention, in particular those forming regular patterns such as lattices. Incremental constructions, although of major practical interest, have received less attention. There exist bounds on the covering radius (or dispersion) for low discrepancy sequences used in Quasi-Monte Carlo methods, but they are extremely pessimistic and the performances of these constructions are rather deceiving. Three incremental constructions will be considered, based on the minimization of a Maximum-Mean-Discrepancy by kernel herding, on the greedy maximization of an integrated covering measure that defines a submodular set function, or on geometrical considerations leading to the greedy-packing algorithm and its boundary-phobic variants. In the later case, performance guarantees can be provided.

D-optimal subsampling design for big data regression
Torsten Reuter, Otto von Guericke University, Magdeburg, Germany

Data reduction is a fundamental challenge of modern technology, where classical statistical methods fail due to computational limitations. Subsampling reduces data size by selecting a subset from the original data. We consider a general linear model for an extraordinarily large number of observations, but only a few covariates. Under distributional assumptions on the covariates, we derive D-optimal subsampling designs for multiple linear and polynomial regression. We make use of fundamental concepts of optimal design theory and an equivalence theorem from convex optimization. We study the shape of the designs and the effect of the subsampling

proportion on them as well as their statistical properties. The obtained subsampling designs provide simple rules on whether to accept or to reject a data point and therefore allow for easy algorithmic implementation. We present a simulation study showing the advantages of our method over the IBOSS method among others and discuss their computing times.

Balancing covariates in randomized experiments with the Gram-Schmidt Walk Design
Fredrik Sävje, Yale University

The design of experiments involves an inescapable compromise between covariate balance and robustness. This paper provides a formalization of this trade-off and introduces an experimental design that allows experimenters to navigate it. The design is specified by a robustness parameter that bounds the worst-case mean squared error of an estimator of the average treatment effect. Subject to the experimenter's desired level of robustness, the design aims to simultaneously balance all linear functions of potentially many covariates. The achieved level of balance is better than what previously was known to be possible and is considerably better than what a fully random assignment would produce. We show that the mean squared error of the estimator is bounded by the minimum of the loss function of an implicit ridge regression of the potential outcomes on the covariates. The estimator does not itself conduct covariate adjustment, so one can interpret the approach as regression adjustment by design. Finally, we provide non-asymptotic tail bounds, conditions for asymptotic normality and a variance estimator, which facilitate the construction of conservative confidence intervals.

Optimal design for generalized linear mixed models based on the penalized quasi-likelihood method
Yao Shi, Qingdao University, China

While generalized linear mixed models are useful, optimal design questions for such models are challenging due to complexity of the information matrices. For longitudinal data, after comparing three approximations for the information matrices, we propose an approximation based on the penalized quasi-likelihood method. We evaluate this approximation for logistic mixed models with time as the single predictor variable. Assuming that the experimenter controls at which time observations are to be made, the approximation is used to identify locally optimal designs based on the commonly used A- and D-optimality criteria. The method can also be used for models with random block effects models. Locally optimal designs found by a Particle Swarm Optimization algorithm are presented and discussed. As an illustration, optimal designs are derived for a study on self-reported disability in older women. Finally, we also study the robustness of the locally optimal designs to mis-specification of the covariance matrix for the random effects.

Systematic enumeration of two-level even-odd designs of strength 3
Eric Schoen, KU Leuven, Belgium

Two-level even designs can be constructed by folding over smaller designs. The number of two-factor interactions that can simultaneously be estimated with such designs cannot exceed half the run size minus one. Even-odd designs cannot be constructed by folding over, but they may permit simultaneous estimation of many more two-factor interactions. We present the first dedicated algorithm to enumerate even-odd designs. We restrict the enumeration to designs with at least one nonzero correlation between a two-factor and a three-factor interaction contrast vector. We enumerate all such designs with up to 56 runs, those with 64 runs and up to 13 factors, and those with 64 runs and more than 13 factors with only partial correlations between two-factor and three-factor interaction contrast vectors. As regards the rank of the matrix of two-factor interaction contrast vectors, our best ranked 64-run designs substantially improve on benchmark designs from the literature.

Framework to design a Bayesian group sequential clinical study
Jinesh Shah, CSL Behring

Bayesian design and analysis of clinical trials have been popularized in the past few years as associated computational challenges become trivial. This presentation will elaborate on design and operating characteristics

of a phase 3 Bayesian group sequential trial through extensive simulations. Prior elicitation of treatment effect from group of experts and calculation of assurance for decision making at different stages of design and financial allocation of company funds will also be discussed.

Design selection for multi- and mixed-level supersaturated designs
Rakhi Singh, Binghamton University

The literature offers various design selection criteria and analysis techniques for screening experiments. Designs used in a screening experiment are often termed supersaturated designs. For two-level supersaturated designs, the Gauss-Dantzig Selector is often preferred for analysis, but it fails to capture differences in screening performance among different designs. Two recently proposed criteria utilizing large-sample properties of the Gauss-Dantzig Selector by Singh and Stufken (Technometrics, 2023) result in better screening designs. Unfortunately, the straightforward extension of these criteria to higher-level designs is not possible. For example, it is unclear if the Gauss-Dantzig Selector is still an appropriate analysis method for multi- and mixed-level designs. In this talk, I will first argue that group LASSO is a more appropriate method to analyze such data. I will then use large sample properties of group LASSO to propose new optimality criteria and construct novel and efficient designs that demonstrate superior screening performance.

Optimal supersaturated designs for lasso sign recovery
Jonathan Stallrich, North Carolina State University

Supersaturated designs aim to identify the relatively few active factors of a system using fewer runs than the number of factors manipulated during the experiment. Designs are often ranked according to some heuristic measure of orthogonality of the design's information matrix. However, the designs are often analyzed using penalized estimation and it is unclear whether optimal designs under the heuristic measures will perform well under such an analysis. This talk introduces new optimal supersaturated design criteria that directly target the screening properties of the lasso estimator, particularly the probability of sign recovery. First, a local optimality approach is taken in which the entire model form and its parameter values are known. Situations are identified in which an orthogonal design is suboptimal even if it were to exist, which contradicts common design intuition. A more practical criterion is then studied that relaxes the degree of prior knowledge. We establish that when there is no prior sign information about the active effects, designs achieving near orthogonality are optimal, but under known sign information, designs having an information matrix with constant positive off-diagonals are superior to orthogonal designs. A design search algorithm is proposed that leverages the computational efficiency of existing heuristics and then implements our criteria as a secondary measure to improve the design rankings.

An overview of statistical challenges in online controlled experiments
Nathaniel T. Stevens, University of Waterloo, Canada

The rise of internet-based services and products in the late 1990's brought about an unprecedented opportunity for online businesses to engage in large scale data-driven decision making. Over the past two decades, organizations such as Airbnb, Alibaba, Amazon, Baidu, Booking, Alphabet's Google, LinkedIn, Lyft, Meta's Facebook, Microsoft, Netflix, Twitter, Uber, and Yandex have invested tremendous resources in online controlled experiments (OCEs) to assess the impact of innovation on their customers and businesses. Running OCEs at scale has presented a host of challenges requiring solutions from many domains. In this talk we discuss the practice and culture of online experimentation, and we review practical challenges that require new statistical methodologies to address them. The goal is to raise academic statisticians' awareness of these new research opportunities so as to increase collaboration between academia and the online industry.

Business policy experiments using factorial designs
Yixin Tang, DoorDash

In a business decision-making process, we aim to find the optimal policy in a huge business policy space. Typically the cardinality of the business space is so high that testing all of them is both time-consuming and requires a lot of manual effort to set up each policy. Inspired by conjoint analysis, the framework we proposed breaks down the policy space into factors. After the factorization, we apply fractional factorial design to the factors generated by the previous step. To verify the correctness of the framework, particularly the additivity assumption we imposed on our selected factors, we conducted a new experiment to validate an out-of-sample policy that did not exist in our original experiment. The main benefit of our framework is to improve the sensitivity or velocity, which can be measured by the improved minimum detectable effects (MDE) of policies given a fixed sample, or by the smaller sample size required to test a certain number of policies.

Cost of sequential adaptations
Sergey Tarima, Medical College of Wisconsin

The possibility of early stopping and/or interim sample size re-estimation lead to random sample sizes. When such interim adaptations are informative, the interim decision becomes a component of the sufficient statistic. We decompose the total Fisher Information (FI) into the design FI and a conditional-on-design FI analogous to Molenberghs et al. (2014). We go further, representing the conditional-on-design FI as a weighted linear combination of FIs conditional on realized decisions. This decomposition is useful for quantifying how much mean-squared error will be lost due to planned-informative adaptations. We use The FI unspent by having a planned-informative adaptation to determine the lower bound on mean squared error of post-adaptation estimators [the Cramer-Rao lower bound (1946) and its sequential version suggested by Wolfowitz (1947) are not applicable to such estimators]. Theoretical results are illustrated with simple normal samples collected according to a two-stage design with a possibility of early stopping.

Enhancing efficient global optimization through a kriging based space reduction
Jose Toledo, University of California, Los Angeles

Efficient Global Optimization (EGO) is a widely used form of Bayesian optimization that has been successfully applied to solve global optimization of black-box problems. However, performing EGO through the entire design space can be computationally expensive and time consuming.
This paper introduces a a Kriging-based space reduction algorithm, to enhance the performance of EGO. Specifically, we adjust the design space in EGO by creating a sub-region centered around the top γ percentage of points obtained through the maximization of an acquisition function. This process is repeated until a stopping criteria is met. Through numerical experiments on global optimization tasks and hyperparameter tuning of machine learning models, we have demonstrated that our algorithm consistently outperforms EGO over the entire design space and can compete with other state-of-the-art black-box optimization methods.

New sample size selection methods for discrete choice experiments
Martina Vandebroek, KU Leuven

Selecting the appropriate sample size for discrete choice experiments (DCE) remains a challenge. Both rules-of-thumb and elaborate power calculations can be found in the literature. The former do not depend on the desired power and significance level and is therefore not very accurate, whereas the latter requires the complete experimental setup which may not yet be known at the planning stage. We investigate a new rule-of-thumb as well as a new regression-based method that requires only a few design characteristics rather than the complete design and takes into account the power and significance level. We compare the sample size determined using the proposed methods with the true required sample size based on the statistical error of the parameter of interest and with the approximations given by the existing rules-of-thumb. The results show that our new rule-of-thumb reduces the overestimation of the existing rules-of-thumb is many realistic settings while providing a

minimum power of 70%. Using the regression-based approach, we are able to approximate the required sample size better than the existing rules-of-thumb when the desired power level is high.

An integer programming algorithm for constructing maximin distance designs from good lattice point sets
Alan R. Vazquez, University of Arkansas

Computer experiments allow us to build computationally-cheap statistical models to study complex computer models. These experiments are commonly conducted using maximin distance Latin hypercube designs (LHDs), which are generated using heuristic algorithms or algebraic methods in the literature. However, the performance of these algorithms deteriorates as the number of factors increases, while the algebraic methods only work for numbers of runs that are of a special kind, say, a prime number. To overcome these limitations, we introduce an integer programming algorithm to construct maximin distance LHDs of flexible sizes. Our algorithm leverages the recent advances in the field of optimization as implemented in commercial optimization solvers. Moreover, it benefits from the attractive algebraic structures given by good lattice point sets and the Williams' transformation. Using comprehensive numerical experiments, we show that our integer programming algorithm outperforms benchmark algorithms and methods for constructing large designs.
References
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Scale-invariant optimal sampling and variable selection with rare-events data
Jing Wang, University of Connecticut

Subsampling is a particularly effective approach to solve the computational challenges with massive rare-events data, with the possibility of a significant reduction in computational burden by little sacrifice on asymptotic estimation efficiency. In case of any estimation efficiency loss due to too aggressive subsampling, an optimal subsampling method can help minimize the information loss. However, optimal subsampling has never been investigated in the context of variable selection. Existing optimal subsampling probabilities depend on the scale of the covariates and may produce inconsistent results for the same data with different scale transforms. This scale dependence issue may cause more serious problems in variable selection when there are inactive covariates, because the contribution of the inactive covariates may be arbitrarily amplified if an inappropriate scale transform. To resolve this issue and fill the aforementioned gap in the literature, we investigate variable selection for rare-events data. We first prove the oracle properties of full data adaptive lasso estimator with massive rare-events data, which justify the usage of subsampling controls. We then propose a scale invariant optimal subsampling function to minimize the prediction error of the inverse probability weighted (IPW) adaptive lasso. Both the optimal subsampling function and the adaptive lasso require a pilot estimator, and the two procedures are naturally integrated. We also propose an estimator based on maximum sampled conditional likelihood with adaptive lasso penalty to further improve the estimation efficiency. The oracle properties of the proposed estimator are also investigated. Numerical experiments based on simulated and real data are carried out to investigate the performances of proposed methods.

A note on centering in subsample selection for linear regression
HaiYing Wang, University of Connecticut

Centering is a commonly used technique in linear regression analysis. With centered data on both the responses and covariates, the ordinary least squares estimator of the slope parameter can be calculated from a model without the intercept. If a subsample is selected from a centered full data, the subsample is typically un-centered. In this case, is it still appropriate to fit a model without the intercept? The answer is yes, and we show that the least squares estimator on the slope parameter obtained from a model without the intercept is unbiased and it has a smaller variance covariance matrix in the Loewner order than that obtained from a model with the intercept. We further show that for noninformative weighted subsampling when a weighted least squares estimator is used, using the full data weighted means to relocate the subsample improves the estimation efficiency.

Group-orthogonal subsampling for non-independent data based on linear mixed models
Lin Wang, Purdue University

Linear mixed model is commonly used for training data with a hierarchical structure. It is computationally expensive to obtain parameter estimates in a linear mixed model with big data. Subsampling techniques have been developed to address computational challenges. However, existing methods typically assume independently distributed data without considering the correlation between observations. We develop a novel group-orthogonal subsampling (GOSS) approach for selecting an informative subsample from hierarchical data. GOSS selects the subsample with sample size balance between groups and combinatorial orthogonality within each group, therefore ensures the selected subsamples are D- and A-optimal for establishing linear mixed models. The estimators of parameters trained on a GOSS subsample is shown to be consistent asymptotic normal. Extensive simulation results show that GOSS outperforms existing methods in minimizing the mean squared errors of the estimated parameters. A real data example is also provided to illustrate the advantages of the GOSS method.

Rerandomization with diminishing covariate imbalance and diverging number of covariates
Yuhao Wang, Tsinghua University

Completely randomized experiments have been the gold standard for drawing causal inference because they can balance all potential confounding on average. However, they may suffer from unbalanced covariates for realized treatment assignments. Rerandomization, a design that rerandomizes the treatment assignment until a prespecified covariate balance criterion is met, has recently got attention due to its easy implementation, improved covariate balance and more efficient inference. Researchers have then suggested to use the treatment assignments that minimize the covariate imbalance, namely the optimally balanced design. This has caused again the long-time controversy between two philosophies for designing experiments: randomization versus optimal and thus almost deterministic designs. Existing literature argued that rerandomization with overly balanced observed covariates can lead to highly imbalanced unobserved covariates, making it vulnerable to model misspecification. On the contrary, rerandomization with properly balanced covariates can provide robust inference for treatment effects while sacrificing some efficiency compared to the ideally optimal design. In this paper, we show it is possible that, by making the covariate imbalance diminishing at a proper rate as the sample size increases, rerandomization can achieve its ideally optimal precision that one can expect with perfectly balanced covariates, while still maintaining its robustness. We further investigate conditions on the number of covariates for achieving the desired optimality. Our results rely on a more delicate asymptotic analysis for rerandomization, allowing both diminishing covariate imbalance threshold (or equivalently the acceptance probability) and diverging number of covariates. The derived theory for rerandomization provides a deeper understanding of its large-sample property and can better guide its practical implementation. Furthermore, it also helps reconcile the controversy between randomized and optimal designs in an asymptotic sense.

An efficient filtering approach for model estimation in sparse regression
Yanran Wei, Virginia Tech

As the technology advances, the scale of data generated is growing exponentially, bringing huge challenges to the storage space and computational resources. To get rid of computational cost while keeping estimation accuracy, subdata selection becomes critical. Traditional methods, like LASSO and Ridge, focus on selecting features. Also, there are other methods, like subsampling techniques, specifying data points to be extracted. However, these methods do not give full consideration to the role of response variable and its relationship with predictor variables. To overcome these shortages, we proposed a method called Filtering Approach for Model Estimation (FAME). The proposed method conducted subsampling after predictor screening. Compared with existing methods, the generated subdataset has a smaller size both in terms of number of features and observations and the computational complexity does not increase. The performance of FAME is measured in several numerical examples. And it can be extended to situations when the predictor is binary or response is binary or both are binary.

Designs for order-of-addition screening experiments
Hongquan Xu, UCLA

When studying the relationship between the order of a set of components and a measured response in an order-of-addition experiment, the number of components may exceed the number of available positions. In this case there is an added layer of complexity in which the experimenter is tasked with locating both the best combination of components and its corresponding best order. Akin to the standard order-of-addition setup, the number of possible sequences grows quickly with the number of components, rendering a brute force approach unfeasible. This necessitates the development of parsimonious designs for these order-of-addition screening experiments. We present a framework for constructing optimal and near-optimal screening designs under adapted versions of several prominent order-of-addition models. We apply our order-of-addition screening designs to job scheduling problems in the context of both a single-shot experiment and an active learning framework for sequential experimentation. The proposed designs not only offer precise effect estimation and accurate predictions, but also facilitate quick convergence to the optimal ordering in sequential experiments.

Comparing supersaturated screening designs using exact screening probabilities
Kade Young, North Carolina State University

Supersaturated screening designs (SSDs) push screening capability to its extremes. In this setting, there are fewer experimental runs than there are factors to screen, and the main effects model is not fully estimable under ordinary least squares. Traditionally, SSDs are analyzed using a penalized regression framework to select which factors drive the response. Several optimal design heuristic criteria exist for SSDs, but comparisons between designs constructed using different heuristic criteria are usually performed via simulation studies that rely on tuning parameter selection techniques and arbitrary thresholds. This work explains the reproducibility and accuracy issues that arise when comparing SSDs via simulation and demonstrates its potential pitfalls. We then propose a different method of comparing SSDs based upon exact local lasso sign recovery probabilities over a range of tuning parameter values. This comparison method is not dependent on a tuning parameter selection strategy or a threshold.

Analysis of order-of-addition experiments
Xueru Zhang, Purdue University

Order-of-addition (OofA) problems have attracted a great deal of attention in many disciplines, especially in the areas of biochemistry, nutritional science, scheduling fields, pharmaceutical company and engineering field. While there have been numerous studies in this area from a statistical perspective, it is too scattered to solve a general OofA problem. To fill this gap, we develop a unified framework to account for a general OofA problem, suitable for both homoscedasticity and heteroscedasticity cases. This framework encompasses data collection (design), test of variance homogeneity, model building, and optimization. Especially for heteroscedasticity cases, we build up the dual response surface optimization with unknown parameters which are derived from the unknown distribution of environmental variables. To learn this distribution, we construct an uncertainty set, which is fully data driven. The proposed dual response surface optimization minimizes the dispersion of response while keeping the location of response close to a given target value under the uncertainty set. We transform the proposed optimization into a tractable and equivalent minimization with a low computational cost. Theoretical supports are obtained to ensure the tractability of the proposed method. Simulation studies are provided to illustrate the effectiveness of the proposed approach. With its solid theoretical support, ease of implementation, and ability to find optimal orders, the proposed approach is a valuable tool for addressing a general OofA problem.

Independence-encouraging subsampling for nonparametric additive models
Yi Zhang, George Washington University

The additive model is a popular nonparametric regression method that can retain modeling flexibility and meanwhile prevent the curse of dimensionality. The backfitting algorithm is an intuitive and easy-to-implement numerical approach to fitting additive models. However, applying the backfitting algorithm to a large dataset may incur a high computational cost. To address this problem, we propose an independence-encouraging subsampling (IES) approach to select an informative subsample from big data such that the predictors are empirically independent and uniform in the subsample.
The IES is inspired by the minimax optimality of an orthogonal array (OA). Asymptotic analyses show that an IES subsample converges to an OA and the backfitting algorithm over the subsample converges to a unique solution even if the predictors are highly dependent in the original data. The IES method is also shown to be numerically appealing via simulation and a real data application.

Thompson sampling with discrete prior
Wei Zheng, University of Tennessee

Thompson sampling is a popular algorithm for multi-armed bandit problems, but its Bayesian posterior update can be computationally expensive for complex reward distributions. Recently, prior discretization has been proposed to address this issue. In this paper, we propose a new prior discretization method that guarantees the same regret rate without requiring the unreasonable assumption that the true value of the parameter is one of the discrete points. Additionally, we introduce a modified posterior update approach that further improves the performance of discrete prior Thompson sampling. We prove that the accumulated regret has $O(\log(T))$ convergence rate with high probability. In addition, we conduct numerical experiments to validate our theoretical analysis and demonstrate that the proposed algorithm outperforms both the standard discrete prior method and the Laplace approximation approach for the continuous prior.

ICODOE 2022
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