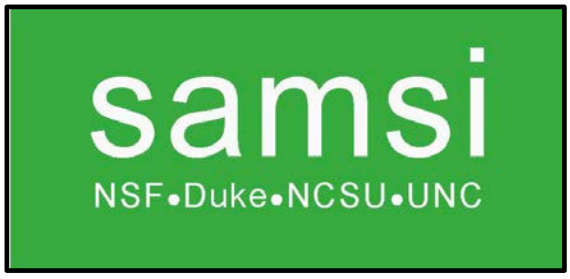
Optimization Under Uncertainty and Data-Driven Science and Engineering

April 13-14, 2017

Ambassador Room, Washington Duke Inn



Duke UNIVERSITY | PRATT SCHOOL *of* ENGINEERING

Optimization Under Uncertainty and Data-Driven Science and Engineering
April 13-14, 2017
Ambassador Room, Washington Duke Inn

Thursday, April 13

8:00 **Registration**
8:40 **Opening**
9:00 **Terry Rockafellar**, Solving Stochastic Variational Inequalities by Progressive Hedging
9:40 **Drew Kouri**, A Data-Driven Approach to PDE-Constrained Optimization under Uncertainty
10:20 Break-Rotunda (open 9-5pm)
10:40 **Guillermo Sapiro**, Learning to Optimize
11:20 **Madeleine Udell**, Sketchy Decisions: Convex Low-Rank Matrix Optimization with Optimal Storage
12:00 Lunch- Buffet
2:00 **Alexander Shapiro**, Computational complexity of stochastic programs
2:40 **Jonathan Mattingly**, Analyzing MCMC and Streaming algorithms in high-dimensions through scaling limits
3:20 Break-Rotunda (open 9-5pm)
3:40 **Stan Uryasev**, Classification with Error Control using Buffered Probability
4:20 **Genetha Gray**, Uncertainty Quantification of Big Data Applied to Autonomous Vehicles
5:00 **Johannes Royset**, Risk-Tuned Prediction and Design
5:40 End of technical talks
6:00 **Poster session**-Ambassador Room: hors d'oeuvres, open bar

Friday, April 14

9:00 **Steven Low**, Optimal Power Flow: Online Algorithm and Fast Dynamics
9:40 **Santiago Grijalva**, Decentralized Coordination in Transactive Energy Prosumer Networks
10:20 Break-Rotunda (open 9-5pm)
10:40 **Lang Tong**, Probabilistic Forecasting and Simulation of Real-time Electricity Markets via Online Dictionary Learning
11:20 **Michael Zavlanos**, Distributed Optimization Algorithms for Networked Systems
12:00 Lunch- Sandwich Cart
2:00 **Ingrid Daubechies**, Bones, Teeth and Animation
2:40 **Noemi Petra**, Mean-variance risk-averse optimal control of systems governed by PDEs with random parameter fields using quadratic approximations
3:20 Break-Rotunda (open 9-5pm)
3:40 **Bart Van Bloemen Waanders**, Data Analysis and Risk Averse Optimization for Additive Manufacturing
4:20 **Sayan Mukherjee**, Inference in Dynamical Systems
5:00 End of workshop

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Terry Rockafellar, University of Washington
Solving Stochastic Variational Inequalities by Progressive Hedging
Variational inequalities are a modeling tool for problems of optimization and equilibrium, but also have a long-standing role in extending partial differential ``equations'' to the possibility of ``inequations'' coming from obstacles. Stochastic variational inequalities incorporate uncertainty and thus have a bearing on uncertainty quantification, but they can stand for optimality and equilibrium conditions in a single-stage or multi-stage environment as well. Besides explaining that framework, this talk will show how, in the presence of monotonicity (in the operator sense), solutions can be obtained by the progressive hedging algorithm.

Drew Kouri, Sandia National Labs
A Data-Driven Approach to PDE-Constrained Optimization under Uncertainty
Many science and engineering applications require the optimal control or design of a physical system governed by partial differential equations (PDEs). More often then not, PDE inputs such as coefficients, boundary conditions and initial conditions are unknown and estimated from noisy, incomplete data. In this talk, I will discuss the theoretical challenges associated with such PDE-constrained optimization problems, including their mathematical formulation and their efficient numerical solution. First, I will assume that the probability distributions characterizing the uncertain PDE inputs are known. For this case, I will review risk measures as a means for quantifying the "hazard" associated with large objective function values. Next, to handle the situation of unknown probability distributions, I will introduce and analyze a distributionally-robust formulation for the optimization problem. To enable numerical solutions, I will present a novel discretization for the unknown probability measure and provide rigorous error bounds for this approximation. I will conclude with numerical results confirming the aforementioned bounds.

Guillermo Sapiro, Duke University
Learning to Optimize
In this talk I will describe some of our early work on how to adapt optimizers to the data and task, achieving orders of magnitude speed-ups. This is joint work with P. Sprechmann and A. Bronstein, with additional theoretical foundation with R. Giryes and Y. Eldar.

Madeleine Udell, Cornell University
Sketchy Decisions: Convex Low-Rank Matrix Optimization with Optimal Storage
In this talk, we consider a fundamental class of convex matrix optimization problems with low-rank solutions. We show it is possible to solve these problems using far less memory than the natural size of the decision variable when the problem data has a concise representation. Our proposed method, SketchyCGM, is the first algorithm to offer provable convergence to an optimal point with an optimal memory footprint. SketchyCGM modifies a standard convex optimization method — the conditional gradient method — to work on a sketched version of the decision variable, and can recover the solution from this sketch. In contrast to recent work on non-convex methods for this problem class, SketchyCGM is a convex method; and our convergence guarantees do not rely on statistical assumptions.

Alexander Shapiro, Georgia Institute of Technology
Computational Complexity of Stochastic Programs
The traditional approach to solving stochastic programming problems involves discretization of the underlying probability distributions. However, the number of required discretization points (called scenarios) grows exponentially both with increase of the number of random parameters and number of stages. In order to deal with this exponential explosion, randomization approaches based on Monte Carlo sampling techniques were developed. In this talk we discuss computational complexity of some of such methods from theoretical and practical points of view.

Jonathan Mattingly, Duke University
Analyzing MCMC and Streaming algorithms in high-dimensions through scaling limits
I will discuss the high dimensional scaling limits of some Markov Chain algorithms in Monte Carlo and streaming applications. The limits will consist of stochastic, as well as deterministic, PDEs and Non-linear PDEs which come from a mean-field limit. The talk will be based on older work with Andrew Stuart (Caltech) and Natesh Pillai (Harvard) and ongoing work with Yue Lu (Harvard) and Chuang Wang (Harvard).

Stan Uryasev, University of Florida
Classification with Error Control using Buffered Probability
We present a new classification paradigm with error control inspired by the Neyman-Pearson (NP) classification. Standard NP classification minimizes False Positive Rate (FPR) with constrained False Negative Rate (FNR). Our approach, which is called bNP classification, is a new counterpart for NP classification. bNP classification is derived from the Buffered Probability of

Uncertainty Quantification of Big Data Applied to Autonomous Vehicles
Determining the likelihood of specific outcomes despite the lack of complete system knowledge is central to the use of predictive simulation. To date, the development of uncertainty quantification (UQ) tools has focused primarily on data-poor application or "small data" environments. However, many of today's problems are characterized by "big data" or collections of data too large and complex for traditional processing techniques. While tools have been developed to analyze big data, the associated uncertainties and their impacts to are yet to be well defined or understood. In this talk, we will consider UQ methodology for applications related to autonomous vehicles (AV). Each hour, an AV can collect one terabyte of heterogeneous data from car positioning to camera images. Such data sets cannot simply be analyzed by applying existing UQ methodologies as the quantity of data can add intractable complexities or impossible computational workload requirements. Moreover, simplistic sampling or down selecting the data may lead to lost information or useless risk assessments. We will review alternative approaches to UQ and describe their importance in the development of AV systems.

Johannes Royset, Naval Postgraduate School
Risk-Tuned Prediction and Design
Engineering decisions are invariably made under substantial uncertainty about current and future system cost and response, including cost and response associated with low-probability, high-consequence events. We review models for decision making based on superquantile risk (s-risk) that comprehensively capture uncertainty, avoid paradoxes, and accrue substantial benefits in risk, reliability, and cost optimization. We describe methods for predicting s-risk at reduced computational cost using multi-fidelity simulations and give examples from earthquake engineering, naval architecture, and energy management.

Steven Low, Caltech
Optimal Power Flow: Online Algorithm and Fast Dynamics
We are at the cusp of a historical transformation of our power systems into a more sustainable, dynamic, and intelligent network with hundreds of millions of distributed energy resources. One of the key challenges in this transformation is the control and optimization of such a large-scale cyberphysical system. The optimal power flow (OPF) problem underlies numerous system operation and planning applications. Traditional OPF algorithms are offline in that they solve power flow equations explicitly or implicitly, and iteratively until the computation has converged before applying the final solution. This is computationally challenging because power flow equations are nonlinear. The grid however implicitly solves power flow equations in real-time at scale for free. We describe two methods to explicitly exploits the network as a power flow solver to carry out part of our optimization algorithm. This approach naturally adapts to evolving network conditions.
Specifically, we present algorithms that adapt controllable devices and interacts continuously with the grid which computes a power flow solution given a control action. Collectively these devices and the grid implement a gradient algorithm in real time. We characterize optimality and tracking performance. We apply this idea to ubiquitous load-side frequency control at a fast timescale that integrates primary frequency regulation, secondary frequency regulation, and congestion management. We prove sufficient conditions under which the algorithm converges to a global optimum.

Santiago Grijalva, Georgia Institute of Technology
Decentralized Coordination in Transactive Energy Prosumer Networks
Energy prosumers are economically motivated subsystems that can consume, produce or store electricity. They emerge naturally from the deployment of distributed energy resources (DERs) such as solar, wind, demand response, energy storage, electric vehicles, etc. Energy prosumers include homes, buildings, microgrids, as well as larger subsystems. Connected through communication networks, and equipped with distributed computing, prosumers become “energy aware” and can locally and intelligently optimize their energy utilization. However, in order to maintain the functionality, security, and resilience of the overall electricity grid, they must coordinate with each other in a decentralized and provable manner. This talk will describe architectures and methods for massively scalable decentralized coordination among energy prosumers at the control and optimization (scheduling) time scales. We will present novel results on algorithmic development and their performance on DER-rich networks, demonstrating scalability. We will describe the elements of transactive energy services platforms to realize decentralized prosumer coordination.

Lang Tong, Cornell University
Probabilistic Forecasting and Simulation of Real-time Electricity Markets via Online Dictionary Learning
The dramatic increase of the behind-the-meter solar integration in recent years has fundamentally changed the overall netload characteristics. In some areas, the traditional load profile is being transformed to the so-called “duck curve” profile where a steep downramp when a large amount of solar power is injected is followed by a steeper up-ramp when the solar power drops sharply in the late afternoon and early evening hours. While the duck curve phenomenon represents an average behavior, it is the highly stochastic and spatial-temporal dependent ramp events that present difficult operational challenges to system operators. In this talk, we consider the problem of online forecasting and simulation of real-time system operations. By online forecasting and simulation we mean in particular using real-time SCADA and PMU measurements to produce conditional probability distributions of future nodal prices, power flows, power dispatch levels, and discrete events such as occurrences of congestion and system contingencies. An online dictionary learning technique is proposed to achieve several orders of magnitude of improvement in computation time over standard Monte Carlo techniques.

Michael Zavlanos, Duke University
Distributed Optimization Algorithms for Networked Systems
Distributed optimization methods allow to decompose an optimization problem into smaller, more manageable subproblems that are solved in parallel. For this reason, they are widely used to solve large-scale problems arising in areas as diverse as wireless communications, optimal control, machine learning, artificial intelligence, computational biology, finance, and statistics, or problems with a separable structure that are amenable to distributed implementations. In this talk we present the Accelerated Distributed Augmented Lagrangians (ADAL) algorithm, a novel decomposition method for optimization problems that involve a separable convex objective function subject to convex local constraints and linear coupling constraints. Optimization using Augmented Lagrangians (ALs) combines the low computational complexity of first order optimization methods with fast convergence speeds due to the regularization terms included in the AL. In its centralized version, optimization using ALs is an excellent general purpose method for constrained optimization problems and enjoys a large amount of literature. However, decentralized methods that employ ALs are few, as decomposition of ALs is a particularly challenging task. We establish convergence of ADAL and show that it has a worst-case O(1/k) convergence rate. Moreover, we show that ADAL converges to a local minimum of the problem when the objective function is non-convex, and that it can handle uncertainty and noise in which case it generates sequences of primal and dual variables that converge to their respective optimal sets almost surely. We provide numerical simulations for wireless network optimization problems that suggest that the proposed method outperforms the state-of-the-art distributed Augmented Lagrangian methods that are known in the literature. Moreover, we present a Random Approximate Projections (RAP) method for decentralized optimization problems with SDP constraints. Unlike other methods in the literature that employ Euclidean projections onto the feasible set, our method is computationally inexpensive as it relies only on subgradient steps in the direction that minimizes the local constraint violation. We show that the algorithm converges almost surely and can also handle inexact problem data. We demonstrate our approach on a distributed estimation problem involving networks of mobile sensors estimating a set of hidden states that are governed by linear dynamics up to a user-specified accuracy.

Ingrid Daubechies, Duke University
Bones, Teeth and Animation
The talk describes new distances between pairs of two-dimensional surfaces (embedded in three-dimensional space) that use both local structures and global information in the surfaces. These are motivated by the need of biological morphologists to compare different phenotypical structures, to study relationships of living or extinct animals with their surroundings and each other. This is typically done from carefully defined anatomical correspondence points (landmarks) on e.g. bones.
Unlike other algorithms presented for morphological correspondences, our approach does not require any preliminary marking of special features or landmarks by the user. It also differs from other seminal work in computational geometry in that our algorithms are polynomial in nature and thus faster, making pairwise comparisons feasible for significantly larger numbers of digitized surfaces. The approach is illustrated using three datasets representing teeth and different bones of primates and humans; it is shown that it leads to highly accurate results.

Noemi Petra, University of California, Merced
Mean-variance Risk-averse Optimal Control of Systems Governed by PDEs with Random Parameter Fields uUsing Quadratic Approximations
We present a method for optimal control of systems governed by partial differential equations (PDEs) with uncertain parameter fields. We consider an objective function that involves the mean and variance of the control objective, leading to a risk-averse optimal control problem. To make the optimal control problem tractable, we invoke a quadratic Taylor series approximation of the control objective with respect to the uncertain parameter field. This enables deriving explicit expressions for the mean and variance of the control objective in terms of its gradients and Hessians with respect to the uncertain parameter. The risk averse optimal control problem is then formulated as a PDE-constrained optimization problem with constraints given by the forward and adjoint PDEs defining these gradients and Hessians. The expressions for the mean and variance of the control objective under the quadratic approximation involve the trace of the (preconditioned) Hessian, and are thus prohibitive to evaluate. To overcome this difficulty, we employ randomized trace estimators. We illustrate our approach with two specific problems: the control of a semilinear elliptic PDE with an uncertain boundary source term, and the control of a linear elliptic PDE with an uncertain coefficient field. For the latter problem, we derive adjoint-based expressions for efficient computation of the gradient of the risk-averse objective with respect to the controls. Our method ensures that the cost of computing the risk-averse objective and its gradient with respect to the control-measured in the number of PDE solves-is independent of the (discretized) parameter and control dimensions, and depends only on the number of random vectors employed in the trace estimation. Finally, we present a comprehensive numerical study of an optimal control problem for fluid flow in a porous medium with uncertain permeability field.

Bart Van Bloemen Waanders, Sandia National Laboratories
Data Analysis and Risk Averse Optimization for Additive Manufacturing
Additive manufacturing (AM) is capable of creating compelling designs at a much faster rate than standard methods. However, achieving consistent material properties at various length scales remains a challenge. In this work, we present risk-averse optimization to produce robust designs by tightly controlling certain features of the dynamics while addressing underlying uncertainties. Aspects of the AM process are emulated with PDEs to mimic the behavior of the material during the processing.

The goal is to control different aspects of the dynamics, such as source terms and boundary conditions, to achieve design targets and simultaneously accomodate uncertainties in different parts of the underlying dynamics.
PDE-constrained optimization methods serve as the foundation for this work with finite element discretizations, adjoint-based sensitivities, trust-region methods, and Newton-Krylov solvers. Our final AM produced parts must achieve tight tolerances for a range of different material properties. Accordingly, risk-averse methods are considered with a specific emphasis on reliability. A numerical example demonstrates that the use of risk measures results in optimal solutions and ensures that worse case scenarios are avoided.

Sayan Mukherjee, Duke University
Inference in Dynamical Systems
We consider the asymptotic consistency of maximum likelihood parameter estimation for dynamical systems observed with noise. Under suitable conditions on the dynamical systems and the observations, we show that maximum likelihood parameter estimation is consistent. Furthermore, we show how some well-studied properties of dynamical systems imply the general statistical properties related to maximum likelihood estimation. Finally, we exhibit classical families of dynamical systems for which maximum likelihood estimation is consistent. Examples include shifts of finite type with Gibbs measures and Axiom A attractors with SRB measures. We also relate Bayesian inference to the thermodynamic formalism in tracking dynamical systems. We state conditions for consistency of a Gibbs distribution using classic ideas from dynamical systems such as topological entropy and pressure.

Posters

Olalekan Babaniyi, Duke University
PDE-Constrained Optimization Techniques for Bio-Mechanical Imaging

Andres Contreras, Duke University
Parallel Domain Decomposition Strategies for Stochastic Elliptic Equations

Henri Gavin, Duke University
Constrained Optimal Control

Dmitry Kalika, Duke University
Adaptive Querying in ERP-based Brain-computer Interfaces Using Maximum Expected Discrimination Gain

Alicia Kim, University of California San Diego
M2DO: Multiscale Multiphysics Design Optimization

Varun Mallampalli, Duke University
Uncertainty and the Green Paradox

Vaishakhi Mayya, Duke University
The P300-based Brain-computer Interface as a Communication Channel with Memory

Matthew Norton, University of Florida
Maximization of AUC and Buffered AUC in Binary Classification

Clay Sanders, Duke University
PDE-Constrained Optimization for the Design of Acoustic Cloaks

Daniel Seidl, Sandia National Laboratories
Multiscale Interfaces for Large Scale Optimization

Matthew Zahr, Lawrence Berkeley National Laboratories
Efficient PDE-Constrained Optimization using Adaptive Model Reduction

Zilong Zou, Duke University
Local Sample-Based Approximations to Partial Differential Equations with Stochastic Parameters

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To Primate Center

To Chapel Hill
US 15-501 & I-40

To I-85

ERWIN ROAD

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RESEARCH DRIVE

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TRENT DRIVE

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OREGON STREET

CAMPUS DRIVE

SWIFT AVENUE

NINTH STREET

MAIN STREET

BROAD STREET

TO EAST CAMPUS

Geneen Auditorium
R. David Thomas Center
Fuqua School of Business
Law School (dining)
Gross Chemical Laboratory
French Science Center (under construction)
Biological Sciences
Physics and Math
Love Auditorium
Levine Science Research Center (dining)
Teer Engineering Library
New ROTC Air Force ROTC
North Bldg.
Hudson Hall Engineering School
CIEMAS
Bryan Research Bldg.
Cancer Research Bldg.
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Eye Center
Seeley Mudd Bldg.
Searle Center
Medical Bookstore
Duke Hospital North
VA Hospital
Brookwood Inn
P Hospital North Parking Deck
Tel-Com Bldg.
Perkins Addition (under construction)
Perkins Library (Main Library)
Political Sciences
Old Chemistry Bldg.
Foreign Language Bldg.
Davison Quad
Duke Hospital South
Davison Bldg.
Medical School
School of Nursing
Hanes House
John Hope Franklin Center
Trent Hall
Hospital South Parking Deck
Pickens Bldg.
Chapel
Divinity School
Yoh Chapel
Gray Bldg.
Registrar's Office
Student Service Center
Allen Bldg. Administration
English
Social Science Bldg.
Sociology/ Psychology Bldg.
Duke Student Health Bldg.
Zener Auditorium
Bryan University Center
Bookstore
Construction
Page Auditorium
Flowers Bldg.
Union Building (dining)
Kilgo Quad
Crowell Quad
Craven Quad
Few Quad
Few Quad
Wannamaker
West Campus Housing Office
The Loop
Duke Card Office
Great Hall Cambridge Inn
James B. Duke Statue
Bus Stop
Women's Center
Keohane Quad
McClendon Tower (dining)
Edens Quad
Shaefer House
Parking Information
Baseball Diamond
Sanford Institute (dining)
Koskinen Stadium
Schwartz-Butters Athletic Center
Cameron Indoor Stadium
Murray Bldg.
Yoh Football Ctr
Aquatic Center
Card Gym
Wilson Recreation Center
Intramural Bldg.
Indoor Outdoor Tennis Ctr
Sheffield Tennis Ctr
Duke TIP Parking
Duke TIP Parking
ENTER HERE FOR DUKE TIP PARKING
Duke University Road Parking Lot
Washington Duke Inn & Golf Club
Duke Gardens
Asiatic Arboretum
Rose Garden
Pergola
Fish Pond
Gardens Info
Doris Duke Center
Central Campus Apartments
Central Campus Pool
Central Campus Apartments
217
218
Undergraduate Admissions
Financial Aid
Latin American Studies
Student Loan Office
International House
Study Abroad
Duke Police
Devil's Den
Freeman Center for Jewish Life
Erwin Mill (Human Resources)
University Development
Alumni Affairs
Public Affairs
Demographic Studies
Asian/Pacific Studies Institute
Asian & African Languages
Nasher Art Museum
North
West
East
South

Map is not to scale

* Information Sessions at Page Auditorium (9:15 a.m. - 11:30 a.m.)

** Awards Ceremony at Cameron Indoor Stadium (1:30 p.m.)

Walking path between Cameron and Page

February 2006