Optimization Under Uncertainty and Data-Driven Science and Engineering

April 13-14, 2017
Ambassador Room, Washington Duke Inn
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and Data-Driven Science and Engineering
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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, TBA
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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and the planning committee: Wilkins Aquino, Robert Calderbank, Drew Kouri, Jianfeng Lu, Michael Zavlanos
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 "inequalities" 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 than 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 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
TBA

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 Exceedance (bPOE), a recently introduced quantification of uncertainty. bNP accounts for the severity of False Positives and False Negatives by utilizing two new performance metrics called the Buffered False Negative Rate (bFNR) and Buffered False Positive Rate (bFPR). A major advantage of bNP classification is that it is a convex (and sometimes even linear) programming
problem. We used regularization and considered a margin maximizing problem that shares strong connections with Support Vector Machines (SVM's). In particular, our formulation is amenable to the kernel trick for non-linear classification.

Genetha Gray, Intel Corporation
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 methodologies 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
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 Using 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 accommodate 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.