Linear and Non-Linear Mixed Integer Optimization
Poster Session Abstracts
Wednesday, March 1, 2023

The Maximum-Entropy Sampling Problem: Hardness and Solvable Cases

Hessa Al-Thani, University of Michigan

The maximum-entropy sampling problem (MESP) is an NP-Hard problem, where we aim to maximize a sub-determinant of some given matrix C. We present some cases where the MESP is efficiently solvable and compare our specialized algorithms performance against state of the art branch-and-bound algorithm that solves the MESP for the general case. In particular in the case where C is tridiagonal we have an exact algorithm that solves the MESP efficiently. We can use this algorithm in the case where C is not tridiagonal by applying a mask M to C and obtaining an upper-bound on the MESP. A mask is a correlation matrix that is intended to impose a certain structure on C, in our work we look at a tridiagonal M and at different choices of off-diagonal elements that minimize the upper-bound for the MESP.

Small Shadows of Lattice Polytopes

Alexander Black, UC Davis

For 75 years, the simplex method has remained one of the most popular methods for solving linear programs, yet much still remains mysterious about its performance. Geometrically, the simplex method optimizes a linear function by tracing a path on the oriented graph of a polyhedron, and the simplex method may only run quickly if this graph has small diameter. It is a fundamental open question to understand whether polyhedra are guaranteed to have polynomially bounded diameters. However, even in cases in which we know bounds on diameters, actually following such short paths with the simplex method has continued to be an additional challenge. My poster will cover a bit about my joint work with Jesús De Loera, Sean Kafer, and Laura Sanità on finding pivot rules for the simplex method guaranteed to match the theoretical best possible bound on diameters for 0/1-polytopes as well as my work on nearly matching the best known bounds for lattice polytopes.

A binary expansion approach for the water pump scheduling problem in large high altitude water distribution networks

Denise Cariaga Sandoval, University of Edinburgh

The water pump scheduling problem is an optimization model determining which water pumps will be turned on or off at each period. In this work, we tackle the optimal operation of the desalinated water system, with reservoirs and pumps that send water to mining companies at high altitudes. The optimization of this process faces several difficulties derived from i) the non-linearities of the friction loss equations along pipes and pumps and ii) many possible combinations of head pressure and flow that leads to high computational costs, which makes it an NP-Hard problem. These limitations prevent solving the problem in a reasonable computational time in water distribution networks with more than two pumps and tanks, as occurs in different networks worldwide. Therefore, in this work, we develop new optimization models of the pump scheduling problem using a binary expansion approach to tackle the non-linearities to minimize the systemic costs and the computational cost of the original MINLP. We tested these models in different network topologies and solved them with Julia and Gurobi.

Keywords: Water supply - Water distribution networks - Nonlinear Optimization

Generalized Scaling for the Constrained Maximum-Entropy Sampling Problem
Zhongzhu Chen, University of Michigan

The best techniques for the constrained maximum-entropy sampling problem, a discrete-optimization problem arising in the design of experiments, are via a variety of concave continuous relaxations of the objective function. A standard bound-enhancement technique in this context is \emph{scaling}. We extend this technique to \emph{generalized scaling}, we give mathematical results aimed at supporting algorithmic methods for computing optimal generalized scalings, and we give computational results demonstrating the usefulness of generalized scaling on benchmark problem instances.

Poisoning Attacks Against Linear Regression Models with Categorical Variables: a Mixed-Integer Nonlinear Bilevel Optimization Approach
Monse Guedes Ayala, University of Edinburgh

Machine Learning (ML) models have become a very powerful tool to extract useful information from large datasets and use it to make accurate predictions and automated decisions. However, ML models can be vulnerable to external attacks, causing them to underperform or to even fully deviate from their expected task. It is possible to anticipate and prepare for such events by designing strong attacks, which are later used for creating and testing defence strategies. One way to attack ML models is by injecting them with poisoning data to mislead the algorithm during the training phase. These problems are usually solved using gradient-based methods that do not explicitly optimize categorical variables. Instead, these variables are treated as numerical variables and then heuristically rounded to meet the binary structure of categorical features. In this paper we propose a poisoning attack for a ridge regression model containing both numerical and categorical variables and explicitly model and optimize categorical variables. We formulate the problem of designing poisoning attacks as a bilevel optimization that is quadratic mixed-integer on the upper-level and unconstrained convex quadratic on the lower-level (MIQP-QP). This poster outlines the mathematical formulation of the problem, introduce a single-level reformulation based on the Karush-Khun-Tucker (KKT) conditions of the lower-level, together with bounds for the lower-level variables that depend on the number of attacked

samples. We also present computational experiments on different datasets and discuss results.

Sculpting polytopes at the Hirsch bound
Fred B. Holt, T-Mobile

We present a set of tools - wedging, truncation, blending - with which we can create polytopes whose diameters are n-d.
Wedging produces slow edges, and once we have a sufficient number of slow edges, we can use blending to produce H-sharp polytopes for any number of facets n for fixed dimension d.
Blending at vertices we can produce H-sharp polytopes for all (d=8, n). Blending at simplex faces we produce H-sharp polytopes for all (d=7,n).

Polyhedral view of Neural Networks: Structure, Complexity and Algorithms
Sammy Khalife, Johns Hopkins University

The class of functions that are representable by linear threshold neural networks can be fully characterized, and two hidden layers are necessary and sufficient to represent any function in the class. This is a surprising result in the light of recent exact representability investigations for neural networks using other popular activation functions like rectified linear units. Nearly tight bounds on the depth and width of the neural networks can be derived using polyhedral combinatorics, as well as an algorithm to solve the empirical risk minimisation (ERM) problem to global optimality for these neural networks with a fixed architecture. The algorithm's running time is polynomial in the size of the data sample, if the input dimension and the size of the network architecture are considered fixed constants. This approach extends to a strict superclass of the rectified linear units (ReLU) neural networks, called shortcut linear threshold networks. These networks have several desirable theoretical properties. In particular, the ERM problem can also be solved to global optimality with a similar algorithm.

Polyhedral and Approximation Aspects of Feedback Vertex Set and PseudoForest Deletion
Shubhang Kulkarni, University of Illinois at Urbana Champaign

A feedback vertex set is a subset of vertices whose deletion makes the graph acyclic. FVS asks for a minimum cost feedback vertex set. A pseudoforest deletion set is a subset of vertices whose deletion ensures that each connected component contains at most one cycle. PFDS asks for a minimum cost pseudoforest deletion set. Both these problems are NP-hard. Approximation algorithms for these problems have relied on the local ratio technique which have subsequently led to primal-dual algorithms via LPs, but these LPs were not known to be solvable efficiently. In this poster, I will discuss polynomial time solvable LPs that achieve

The best possible approximation factor for both FVS and PFDS. I will also present the proof of an extreme point structural result for an associated polyhedra which naturally leads to an iterative-rounding based approximation algorithm.

Based on joint work with Karthekeyan Chandrasekaran, Chandra Chekuri, Samuel Fiorini, and Stefan Weltge.

New Results in the Global Minimization of Molecular Potential Energy Functions
Anatoliy Kuznetsov, Georgia Institute of Technology

Finding global energy minima for clusters of identical atoms is an important problem in chemical physics. In this work, we introduce novel convex relaxations and symmetry elimination constraints for minimization problems involving the Lennard-Jones potential, a common component of molecular potential energy functions. We demonstrate the impact of these techniques with numerical experiments using the Lennard-Jones energy minimization problem as a benchmark and discuss extensions of our results to other applications.

On the Partial Convexification for Low-Rank Spectral Optimization: Rank Bounds and An Effective Algorithm
Yongchun Li, Georgia Tech

The Low-rank Spectral Optimization Problem (LSOP) minimizes a linear objective function over multiple two-sided linear inequalities intersected with a low-rank spectral domain set. Many important problems such as matrix completion, fair PCA, and quadratically constrained quadratic programs fall into our proposed LSOP framework. Although the convexification of the LSOP feasible set, in general, is difficult, recent studies reveal that replacing the LSOP domain set with its convex hull can lead to promising tractable and high-quality relaxation, termed "LSOP-R". This motivates us to study the strength of LSOP-R. Specifically, we prove the rank upper bounds of an optimal solution of LSOP-R. Our rank bound results: (i) are independent of the domain set; (ii) can recover the well-known ones for two LSOP special cases in literature; and (iii) provide sufficient conditions about when LSOP-R yields the same optimal value as the original LSOP. To harvest the promising theoretical results, we develop an efficient column generation algorithm with a vector-based convex pricing oracle for solving LSOP-R, whose output optimal solution can achieve the same rank bounds. Our numerical results demonstrate the effectiveness of the proposed algorithm.

Shortest paths in graphs of convex sets
Tobia Marcucci, MIT

We present a novel modeling and computational framework for optimal decision making in circumstances where discrete and continuous choices have to be made simultaneously. In particular, we study directed graphs where the position of each vertex is a continuous variable constrained in a convex set, and the length of an edge is a convex function of the position of its endpoints. We call these Graphs of Convex Sets (GCS). Many classical problems in graph theory can be extended to GCS in a natural way, yielding a class of problems at the intersection of discrete and continuous optimization with a wide range of applications. For the solution of these problems, we present a unified framework that uses perspective operators to efficiently blend techniques from network-flow and convex optimization. In this poster, we will focus primarily on the shortest-path problem in GCS, and its applications to control and robotics.

Characterizing QUBO Reformulations of the Knapsack Problem and Applications to Quantum Computing.

Rodolfo Alexander Quintero Ospina, Lehigh University

It has been shown that quantum computers can outperform classical computers in solving some instances of NP-hard problems, for instance, the Graph partitioning problem, which motivates the use of quantum-based algorithms to solve applied combinatorial problems and more general integer programs. Many of such algorithms need a Quadratic Unconstrained Binary Optimization (QUBO) formulation of the problem, but, most of the literature regarding QUBO reformulations for constrained optimization problems (COPT) is centered around equality constrained problems, and in general, it is not suitable for problems with inequality constraints. Here, we start by focusing on the "simplest" inequality constrained problem, the knapsack problem (KP), and then consider more general integer programs and the algebraic-combinatorial theory needed to obtain exact QUBO reformulations. In particular, we derive different QUBO formulations for the KP and characterize the range of their associated penalty constants. As a byproduct, we correct some erroneous results regarding QUBO reformulations for the KP reported in the literature. Additionally, we show computational experiments in D-Wave where we benchmark different QUBO formulations for the maximum independent set problem.

Improving Relaxations in Linear Bilevel Optimization

Bárbara Rodrigues, University of Edinburgh

This poster is concerned with linear bilevel optimization problems and their single-level relaxations that are central to solution approaches. The High Point Relaxation (HPR) is the most common single-level relaxation but when it is unbounded, nothing can be concluded about the optimality status of the corresponding bilevel problem. We introduce a new linear optimization model to help detect whether or not the unboundedness of the HPR originates in unboundedness of the corresponding bilevel problem, and present a theorem giving sufficient conditions for bilevel boundedness. We also propose an alternative relaxation to the HPR, and show how it is an improvement on the HPR. Future work will study how to make use of lower-level dual information to further improve single-level relaxations.

Variable Selection for Kernel Two-Sample Tests

Jie Wang, Georgia Institute of Technology

We consider the variable selection problem for two-sample tests, aiming to select the most informative features to best distinguish samples from two groups. We propose a kernel maximum mean discrepancy (MMD) framework to solve this problem and further derive its equivalent mixed-integer programming formulations for linear, quadratic, and Gaussian types of kernel functions. Our proposed framework admits advantages of both computational efficiency and nice statistical properties: (i) A closed-form solution is provided for the linear kernel case. Despite NP-hardness, we provide an exact mixed-integer semi-definite programming formulation for the quadratic kernel case, which further motivates the development of exact and approximation algorithms. We propose a convex-concave procedure that finds critical points for the Gaussian kernel case. (ii) We provide non-asymptotic uncertainty quantification of our proposed formulation under null and alternative scenarios. Experimental results demonstrate good performance of our framework. (This is a joint work with Santanu S. Dey and Yao Xie, link at https://arxiv.org/abs/2302.07415)