
Industrial Mathematics
Mathématiques industrielles

(Org: **Huaxiong Huang** (York), **Michael Lamoureux** (Calgary) and/et **Odile Marcotte** (UQAM))

SEAN BOHUN, University of Ontario Institute of Technology

The Pixel Imaging Mass Spectrometer: towards reconstructing molecules

Pixel Imaging Mass Spectrometry is a new molecular imaging technique that relies on precision laser pulses to both align and strip molecules of their valence electrons thereby causing them to explode. The primary task of this experimental setup is the reconstruction of the disintegrated parent molecule through the systematic collection of the fragments of the explosion. The unique characteristics of the experimental setup provide an unprecedented resolution from other techniques. Experimentally obtained covariance maps reveal a partially hidden rich structure of the parent molecule and fragmentation dynamics. However, for larger molecules, the large number of fragment ions that are produced congest the the resulting time-of-flight spectrum and alternative strategies are required to resolve the structure of the parent molecule.

The underlying mathematical challenges of this problem that are unique to the pixel imaging mass spectrometer will be discussed, and a comparison of the forward model predictions with experimental data for the imaging of 3,5-dibromo-3',5'-difluoro-4'-cyanobiphenyl molecule will be presented. A brief survey of the established reconstruction methods for this type of problem will also be discussed.

MATT DAVISON, University of Western Ontario

Operations Research and Machine Learning combine to solve a Harbour Security Problem

I present a successful application which unites techniques in Operations Research and in Machine learning to attack a problem in national security: How to clear a harbour that has been seeded with naval mines by an adversary. An underwater autonomous vehicle equipped with a sidescan sonar is able to identify possible mine targets. Once identified, targets may be visited by divers for further investigation and, if necessary, disarming. However, the sidescan imaging process returns many false positive contacts that in fact may simply be rocks. As diver resources are scarce and expensive, and as time to clear the harbour is a factor, it makes sense to revisit targets from a different angle to better classify targets at the UAV imaging stage.

How best to do this represents both an interesting problem in data-driven classifier theory (what is the optimal angle relative to the first one for a second or third look at a target) and an interesting travelling salesman problem in a non-traditional space obtained by adjoining 2D spatial coordinates with a view angle coordinate.

I present collaborative work between my team and the Royal Canadian Navy in which we use a unique dataset of sonar images of various real and simulated mine targets and rocks together with operational characteristics of real UAV vehicles to solve both problems.

I discuss the need for increased emphasis on game theory for the analytics toolbox, both for security problems such as this and for more traditional business analytics problems in credit scoring etc.

WENYUAN LIAO, University of Calgary

A Helmholtz-decomposition based numerical method for Elastic wavefield separation

In an elastic migration or inversion problem, the P and S waves are treated separately, thus efficient numerical solver is required to compute P and S wavefields. Direct solution of an Elastic wave equation is computationally costly, as it is a coupled system of partial differential equations (PDE). Numerical solution of such model is of great interests to both Mathematicians and Geophysicists working on a variety of applications, geophysical exploration for instance. In particular numerical modeling of Elastic wave equation is an integral part of full waveform inversion and other wave equation based seismic inversion methods. Here we propose a new method, in which we first use the Helmholtz decomposition to decouple the Elastic wave equation system into four scalar acoustic wave equations, which are then efficiently solved by compact higher-order finite difference

method with high accuracy. Some novel boundary treatments have been developed for the new equations. The numerical solution of the Elastic wave equation is reconstructed from the previously obtained numerical solutions of the four scalar PDEs. Finally numerical examples are solved to demonstrate the efficiency and effectiveness of the newly proposed numerical method.

OSCAR LOPEZ, University of British Columbia

Off-the-Grid Low-Rank Matrix Recovery: Seismic Data Reconstruction

This talk discusses a modified low-rank matrix recovery work-flow that admits unstructured observations. By incorporating a regularization operator which accurately maps structured data to unstructured data, into the nuclear-norm minimization problem, this approach is able to compensate for data irregularity. Furthermore, by construction this formulation yields output that is supported on a structured grid. Recovery error bounds are established for the methodology with matrix sensing and matrix completion numerical experiments including applications to seismic trace interpolation to demonstrate the potential of the approach.

PAUL MCNICHOLAS, McMaster

ARIAN NOVRUZI, University of Ottawa

Modeling, shape analysis and computation of the equilibrium pore shape near a PEM-PEM intersection

We study the equilibrium shape of an interface that represents the lateral boundary of a pore channel embedded in an elastomer. The model representing this phenomena consists of a system of PDEs, comprising a linear elasticity equation for displacements within the elastomer and a nonlinear Poisson equation for the electric potential within the channel (filled with protons and water). To determine the equilibrium interface, a variational approach is employed. We analyze: (i) the existence and uniqueness of the electrical potential, (ii) the shape derivatives of state variables and (iii) the shape differentiability of the corresponding energy and the corresponding Euler-Lagrange equation. The latter leads to a modified Young-Laplace equation on the interface. This modified equation is compared with the classical Young-Laplace equation by computing several equilibrium shapes, using a fixed point algorithm.

VAHKTANG POUTKARADZE, Alberta

ANTHONY WARE, University of Calgary

Energy market modelling and asset valuation: two industry projects

This talk (presented with Matthew Couch) will give an overview of two projects we have conducted with TransAlta Corp., and we will discuss the challenges and opportunities we have encountered in applying mathematical models to real-world problems.

The first project involved the development of stochastic models for natural gas and power prices in the Pacific North West (PacNW) market, for the purpose of derivative valuation. The PacNW options markets are fairly illiquid, thus the available implied volatility data are limited, and so do not necessarily provide a meaningful measure of price uncertainty. This lack of reliable implied volatility data, combined with the complex nature of power prices, motivates the need for models driven by market fundamentals. In order to capture as much market information as possible while retaining tractability, hybrid pricing models in the style of Coulon, Powell and Sircar (2013) and - more generally - Carmona and Coulon (2014) were chosen. The large impact of hydroelectric generation on the PacNW market required significant revisions to their framework.

The second project was concerned with maximizing the long-term value of hydropower generation in the face of uncertain reservoir inflows, potentially variable constraints on outflows, and possibly wildly varying power prices. We present a stochastic dynamic programming approach to the quantification of reservoir reliability (for example, measures of the risk of over-topping

the reservoir or failing to satisfy downstream flow requirements) and a related approach to determining the reservoir flow strategy that maximizes expected revenue, subject to defined target reliability levels

HONGMEI ZHU, York University

Noise Analysis

Noise generally refers to the undesirable part of a signal. However, analyzing noise may reveal hidden information that is useful to monitor operational conditions of a device. For instance, signals routinely acquired from in-core flux detectors in CANDU reactors contain noise, namely, neutron noise. In this talk, we analyze neutron noise using time-frequency techniques. Our findings suggest that neutron noise can measure combined mechanical vibrations from nearby fuel channels. It indicates the potential of using the neutron noise analysis technique to exact vibrating frequencies of fuel channels and to indirectly monitor the operational conditions within a CANDU reactor core.

This is a joint work with Cheng Liu and Andrew C. Wallace, Department of Materials and Major Components, Kinectrics Inc.