Workshop Report 21w5167 Optimization under Uncertainty: Learning and Decision Making in 2021

held virtually Feb 8 - 12 hosted by the Banff International Research Station for Mathematical Innovation and Discovery (BIRS)

Johannes Royset* Lars Ruthotto† Claudia Schillings‡
Thomas M. Surowiec§

January 26, 2023

Subject Area: Control/Optimization
AMS subject code 49J20, 49J55

1 Overview

This workshop brought together researchers in optimization under uncertainty and uncertainty quantification, whose work stands to benefit from cutting-edge machine learning techniques for data-driven differential equations. The workshop focused on mathematical challenges at the interface of applied mathematics, optimization, probability and statistics, and machine learning. Through eleven scientific talks, three panel discussions, and unstructured interactions, the workshop facilitated an exchange of ideas towards new, powerful methods for optimization under uncertainty.

In what follows, we give an overview of the presentations, discussions, and outcomes.

2 Presentations

- **Darinka Dentcheva:** *Subregular Recourse in Multistage Stochastic Optimization*
- **Guzin Bayraksan:** *Data-driven sample average approximation with covariate information*
- **Drew Kouri:** *A primal-dual algorithm for large-scale risk minimization*
- **Youssef Marzouk:** *Transport methods for likelihood-free inference and data assimilation*
- **Georg Stadler:** *Optimal control of PDEs under uncertainty with joint chance state constraints*
- **Peng Chen:** *Taylor approximation for PDE and chance constrained optimization under uncertainty*
- **Bamdad Hosseini:** *Conditional Sampling with Monotone GANs: Modifying Generative Models to Solve Inverse Problems*

*Operations Research Department, Naval Postgraduate School, Monterey, CA, USA joroyset@nps.edu
†Department of Mathematics and Computer Science Emory University Atlanta, GA, USA lruthotto@emory.edu
‡Universität Mannheim, Institut für Mathematik, Germany, c.schillings@uni-mannheim.de
§FB Mathematik und Informatik, Philipps-Universität Marburg, Germany surowiec@mathematik.uni-marburg.de

- **Bodhisattva Sen:** *Nonparametric maximum likelihood estimation in heteroscedastic mixture models: density estimation, denoising and deconvolution*
- **Masoumeh Dashti:** *Posterior consistency in Bayesian inference with exponential priors*
- **Philip Thompson** *Robust Regression*
- **Bart van Bloemen Waanders:** *Hyper-differential sensitivity analysis for control under uncertainty of aerospace vehicles*
- **Elizabeth Newman:** *Train Like a (VarPro): Efficient Training of Neural Networks with Variable Projection*

3 Panel Discussions

- **Computational Methods** The panel discussed current developments and challenges in computational methods for optimization under uncertainty. This includes methods used in machine learning, stochastic programming, PDE-constrained optimization under uncertainty, and inverse problems in uncertainty quantification. The panel addressed questions related to the ideal methods for a given field, how to treat uncertainty in practice, and give some insight on the interpretation of solutions.

  Panelists: Darinka Dentcheva, Güzin Bayraksan, Drew P. Kouri, Suvrajeet Sen. (Online)

  Moderator: Thomas Surowiec

- **PDEs and Machine Learning**

  The panel discussed current developments at the interface of machine learning and partial differential equations (PDE). Recent years have seen increased activity in this area including new machine learning approaches using PDE techniques and machine learning approaches for solving PDE problems. The panel discussed research potential, possible pitfalls, and the impact of those activities on education and training.

  Panelists: Peng Chen, Bamdad Hosseini, Georg Stadler

  Moderator: Lars Ruthotto

- **Statistical Learning in the Context of Shape Constraints, Model Information and Rare Events**

  The panel discussed the role of non-data information about a random phenomenon and how such information can improve predications as well as enable extrapolate beyond the range of available data. Through concrete examples, the panel identified situations in which non-data information can easily be combined with data in statistical (learning) models. The panel also discussed emerging challenges and take questions from the audience.

  Panelists: Omar Ghattas, Youssef M Marzouk, Bodhi Sen

  Moderator: Johannes Royset

4 Outcomes of the Meeting

The major themes of the talks were theory, algorithms, and computational methods for optimization and optimal control problems of ever-increasing complexity, for example, in optimization problems governed by systems of nonlinear differential equations subject to random inputs. The activities underscored several open challenges in this field. For example, the mathematical understanding of machine learning techniques for the approximation of high or infinite dimensional systems and its consequences for optimization under uncertainty is still in its infancy. Also, the incorporation of uncertainties in the optimization of complex systems typically results in high or even infinite dimensional problems in terms of the uncertain parameters as well as the optimization variables. In his talk, van Bloemen Waanders

discussed how to use hyper-differential sensitivity analysis to optimally control a partially known and uncertain system [4].

Another theme of the talks were machine learning methods for solving inverse problems and numerical optimization methods for training deep neural networks. The talks by Marzouk and Hosseini presented new data-driven techniques for solving inverse problems that leverage measure transport and Generative Adversarial Networks (GAN); see [1] and [2] respectively. Newman's talk presented a numerical optimization scheme that improves deep neural network training by exploiting the separable structure provided by most architectures [3]. The panel discussion on PDEs and deep learning highlighted how optimization under uncertainty can benefit from and contribute to the field of machine learning. The discussion also exposed entry barriers for mathematicians in the area of deep learning (e.g., the large translation effort required to read and compare the literature between these fields) and resources that help overcome them.

5 Takeaways from the Virtual Format

Due to the pandemic the workshop was held in a fully virtual format. Although no virtual environment can be compared to an on-site workshop in Banff, the BIRS staff provided excellent support that allowed us to retain many of the key features. For the duration of the workshop, participants could meet in a virtual environment that featured different meeting rooms, lounges, and a main room. The virtual environment was helpful to enable networking and collaboration through screen shares and whiteboards. Talks and panel discussions were held using conference calls and most talks were live streamed to the BIRS website. The program was reduced to accommodate all participants that were scattered across at least nine time zones. An advantage of the virtual format was that more researchers than initially planned could be invited to the program, regardless of space limitations, visa status, travel funding, and family obligations. In particular, a number of early career researchers and graduate students were able to attend the meeting and profit from the lively discussions and presentations on cutting edge research topics.

References

[1] R. Baptista, O. Zahm, and Y. Marzouk. An adaptive transport framework for joint and conditional density estimation. *arXiv preprint arXiv:2009.10303*, 2020.

[2] N. Kovachki, R. Baptista, B. Hosseini, and Y. Marzouk. Conditional sampling with monotone GANs. *arXiv preprint arXiv:2006.06755*, 2020.

[3] E. Newman, L. Ruthotto, J. Hart, and B. van Bloemen Waanders. Train Like a (Var)Pro: Efficient Training of Neural Networks with Variable Projection. *arXiv.org*, July 2020.

[4] I. Sunseri, J. Hart, B. van Bloemen Waanders, and A. Alexanderian. Hyper-differential sensitivity analysis for inverse problems constrained by partial differential equations. *Inverse Problems*, 36(12): 125001, 2020.