Mathematical Foundations & Methodologies for Artificial Intelligence & Data-Driven Scientific Computing
Workshop on Mathematical Approaches to Modern AI Challenges
Abstracts

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Abstracts

TBA

Richard Baraniuk
Rice University, USA

Pending

Rigorous Model-Constrained Scientific Machine Learning for Digital Twins: A Computational Mathematics Perspective

Tan Bui-Thanh
The University of Texas at Austin, USA

Digital twins (DTs) are high-fidelity virtual representations of physical systems and processes. At their foundation lie mathematical and physical models that describe system behavior across multiple spatial and temporal scales. A central purpose of DTs is to enable "what-if" analyses through hypothetical simulations, supporting lifecycle monitoring, parameter calibration against observational data, and systematic uncertainty quantification (UQ). For DTs to serve as a reliable basis for real-time forecasting, optimization, and decision-making, they must reconcile two traditionally competing requirements: mathematical rigor and physical fidelity, and computational efficiency at scale. This has motivated a new generation of approaches that combine classical tools from numerical analysis, partial differential equations, inverse problems, and optimization with the expressive power of Scientific Machine Learning (SciML). In this talk, I will outline a principled pathway from traditional computational mathematics to rigorously grounded SciML. I will then present recent Scientific Deep Learning (SciDL) methods for forward modeling, inverse and calibration problems, and uncertainty quantification, emphasizing mathematical structure, stability, and generalization. Both theoretical results and numerical demonstrations will be shown for representative problems governed by transport, heat, Burgers, Euler (including transonic and hypersonic regimes), and Navier–Stokes equations.

TBA

Won Chang
Seoul National University, S. Korea

Pending

Learning Rates, Restart and Adaptive Acceleration

Alexandre d'Aspermont
Ecole Normale Supérieure, France

We study restart schemes in stochastic optimization problems where the function to minimize is weakly convex and satisfies a Kurdyka-Lojasiewicz inequality. We show that the combination of restarts and KL inequalities yields improved rates of convergence, with acceleration depending explicitly on the KL exponent. Furthermore, optimal restart schemes on SGD define an explicit learning rate schedule akin to Polyak steps. While none of the regularity constants are observed in practice, we prove that restart schemes tend to be robust to a significant misspecification of these constants. We detail numerical experiments on both toy problems where the KL exponent is controlled and LLMs.

Joint work with Ali Elhishi and Christophe Roux

On Preventing Model Collapse in Generative Models

Bahman Gharesifard
Queen's University, Canada

Recursive training on synthetic data can lead to model collapse, a degenerative feedback loop in which models progressively lose information about the underlying data distribution. Incorporating fresh human-generated data alongside synthetic data offers a natural way to mitigate this risk. In this talk, I use a simple generative model to establish theoretical guarantees for the minimum rate of human data needed to prevent model collapse under recursive training. In particular, I characterize the human-to-synthetic data ratio required to maintain training stability by leveraging the information-geometric structure of the probability simplex and analyzing the resulting dynamics under the Fisher-Rao metric.

Optimized Relevance Networks for AI

Alfred Hero

University of Michigan, USA

Optimized relevance networks are probabilistic graphical models optimized for quantifying statistical dependency patterns between multiple covariates. They have been incorporated into AI to reveal groups of influential variables and to identify sources of algorithmic bias. Certain types of structural constraints on relevance network inference can facilitate computation, reduce sample complexity, reflect physical generative mechanisms, or penalize undesirable properties of the model. We will describe how such structural constraints can be used for parsimonious relevance network representation in multiway (spatio-temporal) analysis and in clustering with algorithmic fairness guarantees.

TBA

Tara Javidi

University of Califonia, San Diego, USA

Pending

Sobolev IPM with Graph Metric: Regularization, Scalability, and Applications

Tam Le

The Institute of Statistical Mathematics, Japan

We study the Sobolev IPM problem for probability measures supported on a graph metric space. Sobolev IPM is an important instance of integral probability metrics (IPM), and is obtained by constraining a critic function within a unit ball defined by the Sobolev norm. Particularly, it has been used to compare measures and is crucial for several theoretical works in machine learning. However, there are no efficient algorithmic approaches to compute Sobolev IPM effectively, which hinders its practical applications. We establish a relation between Sobolev norm and weighted Lp-norm, and leverage it to propose a novel regularization for Sobolev IPM. By exploiting the underlying graph structure, we demonstrate that the regularized Sobolev IPM provides a closed-form expression for fast computation. This advancement addresses long-standing computational challenges, and paves the way to apply Sobolev IPM for large-scale applications. Moreover, building upon the insights of tree systems, we

further introduce tree-sliced Sobolev IPM (TS-Sobolev), a tree-sliced metric that aggregates regularized Sobolev IPMs over random tree systems for applications with measures on Euclidean spaces or hyperspheres. Notably, TS-Sobolev admits the tree-sliced Wasserstein (TSW) as its special case. We empirically evaluate the proposed approaches on various tasks, e.g., document classification and topological data analysis for graph-based measures; as well as gradient flows, self-supervised learning, generative modeling, and text topic modeling for measures on Euclidean spaces and hyperspheres.

Nipping the Butterfly Effect in the Bud: Self-Output Fine-Tuning for Autoregressive Weather Prediction

Hsuan-Tien Lin

National Taiwan University, Taipei

Long-horizon weather forecasting is a fundamental challenge in atmospheric science, for which autoregressive Deep Learning Weather Prediction (DLWP) has emerged as the primary paradigm. Although the autoregressive pipeline is highly scalable and flexible, its prediction errors grow rapidly over long forecasting horizons. In this work, we study this error growth phenomenon from both theoretical and empirical perspectives. Our analysis reveals that the growth is driven by a feedback loop between output errors and input distribution shifts. Specifically, the autoregressive process amplifies small initial output errors, which progressively corrupt subsequent input distributions, echoing the butterfly effect in atmospheric science and ultimately deteriorating forecasting accuracy over longer horizons. Furthermore, we show that this distributional shift originates at the earliest stage of inference, with out-of-distribution signatures detectable as early as the first autoregressive step. To mitigate this issue, we propose Self-Output Fine-Tuning (SOFT), a plug-and-play strategy that leverages the model's own one-step predictions to calibrate the biased input distribution encountered at the first step. Extensive experiments demonstrate that, despite its simplicity, SOFT achieves state-of-the-art performance on long-horizon forecasting tasks and substantially reduces both prediction errors and distributional discrepancy. The empirical success of SOFT highlights the importance of reexamining the fundamental pipeline of atmospheric science, representing a critical pipeline advance for atmospheric science.

Instances where Compositional Structure Helps Avoid the Curse of Dimensionality

Mauro Maggioni

Johns Hopkins University, USA

I will discuss instances of multiple problems where function composition can be exploited in statistical models in order to obtain efficient estimators, implemented by efficient algorithms, that avoid the curse of dimensionality:

1. a model of high-dimensional functions that depend only on the projection of the data on a low-dimensional manifold, for which we construct estimators that, under suitable assumptions, provably defeat the statistical and computational curse of dimensionality, and achieve nearly optimal learning rates.

2. the problem of estimating interaction laws in stochastic systems of interacting particles given trajectories, where again considering compositional structure imposed by modeling and symmetries allows one to provably avoid the curse of dimensionality.

3. an application of deep learning in the context of digital twins in cardiology, and in particular the use of operator learning architectures for predicting solutions of parametric PDEs, or functionals thereof, on a family of diffeomorphic domains — the patient-specific hearts – which we apply to the prediction of medically relevant electrophysiological features of heart digital twins.

4. recently-introduced Multiscale Markov Decision Processes (MDPs) in Reinforcement Learning, which enable the efficient solution of Markov Decision Processes (MDPs), where scales represent MDPs at different levels of abstraction, that also provide highly transferable skills to new MDPs (via compositionally).

Numerical Approximation for McKean-Vlasov SDE with Super-linear Growth Coefficients

Hoang Long Ngo

Hanoi National University of Education, Vietnam

We consider the numerical approximation for McKean-Vlasov stochastic differential equations driven by Lévy processes. We propose a tamed-adaptive Euler-Maruyama scheme and consider its strong convergence in both finite and infinite time horizons when applied to certain classes of Lévy-driven McKean-Vlasov stochastic differential equations with non-globally Lipschitz-continuous, super-linear-growth drift and diffusion coefficients.

TBA

Thanh Bình Nguyn
University of Science - VNUHCM, Vietnam

Pending

Tutorial TBA

Tan Minh Nguyen
National University of Singapore, Singapore

Pending

TBA

Tien Trinh Nguyen
Shanghai Jiao Tong University, China

Pending

TBA

Kannan Ramchandran
University of California, Berkeley, USA

Pending

TBA

Robin Walters
Northeastern University, USA

Pending

TBA

Melanie Weber
Harvard University, USA

Pending