Theory and applications of scientific machine learning
Théorie et applications de l'apprentissage automatique scientifique
(Org: **Emmanuel Lorin** (Carleton University) and/et **Sophie Morin** (Polytechnique Montréal))

MATHIEU BAZINET, Université Laval
Introduction to PAC-Bayes theory and its applications

Introduced in 1998 by David A. McAllester, PAC-Bayes theory has found an important place in the field of statistical learning theory. Given a stochastic predictor or a majority vote, PAC-Bayes provides high-probability tail bounds on the true risk of the model. The seminal works of Dziugaite and Roy (2017) and Pérez-Ortiz et al. (2021) demonstrated that it was possible to achieve tight generalization bounds for deep neural networks. This talk aims to be an introduction to PAC-Bayes theory, starting from the basic definitions and building up to the proof of a PAC-Bayesian bound. We will finish this talk with some applications of this framework.

MOHAMMED NYUYDINI KIVEN, Memorial University of Newfoundland
VARIATIONAL MOVING MESH METHODS FOR DIFFERENTIABLE NUMERICAL SOLVERS

Moving mesh methods for partial differential equations (PDEs) are a class of adaptive schemes aiming to optimize accuracy with a fixed number of degrees of freedom by allowing the spatial domain to transform with the solution. Optimal mesh transformations can often require nonlinear equations, even for linear problems, introducing significant computational overhead. Concessions to the mesh optimality can compromise the advantages of these approaches. In this work, we introduce a mesh adaptation strategy leveraging an automatically differentiable moving mesh solver to define schemes which depends on the continuous PDE and its discretization directly. Differentiating through the solver allows for the definition of novel schemes which are parsimonious in their design and exhibit orders of magnitude higher accuracy compared to standard r-adaptive monitor functions. We describe two numerical schemes: (i) using an a posteriori error indicator based on a reference solution, and (ii) a self-supervised scheme based on a prescribed mesh quality function and a parametric mesh transformation. Our methods are applied to several partial differential equations where we study their numerical properties and accuracy benefits.

EMMANUEL LORIN, Carleton University
Informed Normalized Gradient Flow Method for Point Spectrum in Spectral Gaps: Application to Edge-State Computation

This presentation is devoted to the derivation of a physics-informed normalized gradient flow method for the computation of eigenvalues in spectral gaps, namely eigenvalues located between two continuous spectra. We present a mathematical analysis of the algorithm together with numerical experiments in the context of edge-state computation in photonic graphene.

SOPHIE MORIN, Polytechnique Montréal
Conditioning and equivariance in a contact detection problem

In several areas of physical science and engineering involving systems of hard or elastic objects, an essential computational task is to detect contacts and to compute contact forces between objects that are in contact. This is generally done in simulations, for instance via the Discrete Element Method, by allowing the objects to overlap slightly and then computing the elastic force from the overlap distance.

However, given two objects parametrized by relative position, orientation, and relevant shape parameters, the problem of computing the signed distance between them is generally ill-conditioned, and a closed form is unavailable for all but the simplest object geometries. The problem is surprisingly subtle even for ellipses in the plane, creating a nontrivial computational bottleneck for high-precision simulations.

We will discuss ongoing computational and theoretical investigations into this problem from the perspective of equivariant machine learning, focusing on fundamental issues in the application of neural networks to this kind of ill-conditioned problem.

ABANI PATRA, Tufts University, Medford, MA
Neural Operators and Complicated Structures Modeling/ Virtual Sensing

In this talk we will briefly discuss the use of neural operator-based strategies for complex offshore structure models. Significant adaptations are needed to model issues associated with simple loss functions and complicated operating conditions. Discretization errors and errors die to low frequency biases are prevalent and need new strategies to correct.