

# HKUST-KAIST-NUS Joint Workshop in Applied and Computational Mathematics

## Program

24 April 2023, Monday	
Morning Session	
09:00 – 09:10	Opening
09:10 – 09:45	<b>Speaker:</b> Prof. Kim Chuan TOH, NUS <b>Title:</b> An Augmented Lagrangian Method with Constraint Generation for Shape-constrained Convex Regression Problems
09:45 – 11:00	Break (Fire Drill 2023, 10:00 – 10:45 am. Campus tour if possible)
11:00 – 11:35	<b>Speaker:</b> Prof. Chang-Ock LEE, KAIST <b>Title:</b> Individual Tooth Segmentation in Human Teeth Images Using Pseudo Edge-Region Obtained by Deep Neural Networks
11:35 – 12:10	<b>Speaker:</b> Prof. Jianfeng CAI, HKUST <b>Title:</b> Provable Sample-Efficient Sparse Phase Retrieval Initialized by Truncated Power Method
12:10 – 14:00	Lunch
Afternoon Session	
14:00 – 14:35	<b>Speaker:</b> Prof. Yang XIANG, HKUST <b>Title:</b> Deep Operator-Splitting Network for Solving PDEs
14:35 – 15:10	<b>Speaker:</b> Prof. Yeonjong SHIN, KAIST <b>Title:</b> Towards Trustworthy Scientific Machine Learning: Theory, Algorithms, and Applications
15:10 – 15:40	Tea Break
15:40 – 16:15	<b>Speaker:</b> Prof. Weiqing REN, NUS <b>Title:</b> Learning committor function and invariant distribution for randomly perturbed dynamical systems
16:15 – 16:50	<b>Speaker:</b> Prof. Jaekyoung KIM, KAIST <b>Title:</b> Analysis of dynamic data: from molecule to behavior
16:50 – 17:25	<b>Speaker:</b> Prof. Donghwan KIM, KAIST <b>Title:</b> Two-timescale extragradient converges to local minimax points
18:30 -	Banquet
25 April 2023, Tuesday	
Morning Session	
09:00 – 09:35	<b>Speaker:</b> Prof. Mikyung LIM, KAIST <b>Title:</b> Inversion Formula for a Planar Conductivity Inclusion
09:35 – 10:10	<b>Speaker:</b> Prof. Hai ZHANG, HKUST <b>Title:</b> Mathematics of In-gap Interface Modes in Photonic/Phononic Structures
10:10 – 10:40	Tea Break
10:40 – 11:15	<b>Speaker:</b> Prof. Shingyu LEUNG, HKUST <b>Title:</b> Spherical Essentially Non-Oscillatory (SENO) Interpolation
11:15 – 11:50	<b>Speaker:</b> Prof. Zhenning CAI, NUS <b>Title:</b> The Entropic and Moment-preserving Spectral Method for the Boltzmann Equation
12:00 -	Lunch
Afternoon Session	
14:00 – 18:00	Free Discussion
18:30 -	Dinner
26 April 2023, Wednesday	
Morning Session	
09:00 – 09:35	<b>Speaker:</b> Prof. Yuan YAO, HKUST <b>Title:</b> Robust Statistical Learning and Generative Adversarial Networks
09:35 – 10:10	<b>Speaker:</b> Prof. Subhroshekhar GHOSH, NUS <b>Title:</b> Learning under Latent Symmetries: Sparse Multi-reference Alignment, Phase Retrieval, and Uncertainty Principles
10:10 – 10:45	<b>Speaker:</b> Dr. Junsuh PARK, KAIST <b>Title:</b> A Non-intrusive Bi-fidelity Reduced Basis Method for Time-Independent Problems
10:45 – 12:00	Tea Break/ Free Discussion
12:00 -	Lunch [End of the Joint Workshop]

## Abstract

### Speakers from HKUST

#### 1. Provable Sample-Efficient Sparse Phase Retrieval Initialized by Truncated Power Method

Prof Jianfeng CAI

We investigate the sparse phase retrieval problem, which involves recovering an  $s$ -sparse signal of length  $n$  using  $m$  magnitude-only measurements. Recently, two-stage non-convex approaches have gained considerable interest due to their provable linear convergence towards the underlying solution when properly initialized, despite their non-convex nature. However, the sample complexity of these algorithms is often constrained by the initialization stage. Commonly, spectral initialization is employed in the initialization stage, which necessitates  $m = O(s^2 \log n)$  measurements to generate a suitable initial guess. This results in a total sample complexity that is order-wisely higher than necessary. To decrease the required number of measurements, we introduce a truncated power method as a substitute for spectral initialization in non-convex sparse phase retrieval algorithms. We prove that  $m = O(ss*s*\log n)$  measurements, with  $ss$  representing the stable sparsity of the underlying signal, are adequate for generating a desired initial guess. In cases where the underlying signal consists of only a few significant components, our proposed algorithm achieves an optimal sample complexity of  $m = O(s \log n)$ . Numerical experiments further validate the enhanced sample efficiency of our method compared to existing state-of-the-art algorithms.

#### 2. Deep Operator-Splitting Network for Solving PDEs

Prof Yang XIANG

Deep neural networks (DNNs) recently emerged as a promising tool for analyzing and solving complex differential equations arising in science and engineering applications. Alternative to traditional numerical schemes, learning based solvers utilize the representation power of DNNs to approximate the input-output relations in an automated manner. However, the lack of physics-in-the-loop often makes it difficult to construct a neural network solver that simultaneously achieves high accuracy, low computational burden, and interpretability. In this work, focusing on a class of evolutionary PDEs characterized by decomposable operators, we show that the classical "operator splitting" technique can be adapted to design neural network architectures. This gives rise to a learning-based PDE solver, which we name Deep Operator-Splitting Network (DOSnet). Such non-black-box network design is constructed from the physical rules and operators governing the underlying dynamics, and is more efficient and flexible than the classical numerical schemes and standard DNNs. To demonstrate the advantages of our new AI-enhanced PDE solver, we train and validate it on several types of operator-decomposable differential equations. We also apply DOSnet to nonlinear Schrodinger equations which have important applications in the signal processing for modern optical fiber transmission systems, and experimental results show that our model has better accuracy and lower computational complexity than numerical schemes and the baseline DNNs.

#### 3. Mathematics of In-gap Interface Modes in Photonic/Phononic Structures

Prof Hai ZHANG

The developments of topological insulators have provided a new avenue of creating interface modes (or edge modes) in photonic/phononic structures. Such created modes have a distinct property of being topologically protected and are stable with respect to perturbations in certain classes. In this talk, we will report recent results on the existence of a in-gap interface mode that is bifurcated from a Dirac point in a photonic/phononic structure. Both one-dimensional and two-dimensional structures will be addressed.

#### 4. Spherical Essentially Non-Oscillatory (SENO) Interpolation

Prof Shingyu LEUNG

We present two new methods for interpolation on the sphere  $\mathbb{S}^2$ . The first method is called the Spherical Interpolation of order  $n$  (SIDER- $n$ ), which is a simple interpolation technique that produces a  $C^n$  interpolant when  $n \geq 2$ . This method is based on the Bezier curves developed for  $\mathbb{R}^3$ . In the second part, we introduce a new method called Spherical Essentially Non-Oscillatory (SENO) interpolation, which incorporates the ENO philosophy. This method is useful for interpolating curves on  $\mathbb{S}^2$  that have kinks or sharp discontinuities in their higher derivatives. It can reduce spurious oscillations in high-order reconstructions. We provide several examples to demonstrate the accuracy and effectiveness of these methods.

#### 5. Robust Statistical Learning and Generative Adversarial Networks

Prof Yuan YAO

Robust learning under Huber's contamination model has become an important topic in statistics and theoretical computer science. Statistically optimal procedures such as Tukey's median and other estimators based on depth functions are impractical because of their computational intractability. In this talk, we present an intriguing connection between f-GANs and various depth functions through the lens of f-Learning. Similar to the derivation of f-GANs, we show that these depth functions that lead to statistically optimal robust estimators can all be viewed as variational lower bounds of the total variation distance in the framework of f-Learning. This connection opens the door of computing robust estimators using tools developed for training GANs. In particular, we show in both theory and experiments that some appropriate structures of discriminator networks with hidden layers in GANs lead to statistically optimal robust location estimators for both Gaussian distribution and general elliptical distributions where first moment may not exist. Some applications are discussed on robust denoising of Cryo-EM images.

# HKUST-KAIST-NUS Joint Workshop in Applied and Computational Mathematics

## Speakers from KAIST

### 1. Individual Tooth Segmentation in Human Teeth Images Using Pseudo Edge-Region Obtained by Deep Neural Networks

Prof. Chang-Ock LEE

In human teeth images taken outside the oral cavity with a general optical camera, it is difficult to segment individual tooth due to common obstacles such as weak edges, intensity inhomogeneities and strong light reflections. In this talk, we propose a method for segmenting individual tooth in human teeth images. The key to this method is to obtain pseudo edge-region using deep neural networks. After an additional step to obtain initial contours for each tooth region, the individual tooth is segmented by applying active contour models. We also present a strategy using existing model-based methods for labeling the data required for neural network training.

### 2. Towards Trustworthy Scientific Machine Learning: Theory, Algorithms, and Applications

Prof. Yeonjong SHIN

Machine learning (ML) has achieved unprecedented empirical success in diverse applications. It now has been applied to solve scientific problems, which has become an emerging field, Scientific Machine Learning (SciML). Many ML techniques, however, are very complex and sophisticated, commonly requiring many trial-and-error and tricks. These result in a lack of robustness and interpretability, which are critical factors for scientific applications. This talk centers around mathematical approaches for SciML, promoting trustworthiness. The first part is about how to embed physics into neural networks (NNs). I will present a general framework for designing NNs that obey the first and second laws of thermodynamics. The framework not only provides flexible ways of leveraging available physics information but also results in expressive NN architectures. The second part is about the training of NNs, one of the biggest challenges in ML. I will present an efficient training method for NNs - Active Neuron Least Squares (ANLS). ANLS is developed from the insight gained from the analysis of gradient descent training.

### 3. Analysis of Dynamic Data: from Molecule to Behavior

Prof. Jaekyoung KIM

Due to the advances in experimental technique and wearable devices, dynamic time-series data of molecules to human behavior can be easily measured. In this talk, I will talk about how to use mathematical modeling and theory to infer information underlying time-series data. Specifically, I will talk about the inference of regulatory interactions among molecules from time-series. Furthermore, I will also discuss about the inference of sleep pressure, circadian rhythms, and alertness of human from timeseries data measured by smart watch.

### 4. Two-timescale Extragradient Converges to Local Minimax Points

Prof. Donghwan KIM

We show that two-timescale extragradient converges to local minimax points without a nondegeneracy condition on the Hessian with respect to the maximization variable. We then prove that it avoids strict non-minimax points, almost surely with random initialization.

### 5. Inversion Formula for A Planar Conductivity Inclusion

Prof. Mikyoung LIM

The problem of determining electrical conductivity throughout a domain from measurements, often called Calderon's inverse conductivity problem, has been a subject of interest for many years. Despite significant progress in theoretical and numerical methods, developing analytic inversion formulas remains challenging due to the nonlinearity and complexity of the inverse problem. In this talk, we focus on recovery of a planar conductivity inclusion. We apply the conformal mapping technique, a powerful tool for planar inclusion problems, and the concept of the Faber polynomial polarization tensors. Our approach introduces a new factorization method that relates the measurement data to the geometric and material information of the inclusion. This method leads to an analytic inversion formula for recovering the inclusion from multi-static measurements.

### 6. A Non-intrusive Bi-fidelity Reduced Basis Method for Time-independent Problems

Dr. Junsuh PARK

Many scientific, engineering problems involve parametric partial differential equations (PDEs). In applications such as uncertainty quantification (UQ), optimizations, and inverse problems, the parametric PDE has to be solved repeatedly for many different parameters. This procedure is prohibitively expensive especially when the computation of the truth solution requires a large number of degrees of freedom or the problem has nonlinear structures. The reduced basis methods have been successfully applied in this frame to reduce the computation time for each new parameter. However, the reduced order modeling often relies on major modifications of the legacy code to achieve this. This procedure can be complex or impossible when the source code of the legacy solver is not available for modifications. In this work, we develop a new non-intrusive bi-fidelity reduced basis method for solving time-independent parametric partial differential equations. The algorithm only uses the assembly matrices, solutions, and the right-hand sides from the legacy solver. Due to its non-intrusive nature, the algorithm is straightforward and can be applied to general steady-state partial differential equations. The robustness of the algorithm is validated by several benchmark examples including nonlinear and multiscale PDEs.

# HKUST-KAIST-NUS Joint Workshop in Applied and Computational Mathematics

## Speakers from NUS

### 1. An Augmented Lagrangian Method with Constraint Generation for Shape-Constrained Convex Regression Problems

Prof Kim Chuan TOH

Shape-constrained convex regression problem deals with fitting a convex function to the observed data, where additional constraints are imposed, such as component-wise monotonicity and uniform Lipschitz continuity. This paper provides a unified framework for computing the least squares estimator of a multivariate shape-constrained convex regression function in  $\mathbb{R}^d$ . We prove that the least squares estimator is computable via solving an essentially constrained convex quadratic programming (QP) problem with  $(d+1)n$  variables,  $n(n-1)$  linear inequality constraints and  $n$  possibly non-polyhedral inequality constraints, where  $n$  is the number of data points. To efficiently solve the generally very large-scale convex QP, we design a proximal augmented Lagrangian method (proxALM) whose subproblems are solved by the semismooth Newton method (SSN). To further accelerate the computation when  $n$  is huge, we design a practical implementation of the constraint generation method such that each reduced problem is efficiently solved by our proposed proxALM. Comprehensive numerical experiments, including those in the pricing of basket options and estimation of production functions in economics, demonstrate that our proposed proxALM outperforms the state-of-the-art algorithms, and the proposed acceleration technique further shortens the computation time by a large margin.

### 2. Learning Committor Function and Invariant Distribution for Randomly Perturbed Dynamical Systems

Prof Weiqing REN

The committor function is a central object in understanding transitions between metastable states in complex systems. It has a simple mathematical description - it satisfies the backward Kolmogorov equation. However, computing the committor function for realistic systems at low temperature is a challenging task, due to the curse of dimensionality and the scarcity of transition data. In this talk, I will present a computational approach that overcomes these issues and achieves good performance on complex benchmark problems with rough energy landscapes. The new approach combines deep learning, importance sampling and feature engineering techniques. I will also discuss the computation of invariant distributions from short trajectories using deep learning.

### 3. The Entropic and Moment-preserving Spectral Method for the Boltzmann Equation

Prof Zhenning CAI

We present a novel Fourier spectral method that utilizes optimization techniques to ensure the positivity and conservation of moments in the space of trigonometric polynomials. We rigorously analyze the accuracy of the new method and prove that it maintains spectral accuracy. To solve the optimization problem, we propose an efficient Newton solver that has quadratic convergence rate. The method is applied to the spatially homogeneous Boltzmann equation and further regularized to guarantee the entropy inequality.

### 4. Learning under Latent Symmetries: Sparse Multi-reference Alignment, Phase Retrieval, and Uncertainty Principles

Prof Subhroshekhhar GHOSH

Motivated by cutting-edge applications like cryo-electron microscopy (cryo-EM), learning problems in the presence of latent symmetries has gained salience in recent years. Such latent symmetries preclude the possibility of having many repeated measurements of the exact same object, and pose a fundamental challenge for statistical learning. We will start with a gentle introduction to the problem of learning under latent symmetries, focussing on the setting of Multi Reference Alignment (MRA). Despite significant interest, a clear picture for understanding rates of estimation in this model has emerged only recently, especially in the practically important regime of high ambient noise ( $\sigma \gg 1$ ), where the best known results exhibit an asymptotic sample complexity of order  $\sigma^6$ , whereas in the absence of latent symmetries it is known to be of order  $\sigma^2$ . In recent work, we investigate this problem for sparse signals, where we unveil a remarkable intermediate sample complexity of order  $\sigma^4$ . Our results explore and exploit connections to classical topics, such as crystallographic phase retrieval, the beltway problem from combinatorial optimization, and uniform uncertainty principles from harmonic analysis. Based on joint work with P. Rigollet.