北京大学数学科学学院
School of Mathematical Sciences
Peking University

北京国际数学研究中心
BEIJING INTERNATIONAL CENTER FOR
MATHEMATICAL RESEARCH

2019 Applied Math Youth Forum

December 21-22, 2019

Peking University

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2019 Applied Math Youth Forum

Time： December 21-22, 2019

Venue: Lecture Hall, Jiayibing Building, Jingchunyuan 82, BICMR, Peking University

Organizing Committee

Tiejun Li	(Peking University)
Ming Jiang	(Peking University)
Lan Wu	(Peking University)
Jingping Yang	(Peking University)

Sponsors

School of Mathematical Sciences

Beijing International Center for Mathematical Research

Invited Speakers

Guangdong Bai	(University of Queensland)
Zecheng Gan	(NYU Courant Institute of Mathematical Sciences)
Tingran Gao	(University of Chicago)
Wuchen Li	(University of California, Los Angeles)
Yinan Li	(Centrum Wiskunde & Informatica)
Yulong Lu	(Duke University)
Peng Luo	(University of Waterloo)
Sui Tang	(Johns Hopkins University)
Xiaochuan Tian	(University of Texas at Austin)
Yunan Yang	(NYU Courant Institute of Mathematical Sciences)
Junyu Zhang	(University of Minnesota Twin Cities)

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Workshop Schedule

Time： December 21-22, 2019

Venue: Lecture Hall, Jiayibing Building, Jingchunyuan 82, BICMR, Peking University

Dec. 20, 2019

15:00-17:00	Registration（Beijing Friendship Hotel）

Dec. 21, 2019

Time	Speakers	Titles /Activities
9:00-9:15	**Opening Remark**	
Session 1	**Chair: Tiejun Li**	
9:15-9:55	Xiaochuan Tian	Analysis and computation of nonlocal models
10:00-10:40	Yunan Yang	Inverse Data Matching in Weak Norms
10:40-11:10	**Group Photo & Coffee Break**	
Session 2	**Chair: Ruo Li**	
11:10-11:50	Zecheng Gan	Self-assembly of charged colloidal spheres: fast algorithms and computer simulations
11:50-14:00	**Lunch (Jiayibing Building)**	
Session 3	**Chair: Xue Cheng**	
14:00-14:40	Peng Luo	An FBSDE approach to market impact games with stochastic parameters
14:45-15:25	Yinan Li	Bipartite perfect matching, (non)commutative rank, and their applications in entanglement transformation
15:25-15:45	**Coffee Break**	

Session 4	Chair: Bican Xia	
15:45-16:25	Junyu Zhang	Robust stochastic optimization with ProxBoost
16:30-17:10	Guangdong Bai	Scrutinizing Security Software and Protocols with Formal Methods
18:00	**Dinner (Huajiayiyuan)**	

Dec. 22, 2019

Session 5	Chair: Lei Zhang	
Time	**Speakers**	**Titles /Activities**
9:00-9:40	Sui Tang	Learning interaction kernels in agent-based systems
9:45-10:25	Yulong Lu	Understanding and Accelerating Statistical Sampling via PDEs and Deep Learning
10:25-10:45	**Coffee Break**	
Session 6	**Chair: Bin Dong**	
10:45-11:25	Wuchen Li	Accelerated Information Gradient flow
11:30-12:10	Tingran Gao	Gaussian Process Landmarking on Manifolds
12:10-14:00	**Lunch (Shao Yuan Dining Hall)**	
Session 7		
14:00-16:00	**Meeting with school dean (Room 1560, Sciences Building No. 1)**	

Abstracts

Analysis and computation of nonlocal models

Xiaochuan Tian

Nonlocal models are experiencing a firm upswing recently as more realistic alternatives to the conventional local models for studying various phenomena from physics and biology to materials and social sciences. In this talk, I will describe our recent effort in taming the computational challenges for nonlocal models. I will first highlight a family of numerical schemes -- the asymptotically compatible schemes -- for nonlocal models that are robust with the modeling parameter approaching an asymptotic limit. Second, fast algorithms will be presented to reduce the high computational cost from the numerical implementation of the nonlocal operators. Although new nonlocal models have been gaining popularity in various applications, they often appear as phenomenological models, such as the peridynamics model in fracture mechanics. Here we will try to provide better perspectives of the origin of nonlocality from multiscale modeling and homogenization, which in turn may help the development of more effective numerical methods for homogenization.

Inverse Data Matching in Weak Norms

Yunan Yang

For many problems in modern science and engineering that involve optimization, the residual or the so-called objective/loss/misfit function is essential to characterize the similarity and dissimilarity between two objects. In particular, the choice of a proper measure of data discrepancy affects the accuracy, convergence rate, and stability for computational solutions of inverse problems. We will have a closer look at the three outstanding benefits of optimization driven by the weak norms. First, it offers a more convex optimization landscape that mitigates the local-minima issues the traditional least-squares norm has. Second, it preconditions the iterative process of updating the solution, which improves general stability. Third, when used as the likelihood function in Bayesian inversion, it accounts for a broader range of noise than purely additive Gaussian. The discussion will be mainly focused on the quadratic Wasserstein distance and the negative Sobolev norm.

Self-assembly of charged colloidal spheres: fast algorithms and computer simulations

Zecheng Gan

Modern particle-based simulations increasingly incorporate polarization charges arising from spatially nonuniform permittivity, for the study ranging from colloidal suspensions to protein-protein interactions, etc. Numerical calculation of these induced many-body effects typically requires large amount of computational effort. For the special case of dielectric spheres, we will present a novel approach for solving the 3D Poisson equation, which is a semi-analytical hybrid method that combines the method of images and method of moments. Singularity in the multipole expansion is removed through the addition of image charges for close sphere pairs, making the problem well-conditioned. We further use our methods to explore the role of dielectric effect in the interaction between charged dielectric spheres. Through a few concrete numerical examples, we will show that the dielectric effect can lead to interesting phenomena such as like-charge attraction and qualitatively different self-assembled structures.

An FBSDE approach to market impact games with stochastic parameters

Peng Luo

We consider n risk averse agents who compete for liquidity in illiquid markets with both instantaneous and persistent price impact. In our model, the asset price has stochastic drift and diffusion coefficients and the agents don't need to close their positions in the end. Our problem can be described as a Nash equilibrium for a stochastic linear quadratic differential game. Using a martingale method, we characterize the Nash equilibrium in terms of a fully coupled FBSDE. We investigate the existence of the solution of the corresponding FBSDE which implies the existence of Nash equilibrium.

Bipartite perfect matching, (non)commutative rank, and their applications in entanglement transformation

Yinan Li

A perfect matching of a graph is a subset of edges in which every vertex is incident to exactly one edge. The celebrated Hall's marriage theorem states that a bipartite graph has a perfect matching if and only if it has no shrunk subset, that is, a subset of vertices (on one side) which has cardinality strictly larger than the cardinality of their neighbours. These two historical graph-theoretic notions are closely connected with the commutative and noncommutative rank of linear matrices (matrices whose entries are linear forms). In this talk, I will review these connections and recent (algorithmic) progress on the noncommutative rank problem. Then I will apply these results to study the asymptotic entanglement transformation.

Robust stochastic optimization with ProxBoost

Junyu Zhang

Standard results in stochastic convex optimization bound the number of samples that an algorithm needs to generate a point with small function value in expectation.
More nuanced high probability guarantees are rare, and typically either rely on “light-tail” noise assumptions or exhibit worse sample complexity. In this work, we show that a wide class of stochastic optimization algorithms for strongly convex problems can be augmented with high confidence bounds at an overhead cost that is only logarithmic in the confidence level and polylogarithmic in the condition number. The procedure we propose, called proxBoost, is elementary and builds on two well-known ingredients: robust distance estimation and the proximal point method. We discuss consequences for both treaming (online) algorithms and offline algorithms based on empirical risk minimization.

Scrutinizing Security Software and Protocols with Formal Methods

Guangdong Bai

This talk will brief our research results on applying formal methods for security analytics. It will show how formal analysis identifies logic flaws from various real-world applications, including web authentication, online payment and mobile apps. This talk will then focus on our approach that uses software model checking technique to verify Android apps. We have built a general framework named DroidPF which enables to explore the concrete state spaces, addresses the challenge caused by event-driven execution paradigm, and alleviates state space explosion.

Learning interaction kernels in agent-based systems

Sui Tang

Agent-based systems are ubiquitous in science, from the modeling of particles in Physics to prey-predator in Biology, to opinion dynamics in economics and social sciences, where the interaction law between agents yields a rich variety of collective dynamics. Inferring the interaction laws between agents from observational trajectory data is a fundamental task for modeling and prediction, yet challenging due to the implicit nonlinear forward map of the system and high dimensionality of the state space. Consequently, the algorithms often offer no guarantees and the resulting discoveries of interaction laws need external human validation.
Given abundant data sampled from multiple trajectories, we use tools from statistical/machine learning to construct estimators for interaction kernels with provably good statistical and computational properties, under the minimal assumptions that the interaction kernels only depend on pairwise distance. Numerical simulations on a variety of examples suggest the learnability of kernels in models used in practice, and that our estimators are robust to noise, and produced accurate predictions of collective dynamics in relative large time intervals, even when they are learned from data collected in short time intervals.

Understanding and Accelerating Statistical Sampling via PDEs and Deep Learning

Yulong Lu

A fundamental problem in Bayesian inference and statistical machine learning is to efficiently sample from probability distributions. Standard Markov chain Monte Carlo methods could be prohibitively expensive due to various complexities of the target distribution, such as multimodality, high dimensionality, large datasets, etc. To improve the sampling efficiency, several new interesting ideas/methods have recently been proposed in the community of machine learning, whereas their theoretical analysis are very little understood.

In the first part of the talk, I aim to demonstrate show how PDE analysis can be useful to understand some recently proposed sampling algorithms. Specifically, I will focus on the Stein variational gradient descent (SVGD), which is a popular particle sampling algorithm used in the machine learning community. I justify rigorously SVGD as a sampling algorithm through a mean field analysis. I will also introduce a new birth-death dynamics, which can be used as a universal strategy for accelerating existing sampling algorithms. The acceleration effect of the birth-death dynamics is examined carefully when applied to the classical Langevin diffusion. For both SVGD dynamics and the birth-death dynamics, I will emphasize the (Wasserstein) gradient flow structure and the convergence to the equilibrium of the underlying PDE dynamics.

The second part of the talk devotes to learning implicit generative models for sampling. Generative model such as Generative Adversarial Network (GAN) provides an important framework for learning and sampling from complex distributions. Despite the celebrated empirical success, many theoretical questions remain unsolved. A fundamental open question is: how well can deep neural networks express distributions? I will answer this question by proving a universal approximation theorem of deep neural networks for generating distributions.

Accelerated Information Gradient flow

Wuchen Li

We present a systematic framework for the Nesterov's accelerated gradient flows in the spaces of probabilities embedded with information metrics. Here two metrics are considered, including both the Fisher-Rao metric and the Wasserstein-2 metric. For the Wasserstein-2 metric case, we prove the convergence properties of the accelerated gradient flows, and introduce their formulations in Gaussian families. Furthermore, we propose a practical discrete-time algorithm in particle implementations with an adaptive restart technique. We formulate a novel bandwidth selection method, which learns the Wasserstein-2 gradient direction from Brownian-motion samples. Experimental results including Bayesian inference show the strength of the current method compared with the state-of-the-art.

Gaussian Process Landmarking on Manifolds

Tingran Gao

Fibre bundles serve as a natural geometric setting for many learning problems involving non-scalar pairwise interactions. Modeled on a fixed principal bundle, different irreducible representations of the structural group induce many associated vector bundles, encoding rich geometric information for the fibre bundle as well as the underlying base manifold. An intuitive example for such a learning paradigm is phase synchronization---the problem of recovering angles from noisy pairwise relative phase measurements---which is prototypical for a large class of imaging problems in cryogenic electron microscopy (cryo-EM) image analysis. We propose a novel nonconvex optimization formulation for this problem, and develop a simple yet efficient two-stage algorithm that, for the first time, guarantees strong recovery for the phases with high probability. We demonstrate applications of this multi-representation methodology that improve denoising and clustering results for cryo-EM images. This algorithmic framework also extends naturally to general synchronization problems over other compact Lie groups, with a wide spectrum of potential applications.

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Accommodation and Traffic

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