ABSTRACTS

2022 Center for AI and Natural Sciences Workshop

August 31 (Wed) ~ September 2 (Fri), 2022

Sono belle Resort, Jeju

2022 CAINS Summer Workshop Schedule

<table>
<tr><th></th><th>August 31 (Wed)</th><th>September 1 (Thu)</th><th>September 2 (Fri)</th></tr>
<tr><td>07:00-09:00</td><td rowspan="9">Airport -> Resort (Sono Belle, Jeju)</td><td>Breakfast</td><td>Breakfast</td></tr>
<tr><td>09:00-10:00</td><td>Seminar
(30min x 2)</td><td>Seminar
(30min x 2)</td></tr>
<tr><td>10:00-10:15</td><td>Break</td><td>Break</td></tr>
<tr><td>10:15-11:15</td><td rowspan="3">Seminar
(30min x 3)</td><td>Seminar
(30min x 2)</td></tr>
<tr><td>11:15-11:30</td><td>Break</td></tr>
<tr><td>11:30-11:45</td><td rowspan="3">Seminar
(30min x 2)</td></tr>
<tr><td>11:45-12:30</td><td rowspan="2">리조트 -> 성산항 이동</td></tr>
<tr><td>12:30-13:00</td><td rowspan="2">Lunch</td></tr>
<tr><td>13:00-14:00</td><td>Lunch</td></tr>
<tr><td>14:00-15:00</td><td rowspan="2">Self Check-in (14:00 -)
& Registration</td><td rowspan="6">Excursion
우도
(Jeju Udo Island)
성산항<->우도
*신분증 지참, 승선신고서 작성 필수</td><td rowspan="6">Resort (Sono Belle, Jeju)
->Airport</td></tr>
<tr><td>15:00-16:30</td></tr>
<tr><td>16:30-17:30</td><td rowspan="2">Seminar
(30min x 3명)</td></tr>
<tr><td>17:30-18:00</td></tr>
<tr><td>18:00-18:30</td><td rowspan="2">Dinner</td></tr>
<tr><td>18:30-20:00</td><td>Banquet</td></tr>
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Talk Schedule

August 31, 2022 (Wed)

Chair				
Chang bong Hyeon		16:30-17:00	Yung-Kyun Noh	Construction of estimators for f-divergences
		17:00-17:30	Jiwon Yoon	Side Channel Analysis to extract spatio-temporal information from multimedia signals
		17:30-18:00	Jaewoong Choi	Diffusion Generative Model

September 1, 2022(Thu)

Kimyeong Lee		09:00-09:30	Junghyo Jo	Mirror descent for machine learning
		09:30-10:00	Sungyoon Lee	Implicit Bias in X: from Least Squares to Deep Neural Networks
		10:00-10:15	Break	
Young-Woo Son		10:15-10:45	Wooseok Jeong	Machine Learning Potentials Based on Hybrid Multilevel Simulations for Molecular Simulations
		10:45-11:15	Daeseong Yong	Accelerating Simulation of Polymer Melts with Deep Learning

September 2, 2022(Fri)

Hyunggyu Park		09:00-09:30	Kyungwoo Song	Contrastive Learning and Multimodal Mixup
		09:30-10:00	EunSol Kim	Structural Semantic Alignment for Multimodal Compositional Reasoning
		10:00-10:15	Break	
Jae Sung Lee		10:15-10:45	Thomas Dieter Flacke	ML enhanced search strategies for BSM di-bosons at the LHC
		10:45-11:15	DongKyum Kim	Working and reference memory in transformers on a navigation task
		11:15-11:30	Break	
Deok-Sun Lee		11:30-12:00	Jaeyong Lee	Learning solution operators of partial differential equations
		12:00-12:30	Eunho Koo	Multifaceted enhancement of neural network learning strategy for the river water level prediction

Talk No.1

Construction of estimators for f-divergences

Yung-kyun Noh

Hanyang University, Seoul, Korea

It is typically inevitable to use an appropriate discrepancy measure between the data of different kinds in producing machine learning algorithms. Among many discrepancy measures, special kinds of functionals constitute a set of f-divergences with a convex function associated with each. In this talk, a novel and systematic way of constructing estimators for the f-divergence will be introduced generalizing the well-known Kozachenko-Leonenko estimator. These estimators use nearest neighbor information from the motivation that the density information is directly encoded within the distance to the nearest neighbors. The convergence and usefulness can easily be checked by the proposed methods. I will also provide a discussion of how the proposed method can be used in constructing novel machine learning algorithms.

Talk No.2

Side Channel Analysis to extract spatio-temporal information from multimedia signals

Jiwon Yoon

School of Cybersecurity and Cyber Defense Department, Korea University, South Korea

Recently, research on power-related signals called ENF (Electronic Network Frequency) has been conducted in various fields including power grid (SCADA), digital forensics, disaster prediction and so on.

In particular, ENF can be regarded as priceless side channel information which is obtained from various multimedia such as images, video, and audio. Because of this characteristics, ENF is now used for digital forensics which locate venues and identify targets.

In this presentation, I will introduce the basics concept of ENF, explain how it is used in the digital forensics field, and introduce various extraction techniques which my team has invented.

Talk No.3

Diffusion Generative Model

Jaewoong Choi

Korea Institute for Advanced Study, Seoul 02455, Korea

Recently, diffusion models have emerged as powerful generative models. Diffusion models achieved impressive success in high-fidelity image synthesis comparable to Generative Adversarial Networks (GANs), while offering strong sample diversity. The limited sample diversity has been considered a major challenge for GAN models. However, the slow sampling is still the main weakness of diffusion models. The diffusion models are described by two Stochastic Differential Equations (SDEs). The forward SDE defines a diffusion process from the data distribution to the noise distribution. Then, the corresponding reverse SDE expresses the dynamics from the noise to the data distributions. The score function in reverse SDE is parametrized and learned by neural networks. In this talk, I will introduce the diffusion models and many attempts to overcome their slow sampling problem.

Talk No.4

Mirror descent for machine learning

Junghyo Jo

Seoul National University, Seoul, Korea

Mirror descent is a gradient descent method using a dual space of parametric models. In this talk, I will briefly introduce various gradient descent methods including the mirror descent. These methods have been intensively studied in convex optimization problems, but not yet applied much in machine learning. I will demonstrate how effectively the mirror descent can train the Boltzmann machine, a representative generative model, and discuss its applicability into general deep learning.

Talk No.6

Implicit Bias in X: from Least Squares to Deep Neural Networks

Sungyoon Lee

Korea Institute for Advanced Study, Seoul 02455, Korea

Training a deep neural network is generally an underdetermined problem with multiple global minima. However, basic optimization algorithms are often biased to a certain set of "good" minima. We study why this is the case from least squares to deep neural networks.

Talk No.7

Machine Learning Potentials Based on Hybrid Multilevel Simulations for Molecular Simulations

Wooseok Jeong

Korea Institute for Advanced Study, Seoul 02455, Korea

Accurate descriptions of host-guest interactions are an essential step to understand gas adsorption phenomena for applications in catalysis and gas storage/separation. As promising heterogeneous catalysts and gas adsorbents, nanocrystalline porous materials such as zeolites and metal-organic frameworks (MOFs) have been attracted much interest since its unique host-guest chemistry. Due to the relatively large system size of the porous materials compared to molecular systems, computationally inexpensive classical force-field methods combined with molecular simulations are commonly used to compute gas adsorption and diffusion properties that can be directly compared with experimental data. However, this approach is limited to cases in which the host-guest interactions are more like physisorption, e.g., gas adsorption of small gases (H2 and CH4, CO2) at weak binding sites. In this talk, I will present how to develop machine learning potentials that can be interface with molecular simulations to study host-guest systems. To compute interaction energies accurately for strong adsorption sites where charge-transfer may occur, different levels of theory calculations can be performed on a host cluster–gas system to obtain hybrid multilevel data, motivated by the hybrid high-level–low-level quantum method developed by Prof. Joachim Sauer's group. As a first step, I will deal with interaction energy calculations for various dimer systems using an automated protocol to develop machine learning potentials.

Talk No.8

Accelerating Simulation of Polymer Melts with Deep Learning

Daeseong Yong

Korea Institute for Advanced Study, Seoul 02455, Korea

Langevin field-theoretic simulation (L-FTS) is a promising tool that can explain statistical behavior of incompressible polymer melts. However, L-FTS is a computationally expensive tool, and it may take more than a week to accurately calculate ensemble averages of thermodynamic quantities. It requires to find the pressure field that satisfies the incompressibility condition for each Langevin step. The conventional approach for finding the pressure field is utilizing an iterative method, since no closed-form solution is known. In this talk, I introduce a deep learning (DL) method that can boost the iteration process by predicting the error of pressure field. This DL approach can achieve speedup of factor 6 or more compared to the conventional relaxation method without compromising accuracy.

Talk No.9

Contrastive Learning and Multimodal Mixup

Kyungwoo Song

Seoul National University, Seoul, Korea

Pre-trained large-scale models by contrastive learning provide a transferable embedding, and they show comparable performance on the diverse downstream task. However, the transferability of multi-modal learning is restricted, and the analysis of learned embedding has not been explored well. Less robust embedding might restrict the transferability of the representation for the downstream task. In this presentation, I provide a perspective to understand multi-modal embedding and contrastive learning. Besides, I present a multi-modal Mixup that mixes the representation of image and text to generate the hard negative samples on the sphere for robust representation learning.

Talk No.10

Structural Semantic Alignment for Multimodal Compositional Reasoning

Eunsol Kim

Hanyang University, Seoul, Korea

In this talk, we propose a new machine learning algorithm for visual commonsense reasoning (VCR) tasks. While most of the methods for the VCR tasks are trained to predict answers by combining multiple feature vectors, we suggest to represent the semantics of the inputs using neuro-symbolic graphs and combine the graphs for the reasoning. Here, we introduce a novel graph neural network method, which is called SSA-MCR. The suggested method constructs multiple semantic graphs and combines them by applying cross-attention over multiple graphs. With our experiments using Visual Commonsense Reasoning dataset, we show that the suggested method has advantages for complex reasoning problems requiring multihop reasoning processes.

Talk No.11

ML enhanced search strategies for BSM di-bosons at the LHC

Thomas Dieter Flacke

Korea Institute for Advanced Study, Seoul 02455, Korea

Many extensions of the Standard Model of particle physics predict new bosons which can be pair-produced at the Large Hadron Collider (LHC). We investigate the multitude of new final states which can arise from the decay these di-bosons and study prospects of ML enhanced search strategies which aim to distinguish rare potential BSM signal events from the large background of Standard Model events.

Talk No.12

Working and reference memory in transformers on a navigation task

Dongkyum Kim

Institute for Basic Science, Daejeon, Korea

A relationship between self-attention mechanism of transformers and hippocampal models from neuroscience has recently been shown to be mathematically similar and also resemble firing pattern of neurons in the brain. In particular, the transformer model, which is trained for a navigation task, replicates place and grid cells which are spatially tuned neural activity. In this work, we investigate properties of two memory types in transformer blocks: working memory in self-attention block and reference memory in point-wise feed-forward networks (FFN). We discover that place cells are formed in FFN while the previous work found the place cells in self-attention blocks. Furthermore, we have demonstrated that non-linearity in FFN is essential for forming reference memory.

Talk No.13

Learning solution operators of partial differential equations

Jaeyong Lee

Korea Institute for Advanced Study, Seoul 02455, Korea

Many differential equations and partial differential equations (PDEs) are being studied to model physical phenomena in nature with mathematical expressions. Recently, operator learning using neural networks has been studied to approximate a PDE solution operator, which is an operator from the parameters of the PDE to its solution. In this talk, I will introduce several recently proposed architectures for operator learning and my research related to them.

Talk No.14

Multifaceted enhancement of neural network learning strategy for the river water level prediction

Eunho Koo

Korea Institute for Advanced Study, Seoul 02455, Korea

A properly designed network structure and initialization scheme are essential factors
in ensuring a better performance of an artificial neural network.
In this study, we investigate a learning strategy for neural networks-based time-series prediction
to predict the water level of Hangang (Han-river) using various local climate data.
Evolving Sequential Structure (ESS) is proposed to intervene in the learning process
with recursively increasing ratio of reliable information.
In addition, to have a similar statistical character between label and input data,
we propose a non-linear transformation technique derived from a domain specific physics,
mass balance equation of land hydrology: exponential filtering (EF).
Furthermore, we equip the networks with an objective function Weighted Empirical Stretching (WES)
which penalizes errors against the probability density of label
to enlarges the overlapping area between the label and prediction distributions.
Newly proposed set of algorithms have been tested on Long Short-Term Memory (LSTM).
We evalueate the effect of the proposed strategy in terms of various error metrics.