NSF AI Institute for Artificial Intelligence and Fundamental Interactions (IAIFI /aɪ-faɪ/)

Advance physics knowledge—from the smallest building blocks of nature to the largest structures in the universe—and galvanize AI research innovation





Al Foundations: Power of machine learning to process large, rich data sets



Physics Theory & Experiment: First principles and best practices from fundamental interactions



Enable physics discoveries by developing and deploying the next generation of AI technologies Galvanize AI research innovation by incorporating physics intelligence into artificial intelligence



- Physicists have been at the forefront of applying AI methods to investigate fundamental questions about the universe. Further progress requires a revolutionary leap in AI as both the complexity of physics problems and the size of physics datasets continue to grow.
- IAIFI research focuses on the intersection of Physics and AI, advancing knowledge of fundamental interactions using innovative methods in AI built upon physics principles while simultaneously advancing the foundations of AI through physics-inspired investigations.
- The IAIFI is coordinating activities to make the Institute more than the sum of its parts and serve as a nexus point for Physics and AI research in the Boston area and beyond, including training the next generation of talent through its IAIFI Postdoctoral Fellowship program.







The Problem

- Approximating "values" via neural networks is a key component in deep reinforcement learning and "Al"
- We identify *underfitting* due to poor learning dynamics as a key bottleneck in deep reinforcement learning

The Solution

We use spectral analysis and neural tangent kernels (NTK) to improve learning, thus prevent underfitting from happening during this process

 $RFF(x) = \sin(Wx + b)$ $W \sim 2\pi N\left(0, \frac{b}{\dim(x)}\right)$ $b \sim U(-\pi, \pi)$

NN-QFT Correspondence

Neural networks (NNs) in the finite-width regime behave as close-to-Gaussian processes.

Which connects NN to perturbative quantum field theory, where interactions are modeled via non-gaussianity!



Ge Yang (IAIFI Fellow), Anurag Ajay, Pulkit Agrawal





Piecewise-Linear Manifold Approximation with K-Deep Simplices (KDS, <u>2012.02134</u>) Well-Defined Metric on Particle Collisions using Energy Mover's Distance (EMD, 2004.04159)



Manifold Learning with Physics-inspired Constraints

$$\begin{split} \mathcal{L}_{\text{KDS}}[a, x] &= \sum_{y} \left[\sum_{i} x_{i}^{(y)} |\vec{y} - \vec{a}_{i}|^{2} + \frac{1}{2\lambda} |\vec{y} - \sum_{i} x_{i}^{(y)} \vec{a}_{i}|^{2} \right] \\ \text{Subject to } \sum_{i} x_{i}^{(y)} &= 1 \\ \mathcal{L}_{\text{EMD}}[a, x] &= \sum_{y} \left[\sum_{i} x_{i}^{(y)} \frac{|\vec{y} - \vec{a}_{i}|^{2}}{R^{2}} \right] \\ \text{Subject to } \sum x_{i}^{(y)} &= z_{y}, \sum x_{i}^{(y)} = z_{i}, \text{ and } \sum x_{i}^{(y)} = 1 \end{split}$$

$$\text{Subject to } \sum_i x_i^{(y)} = z_y, \sum_y x_i^{(y)} = z_i, \text{ and } \sum_{i,y} x_i^{(y)} = 1$$

• KDS learns piecewise linear manifolds

- New class of EMD-based jet observables, calculated using KDS
- Respects physical symmetries and constraints (IRC Safety, Permutation Invariance)
- Generalization of point-like jet algorithms to higher dimensional structures

Demba Ba (), Akshunna Dogra (), Rikab Gambhir (), Jesse Thaler (),





NN-QFT correspondence: Progress by considering one from the other's perspective

QFT ideas for NNs: [Halverson, Maiti, Stoner] 2020 Modeling NN Densities

- Non-Gaussian phenomenological model of NN density.
- Compute NN ensemble correlations with Feynman diagrams.
- RG flow arises in some density models.
- Agreement with NN experiments.

QFT ideas for NNs: [Halverson, Maiti, Stoner] 2021 Symmetry-via-Duality 2021

- Deduce symmetries of NN actions by study of correlations computed in parameter space.
- Input / output symmetries of NN are analog of spacetime / internal symmetries in QFT.
- Both continuous and discrete symmetries, Abelian and non-abelian.

NN ideas for QFTs: [Halverson] in progress Building Quantum Fields out of Neurons

- Reframe randomness of QFs in parameter-space; How we build fields, not how we draw them.
- Use NNs to define Lorentz-invariant, unitary QFTs.
- Explains prevalence near-Gaussianity in QFT.

Other work progress:

[Gukov, Halverson], [Halverson, Maiti, Stoner, Schwartz] See also: [Roberts, Yaida], [Erbin, Lahoche, Samary]





Symmetry structure of the Standard Model of particle physics



 $f^{-1}(z)$

Generative models

based on normalizing flows

Development of machine learning frameworks for efficient sampling in lattice quantum field theory

- Series of papers developing generative flow models on compact domains, and on U(n) and SU(n) Lie group variables
- Proof-of-principle demonstration of orders-of-magnitude acceleration over traditional sampling approaches
- Roadmap to QCD for state-of-the-art nuclear/particle physics studies
 - Architectures for compact variables
 - Incorporation of gauge symmetry
 - 🔽 Non-Abelian groups
 - Fermions

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Scaling to state-of-the-art, exascale hardware

[PRD 103, 074504 (2020), PRL 125, 121601 (2020), ICML, PMLR 8083-8092 (2020), 2107.00734 (2021) 2106.05934 (2021), 2101.08176 (2021)]

Shanahan group (MIT) + Industry Partners (Google DeepMind)





Convolutional Neural Nets (CNNs) plus Physically Modelled Inputs



The Cosmic Density Field as a Probe of Cosmological Physics

Reconstructing the Cosmic Initial Density Field from Galaxy Redshift Surveys



DESI Large-Scale Structure (0.9<z<0.95



- The galaxy density field is a non-linear mapping of the initial matter density field.
- We model this gravitational process with N-body simulations, plus galaxy models.
- Upcoming observational programs such as DESI will produce gigantic maps.
- We will enhance the cosmological value of these maps by using CNNs to reconstruct the initial density field from the sparse and non-linearly evolved galaxy field.

Daniel Eisenstein, Chris Shallue (Harvard), Sihan Yuan (Harvard, SLAC) , Lehman Garrison (Flatiron/CCA)











Reinforcement learning (RL) agents able to optimally tune systems

Squeezed light to improve LIGO sensitivity to gravitational waves

New RL methods with potential to optimize LIGO squeezing performance over long periods of time



- Used deep learning to understand causes of squeezing degradation on past data
- Made progress in predicting squeezing levels based on a large set of auxiliary channels, selecting those with predictive power
- Built a simulation environment to train a Deep-Q-Network (DQN) RL Agent on simple versions of the
 optimization problem, specifically how to optimize mirror alignment with 2 and 4 degrees of freedom
- The far reaching goal is to create an agent able to observe the system and react to keep it on its optimal state by modifying a variety of parameters

C. Whittle, D. Ganpathy, Ge Yang, P. Agrawal, M. Evans, L. Barsotti





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Katherine Frase

IAIFI Early Career and Equity

Committee Membe





Committee Membe

Committee Membe

• Includes a faculty chair, a second faculty member, five postdocs and graduate students, and the IAIFI Project Manager

Harold Erbir

IAIFI Early Career and Equity

Committee Member

- Serves as advisory board to IAIFI Management on aspects related to early career researchers and diversity, equity, and inclusion (DEI)
- **Developed a Code of Conduct** for IAIFI members in conjunction with MIT Office of General Counsel, which will serve as an example for similar awards at MIT in the future
- Established an anonymous form for IAIFI members to submit feedback
- Held Early Career Town Hall and compiled suggestions for management based on discussion
- **Reviews IAIFI invitation lists** (i.e. Fellow interviews, External Advisory Board, speakers) with DEI considerations in mind

IAIFI Code of Conduct and Related Policies

Code of Conduct:

Regardless of their position or seniority, members of the IAIFI and participants in IAIFI activities are expected to:

-Act in an ethical and collaborative manner at all times and abide by the MIT Physics Community Values

-Work with the utmost scientific integrity and respect the confidentiality of information and work presented at internal IAIFI meetings

-Treat each other with dignity and respect, support and encourage each other's growth, and step in as needed to maintain an environment free of discrimination, harassment, and bullying

Furthermore, members of the IAIFI and participants in IAIFI activities may not engage in retaliation against anyone for objecting to a behavior that may violate this Code of Conduct, reporting a violation of the Code of Conduct, or participating in the resolution of such a complaint.

Related Policies:

In addition to this Code of Conduct, members of the IAIFI and participants in IAIFI activities are required to comply with MIT's Non-Discrimination Policy, and MIT's Policy prohibiting Discriminatory Harassment, including Sexual Harassment, Sexual Misconduct, Gender-Based Harassment, and Title IX Sexual Harassment (see https://iaifi.org/code-of-conduct.html for further information). IAIFI members must also be aware of and abide by their institutions' policies against research misconduct.

Suggestion box for the IAIFI

This form is anonymous; if you want us to get back to you, please put your contact information in the optional question below. Your input will go to the Early Career and Equity Committee (ECEC) for review, and may then be shared more widely, with any identifying information removed.







IAIFI Fellowship Program

- To recruit and train the most talented, promising, and diverse group of early-career researchers and spark vital interdisciplinary, multi-investigator, and multi-subfield collaborations
- Launched the IAIFI Fellowship program with the selection of our first 4 IAIFI Fellows for 2021-2024
- Developed interdisciplinary postdoctoral mentoring plan for Fellows
- In the first year of IAIFI, 6 research projects involved direct collaboration and/or discussion with IAIFI Fellows (1 Fellow started in April and the rest started in September)





Top left: Anna Golubeva; Top right: Di Luo; Bottom left: Siddharth Mishra-Sharma; Bottom right: Ge Yang



IAIFI Fellows serve as "gluons" for the Institute







Interdisciplinary PhD Program

- <u>Physics, Statistics, and Data Science (PhysSDS)</u> PhD program at MIT is a **collaboration** between IAIFI, the MIT Physics Department, and the MIT Statistics and Data Science Center (SDSC)
- Establishes a **verifiable credential** that helps Physics students pursue careers in the fields of data science and Artificial Intelligence
- Open to **current MIT Physics PhD students**; the first 5 students were admitted to the program in December 2020
- Nine IAIFI Senior Investigators are serving on the PhysSDS Committee, including Jesse Thaler and Mike Williams who are the Program Chairs





IAIFI member Constantin Weisser became the first recipient in May 2021 with his thesis "Search for Dark Photos at LHCb and Machine Learning in Particle Physics." He is now a Data Science Consultant at QuantumBlack and also had a short internship at NASA.







IAIFI Colloquia, Seminars, and Journal Club

- Colloquia (public) and Discussion Seminars (internal) are held on alternating weeks during the academic year
- The Journal Club is held biweekly and organized by IAIFI Junior Investigators
- The Colloquia are simultaneously broadcast on YouTube and saved on the IAIFI YouTube channel
- Virtual colloquia allow us to broaden our reach
 - YouTube comment: "I am...a physics undergrad. Today I am attending 3rd talk in this Colloquium series. I really appreciate the opportunity to attend these talks from half the way across the world from India."



- Public colloquia are attended by an average of 83 live participants and have an average of 370 views on YouTube
- Discussion seminars are attended by an average of 29 live participants
- Journal Clubs are attended by an average of 17 live participants



IAIFI Colloquium Series: ML-discovery of equations, conservation laws and useful degrees of freedom