

Alexander Shmakov

Artificial Intelligence Scientist

☎ +1 408 571 9059 | @ ashmakov@uci.edu | G Scholar | GitHub

I am a 5th Year Ph.D. candidate at the University of California, Irvine with over 6 years of experience in deep learning and artificial intelligence. I specialize in applying generative AI to scientific challenges and leveraging reinforcement learning for planning. I employ state-of-the-art AI techniques to address challenging, real-world problems across various scientific disciplines by developing innovative solutions and fostering strategic interdisciplinary collaborations.

EDUCATION

University of California Irvine

Ph.D. in Computer Science | **4.00 GPA**

B.S. in Computer Science | *Cum Laude* | **3.92 GPA**

B.S. in Mathematics | *Magna Cum Laude* | *Honors* | **3.88 GPA**

Irvine, CA, USA

Jun 2020 – Dec 2025 (*Expected*)

Sep 2015 – Mar 2020

Sep 2015 – Mar 2020

EXPERIENCE

ATLAS Collaboration at CERN

Reconstruction and Tracking Groups Member

European Organization for Nuclear Research (CERN)

Jan 2023 – Present

- Pioneering machine learning and generative AI innovations in high-energy physics to enhance detection of rare interaction involving the Higgs Boson and potential new discoveries beyond the standard model.
- Integrating physical symmetries into state-of-the-art transformer and diffusion models to improve the precision of complex classification tasks and inverse problems.
- Developing software libraries which are widely employed across CERN to accelerate the search for new physics and improve our understanding of the universe.

Artificial Intelligence in Science Institute

Graduate Student Researcher in Deep Learning

University of California Irvine (UCI)

Jan 2018 – Present

- Conducting advanced AI research with applicability in particle physics, chemistry, astronomy, and biology under the mentorship of Distinguished Professor Pierre Baldi.
- Inventing novel neural network architectures that incorporate physical symmetries and domain insights, leveraging cross-disciplinary knowledge from domain experts to produce state-of-the-art results.
- Spearheading the development and execution of deep learning experiments, managing intricate cross-domain data sets, and efficiently employing large-scale compute clusters.

Intelligent Dynamics Lab

Graduate Student Researcher in Reinforcement Learning

University of California Irvine (UCI)

Jun 2020 – Present

- Conducting in-depth research in deep reinforcement learning, targeting its practical applications in robotics, planning, and competitive multi-agent environments.
- Produced headlining results by engineering the first RL agent capable of learning to solve the Rubik's Cube without reliance on human knowledge.
- Leading the development of advanced reinforcement learning software, incorporating long-term memory, and devising complex environments for rigorous evaluation of these agents' performance.

Amazon, Buyer Risk Prevention

Applied Science Intern

Jun 2024 – Dec 2024

Amazon.com Inc

- Developing fully automated AI solutions to detect and adapt to fraud on a global scale.
- Designing innovative reinforcement learning techniques to identify shifts in customer behavior and swiftly adjust strategies to prevent losses.
- Leading the implementation of interpretable fraud AI systems, ensuring human-understandable adjustments and reliability in unforeseen scenarios.

Hewlett Packard Labs

Artificial Intelligence Research Associate

Hewlett Packard Enterprise (HPE)

Jun 2021 – May 2023

- Pioneered the design of advanced multi-agent reinforcement learning systems, targeting enhancements in green energy solutions and industrial control mechanisms.
- Achieved breakthroughs in ensuring the safety and reliability of AI implementations, significantly reducing the cost of energy from wave-powered renewable energy sources.
- Drove the development of innovative reinforcement learning agents, emphasizing the integration of long-term memory, AI safety, and multi-agent cooperation.

SELECTED PUBLICATIONS

End-To-End Latent Variational Diffusion Models for Inverse Problems in High Energy Physics

Shmakov A[†], Greif K[†], Fenton M, Ghosh A, Baldi P, Whiteson D

NeurIPS, 2023, [www.arxiv.org/abs/2305.10399](https://arxiv.org/abs/2305.10399)

SPANet: Generalized Permutationless Set Assignment for Particle Physics using Symmetry Preserving Attention

Shmakov A[†], Fenton M[†], Ho TW, Hsu SC, Whiteson D, Baldi P

SciPost, 2022, www.scipost.org/SciPostPhys.12.5.178

Reconstruction of unstable heavy particles using deep symmetry-preserving attention networks

Fenton M[†], Shmakov A[†], Okawa H, Li Y, Hsiao KY, Hsu SC, Whiteson D, Baldi P

Nature Communications Physics, 2024, www.nature.com/articles/s42005-024-01627-4

Solving the Rubik's Cube with Deep Reinforcement Learning and Search

Agostinelli F[†], McAleer S[†], Shmakov A[†], Baldi P

Nature Machine Intelligence, 2019, www.nature.com/articles/s42256-019-0070-z

Multi-agent reinforcement learning controller to maximize energy efficiency for multi-generator industrial wave energy converter

Sarkar S, Gundecha V, Shmakov A, Ghorbanpour S, Babu AR, Faraboschi P, Cocho M, Pichard A, Fievez J

AAAI, 2023, ojs.aaai.org/index.php/AAAI/article/view/21473

AI for Interpretable Chemistry: Predicting Radical Mechanistic Pathways via Contrastive Learning

Tavakoli M, Baldi P, Carlton AM, Chiu Y, Shmakov A, Vranken DV

NeurIPS, 2023, neurips.cc/virtual/2023/poster/72740

Deep learning for drug discovery and cancer research: Automated analysis of vascularization images

Urban G, Bache K, Phan D, Sobrino A, Shmakov A, Hachey S, Hughes C, Baldi P

IEEE/ACM, 2018, <https://ieeexplore.ieee.org/abstract/document/8368281>

AWARDS

IEEE CASE Best Application Paper Awarded for my work in harnessing multi-agent reinforcement learning to optimize the control mechanisms of wave energy converters, a major improvement in the realm of sustainable energy.

NSF Machine Learning and Physical Sciences (MAPS) Fellowship Granted in recognition of my cutting-edge contributions to the application of deep learning within high-energy physics, supporting pivotal research in the field.

PROJECTS

SPANet, Symmetry Preserving Attention Networks

github.com/Alexanders101/SPANet

- Developed an accessible and actively used Python library based on my innovative research paper, enabling symmetry-preserving attention networks for enhanced event reconstruction at the Large Hadron Collider.
- Designed a universal, group-theoretic algorithm to dynamically generate transformer attention networks which are uniquely tailored to preserve symmetries in high-energy physics classifications tasks.

ColosseumRL, Multi-Agent RL Library

github.com/colosseumrl/colosseumrl

- Developed a robust suite of multi-agent reinforcement learning environments and distributed tournament routines to explore cooperative and competitive AI behaviors.
- Managed competitions and guided students through hands-on, project-based learning experiences, nurturing a deeper understanding and passion for reinforcement learning and multi-agent dynamics.

SKILLS

Programming: Python, C++, Git, Docker, Linux, HPC

Libraries: PyTorch, Jax, PyMC, Hugging Face, RLLib, Scikit-Learn

AI Techniques: Attention, Transformers, Generative AI, Diffusion Models, Physics-informed Machine Learning, Computer Vision, Reinforcement learning, Bioinformatics, Computational Chemistry, Scientific Computing