Stanislav Chekmenev

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Profile

Machine Learning Researcher with expertise in geometric deep learning, generative models, and reinforcement learning. Background in particle physics and experience with symmetry-aware models for molecular and protein ML applications through independent research and student supervision. Passionate about advancing computational biology with innovative ML approaches.

Work Experience

2020-06 – present **Instructor & Mentor**, Data Science Retreat, Berlin, Germany.

- Designed and taught courses on geometric deep learning (GDL), reinforcement learning (RL), and practical debugging of deep neural networks.
- Supervised and mentored students on applied research portfolio projects, including ADMET molecular property prediction with equivariant GNNs and DNA-protein binding affinity modeling using state-of-the-art architectures (e.g. ATOMICA).
- Guided students through the research workflow, from literature review to model development, evaluation, and presentation of results.

2024-01 – 2024-07 **Founding Machine Learning Scientist**, Qypt GmbH, Berlin, Germany.

- Led the development of generative AI solutions at the intersection of large language models (LLMs) and cyber security.
- Designed and implemented a proof-of-concept language system leveraging a modern LLM backbone, deployable locally on mobile devices with backend infrastructure in Rust.
- Developed and applied a novel data weighting approach for LLM finetuning across multiple datasets, achieving a 20% performance improvement over baseline.
- Enabled the company's first product launch by delivering an efficient LLM-powered app as the technical foundation for future development.
- Conducted R&D on generative text models and explored the integration of fully homomorphic encryption for privacy-preserving inference.

2022-06 – 2022-12 **Machine Learning Scientist**, Hella Aglaia Mobile Vision, Berlin, Germany.

- Developed a computer vision prototype for automated tiny defect detection on automotive door panels, combining self-supervised learning with generative modeling (normalizing flows).
- Enabled deployment of a real-time anomaly detection system, successfully implemented at Hella Aglaia production plants, improving quality control and reducing manual inspection requirements.
- Mentored a junior data scientist throughout the whole project, providing guidance in ML modeling and dataset creation.
- Delivered graph neural network (GNN) training sessions to the ML teams distributed throughout Germany and India.

2020-02 – 2022-04 **Machine Learning Researcher**, Certainty Lab, Berlin, Germany.

- Collaborated on the development and implementation of a real-world reinforcement learning (RL) system for adaptive traffic light control.
- Co-designed and implemented a scalable GNN based architecture, achieving a 10× speedup in training and enabling agent transferability to new intersections without retraining.
- Co-developed a parallelized version of MuZero algorithm, specifically adapted for traffic signal optimization, significantly improving sample efficiency.
- Built generative vision models (VAE) to reconstruct occluded objects in video feeds, enhancing traffic situation assessment and system robustness.
- Contributed several key modules to the production traffic light control system, including near real-time model evaluation.
- Mentored a master student in explainable AI, applying Integrated Gradients for model interpretability.

2019-09 **Student**, Data Science Retreat, Berlin, Germany.
2019-12
- Developed a portfolio project for autonomous driving at the intersection of computer vision and reinforcement learning, based on the World Models RL algorithm.
- Enhanced World Models with the Proximal Policy Optimization (PPO) algorithm, resulting in improved sample efficiency for control policies.

2018-12 **Data Scientist**, Looping PowerRoom Berlin, Berlin, Germany.
2019-08
- Developed and deployed natural language processing (NLP) solutions for emotion recognition in text, leveraging LSTMs.
- Proposed the ideas and lead the implementation from scratch of several data based products.
- Mentored and provided technical guidance to two junior data scientists.

2016-06 **Data Scientist**, HeilpflanzenWohl GmbH, Berlin, Germany.
2018-10
- Designed and implemented linear and nonlinear machine learning models for accurate sales forecasting and business planning.
- Initiated and led the development of several data driven product features, overseeing the entire process from ideation to production deployment.
- Built interactive dashboards for marketing analytics, providing improved brand strategy insights.

Research Projects

2024-10 **Self-initiated research project:**
2025-07 **Learning SE(3) Flow Matching for Protein Structure Generation**.
- Adapted and extended an SE(3) Flow Matching model for protein structure generation, augmenting its architecture with an SE(3) equivariant GNN.
- Explored geometric deep learning techniques in combination with recent generative models for protein discovery tasks.
- Demonstrated understanding of group theory and generative models operating on SE(3) group manifold within the context of protein design.
- Documented learning process and technical deep dives in a detailed blog post. `https://chekmenev.me/posts/protein_discovery/`.

Education

2012–2016 **PhD in Physics**, *RWTH Aachen University*, Aachen, Germany, *Excellent (1.0)*.
Specialized in Particle Physics and Accelerator Physics.

2006–2012 **Master of Physics**, *State Polytechnic University*, Saint-Petersburg, Russia, *Very good (1.5)*.
Specialized in Particle Physics.

Skills

Programming & Research Tools.
- **Languages/Frameworks:** Python, PyTorch, PyTorch Geometric, TensorFlow, HuggingFace Transformers, Rust, NumPy, Pandas, scikit-learn, R, SQL, MATLAB.
- **Parallel Computing:** Ray, PySpark.
- **Visualization/Dashboards:** Matplotlib, Plotly, Shiny Dashboards.
- **Cloud & DevOps:** GCP, AWS, Azure, Docker, CI/CD best practices.

Technical Knowledge & Research Expertise.
- **Core Machine Learning:** Linear algebra, probability, optimization, supervised/unsupervised/self-supervised learning, model evaluation.
- **Deep Learning:** Generative models (VAEs, normalizing flows, diffusion/flow matching), graph neural networks, geometric deep learning, transformers, large language models.
- **Reinforcement Learning:** Deep RL (MuZero, PPO, World Models), real-world and simulation-based applications.
- **Scientific ML:** Molecular modeling, protein structure generation, ADMET prediction, DNA-protein affinity prediction.
- **Computer Vision:** Anomaly detection, self-supervised techniques, generative vision models.

Research, Collaboration & Communication.
- Academic writing (lead author or essential contributor), publication and conference participation (e.g. International Symposium on Spin Physics).
- Extensive teaching and mentoring experience, including supervision of applied ML and GNN research projects.
- Strong written and oral presentation skills for technical and non-technical audiences.

Additional Skills

Languages.

- English: fluent (C2) | German: upper intermediate (B2) | Russian: native

Personal Skills.

- Self-motivated and able to prioritize tasks effectively in both independent and collaborative settings.
- Strong communication and teamwork skills, with a proven ability to collaborate in interdisciplinary teams.
- Consistent practice of writing clear, maintainable code with thorough documentation.
- Quick learner, adaptable to new domains, and able to perform under pressure and meet tight deadlines.

Interests.

- Handpan and oriental percussion, surfing, qigong, tai chi, and meditation.

Courses & Continuous Education

2017 – present **Online & Offline Courses**.

- Deep Learning Specialization, Reinforcement Learning Specialization, Machine Learning, Bayesian Statistics I & II, Graph Neural Networks, Transformers, Geometric Deep Learning, Cyber Security.

Volunteering

2023-01 – 2023-11 **Temple Volunteer**, *Shaolin Temple Europe*, Otterberg, Germany.

- Practiced qigong, tai chi, kung fu, and meditation as part of the temple community.
- Contributed to essential daily operations, including kitchen work, animal care, and gardening.

This experience strengthened my ability to approach problems from new perspectives and stay focused under challenging conditions.