Pengfei Zhang

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Summary

Self-motivated **Computer Science Ph.D. Candidate** specializing in **Generative AI**, **LLMs**, and **Reinforcement Learning from Human/AI Feedback (RLHF/RLAIF)**. Strong background in developing and optimizing ML models, with experience applying generative AI techniques to research and real-world problems. Skilled in building reproducible ML pipelines and scalable workflows. Proficient in Python, PyTorch, TensorFlow. Expertise includes:

- **Generative AI**: Adapted GPT-based LLMs for sequence generation with metrics to curb hallucination.
- **Reinforcement Learning**: Reframed RLHF/RLAIF to expose reward model flaws and improve alignment.
- **Representation Learning**: Built context-aware embeddings to boost prediction on complex bio data.

Education

Arizona State University	*08/2019 – 04/2026*
Ph.D. in Computer Science, GPA: 3.9/4.0	*(expected)*
Arizona State University	*08/2019 – 12/2022*
M.S. in Computer Science	
Changchun University of Science and Technology	*09/2015 – 06/2019*
B.E. in Optoelectronic Engineering (with honors)	

Selected Projects

Protein Language Models and Generative Models — *05/2023–Present*
3 first-author papers delivered

- Adapted generative model training to an **in-context learning** approach, enabling immune T cell receptor design conditioned on novel target binding sequences and few-shot prompting.
- Developed an automated **chain-style, self-contemplating prompting** method that eliminated the need for human-fed few-shot examples without compromising model performance.
- Fine-tuned and deployed protein language models with reinforcement learning from AI feedback (RLAIF) to **attack and defend reward models** (biological prediction models), increasing model robustness **fivefold**.
- Designed a modular **reward hacking mitigation framework** for conditional protein generation, incorporating reward smoothing, ensemble rewards, and distributional regularization to preserve biological authenticity during RL.

Data-Efficient Machine Learning for Biological Prediction — *12/2022–04/2023*
1 first-author papers delivered

- Designed **active learning** frameworks using innovative entropy-based query strategies to optimize data selection.
- Reduced **50% annotation costs** for unlabeled pairs and minimized **40% data redundancy** among annotated pairs.

Representation Learning for Protein Sequences — *05/2021–02/2022*
2 first-author papers and 1 US patent delivered

- Developed **context-aware embedding models** for amino acid and protein sequences using bidirectional LSTM and self-attention, optimized for immune receptors.
- Benchmarked against traditional embedding methods like BLOSUM, word2vec, and Bert, achieving superior performance in predictive accuracy and cluster quality across supervised and unsupervised tasks.
- Enhanced sequence binding predictions by over **20% in AUC scores** and reduced data requirements by **93%**.

Technical Skills

- ○ **Programming Languages**: Python, R, SQL, Java, C++, Bash
- ○ **Machine Learning Frameworks**: TensorFlow, PyTorch, Keras, Scikit-Learn, Transformers, TRL
- ○ **Data Analysis**: NumPy, Pandas, Seaborn, Matplotlib
- ○ **Cloud Platforms**: AWS SageMaker, Google Cloud Platform
- ○ **Version Control**: Git, GitHub, GitLab

Selected Publications

LLMs and Generative Models

- ○ **P. Zhang**, S. Bang, and H. Lee, "Self-Contemplating In-Context Learning Enhances T Cell Receptor Generation for Novel Epitopes", in *Machine Learning in Computational Biology (MLCB)* 2025.
- ○ **P. Zhang**, H. Mei, S. Bang and H. Lee, "Iterative Attack-and-Defend Framework for Improving TCR-Epitope Binding Prediction Models", in *Intelligent Systems For Molecular Biology (ISMB)* 2025.
- ○ **P. Zhang**, F. Guan, X. He, H. Mei, G. Grama, S. Bang, and H. Lee, "Mitigating Goodhart's Law in Epitope-Conditioned TCR Generation Using Plug-and-Play Reward Designs," submitted to *International Conference on Research in Computational Molecular Biology (RECOMB)* 2025.

Representation Learning

- ○ **P. Zhang**, S. Bang, M. Cai and H. Lee, "Context-Aware Amino Acid Embedding Advances Analysis of TCR-Epitope Interactions", in *eLife* 2024.
- ○ **P. Zhang**, S. Bang and H. Lee, "PiTE: TCR-epitope Binding Affinity Prediction Pipeline using Transformer-based Sequence Encoder", in *Pacific Symposium on Biocomputing (PSB)* 2022.

Data-Efficient Machine Learning

- ○ **P. Zhang**, S. Bang and H. Lee, "Active Learning Framework for Cost-Effective TCR-Epitope Binding Affinity Prediction", in *IEEE International Conference on Bioinformatics and Biomedicine (BIBM)* 2023.
- ○ M. Cai, S. Bang, **P. Zhang** and H. Lee, "ATM-TCR: TCR-Epitope Binding Affinity Prediction Using a Multi-Head Self-Attention Model", in *Frontiers in Immunology* 2022.

Patents

- ○ H. Lee, **P. Zhang**, M. Cai, and S. Bang, "Systems and methods for a bidirectional long short-term memory embedding model for T-cell receptor analysis", *US Patent US20240339173*, filed on April 10, 2024.

Awards

- ○ *ACM-ASU Research Symposium and Competition, 1st place in graduate group*, 2025.
- ○ *ASU Outstanding Research Award*, 2024.
- ○ *PSB 23 Travel Award*, 2023.
- ○ *ASU GPSA Travel Grant Individual Award*, 2022.
- ○ *ASU Biodesign Travel Award*, 2022.
- ○ *ASU SCAI Travel Award*, 2022.