Jiaqing Chen

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PROFESSIONAL SUMMARY

- Research Focus: AI4Science, Scientific Machine Learning (SciML), Topological Data Analysis (TDA), High-dimensional Data and Model Visualization, Trustworthy & Explainable AI (XAI).
- Core Expertise: Developing scalable, interpretable ML models for large-scale scientific data. Specialized in loss landscape analysis, uncertainty quantification, and adversarial robustness.
- Research Impact: Authored 8 publications in top-tier conferences (e.g., FPGA, VLDB) and journals (e.g., PMLR, CG&A); developed novel visual analytics tools (e.g., LossLens, Landscaper).
- Collaboration: Successful interdisciplinary collaborations with Lawrence Berkeley National Lab (LBNL), applying ML to diverse domains including computational chemistry, physics, and autonomous systems.

EDUCATION

Arizona State University (ASU)
Ph.D., Computer Science Jan 2021 - Present
Areas of Expertise: AI4Science, Scientific Machine Learning, Topological Data Analysis, High-dimensional Data and Model Visualization, Trustworthy & Explainable AI.

University of California, Riverside (UCR)
M.S., Computer Science Sep 2018 - Mar 2020
Areas of Expertise: Big Data Management & Systems, Spatial & Geospatial Data Analytics, Distributed Data Processing, Data Engineering & Pipeline Development, Data Visualization & Exploration.

University of California, Riverside (UCR)
GPP-E Exchange Student, Computer Science Sep 2017 - Jun 2018
Areas of Expertise: Full-Stack Android Development, Mobile-Centric Architecture, API Integration & Geolocation Services, Stakeholder Collaboration & Civic Technology, User Experience (UX) Design.

Wuhan University of Technology, China (WHUT)
B.E., Computer Science and Technology Sep 2014 - Jun 2018
Areas of Expertise: Full-Stack Mobile Development, Backend Development & Architecture, Database Management, Cross-Platform Programming & Problem-Solving, Collaborative Software Engineering.

NATIONAL LAB EXPERIENCE

Graduate Researcher, Usable Data Systems Group, LBNL May 2025 - Aug 2025
Project: *ManifoldGMM: A Hybrid Framework for Analyzing Multimodal 3D GNN Latent Spaces*

- Investigated the **latent spaces of 3D Graph Neural Networks (GNNs)** applied to real-world molecular tasks, specifically for predicting outcomes in the industrially critical Olefin Hydroformylation reaction.
- Pioneered **a novel hybrid analytical framework** combining Gaussian Mixture Models (GMMs) to capture discrete, multimodal clusters and manifold techniques (Jacobian analysis, pullback metrics) to model smooth, continuous geometric structures.
- Addressed a key challenge in **ML interpretability** by moving beyond standard Euclidean analysis to use manifold-aware distances, which are critical for accurate representation of non-Euclidean molecular data like conformations and reaction pathways.
- Enabled **powerful interpretation of the model's reasoning** by correlating discovered latent structures (GMM clusters, manifold trajectories) with experimental chemical properties, such as product selectivity.
- Provided a **generalizable methodology** for latent space analysis that can be extended to other 3D GNN architectures (SchNet, PaiNN) and molecular applications, from catalysis to protein-ligand binding.

Graduate Researcher, Machine Learning & Analytics Group, LBNL May 2024 - Aug 2024

Project: *Visualizing Loss Functions as Topological Landscape Profiles*

- Introduce a new representation based on topological data analysis that enables the visualization of higher-dimensional loss landscapes named **1D profile landscapes**, to combine key information in both **merge trees** and **persistence barcodes** in higher dimensions.
- Use an **unstructured grid representation** of the loss landscape for **visualization** and further **TDA quantitative analysis**.
- Show how the shape of loss landscapes can reveal new details about **model performance** and **learning dynamics**, highlighting several use cases.
- Provide new insights into how loss landscapes vary across distinct **hyperparameter spaces**.

Graduate Researcher, Machine Learning & Analytics Group, LBNL May 2023 - Aug 2023

Project: *Evaluating Loss Landscapes from a Topology Perspective*

- Architected a novel **quantitative visualization framework** using Topological Data Analysis (TDA) to characterize the underlying topology and structure of high-dimensional neural network loss landscapes.
- Established and implemented three core principles for actionable analysis: **scalability** (via a coordinate-based method), **high-fidelity representation**, and **quantifiability** (using topological data structures).
- Leveraged advanced topological constructs, including **persistence diagrams** and **merge trees**, to efficiently quantify and summarize complex landscape features in a reproducible manner.
- Correlated topological features with machine learning performance by integrating traditional metrics (accuracy, error) and **Hessian-based analyses** (trace, density) to characterize local landscape structure.
- Engineered intuitive visualizations, such as contour plots embedded with topological structures, to clearly communicate complex, high-dimensional insights to diverse audiences.

RESEARCH EXPERIENCE

Graduate Researcher, VADER Lab, SCAI, ASU Jun 2022 - Present

Project: *Landscaper: Visualizing and Quantifying Loss Geometry*

- Introduce Landscaper, which is an **open-source Python package** for **multi-dimensional** loss landscape analysis in **scientific machine learning**.
- Present the first topological study of **3D GNN loss landscapes** in a real-world chemistry task.
- **Novel TDA-based tools** reveal structural patterns invisible to traditional visualization methods.
- Introduce **SMAD**, a metric that quantifies loss landscape smoothness and generalization potential.
- Our findings show that domain-guided data augmentation improves optimization more effectively than manual input design.

Project: *AmigoLUT: Enabling Large-Scale LUT-NNs for Low-Latency Applications*

- Pioneered **AmigoLUT**, a novel ensemble method for lookup-table-based neural networks (LUT-NNs) to overcome the exponential FPGA resource scaling limitations of existing designs like LogicNets.
- Engineered a scalable architecture that linearly increases LUT usage with the number of models, enabling larger and more performant networks while reducing resource consumption by **up to an order of magnitude**.
- Targeted and achieved **nanosecond-scale, low-latency inference** critical for high-performance computing applications in domains like high-energy physics and cybersecurity.
- Optimized the mapping of neural network models directly to FPGA LUTs, maximizing hardware efficiency and throughput for extremely low-latency requirements.

- Addressed the fundamental challenge of neuron fan-in, allowing for the construction of more complex LUT-NNs without exceeding the physical constraints of available FPGA hardware.

Project: *Diagnostics for Machine Learning Models through Loss Landscape Visual Analytics*

- Designed and implemented a novel **multi-scale visual analytics framework** to intuitively explore and diagnose the structure of neural network loss landscapes at **global, semi-global, and local scales**.
- Engineered a unified visual representation that seamlessly integrates metrics from different scales, enabling researchers to identify issues related to model optimization and generalization quickly.
- Validated the framework's **effectiveness and flexibility** through three comprehensive case studies across diverse model architectures and stages of the ML pipeline.
- Applied the diagnostic tool to analyze: **Vision Transformers (ViT)** on corrupted datasets (CIFAR10-C), the impact of **ResNet residual connections**, and failure modes in **Physics-Informed Neural Networks (PINNs)**.
- Provided critical insights into how architectural choices and data quality manifest in the loss landscape, directly linking landscape structure to model performance and robustness.

Project: *High-Performance ONNX Runtime Compiler via MLIR/LLVM*

- Designed and implemented **a compiler pipeline** to parse and transform standard **Open Neural Network Exchange (ONNX)** computational graphs into highly optimized, standalone native code.
- Leveraged the **MLIR (Multi-Level IR) and LLVM compiler frameworks** to perform graph-level optimizations, lower operations to intermediate representations (IR), and generate efficient target-specific machine code for CPU and GPU.
- **Eliminated dependency on a heavyweight runtime engine** by specializing the compiled code for a specific model, resulting in a minimal memory footprint and reduced overhead for embedded and edge computing deployments.
- Implemented a suite of **model-specific optimizations**, such as constant folding, kernel fusion, and static memory planning, to achieve performance comparable to or exceeding that of traditional just-in-time (JIT) inference runtimes.
- Contributed to the **open-source MLIR/LLVM ecosystem** by developing new lowering passes or dialects to bridge the ONNX operator set to existing compiler infrastructure.

Graduate Researcher, CACTUS Data-intensive Systems Lab, SCAI, ASU Jan 2021 - May 2022

Project: *A Comparison of Decision Forest Inference Platforms from A Database Perspective*

- Investigated the performance gap between **standalone ML frameworks (ONNX, TreeLite, TF-DF, HummingBird)** and **integrated in-database** inference by designing and executing a comprehensive benchmark for RandomForest, XGBoost, and LightGBM models.
- Proposed and integrated **a novel "relation-centric" data representation** that significantly optimized processing and memory handling for large-scale models within the database engine.
- Devised **a "model reuse" optimization technique** that drastically accelerated inference on small-scale datasets by minimizing redundant computation, achieving performance gains of up to hundreds of times speedup.
- Authored **a seminal performance analysis**, identifying the ideal use cases for in-database inference: netsDB excels with small models on large datasets and all models on small datasets, providing critical design guidance for the field.

Project: *Serving Deep Learning Models with Deduplication from Relational Databases*

- Pioneered **novel storage optimization techniques**—including duplication detection, page packing, and caching—specifically designed for serving deep learning models within a relational database, addressing the unique challenges of tensor blocks and database page inconsistency.
- Invented **a model deduplication method** that significantly reduced storage space, memory footprint, and cache misses, thereby directly improving inference latency without impacting model accuracy.
- Leveraged the **integrated data management of relational databases** to enable continuous model serving even when working sets exceeded available memory, a key advantage over decoupled deep learning systems like TensorFlow or PyTorch.
- Implemented and validated the **proposed techniques in netsDB**, an object-oriented relational database, demonstrating **a seamless integration of model** serving with core database query processing and storage hierarchy management.
- Proved **superior performance through comprehensive evaluation**, showing that the enhanced database system outperformed standalone deep learning frameworks in storage efficiency and inference latency, particularly for memory-intensive workloads.

Graduate Researcher, The Big Data Lab, BCOE, UCR Jan 2019 - Mar 2020

Project: *Interactive Visualization Server for Geospatial Data Exploration*

- Architected and implemented **an intermediate caching layer** for UCR-STAR to dramatically accelerate response times by storing frequently accessed small images in memory, significantly reducing computational overhead and server load.
- Engineered **a scalable, automated pipeline** for ingesting and visualizing new user-submitted datasets by orchestrating backend processing operations, seamlessly integrating them into the live system without manual intervention.
- Designed and deployed a **NoSQL database solution using MongoDB** to manage metadata for a high volume of datasets efficiently, ensuring rapid retrieval and providing essential dataset information to the frontend upon request.
- **Enhanced overall system performance and user experience** by reducing latency for data visualization requests through strategic caching and optimized database management.

Undergraduate Researcher, Networks and Communications lab, BCOE, UCR Sep 2017 - Aug 2018

Project: *R'Home: A Lightweight Platform for Homeless Community Support*

- **Co-developed "R'Home," a lightweight, dual-client Android application** in collaboration with the Riverside government to provide intuitive support and resources for the local homeless community.
- Engineered **core functionalities using Java and Android Studio**, including real-time user positioning via Google Maps API and a platform for publishing and querying critical information.
- Designed **a fully mobile-centric system** where all operations for both service providers and consumers are performed directly on the Android client, eliminating the need for a complex backend and maximizing accessibility.
- **Focused on user experience and efficiency** to create an intuitive tool that connects individuals with essential services, directly addressing community needs.

Undergraduate Researcher, Wuhan University of Technology (WHUT) Sep 2015 - Jun 2017

Project: *FindNow: An Integrated Intelligent Urban Lifestyle Android Platform*

- **Led the full-stack development of "FindNow," a multi-client Android platform** using Java and Android Studio, designed to streamline daily city life by integrating geolocation services with aggregated e-commerce data.

- Engineered **core functionalities by leveraging Baidu Maps API** for precise positioning and map-based search, creating an intuitive interface for users to navigate and discover local services and online shopping options seamlessly.
- Architected and managed the **backend data infrastructure** using MySQL to efficiently handle big data analysis, user information, and geographic data, ensuring robust performance and scalability.
- **Spearheaded the project's success in national competitions**, securing the **highest prize in the iSoftStone & Y.E.S Software Programming Competition** and the **"Best Smart City Design Award"** for its innovative contribution to intelligent urban design.
- **Delivered a commercially viable product** that received official **software copyright certification** in P.R. China, validating the project's originality, technical execution, and market potential.

Project: *HealthBand: An Advanced Fall Detection & Alert System for Wearables*

- Designed and implemented **a novel fall-detection algorithm** utilizing the Microsoft Band API, processing accelerometer and gyroscope data to accurately distinguish falls from daily activities, now applied in multiple commercial wearable products.
- Engineered a **full-featured Android application in Java** that seamlessly integrated with the wearable to automatically trigger emergency protocols—including retrieving geographic location via Android APIs and initiating automated phone calls and SMS alerts to pre-set contacts.
- Pioneered a **software solution that achieved official software copyright certification** in P.R. China, demonstrating significant novelty and technical execution in the field of health informatics.
- **Garnered top awards at multiple tiers of national independent innovation project competitions**, recognized for the project's practical application, algorithmic innovation, and potential for social impact in elderly care and personal safety.

SCHOLARSHIPS & AWARDS

- ASU Engineering Graduate Fellowship (2025)
- ASU Engineering Graduate Fellowship (2023)
- Third-Class Scholarship(Top 7.8%in Computer Science) (2017)
- Hardworking Advanced Individual (2017)
- Highest Prize in iSoftStone & Y.E.S Software Programming Competition (2017)
- National Scholarship (Top 1 in Computer Science) (2016)
- Merit Student (Top 2% in Computer Science) (2016)
- First-Class Scholarship (Top 1.2% in Computer Science) (2015)
- Merit Student (Top 2% in Computer Science) (2015)
- Third-class Prize in ACM Programming Contest (2015)

TEACHING EXPERIENCE

Teaching Assistant, UCR Sep 2019 - Dec 2019
Software Construction (CS100)

- Mentored students in software engineering best practices, including OOP, design patterns, Git, debugging, and unit testing for real-world projects.
- Provided detailed feedback on code quality, optimization, and architecture to ensure the development of clean, maintainable software.
- Strengthened expertise in scalable software systems and ability to communicate complex technical concepts clearly.

Teaching Assistant, ASU Jan 2022 - May 2022
Database Management (CSE412)

- Instructed students on core database principles, including relational design, SQL optimization, normalization, and transaction management.
- Evaluated assignments and provided detailed feedback on database schemas, query performance, and analytical problem-solving with large datasets.
- Supported the development of robust database management systems (DBMS) by teaching troubleshooting and industry best practices.

TECHNICAL SKILLS

Programming Languages:
Python (Expert), Java (Proficient), C/C++ (Proficient), SQL (Expert), R (Familiar), PHP (Familiar), JavaScript (Familiar), MATLAB (Familiar)

Machine Learning & Deep Learning:
- Core: Scientific Machine Learning (SciML), Topological Data Analysis (TDA), Explainable AI (XAI), Trustworthy ML, Uncertainty Quantification, Adversarial Robustness, Loss Landscape Analysis, Model Diagnostics
- Architectures: Graph Neural Networks (GNNs: SchNet, PaiNN), Vision Transformers (ViT), Physics-Informed Neural Networks (PINNs), ResNets, Lookup-Table Neural Networks (LUT-NNs), Decision Forests (RandomForest, XGBoost, LightGBM)
- Libraries: PyTorch, TensorFlow, Scikit-learn, JAX, ONNX Runtime, HummingBird

Data Engineering & Systems:
- Databases: Relational Databases (MySQL, PostgreSQL), NoSQL (MongoDB), In-Database Inference, Database Management Systems (DBMS)
- Big Data & Distributed Systems: Distributed Data Processing (Spark, Hadoop), Big Data Analytics, Data Pipeline Development, netsDB
- Compilers & High-Performance Computing: MLIR, LLVM, FPGA Programming, High-Latency/Low-Latency Systems, Code Optimization, Native Code Generation

Scientific Computing & Visualization:
- Tools: NumPy, SciPy, Pandas, Matplotlib, Seaborn, Plotly, Paraview, VTK
- Concepts: High-dimensional Data Visualization, Model Interpretation, Geometric Data Analysis, Manifold Learning, Gaussian Mixture Models (GMM)

Software & Tools:
- Development: Git, Docker, Android Studio, Linux/Unix, Bash Scripting
- Cloud & Lab: Experience with HPC clusters (NERSC), Google Cloud Platform (GCP) services

Domain Expertise:
- AI4Science: Computational Chemistry, Molecular Modeling, Catalysis, Physics Simulations
- Geospatial Analytics: Spatial Data Processing, GIS, Google Maps API, Baidu Maps API
- Mobile & Web: Full-Stack Android Development, API Integration, Geolocation Services, UX Design

CERTIFICATE & SPECIALIZATION

- IBM Data Science Professional Certificate
- IBM Applied AI Professional Certificate
- IBM Introduction to Data Science Specialization
- IBM Applied Data Science Specialization
- IBM AI Foundations for Everyone Specialization

SELECTED PUBLICATION

- **Jiaqing Chen***, Nicholas Hadler*, Tiankai Xie*, Rostyslav Hnatyshyn, Caleb Geniesse, Yaoqing Yang, Michael W. Mahoney, Talita Perciano, John Hartwig, Ross Maciejewski, Gunther H. Weber. ”Landscaper: Understanding LossLandscapes Through Multi-Dimensional Topological Analysis” Under Review.
- Nicholas Hadler, N. Ian Rinehart, Masha Elkin, Jeremy Nicolai, Golsa Gheibi, **Jiaqing Chen**, Matthew Avaylon, Ross Maciejewski, Gunther H. Weber, Michael W. Mahoney, Talita Perciano, and John F. Hartwig. ”A 3D, Structure-Based, Deep Learning Approach for Predicting the Regioselectivity of Transition-Metal Catalysis” Under Review.
- Olivia Weng, Andres Meza, **Jiaqing Chen**, Caleb Geniesse, Nhan Tran, and Ryan Kastner. ”PrioriFI: Efficient Fault Injection for Edge Neural Networks” Under Review.
- Olivia Weng, Marta Andronic, Danial Zuberi, **Jiaqing Chen**, Caleb Geniesse, George A Constantinides, Nhan Tran, Nicholas Fraser, Javier Duarte, and Ryan Kastner. ”Greater than the Sum of its LUTs: Scaling Up LUT-based Neural Networks with AmigoLUT” ACM/SIGDA International Symposium on Field-Programmable Gate Arrays (2025)
- Tiankai Xie*, **Jiaqing Chen***, Yaoqing Yang*, Caleb Geniesse*, Ge Shi, Ajinkya Jeevan Chaudhari, John Kevin Cava, Michael W. Mahoney, Talita Perciano, Gunther H. Weber, and Ross Maciejewsk. ”LossLens: Diagnostics for Machine Learning Models through Loss Landscape Visual Analytics.” IEEE Computer Graphics and Applications (2024)
- Caleb Geniesse*, **Jiaqing Chen***, Tiankai Xie*, Ge Shi, Yaoqing Yang, Dmitriy Morozov, Talita Perciano, Michael W. Mahoney, Ross Maciejewski, and Gunther H. Weber. ”Visualizing Loss Functions as Topological Landscape Profiles.” NeurIPS 2024 Workshop on Symmetry and Geometry in Neural Representations (NeurReps).
- Tiankai Xie*, Caleb Geniesse*, **Jiaqing Chen***, Yaoqing Yang, Dmitriy Morozov, Michael W. Mahoney, Ross Maciejewski, and Gunther H. Weber. ”Evaluating Loss Landscapes from a Topology Perspective.” NeurIPS 2024 Workshop on Scientific Methods for Understanding Deep Learning (SciForDL).
- Lixi Zhou, **Jiaqing Chen**, Amitabh Das, Hong Min, Lei Yu, Ming Zhao, and Jia Zou. ”Serving Deep Learning Models with Deduplication from Relational Databases.” VLDB 2022, PVLDB Volume 15 Issue 10.