Kian Maleki — Research Scientist | Machine Learning | Scientific Computing | Physics PhD

+1 (737) 600 9803 | kian@drkianmaleki.com | drkianmaleki.com | linkedin.com/in/kian-maleki-phd | github.com/drkianmaleki

University of Iowa (2026) PhD in Physics (GPA: 4.03) | Creighton University (2017) MS in Physics (GPA: 4.00)

Research Profile

- Research scientist with a PhD in physics and experience in mathematical modeling, scientific computing, machine-learning methodology, and high-dimensional data analysis.
- Developed reproducible computational frameworks for complex physical systems, classifier evaluation, uncertainty/ambiguity analysis, learning-curve extrapolation, and document intelligence.
- Published peer-reviewed research in *Physical Review B* and *Nano Letters*; current machine-learning research focuses on diagnostic evaluation of classifiers and conservative prediction of gradient-boosting learning curves.

Research Experience

University of Iowa | Graduate Research Assistant, Physics Aug 2018 – Aug 2025

- Developed high-dimensional numerical models for complex physical systems, combining statistical inference, optimization, and large-scale simulation.
- Optimized computational workflows, reducing simulation runtime from days to under one hour through algorithmic improvements and efficient implementation.
- Analyzed noisy, high-dimensional experimental and simulation data to identify structure, extract signal, and validate theoretical predictions.
- Contributed to peer-reviewed publications in condensed matter physics, quantum materials, and solid-state integration of quantum devices.

Creighton University | Graduate Research Assistant, Physics Aug 2015 – Aug 2018

- Built simulation-based models for physical systems using Python and Fortran, including N-body simulations and molecular dynamics.
- Designed parallelized computation pipelines for large-scale simulations, improving scalability with HPC resources.
- Developed interactive scientific software tools for simulation and analysis, enabling user-driven exploration of model behavior.

Creighton University | Assistant Professor of Physics Aug 2025 – Present

- Teach undergraduate physics courses emphasizing quantitative reasoning, modeling, optics, electronics, and applied problem-solving.
- Developed interdisciplinary lab curriculum integrating AI tools and chatbots into scientific workflows while emphasizing responsible and ethical use.
- Supervise and mentor teaching assistants across large-enrollment courses.

Machine Learning and Applied AI Research

Sequence Acceleration Benchmark for Gradient Boosting 2026

Tech: Python, XGBoost, Scikit-Learn, NumPy, Statistical Testing, Reproducible Benchmarking

link: https://github.com/drkianmaleki/sequence-acceleration-benchmark

- Developed a benchmark for finite-horizon learning-curve prediction in gradient boosting, evaluating 51 sequence-acceleration methods from 13 families across 18 synthetic convergence regimes.
- Studied regime dependence, failure detection, perturbation diagnostics, adaptive selection, and conservative extrapolation rules for reliable learning-curve forecasts.
- Submitted the associated manuscript to *Machine Learning*: "Finite-Horizon Learning-Curve Prediction for Gradient Boosting: Regime Dependence, Failure Detection, and Conservative Extrapolation Rules."

Ambiguity Range Framework 2026

Tech: Python, Scikit-Learn, XGBoost, PyTest, Statistical Testing, Model Evaluation

link: https://github.com/drkianmaleki/ambiguity-framework

- Developed a model-agnostic diagnostic framework for evaluating binary classifiers beyond global metrics such as AUC-ROC.
- Introduced ambiguity-focused metrics that quantify prediction concentration near decision boundaries and threshold-sensitive degradation in precision, recall, and F1.
- Built reproducible experiments with calibration analysis, bootstrap confidence intervals, paired statistical tests, and automated test coverage.

PDF Document Intelligence Extractor 2026

Tech: Python, NLP, Regex, Pandas, PDF Text Extraction, RAG

link: https://github.com/drkianmaleki/PDF-Document-Intelligence-Extractor

- Built a document intelligence pipeline to extract structured regulatory information from PDFs using native text-layer parsing.
- Developed rule-based and NLP extraction methods to identify, normalize, and structure information from semi-structured documents.

RAG-Powered Knowledge Assistant 2026

Tech: Python, PyTorch, Transformers, NLP, Docker

link: https://github.com/drkianmaleki/RAG-Powered-Knowledge-Assistant

- Built a local retrieval-augmented generation system for document question answering with context-aware responses.
- Designed chunking and retrieval strategies to preserve semantic continuity across long documents and reduce unsupported responses.

Technical Expertise

- **Research Methods:** Mathematical modeling, statistical inference, uncertainty analysis, hypothesis testing, bootstrap confidence intervals, paired statistical tests, Monte Carlo simulation.
- **Machine Learning:** Scikit-Learn, XGBoost, PyTorch, TensorFlow, Transformers, calibration analysis, model evaluation, NLP, RAG, MLflow.
- **Scientific Computing:** Python, NumPy, Pandas, Polars, Numba, Fortran, Linux/Bash, HPC, MPI, multithreading, numerical optimization.
- **Engineering and Reproducibility:** Git, GitHub Actions, pytest, Docker, DVC, FastAPI, Pydantic, AWS S3/EC2, reproducible experiment design.

AI and Machine Learning Training

TripleTen | AI & Machine Learning Program 2026

- Completed project-based training in supervised and unsupervised learning, deep learning, NLP, computer vision, feature engineering, and model evaluation.
- Built end-to-end machine-learning projects using Scikit-Learn, Python, SQL, Git, and modern ML workflows.

Extern, Pfizer | AI-Powered Document Intelligence Externship 2026

- Developed document intelligence workflows for healthcare documents using native PDF text extraction, advanced OCR-aware workflows, LLMs, and RAG architectures.
- Built retrieval-augmented pipelines to improve accuracy and reduce hallucinations in document-based question-answering systems.

Selected Publications

- Maleki, K. (2026). "Finite-Horizon Learning-Curve Prediction for Gradient Boosting: Regime Dependence, Failure Detection, and Conservative Extrapolation Rules." *Machine Learning*, submitted.
- Maleki, K. (2026). "The Ambiguity Range Framework: A Diagnostic Toolkit for Operational Evaluation of Binary Classifiers." Manuscript under review.
- Maleki, K. et al. "Crystal fields, exchange and dipolar interactions..." *Physical Review B*, 2025.
- Maleki, K. et al. "A General and Modular Approach to Solid-State Integration..." *Nano Letters*, 2025. Related to a patented quantum device.