

Taiwo A. Adebiyi

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Education

University of Houston

PhD, Civil Engineering (Focus: Probabilistic Machine Learning & Optimization)

Houston, TX, USA

August 2022—May 2027 (Expected)

- Thesis: “Towards Smart Infrastructure: Digital Twins, Bayesian Optimization and Large Language Models as Key Enablers”
- GPA: 3.94/4.00 | Advisor: Dr. Ruda Zhang

Nigerian University of Technology and Management

PG Cert., Technology, Entrepreneurship, & Design

Lagos, Nigeria

August 2021—August 2022

- Distinction | Overall Best in All-round Academic Excellence

University of Lagos

BSc., Civil Engineering

Lagos, Nigeria

December 2015—September 2021

- First Class (Honors) | Vice Chancellor’s Overall Best Student in Service Delivery

Research Experience

Uncertainty Quantification Lab—University of Houston

Houston, TX, USA

Graduate Research Assistant

August 2022—Present

- Conducting research in Bayesian optimization, Gaussian processes, and foundation models with applications in high-risk decision-making.
- Developing uncertainty-aware training methods for foundation models, improving robustness for forecasting and risk detection.
- Building scalable ML algorithms for optimization under uncertainty, bridging academic ML to real-world infrastructure systems.
- Open-source ML libraries creation and contributions:
 - TSRoots: Python package for Gaussian Process Thompson Sampling via rootfinding for improved Bayesian optimization.
 - BoTorch (Meta): Contributed to the pathwise sampling features in the popular PyTorch-based Bayesian optimization library.

Chevron | UH Energy

Houston, TX, USA

Graduate Research Fellow

August 2025—Present

- Applying probabilistic machine learning and optimization to quantification of geologic hydrogen.
- Integrating Bayesian models into risk and resource forecasting frameworks.

Nigerian University of Technology & Management | First E & P Development

Lagos, Nigeria

Visiting Graduate Research Scholar

May 2022—July 2022

- Investigated digital twin frameworks for large-scale engineering systems with simulation-driven decision optimization.

Software & Technical Contributions

BoTorch (Meta AI): Rebased pathwise condition sampling features for Bayesian optimization in PyTorch ([GitHub link](#))

2025

TSRoots: Python package for efficient Gaussian process Thompson sampling in Bayesian optimization via rootfinding ([GitHub link](#))

2024

LS-DYNA-GPS: Automated LS-DYNA Keyword file changes using QD Library ([GitHub link](#))

2023

GPyS: Gaussian Process Subspace Prediction, a Python Implementation ([GitHub link](#))

2022

Publications (Selected)

1. **Adebiyi, T.A.**, Do, B., & Zhang, R. (2025). Optimizing Posterior Samples for Bayesian Optimization via Rootfinding. In *Proceedings of the Thirteenth International Conference on Learning Representations (ICLR)*, 2025. ([link](#))
 - Average rating: 7.0 (top 8% out of over 11,000 submissions).
2. **Adebiyi, T.A.**, Do, B., & Zhang, R. (2024). Gaussian Process Thompson Sampling via Rootfinding. In *Proceedings of the NeurIPS 2024 Workshop on Bayesian Decision-making and Uncertainty (BDU)*. ([link](#))
 - Oral presentation (1 of 6; top 5% of accepted papers).
3. **Adebiyi, T. A.**, Ajenifuja, N. A., & Zhang, R. (2024). Digital Twins and Civil Engineering Phases: Reorienting Adoption Strategies. *Journal of Computing and Information Science in Engineering*. ([link](#))
4. Do, B., Ajenifuja, N. A., **Adebiyi, T. A.**, & Zhang, R. (2025). Sampling from Gaussian Processes: A Tutorial and Applications in Global Sensitivity Analysis and Optimization. arXiv preprint (under review @ Springer Nature SMO – [link](#))
5. Do, B., **Adebiyi, T.A.**, & Zhang, R. (2024). Epsilon-Greedy Thompson Sampling to Bayesian Optimization. *Journal of Computing and Information Science in Engineering*. ([link](#))

6. Do, B., Ghalekohneh, SJ., Adebiyi, T.A., Zhao, B., Zhang R. (2024). Automated Design of Nonreciprocal Thermal Emitters via Bayesian Optimization. *Journal of Quantitative Spectroscopy and Radiative Transfer*. ([link](#))

Academic Presentations

Optimizing Posterior Samples for Bayesian Optimization via Rootfinding

International Conference of Learning Representation (Top 8% Poster @ Main Conference Track)

Singapore Expo, Singapore

April 24—28, 2025

Gaussian Process Thompson Sampling via Rootfinding

NeurIPS 2024 Workshop on Bayesian Decision-making and Uncertainty (Oral)

Vancouver, BC, Canada

December 10—15, 2025

Optimizing ADCIRC simulations using AI/ML-Based Surrogates

NHERI Computational Academy at Texas Advanced Computing Center

Austin, TX, USA

July 23—26, 2024

Digital Twin and Civil Engineering Phases: Reorienting Adoption Strategies

Engineering Mechanics Institute Conference and Probabilistic Mechanics & Reliability Conference 2024

Chicago, IL, USA

May 26—31, 2024

Core Skills

Machine / Deep Learning:

- ❖ Bayesian Optimization, Gaussian Processes, LLMs, Scientific Foundation Models (ViTs), Probabilistic ML (GANs, VAEs)

Programming Languages & Libraries:

- ❖ Python (NumPy, Pandas, scikit-learn, PyTorch, TensorFlow, JAX), Scala/Spark (familiarity), MATLAB, R, C

Software Development:

- ❖ Git/GitHub, HPC & distributed computing, Code Coverage and Testing, Linux

Applications:

- ❖ Adaptive Experimentation, Resource Forecasting, Algorithmic Development, Optimization

Fellowships / Grants / Awards (Selected)

Chevron – UH Energy Graduate Fellowship (<i>Research Grant</i>)	2025
ICLR Travel Award (<i>Travel Grant</i>)	2025
NeurIPS BDU Google Travel Award (<i>Travel Grant</i>)	2024
Jimmie A. Schindewolf Academic and Research Scholarship (<i>Study Grant</i>)	2024
NSF DesignSafe CI Travel Grant, University of Texas at Austin (<i>Travel Grant</i>)	2024
Cullen Fellowship Travel Grant, University of Houston (<i>Travel Grant</i>)	2024
Fellow, Blue Innovation Partnerships Consortium, Purdue University & University of Puerto Rico (<i>Research Fellowship</i>)	2023
Inclusive Excellence Admission Scholarship, University of Toronto (<i>Study Grant</i>) – Declined	2022
Winner, Circular Economy Innovation Partnership Looplab Incubation Challenge (<i>Business Grant</i>)	2022
Winner, Nigerian Institute of Civil Engineers Open Defecation Design Challenge (<i>Research Grant</i>)	2021
Winner, Sixth Annual Millennium Oceans Prize (<i>Research Grant</i>)	2021
NNPC/Chevron JV Scholarship (<i>Study Grant</i>)	2017–2021
Federation of Construction Scholarship (<i>Study Grant</i>)	2017–2021

Teaching Experience

Structural Analysis (CIVE 3337: University of Houston)	2023—2025
Professional Practice in Civil Engineering (CIVE 4311: University of Houston Dalian Maritime Institute)	2024

Volunteering / Leadership Experience

Vice President, Civil Engineering Graduate Students Organization (University of Houston)	2024–2025
Tertiary Officer, Redeemed Christian Church of God JPFAN (University of Houston)	2024
President, Nigeria Institute of Civil Engineering Students' Association (UNILAG)	2020–2021
President, Sustainable Development Advocates	2019–2021
Africa Team Lead, Millennium Fellowship Global Admission Committee	2020
Campus Director, United Nations Academic Impact Millennium Fellowship	

Academic and Professional Affiliations

United States Association for Computational Mechanics (USACM). *Technical Thrust Area in Uncertainty Quantification and Probabilistic Modeling. Graduate Student Member.*

Society for Industrial and Applied Mathematics (SIAM). *Graduate Student Member.*