ABIN SHAKYA

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EDUCATION

Louisiana State University, Baton Rouge — *Advisor: Dr. Bijaya Karki*
PhD in Computer Science : 4.062/4.0 GPA — *Aug 2021 - May 2026 (Expected)*
Relevant Courses : Applied Deep Learning, Bayesian Data Analysis,
Machine Learning, Big Data Analysis, Statistics 7004, Statistics 7014, Algorithm Design and Analysis

Tribhuvan University, Kathmandu, Nepal — *Advisor: Dr. Subarna Shakya*
BE in Computer Engineering: 3.6 GPA (US Scale) — *Nov 2013 - Nov 2017*

EXPERIENCES

Louisiana State University, Baton Rouge
Position: Research Assistant — *Aug 2021 - Present*

- Working on **Geometric Generative Modeling** to create precise atomic configurations, maintaining structural integrity and compliance with essential physical constraints.
- Building **Graph Neural Network-accelerated** Molecular Dynamics to explore atom distribution in Earth's core.
- Designed an active learning framework for molecular dynamics, utilizing iterative data sampling and model training cycles to continuously enhance model accuracy.
- Developed deep learning-based potential energy models for molecular dynamics, facilitating simulations of Earth's interior, and authored the paper **Insights into core-mantle differentiation from bulk Earth melt simulations**. DOI: 10.1038/s41598-024-69873-8
- Conducted binning analysis to identify bimodal distribution and verify core-mantle segregation using strongly connected components. Also created a 3D convex hull to model the Earth's core boundary, employing various methods for validation.
- Developed a **transformer-based generative AI model** that composes original piano music, crafting expressive and dynamic melodies for an immersive listening experience.
- Implemented a state-of-the-art Bayesian Neural Network architecture to address prediction uncertainty in X-ray dataset, contributing to more reliable and robust predictions.

Sparrow Private Limited, Lalitpur, Nepal — *Oct 2017 - Sep 2021*
Position: Software Engineer

- API Integration: Developed a middleware layer to integrate multiple SOAP and REST APIs into a unified REST API, facilitating applications for flight and hotel bookings, and implementing secure online payment solutions.
- Performance Optimization: Enhanced a flight search engine using caching and parallel programming techniques, significantly improving search efficiency and user experience.
- Automation and Code Maintenance: Build task schedulers for automating financial reporting and transactions, **led the migration of the codebase from Django 1.8 to 2.2**, and documented APIs in Swagger.

SKILLS

Programming Language:	**Python**, **R**, JAVA, C, C++, SML, SAS, SQL, MATLAB
Frameworks/Libraries:	**Pytorch, Tensorflow**, Django/DRF, PySpark, Keras, Pandas, Numpy, Scikit-Learn, Matplotlib, PyG, HPC, Seaborn
Tools, Technologies, DB:	PostgreSQL, MongoDB, SparkSQL, PySpark, Apache Kafka, Apache Hadoop Amazon S3, Nginx, Redis, RabbitMQ, Latex
ML skills:	**Graph Learning, Representation Learning**, Generative AI, Transformers, GANs, Variational Auto Encoders, Stable Diffusion, LLMs, PINN, Model Optimization for Edge, Fine-Tuning LLMs
Time Series Analysis / Statistics:	ARIMA, SARIMA, GARCH, Exponential Smoothing, Gibbs sampling, MCMC, PCA, SVD, A/B testing, ANOVA analysis

PAPERS, AWARDS AND RECOGNITIONS

- **Shakya, A.*, Ghosh, D.B., Jackson, C., Morra, G., Karki, B.B. (2024). Insights into core-mantle differentiation from bulk Earth melt simulations. Scientific Reports. DOI: 10.1038/s41598-024-69873-8.**
- Shakya, A.*, Pokharel, A., Bhattarai, A., Sitikhu, P., Shakya, S. (2018). Real-Time Stock Prediction Using Neural Network. 8th International Conference, Confluence 2018— IEEE. ISBN: 978-1-5386-1720-5.
- Enrolled in a fully Funded PhD Program : NASA Emerging Worlds Research Grant, Computer Science, LSU, 2021/22
- Enrolled in a fully funded Bachelor's Program: Merit based scholarship for securing 26th Rank in Engineering Entrance Examination (From a pool of 15000+ applicant)