PADAVINANGADY NAKUL BHAT

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⌱ GitHub   in LinkedIn   ⚙ Scholar   🔗 Website

Education

B. Tech (Hons.), Computer Science and Engineering (AI & ML)   Jul. 2023—May 2027
Manipal Institute of Technology, Manipal, India   CGPA: 8.56/10.00 (3.42/4.00)

Skills & Tools

Programming & Core: Python; C++; C; Java; SQL; Lua; Nix; Shell scripting; Git
Machine Learning & AI: scikit-learn; XGBoost; SHAP; QLattice; PyTorch; OpenCV
Specialized Tools: LaTeX; RDKit; Flask; Hugo; pybind11; Docker

Relevant Experience

Summer Research Fellow   May 2025—July 2025
Indian Institute of Science, Bengaluru

- Selected for the prestigious IASc-INSA-NASI Summer Research Fellowship, a program with <5% acceptance rate, based on academic merit and research proposal.
- Advanced the GenetiGraph project under Dr. Debnath Pal through the development of a supporting library and completion of my fellowship thesis.

Featured Projects

GenetiGraph: A Genetics Framework For AI   Sep. 2024—Present
Tools: C++, Python, pybind11, Git, Github Actions

- Designed and implemented an efficient binodal mixed-graph data structure to represent complex genetic pedigrees, supporting remarriage, sibling ordering, and rich genotypic annotations. [Patent Pending]
- Invented a modular, partner-independent mathematical model enabling constant-time $\mathcal{O}(1)$ inheritance simulation across arbitrary family structures, with robust handling of incomplete or missing pedigree data. [Preprint. Publication Pending]
- Secured institutional ethical clearance for primary data collection to validate the mathematical model as well as library performance.

ToxiTox: Structure-Based Toxicity Prediction   Jul. 2024—Present
Tools: Python, Flask, RDKit, Git, PubChem API

- Designed, built, and deployed a full-stack cheminformatics web application for structure-based molecular toxicity prediction using a proprietary fuzzy-matching algorithm.
- Generated a custom, benchmark-ready dataset by applying the prediction tool's structure-matching results, creating a novel resource to advance toxicity research [Preprint in progress].

AI Framework for Hypothesis Generation in CKD Diagnosis   Aug. 2024—Present
Skills & Tools: Python, scikit-learn, XGBoost, SHAP, ELI5, QLattice, Git

- Engineered an AI framework for CKD diagnosis; evaluated 22 models across multiple datasets and achieved 99.5% accuracy using Stratified K-Fold Cross-Validation.
- Leveraged Explainable AI (XAI) to identify key clinical features and data patterns, generating novel, clinically-validated diagnostic hypotheses for Chronic Kidney Disease [Paper Under Review].

Featured Publications

Bhat, P. N., S. Balaji, and P. Shapshak, A Review of AI Tools in Molecular Biology and Virology. In: P. Shapshak et al. (eds.), *Global Virology V: 21st Century Vaccines and Viruses.* Springer Nature Switzerland, Cham, pp. 739–759, 2025. doi: 10.1007/978-3-031-77911-4_30

Bhat, P. N. and D. Pal, Genetic Expectations in Inheritance: A Probabilistic Algebraic Framework. *bioRxiv*, 2025. doi: 10.1101/2025.06.12.659255