

Chitra Karki

Department of Mathematical Sciences

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CURRICULUM VITAE

Education

The University of Texas at El Paso | El Paso, TX

Ph.D., Candidate | Data Science

- Dissertation: "A Robust Elastic-Net Logistic Regression Framework for Classification with Contamination."

M.S., Computational Science | 08/2021

- Thesis: "Interaction of Kinesin-5 Motor Domain with Tubulin Dimer."

M.S., Physics | 08/2019

- Thesis: "Computational Study of Disease-Related Proteins from an Electrostatic Point of View."

Research Experience

Graduate Research Assistant | The University of Texas at El Paso | Various Semesters | 08/2019 - Present

- Developed robust elastic-net logistic regression methods for high-dimensional classification with contaminated data.
- Investigated environmental drivers of West Nile virus mosquito vectors' abundance using zero-inflated mixed models, informing public health monitoring.
- Applied advanced statistical and computational methods (PCA, probability modeling, etc.) to analyze protein structure and energy fluctuations in large-scale simulation data.
- Conducted computational studies of protein interactions (TB, SARS-CoV-2, Dengue, molecular motors, etc.)
- Built custom analysis pipelines and bioinformatics tools in R, Python, and Bash ([Structure Manipulation Tool](#), [Bound Ions Prediction](#)).
- Mentored five students (four undergraduate, one graduate), leading to four co-authored peer-reviewed publications and one completed master's thesis.
- Published findings in 13 peer-reviewed journals and presented at multiple national conferences.

Publications

1. Vera AJ, Soliz AG, Vera KR, Ortega OJ, **Karki CB**, Su X, Lavretsky P, de la Mora-Covarrubia A, Watts DM. "Meteorological Effects on the Abundance of West Nile Virus Mosquito Vectors in Two Communities Located on the Texas-Mexico Border in the Northern Chihuahuan Desert". *Vector Borne Zoonotic Dis.* 2025 Sep 24. doi: 10.1177/15303667251382345. Epub ahead of print. PMID: 40991427.
2. Sun Shengjie, **Chitra Karki**, Bruce Z. Gao, and Lin Li. "Molecular mechanisms of cardiac actomyosin transforming from rigor state to post-rigor state." *The Journal of Chemical Physics* 156, no. 3, 2022.
3. Sun Shengjie, **Chitra Karki**, Javier Aguilera, Alan E Lopez Hernandez, Jianjun Sun, and Lin Li. "Computational Study on the Function of Palmitoylation on the Envelope Protein in SARS-CoV-2." *Journal of Chemical Theory and Computation* 17, no. 10, 2021.

4. Xie, Yixin, **Chitra B Karki**, Jiawei Chen, Dongfang Liu, and Lin Li. "Computational Study on DNA Repair: The Roles of Electrostatic Interactions between Uracil-DNA Glycosylase (Udg) and DNA." *Frontiers in Molecular Biosciences* 8, 2021.
5. Xian Yuejiao, Yixin Xie, Sebastian Miki Silva, **Chitra B Karki**, Weihong Qiu, and Lin Li. "Structureman: A Structure Manipulation Tool to Study Large Scale Biomolecular Interactions." *Frontiers in Molecular Biosciences* 7, 2021.
6. Sun Shengjie, **Chitra Karki**, Yixin Xie, Yuejiao Xian, Wenhan Guo, Bruce Z Gao, and Lin Li. "Hybrid Method for Representing Ions in Implicit Solvation Calculations." *Computational and Structural Biotechnology Journal* 19, 2021.
7. Xie Yixin, Dan Du, **Chitra B. Karki**, Wenhan Guo, Alan E. Lopez-Hernandez, Shengjie Sun, Brenda Y. Juarez, Haotian Li, Jun Wang, and Lin Li. "Revealing the mechanism of SARS-CoV-2 spike protein binding with ACE2." *Computing in Science & Engineering* 22, no. 6, 2020.
8. Xie Yixin, **Chitra B. Karki**, Dan Du, Haotian Li, Jun Wang, Adebiyi Sobitan, Shaolei Teng, Qiyi Tang, and Lin Li. "Spike proteins of SARS-CoV and SARS-CoV-2 utilize different mechanisms to bind with human ACE2." *Frontiers in Molecular Biosciences*, 2020
9. Wang Jun, **Chitra Karki**, Yi Xiao, and Lin Li. "Electrostatics of Prokaryotic Ribosome and Its Biological Implication." *Biophysical Journal*, 2020.
10. Aguilera Javier, **Chitra B Karki**, Lin Li, Salvador Vazquez Reyes, Igor Estevao, Brian I Grajeda, Qi Zhang, Chenoa D Arico, Hugues Ouellet, and Jianjun Sun. "Na-Acetylation of the Virulence Factor EsxA Is Required for Mycobacterial Cytosolic Translocation and Virulence." *Journal of Biological Chemistry* 295, no. 17, 2020.
11. **Karki Chitra**, Yuejiao Xian, Yixin Xie, Shengjie Sun, Alan E Lopez-Hernandez, Brenda Juarez, Jun Wang, Jianjun Sun, and Lin Li. "A Computational Model of Esat-6 Complex in Membrane." *Journal of Theoretical and Computational Chemistry*, 2020.
12. Salas Gicela G. Saucedo, Alan E. Lopez Hernandez, Jiadi He, **Chitra Karki**, Yixin Xie, Shengjie Sun, Yuejiao Xian, and Lin Li. "Using Computational Approaches to Study Dengue Virus Capsid Assembly." *Computational and Mathematical Biophysics* 7, no. 1, 2019.
13. Y Xian, **C karki**, Lin Li. "Revealing the essential role of protein-protein interactions in viral capsid assembly." Abstracts of Papers of the *American Chemical Society*, 258, 2019
14. (Cover figure paper) Xian, Yuejiao†, **Chitra B Karki**†, Sebastian Miki Silva, Lin Li, and Chuan Xiao. "The Roles of Electrostatic Interactions in Capsid Assembly Mechanisms of Giant Viruses." *International journal of molecular sciences* 20, no. 8, 2019 († these authors contribute equally).

Ongoing Projects

- **Methodological:** Evaluating performance of the robust elastic-net logistic regression framework via comprehensive simulation studies (with Dr. Xiaogang Su).
- **Applied Machine Learning:** Building predictive models (Logistic Regression, Random Forest, SVM, ANN, etc.) to investigate the effects of point mutation on protein binding energy (with Dr. Xiaogang Su, Dr. Lin Li).
- **Predictive Analytics:** Developing predictive models, ensembles, and survival analyses to improve graduate student retention and graduation outcomes at UTEP (with Dr. Xiaogang Su, Dr. Stephen Crites).

Software and Visualization Projects

- **RobENetLog** | Method Development | R Package | github.com/cbkarki/RobENetLog
Created a GitHub repository with helper functions and ongoing method development – a robust elastic-net logistic regression framework to handle feature and response space contamination in high/low-dimensional data.
- **gradUtilities** | R Package | github.com/cbkarki/gradUtilities
Developed a collection of custom R functions for student data processing, cleaning, wrangling, and automation.

- **Projects Repository** | Interactive Data Visualization and Teaching Apps | github.com/cbkarki/Projects
- **Central Limit Theorem Visualizer:** Created an interactive R Shiny app illustrating the Central Limit Theorem through real-time sampling simulations and distribution plots.
- **Monte Carlo π Estimation:** Developed an interactive R Shiny app that visualizes the Monte Carlo simulation process for estimating π .
- **UTEP Food Pantry Dashboard:** Designed an interactive R Shiny dashboard to study how the federal aid usage relates to student food insecurity and academic progress, identifying patterns across gender and ethnicity.

Teaching Experience

Graduate Teaching Assistant and Math Tutor | The University of Texas at El Paso | Various Semesters | 08/2017 - 05/2023

- Led workshops, computer labs, and office hours for graduate and undergraduate students, including Data Mining, Statistical Inference, Differential Equations, and Applied Mathematics.
- Tutored students in Statistics, Linear Algebra, and Calculus; advised projects in R, Excel, and Python.
- Assisted faculty in course administration, grading, and providing constructive feedback to enhance student learning outcomes.

Physics Lecturer | Liverpool International College | Kathmandu, Nepal | 06/2016 – 06/2017

- Independently designed and delivered lectures on Mechanics, Optics, and Electromagnetism.
- Supervised laboratory sessions, managed course assessments, and provided individualized academic support to students.

Professional Experience

Doctoral Assistant | Graduate School | The University of Texas at El Paso | 06/2023 - Present

- Developed interactive Power BI dashboards tracking the admissions funnel, from applications to enrollments, as well as graduation indicators.
- Automated ETL workflows in R and Power BI, reducing reporting time by over 70%.
- Trained one staff member and three student hires in data cleaning, visualization, and automated reporting workflows.
- Produced ad-hoc data reports for Graduate School leadership and the Provost's Office.
- Ensured reproducibility through proper project documentation.

Skills

- **Programming and Analysis:** R | Python | SQL | Bash | C | MATLAB | Excel
- **Computational Modeling:** NAMD | VMD | Chimera | Delphi | Charmm-GUI
- **Data Visualization and Reporting:** Power BI | R (Shiny, Markdown) | LaTeX | GitHub
- **Databases:** PostgreSQL
- **HPC:** HPC clusters TACC
- **Operating Systems:** Unix | Windows

Certifications and Professional Development

- Excel Essentials for Data Analytics | Excel Essentials for Statistics Coursera (2025)
- Querying Databases with SQL | Relational Databases (RDBMS) Essentials Coursera (2025)

Awards and Scholarships

- Best Oral Presentation Award, 11th International Conference, New Mexico State University, 2019.
- C. SHARP COOK GRADUATE SCHOLARSHIP FUND, 2019 – 2020.

Presentations

Oral

- **Chitra Karki**, Yuejiao Xian, Virginie Oxaran David, Jianjun Sun, Lin Li. Study of key proteins in Mycobacterium Tuberculosis. *24th joint NMSU/UTEP workshop on Mathematics, Computer Science and Computational Sciences*, New Mexico State University, Las Cruces, NM, April 6, 2019.
- **Chitra Karki**, Yuejiao Xian, Virginie Oxaran David, Jianjun Sun, Lin Li. Effect of pH on the complex of ESAT-6/CFP-10: VdW energy compensates electrostatic energy. 11th International Conference on "Science for all: Role towards Development of Modern World", New Mexico State University, Las Cruces, NM, March 23, 2019.
- **Chitra Karki**, Lindsay Voglewede, Jianjun Sun, Lin Li. Role of Esat-6 in the virulence of Mycobacterium Tuberculosis. *22nd joint NMSU/UTEP workshop on Mathematics, Computer Science and Computational Sciences*, New Mexico State University, Las Cruces, NM, April 7, 2018.

Poster

- **Chitra Karki**, Lin Li. Interactions of the kinesin-5 motor domain and tubulins. *ACS FALL 2021, RESILIENCE OF CHEMISTRY*, Georgia World Congress Center (GWCC), Atlanta, GA, August 22-26, 2021.
- **Chitra Karki**, Lin Li. pH dependency of ESAT-6/CFP-10 in the virulence of Tuberculosis. *RCMI 2019 National Conference on "Collaborative Solutions to Improve Minority Health & Reduce Health Disparities"*, Bethesda Marriott Hotel in Bethesda, MD, December 15-17, 2019.
- Yuejiao Xian, **Chitra Karki**, Sebastian M. Silva, Lin Li, Chuan Xiao. Electrostatics-driven capsid assembly and disassembly of giant viruses. *Graduate Research Expo*, The University of Texas at El Paso, El Paso, TX, November 8-9, 2018.
- **Chitra Karki**, Jianjun Sun, Lin Li. Membrane interaction of ESAT-6 and its role in the pathogenesis of Mycobacterium Tuberculosis. *10th International Conference on "Transforming Lives through Technology and Empowerment"*, New Mexico State University, Las Cruces, NM, March 31, 2018.

Leadership

President | Nepali Student Association | The University of Texas at El Paso | 05/2023 – 08/2024

- Promoted community engagement and cultural exchange through event organizations and collaboration with diverse student organizations.
- Participated in leadership training and provided mentorship to fellow students.