RAVITEJA VANGARA

Contact: 505-488-1420 | **E-mail**: rvangara.phd@gmail.com | **Linkedin**-ravitejavangara |**Present Location**: Los Alamos NM, U.S.A

Motivated researcher *with experience in planning and executing novel high-impact research projects; worked extensively on developing large scale* ***computational*** *models and incorporating* ***machine learning*** *in scientific applications in Physics, Chemistry and Biology. Expert in pattern recognition and feature extraction in unstructured and unlabelled data.*

Postdoctoral Research Associate ***at Los Alamos National Laboratory,*** *PhD in Engineering with Distinction;*

PROFILE SYNOPSIS

- Hands-on 3+ years' experience in implementing machine learning optimizations for unsupervised machine learning; introduced new feature extraction techniques with multiple factor analyses with machine learning and graph clustering methods.
- Experience in working and leading interdisciplinary research teams and executing projects out of my areas of expertise in these collaborations.
- Professional expertise in unsupervised machine learning, with strong foundations of Tensor and matrix decompositions.
- Developed various scientific applications with unsupervised machine learning for pattern recognition and data mining and successfully applied in Physics, Chemistry, Climate and Biology.
- Experience in working under high-paced mission critical projects at Los Alamos National Laboratory with precise timelines and deliverables.
- Published scientific papers in reputed international journals on machine learning applications and a main team member in development teams to produce two opensource softwares and others are on the way:
  - ✓ Non-negative matrix factorization with distributed memory (GitHub: lanl/DnMFk , lanl/pyDnMFk
  - ✓ Symmetric non-negative matrix factorization for unsupervised graphical clustering.
  - ✓ Non-negative matrix factorization with non-linear kernel: *Identification of Anomalous Diffusion* and 1 patent application - *integral transforms through non-linear kernel*.
  - ✓ Semantic NMFk: A Completely unsupervised approach for topic modelling in Natural Language processing, with determination of number of topics with joint factorization technique from nine real world corpuses of BBC, BBC sport, Reuters, Guardian and Newsgroups.
  - ✓ NTFk: Understanding Complex Chemical Reaction Processes by Non-negative Tensor Decompositions

Core Competencies

Machine Learning	Data Collection & Management
Computational Modelling	Data Processing & Analysis
Python programming	Software Development
Tensor and Matrix Factorizations	Team Coordination
	Exploratory data analysis
ML applications for science and technology	High Performance computing

Technical Skills

Python	Parallel Computing
Matlab	Shared and Distributed
Julia	Memory Implementations
LateX & Linux	

EDUCATIONAL QUALIFICATION

2019 **Ph.D. (Engineering)** from University of New Mexico Albuquerque, NM | GPA; 4.04/4.0
2017 **M.S in (Chemical Engineering)** from University of New Mexico Albuquerque, NM | GPA: 4.04/4.0
2015 **B.tech (Chemical Engineering)** from National Institute of Technology, Warangal India | GPA: 7.33/10

EXPERIENCE

Post-Doctoral Research Associate ▸ Los Alamos National Laboratory | Mar 2020 – Present

Projects: (a)Predicting noncoding variants that affect TF-DNA binding and (b) Tensor Networks: Robust Unsupervised Machine Learning for Big-Data Analytics

Role: Markov chain Monte Carlo simulations of DNA, Scientific Machine Learning Developer

- ➢ Large-scale simulations and computations to extract dynamical and structural properties of DNA, from publicly available genomic datasets and development of supervised machine learning tool with multimodal deep neural nets fusion to predict mutations affecting TF-binding which help in formulating biological hypotheses, facilitating the development of targeted therapeutics.
- ➢ Developed various non-negative matrix and tensor factorization techniques using chemical graph theory.

Graduate Research Assistant ▸ Los Alamos National Laboratory | Apr. 2018 – Mar 2020

Project: Development of novel matrix and tensor factorization techniques for applications in chemo metrics and phase transitions

Role: Scientific Machine Learning Developer using Matlab, Julia, Python, C++, bash scripting, and unsupervised learning graphical clustering methods.

Research Brief:
Design & Development of Scalable machine learning developer for high performance computing systems involving shared and distributed memory applications on LANL supercomputers;

Graduate Research Assistant ▸ University of New Mexico, Albuquerque | Dec. 2015 – Apr. 2018

Supervisor: Prof. Dimiter Petsev and Dr. Frank van Swol,
Research Brief:

- Developing density functional models for charged interfaces involving electrolyte solutions; Built a python framework for classical density functional theory coupled with surface charge regulation; model treats solvent explicitly and accounts surface charge basing on thermodynamic chemical equilibrium.
- Observed new physical insights and the steps for a molecular theory to address important features like the role of non-columbic interactions - ionic solvation and surface-ion interactions, on the actual electrostatics of the system i.e. the electric double layer.
- Published six research papers in reputed scientific peer reviewed journals, two conference papers, and two more in preparation.

PUBLICATIONS (Google Scholar)

Unsupervised machine learning:

- Chennupati, Gopinath, **Raviteja Vangara**, Erik Skau, Hristo Djidjev, and Boian Alexandrov. "Distributed non-negative matrix factorization with determination of the number of latent features." The Journal of Supercomputing (2020): 1-31.
- Manish Bhattarai, Gopinath Chennupati, Erik Skau, **Raviteja Vangara**, Hristo Djidjev and Boian Alexandrov "Distributed Non-Negative Tensor Train Decomposition", 2020 IEEE High Performance Extreme Computing.
- **Raviteja Vangara**, Kim Ø. Rasmussen, Dimiter N. Petsev, Golan Bel, and Boian S. Alexandrov. "Identification of anomalous diffusion sources by unsupervised learning." Physical Review Research 2, no. 2 (2020): 023248.
- Akhter, Nasrin, **Raviteja Vangara**, Gopinath Chennupati, Boian S. Alexandrov, Hristo Djidjev, and Amarda Shehu. "Non-Negative Matrix Factorization for Selection of Near-Native Protein Tertiary Structures." In 2019 IEEE International Conference on Bioinformatics and Biomedicine (BIBM), pp. 70-73. IEEE, 2019.
- Akhter, Nasrin, Gopinath Chennupati, **Raviteja Vangara**, Boian S. Alexandrov, Hristo Djidjev, and Amarda Shehu. "Improved Protein Decoy Selection via Non-Negative Matrix Factorization" accepted in IEEE/ACM TCBB.
- Kazi Lutful Kabir, Gopinath Chennupati, **Raviteja Vangara**, Hristo Djidjev, Boian Alexandrov, and Amarda Shehu. "Decoy Selection in Protein Structure Determination via Symmetric Non-negative Matrix Factorization", In 2020 IEEE International Conference on Bioinformatics and Biomedicine (BIBM)
- **Raviteja Vangara**, Erik Skau , Gopinath Chennupati , Hirsto Djidjev , Thomas Tierney , James Smith , Manish Bhattarai , Valentin Stanev , Boian Alexandrov " Semantic Nonnegative Matrix Factorization with Automatic Model Determination for Topic Modeling" in 19th IEEE International Conference On Machine Learning And Applications.

Supervised machine learning / Deep Learning:

- Nebgen, Benjamin, **Raviteja Vangara**, Miguel A. Hombrados-Herrera, Svetlana Kuksova, and Boian Alexandrov. "A neural network for determination of latent dimensionality in Nonnegative Matrix Factorization." Machine Learning: Science and Technology (2020).

Computational Chemistry:

- **R. Vangara**, D.C.R. Brown, F. van Swol, D.N. Petsev, 'Electrolyte Solution Structure and Its Effect on the Properties of Electric Double Layers with Surface Charge Regulation'. JCIS 488, Oct 2016.
- **R. Vangara**, Frank van Swol, and Dimiter Petsev, 'Ionic Solvation and Solvent-Solvent Interaction Effects on the Charge and Potential Distributions in Electric Double Layers', Journal of Chemical Physics.
- **R. Vangara**, Frank van Swol, and Dimiter Petsev, 'Solvophilic and Solvophobic Surfaces and Non-Columbic Surface Interactions in Charge Regulating Electric Double Layers', Journal of Chemical Physics.
- **R. Vangara**, D.C.R. Brown, D.J. Prakash, D.N. Petsev, and F. Van Swol. 'Corrosion and surface charge in electric double layers by classical density functional theory', 2017 Dept. of Defense – Allied Nations Technical Corrosion Conference. 2017. Birmingham, AL.
- **R. Vangara**, F. van Swol, and D.N. Petsev, 'Coulombic and non-Coulombic effects in charge-regulating electric double layers', 2019 Mater. Res. Express 6 086331
- D. J. Prakash, L. Denoyer, **R. Vangara** , J. M. Baca , F. van Swola, and D. N. Petsev 'Classical density functional analysis of the ionic size effects on the properties of charge regulating electric double layers', 2021 Molecular Physics.

Invention Disclosures: Integral transforms through non-linear kernel: Joint disclosure filing between LANL and UNM.

Scholastic Activities

Peer Reviewer for many reputed scientific journals: IOP Machine Learning for Science and Technology, PLOS ONE, Journal of Physical Chemistry, ACS Langmuir, Journal of Contaminant Hydrology and IEEE Access.

Lead PI for Institutional Computing proposal at LANL to perform large scale high-performance computing calculations of non-linear breathing dynamics of DNA, awarding 4.5 million core hours on LANL HPC clusters.

Milton Levy Award of Corrosion Science for poster presented in 2017, DOD Allied Nations Technical Corrosion Conference.

Awarded **International Amigo Scholarship** for graduate studies at UNM

Awarded **Prime Minister (of India) Merit Scholarship (PMSS)** for my under-graduation studies at NIT Warangal, India.

Mentored **two** undergraduate students, **two** Ph.D. interns into to four publications.