Krishnan **Raghavan**

Assistant Computational Mathematician

Mathematics and Computer Science, Argonne National Laboratory

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Summary

My primary research agenda is to develop a mathematical characterization of machine learning (ML) models, their learning/training behavior and the associated precision achieved by them. Towards this end, I study the two broad facets of ML: theory; through the eyes of tools from systems theory, statistics and optimization; and applied; by building AI/ML models to solve key problems in nuclear physics, material science, HPC and more recently climate. I have a strong publication record in the field of ML including 9 journal papers and 12 conference papers and 3 published book chapters with 4 additional publications under review. I also have a strong track record of grants and have been involved in 18 grant proposals, many of them multi-institutional. I am presently a principal investigator on funded multi-institutional proposals worth $\$12M$ (my share $\$5M$) with and my lifetime total of grant awarded amounts to $\$18M$.

Work Experience

Present – 2022 | **Assistant Computational Mathematician, Argonne National Laboratory, Mathematics and Computer Science (MCS)**
Supervisor: Dr. Prasanna Balaprakash.
Continual Learning · Graph Theory · Deep Learning · Optimization

2022 – 2019 | **Postdoctoral Appointee, Argonne National Laboratory, Mathematics and Computer Science (MCS)**
- Scientific Machine Learning.
- Supervisor: Dr. Prasanna Balaprakash.

Deep Learning · Optimization · Statistics · AI for Science

2019 – 2013 | **Graduate Research Assistant, Missouri University of Science & Tech (S&T), Electrical and Computer Engineering (ECE)**
- RFID-based Localization.
- RFID-based Strain Analysis in Composite Materials.
- A Fuzzy Logic-based Controller for PV Shaded Array Using MPPT in MATLAB Simulink.
- Computer Vision-based Asset Tracking.
- A Face Recognition/object Recognition Software using MATLAB.
- A 3D Model Rendering Software Using OpenCV and C++.
- Android App Development for Asset Tracking and Monitoring using QR codes.

Android · RFID · Computer-vision · Matlab · C++ · Python

2018 – 2013 | **Graduate Teaching Assistant, S&T, ECE**
- Control Systems Laboratory.
- Introduction to Electronics.
- Intro to Computer Engineering.

Education

2019 – 2015 | **Ph.D., S&T, Computer Engineering**
- **Dissertation Title:** *Deep Neural Network Learning-based Classifier Design for Big-data Analytics.*
- Supervisor: Prof. Jagannathan Sarangapani.

Deep Neural Networks · Learning-systems · Optimization · Statistics · Dimension-reduction

2014 – 2012 | **M.S., S&T, Computer Engineering**
- **Thesis Title:** *Computer Vision Libraries for Trailer Truck Test Bed.*
- Supervisor: Prof. Levent Acar.

Robotics · Control · Computer vision · Unix

2012 | B.E., V.E.S. Institute of Technology (VESIT), University of Mumbai, India, Instrumentation and Control Engineering

2008 | › Thesis Title: *Modbus Protocol Implementation with ARM7.*
› Supervisor: Prof. Deepthi Khimani.
Robotics | Embedded Systems | Process Control

Grants and Proposals

Funded

6. $8.75M ($1.875M), PI (Argonne), DOE ASCR, Exploring the Power of Distributed Intelligence for Resilient Scientific Workflows, 07/23-06/28.
5. $3.75M ($1.05M), PI (Argonne), DOE ASCR, Platform for Explainable Distributed Infrastructure (PosEiDon), 10/21–9/24.
4. $13M ($525K), Senior Personnel, DOE ASCR, SciDAC-5 Nuclear Computational Low Energy Initiative (NUCLEI), 10/22–9/27.
3. $25k, PI, Argonne National Laboratory Directed Research and Development, Accelerating inversion of nuclear responses with uncertainty quantification, 2021.
2. $2.1M, Co-PI, Argonne National Laboratory Directed Research and Development, Nuclear Quantum Monte Carlo methods for ML and AI techniques, 10/20-9/23.
1. $28,75M, Senior personnel, DOE ASCR, SciDAC-5 Rapids2 Institute.

Pending

2. $3.07M, PI (Argonne), DOE FES, Machine Learning for Advanced Diagnostics and Accelerated Plasma Turbulence Simulations (ML-ADAPTS), 07/23- 06/26.
1. $547,179, Co-PI, DOE SC, Machine Learning Methods for Active target detectors at ATLAS, 09/23- 08/25.

Unfunded

10. Senior Personnel, DOE ASCR, Randomized Algorithms for Continually-Learning Higher-Order Graph Neural Networks, 10/22–9/25.
9. Senior Personnel, DOE HEP, Advancing Uncertainty Quantification and Interpretability of AI models in HEP, 10/22–9/25.
8. Co-PI, Batch Error-driven learning for Accelerating Scientific ML,2021.
7. Co-PI, Federated Neural Architecture Search for Privacy-Preserving AI/ML, 2021.
6. Co-PI, Argonne National Laboratory Directed Research and Development, Hybrid Mixed Integer Programming – Deep Reinforcement Learning Framework for Systematic Process Intensification, 2021.
5. Co-PI,Argonne National Laboratory Directed Research and Development, A Hybrid Approach for Interpretable Modelling of Spatiotemporal Data, 2021.
4. PI, Argonne National Laboratory Directed Research and Development, Continual Domain-adaptation for Simulation Calibration, 2021.
3. Co-PI, Argonne National Laboratory Directed Research and Development, Machine Learning-based Design Optimizer for Molten Salt Reactor, 2020.
2. Senior personnel, DOE ASCR, FAIR Automated Machine Learning for Scientific Data, 2020.
1. Senior personnel, DOE SC, Machine Learning Methods for Nuclear Physics Detectors, 2020.

Publications

Journal Articles IF: Impact Factor

[J9] Hongwei Jin, **Krishnan Raghavan**, George Papadimitriou, Cong Wang, Mandal Anirban, Kiran Mariam, Deelman Ewa, and Prasanna Balaprakash. “Graph Neural Networks for Detecting Anomalies in Scientific Workflows”. In: **International Journal of high performance computing applications (IF:2.457)** (2023). https://journals.sagepub.com/doi/abs/10.1177/10943420231172140?journalCode=hpcc.

[J8] **Krishnan Raghavan**, Melina L. Avila, Prasanna Balaprakash, Heshani Jayatissa, and Daniel Santiago-Gonzalez. “Classification of Events from $\backslashalpha $-Induced Reactions in the MUSIC Detector via Statistical and ML Methods”. In: **Nuclear Inst. and Methods in Physics Research, A (IF: 1.335), Accepted** (2023). https://arxiv.org/pdf/2204.03137.pdf.

[J7] **Krishnan Raghavan**, Vignesh Narayanan, and Sarangapani Jagannathan. "Cooperative Deep Q -Learning Framework for Environments Providing Image Feedback". In: **IEEE Transactions on Neural Networks and Learning Systems (IF:11.683), Accepted** 0.0 (2023), p. 0. DOI: AcceptedforPublicatioin. https://ieeexplore.ieee.org/abstract/document/10012540.

[J6] **Krishnan Raghavan**, Prasanna Balaprakash, Alessandro Lovato, Noemi Rocco, and Stefan M. Wild. "Machine-Learning-Based Inversion of Nuclear Responses". In: **Physical Review C (IF: 3.09)** 103.3 (2021), p. 035502. https://journals.aps.org/prc/abstract/10.1103/PhysRevC.103.035502.

[J5] **Krishnan Raghavan**, Sarangapani Jagannathan, and V. A. Samaranayake. "A Game Theoretic Approach for Addressing Domain-Shift in Big-Data". In: **IEEE Transactions on Big Data (IF: 4.27)** 8.6 (2021), pp. 1610–1621. https://ieeexplore.ieee.org/abstract/document/9424459.

[J4] **Krishnan Raghavan**, Shweta Garg, Sarangapani Jagannathan, and V. A. Samaranayake. "Distributed Min–Max Learning Scheme for Neural Networks With Applications to High-Dimensional Classification". In: **IEEE transactions on neural networks and learning systems (IF:11.623)** 32.10 (2020), pp. 4323–4333. https://ieeexplore.ieee.org/abstract/document/9199282.

[J3] **Krishnan Raghavan**, Sarangapani Jagannathan, and V. A. Samaranayake. "Direct Error-Driven Learning for Deep Neural Networks with Applications to Big Data". In: **IEEE Transactions on Neural Networks and Learning Systems (IF:11.623)** 31.5 (2019), pp. 1763–1770. https://ieeexplore.ieee.org/abstract/document/8763927.

[J2] **Krishnan Raghavan**, V. A. Samaranayake, and S. Jagannathan. "A Hierarchical Dimension Reduction Approach for Big Data with Application to Fault Diagnostics". In: **Big Data Research (IF: 3.739)** 18.0 (2019), p. 100121. https://www.sciencedirect.com/science/article/pii/S2214579619302102.

[J1] **Krishnan Raghavan**, V. A. Samaranayake, and Sarangapani Jagannathan. "A Multi-Step Nonlinear Dimension-Reduction Approach with Applications to Big Data". In: **IEEE Transactions on Knowledge and Data Engineering (IF: 9.235)** 31.12 (2018), pp. 2249–2261. https://ieeexplore.ieee.org/abstract/document/8496836.

Conference Proceedings AR: Acceptance Rate

[C12] Manisha Garg, Tyler Chang, and **Krishnan Raghavan**. "SF-SFD: Stochastic Optimization of Fourier Coefficients to Generate Space-Filling Designs". In: **Winter Simulation Conference, Accepted**. 2023. https://arxiv.org/abs/4905322.

[C11] Romain Egele, Romit Maulik, **Krishnan Raghavan**, Bethany Lusch, Isabelle Guyon, and Prasanna Balaprakash. "Autodeuq: Automated Deep Ensemble with Uncertainty Quantification". In: **26th International Conference on Pattern Recognition (ICPR)**. IEEE, 2022, pp. 1908–1914. https://ieeexplore.ieee.org/abstract/document/9956231.

[C10] Hongwei Jin, **Krishnan Raghavan**, George Papadimitriou, Cong Wang, Anirban Mandal, Patrycja Krawczuk, Loïc Pottier, Mariam Kiran, Ewa Deelman, and Prasanna Balaprakash. "Workflow Anomaly Detection with Graph Neural Networks". In: **IEEE-ACM Workshop on Workflows in Support of Large-Scale Science (WORKS)**. Nov. 2022, pp. 35–42. DOI: 10.1109/WORKS56498.2022.00010.

[C9] **Krishnan Raghavan** and Prasanna Balaprakash. "Continual Learning via Dynamic Programming". In: **International Conference on Pattern Recognition**. 2022. https://ieeexplore.ieee.org/document/9956042.

[C8] Orcun Yildiz, Henry Chan, **Krishnan Raghavan**, William Judge, Mathew J. Cherukara, Prasanna Balaprakash, Subramanian Sankaranarayanan, and Tom Peterka. "Automated Continual Learning of Defect Identification in Coherent Diffraction Imaging". In: **IEEE/ACM International Workshop on Artificial Intelligence and Machine Learning for Scientific Applications (AI4S)**. Nov. 2022, pp. 1–6. https://ieeexplore.ieee.org/document/10027574.

[C7] **Krishnan Raghavan** and Prasanna Balaprakash. "Formalizing the Generalization-Forgetting Trade-off in Continual Learning". In: **Advances in Neural Information Processing Systems (AR:20)**. Vol. 34. 2021, pp. 17284–17297. https://proceedings.neurips.cc/paper/2021/hash/901797aebf0b23ecbab534d61ad33bb1-Abstract.html.

[C6] Shweta Garg, **Krishnan Raghavan**, Sarangapani Jagannathan, and V. A. Samaranayake. "Distributed Learning of Deep Sparse Neural Networks for High-Dimensional Classification". In: **IEEE International Conference on Big Data (AR:18.7)**. IEEE, 2018, pp. 1587–1592. https://ieeexplore.ieee.org/abstract/document/8621888.

[C5] **Krishnan Raghavan**, Sarangapani Jagannathan, and V. A. Samaranayake. "A Minimax Approach for Classification with Big-data". In: **IEEE International Conference on Big Data (AR: 18.7)**. IEEE, 2018, pp. 1437–1444. https://ieeexplore.ieee.org/abstract/document/8622564.

[C4] **Krishnan Raghavan**, Sarangapani Jagannathan, and V. A. Samaranayake. "Direct Error Driven Learning for Deep Neural Networks with Applications to Bigdata". In: **International Conference on Big Data and Deep Learning**. Vol. 144. Elsevier, 2018, pp. 89–95. https://link.springer.com/chapter/10.1007/978-3-030-31764-5_1https://link.springer.com/chapter/10.1007/978-3-030-31764-5_1.

[C3] **Krishnan Raghavan**, V.A. Samaranayake, and S. Jagannathan. "A Multi-Step Nonlinear Dimension-Reduction Approach with Applications to Bigdata". In: **INNS Conference on Big Data and Deep Learning**. Vol. 144. 2018, pp. 81–88. DOI: 10.1016/j.procs.2018.10.507. https://www.sciencedirect.com/science/article/pii/S1877050918322166.

[C2] **Krishnan Raghavan**, Sarangapani Jagannathan, and V. A. Samaranayake. "Deep Learning Inspired Prognostics Scheme for Applications Generating Big Data". In: **International Joint Conference on Neural Networks (AR:15)**. IEEE, 2017, pp. 3296–3302. https://ieeexplore.ieee.org/abstract/document/7966269.

[C1] **Krishnan Raghavan** and Sarangapani Jagannathan. "Hierarchical Mahalanobis Distance Clustering Based Technique for Prognostics in Applications Generating Big Data". In: **IEEE Symposium Series on Computational Intelligence**. IEEE, 2015, pp. 516–521. https://ieeexplore.ieee.org/abstract/document/7376655.

Book Chapters

[B3] Yixuan Sun, **Krishnan Raghavan**, and Prasanna Balaprakash. "Introduction to Reinforcement Learning". In: **Autonomous Experimentation Book, Accepted**. Taylor & Francis.

[B2] Rohollah Moghadam, S. Jagannathan, Vignesh Narayanan, and **Krishnan Raghavan**. "Optimal Adaptive Control of Partially Uncertain Linear Continuous-Time Systems with State Delay". In: **Handbook of Reinforcement Learning and Control**. Springer, 2021. https://link.springer.com/chapter/10.1007/978-3-030-60990-0_9.

[B1] **Krishnan Raghavan**, S. Jagannathan, and V. A. Samaranayake. "Direct Error Driven Learning for Classification in Applications Generating Big-Data". In: **Development and Analysis of Deep Learning Architectures**. Springer, 2020, pp. 1–29. https://www.sciencedirect.com/science/article/pii/S1877050918322178.

In Review

[P3] Romit Maulik, Romain Egele, **Krishnan Raghavan**, and Prasanna Balaprakash. *Quantifying Uncertainty for Deep Learning Based Forecasting and Flow-Reconstruction Using Neural Architecture Search Ensembles*. DOI: PhysicaD:NonlinearPhenomena. http://arxiv.org/abs/2302.09748. preprint.

[P2] **Krishnan Raghavan** and Prasanna Balaprakash. *Learning Continually on a Sequence of Graph – The Dynamical System Way*. 2023. DOI: SIAMJournalonMathematicsofDataScience. https://arxiv.org/abs/2305.12030. preprint.

[P1] **Krishnan Raghavan**, Vignesh Narayanan, and Jagannathan Saraangapani. *Learning to Control Using Image Feedback*. 2023. https://arxiv.org/abs/2110.15290. preprint.

Thesis

[T2] **Krishnan Raghavan**. "Deep Neural Network Learning-Based Classifier Design for Big-Data Analytics". Missouri University of Science and Technology, 2019.

[T1] **Krishnan Raghavan**. "Computer Vision Libraries for Trailer Truck Testbed Using Open Source Computer Vision Libraries". Missouri University of Science and Technology, 2014.

Invited Talks and Lectures

11. A Dynamical System View of Continual Learning, Department of Mechanical Engineering, Brown University, April 2023.
10. Continuosly Detecting Workflow Anomalies using Graph Neural Networks – Lessons Learnt, Dagstuhl Seminar on Future perspectives in continuous monitoring of HPC system, Schloss Dagstuhl, April 2023.
9. Continual learning for adapting digital twins to modifying environments, Artificial Intelligence for Robust Engineering & Science, Oakridge National Laboratory, April 2023.
8. Advanced Mathematical Tools and Applications, PK Honorarium lecture, Madras Institute of Technology, Feb 2023.
7. Model Parallelization in Deep Neural Networks, Split-learning Workshop, Massachusetts Institute of Technology, February 2021.
6. Machine Learning-based Inversion of Nuclear Responses, Advances in Many Body Theories: From First Principle Methods to Quantum Computing and Machine Learning, Nov. 2020.
5. Generalization As a Tool to Understanding Neural Network Optimization, Keynote Lecture, Madras Institute of Technology, April 2020.
4. Introduction to Generalization, Guest Lecture on Adaptive Dynamic Programming at S & T, March 2020.
3. Distributed Learning with Deep Neural Networks, Washington University in St. Louis, March 2019.
2. Learning to Generalize through Deep Neural Network, Qualcomm AI Research in San Diego, July 2019.
1. Deep Learning-based Classifier Design, Argonne National Laboratory, July 2019.

Conference and Workshop Presentations

17. The Pitfalls of Backpropagation – Some Perspectives and Alternatives, Forward Alternatives to Back-Propagation in ML and Science, SIAM-CSE, Feb 2023.
16. Learning as a Dynamical System, Laboratory for Applied Mathematics, Numerical Software, and Statistics Seminar, November 2021.
15. Meta-continual Learning via Dynamic Programming, Train Once Use Forever: Transferable Deep Models for Accelerating Scientific Computing Mini-symposium in SIAM Computational Science and Engineering, February 2021.
14. Machine Learning-based Inversion of Nuclear Responses, SciDAC-Nuclei Meeting, April 2021.
13. Machine Learning-based Inversion of Nuclear Responses, Advances in Many Body Theories: From First Principle Methods to Quantum Computing and Machine Learning, Nov. 2020.

12. Distributed Learning of Deep Sparse Neural Networks for High-dimensional Classification, IEEE Conference on Big Data, December 2018.
11. A Minimax Approach for Classification with Big-data, IEEE Conference on Big Data, December 2018.
10. Mitigating Heterogeneity and Data-noise of Big-data using Deep Neural Network Learning based Analytics, Intelligent Systems Center, S & T, September 2018.
9. A Multi-step Nonlinear Dimension-reduction Approach with Applications to Big-data, International Neural Network Society's Conference on Big-data and Deep Learning, March 2018.
8. Direct Error-driven Learning for Deep Neural Networks with Applications to Big-data, International Neural Network Society's Conference on Big-data and Deep Learning, March 2018.
7. A Minimax Approach for Classification with Applications to Big-data, Intelligent Systems Center, S & T, February 2018.
6. A Direct Error-Driven Learning Approach with Applications to Big-data, Intelligent Systems Center, S&T, September 2017.
5. Deep Learning Inspired Prognostics Using Big-data, Intelligent Maintenance Systems Center –Industry Advisory Board Meeting, May 2017.
4. Introduction to Neural Networks, Lecture for EE 5320: Neural Networks Control and Application, Missouri University of Science and Technology (MST), Rolla, March 2017.
3. Camera as a Sensor for Asset Management, Intelligent Maintenance Systems Center – Industry Advisory Board Meeting, March 2017.
2. A Nonlinear Hierarchical Dimension Reduction Approach for Diagnostics in Big-data Generating Applications, Intelligent Maintenance Systems Center – Industry Advisory Board Meeting, September 2016.
1. Hierarchical Mahalanobis Distance Clustering Based Technique for Prognostics in Applications Generating Big-data, IEEE Symposium Series on Computational Intelligence, December 2015.

Posters

4. Formalizing the Generalization – Forgetting Tradeoff in Continual Learning, Neural Information Processing Systems, December 2021.
3. Learning as a Dynamical Systems, Postdoctoral Symposium, Argonne National Laboratory, November 2021.
2. Game Theory for Generalization in Machine Learning, Midwest Workshop on Control and Game Theory, Washington University at St. Louis, April 2019.
1. Deep Learning Inspired Prognostics Scheme for Applications Generating Big-data, IEEE International Joint Conference on Neural Networks, May 2015.

Other Activities

Present – 2017 | **Services, Reviewer, Argonne National Laboratory and S & T**

- IEEE Transactions on System, Man and Cybernetics.
- IEEE Transactions on Knowledge and Data Engineering.
- IEEE Transactions on Neural Networks and Learning Systems.
- Neural Computing and Applications.
- International Conference on Control, Automation, Robotics and Vision.
- Parallel AI and Systems for the Edge.
- International Conference on Parallel Processing.
- Super Computing Conference.

Present 2017 — Services, Supervision, Argonne National Laboratory and S & T

- **Yuxin Zi, Ph.D. Student**, Givens Fellow, *Project Title: Continual Molecular Property Prediction.*
- **Haoyang Zheng, Ph.D. Student**, Givens Fellow, *Project Title: Thompson Sampling to Improve Sample Efficiency of Proximal Policy Gradients.*
- **Karen Medlin, Ph.D. Student**, NSF-MSGI Fellow, University of North Carolina – Charlotte, summer-2022, *Project Title: Analysing Imbalanced-data using MCMC.*
- **Himali Kalanchige, Ph.D. Student**,NSF-MSGI Fellow, *Project Title: Analysing Imbalanced-data with Neural Networks.*
- **Phanindra Raja Chava, BS**, *Project Title: Indoor Localization using Bluetooth Low Energy*.
- **Shweta Garg, BS**, *Project Title: Parallelized Implementation of Deep Neural Networks in Tensorflow and Python.*
- **Shameeya Airhart, High School (ACT-SO)**, *Project Title: Using Machine Learning to predict retention time of a molecule*.
- **Taree Evans, High School (ACT-SO)** , *Is there a correlation between gut microbiota and acute stress?*

2019 2008 — Services, Leadership, S&T and VESIT

- 2018–2012, *Coordination Committee Lead*, Diwali – 1000 participants.
- 2014–2012, *Coordination Committee*, International Students Day – 600 participants.
- 2014, Winter Social Organization Committee, Leadership and Cultural Programs.
- 2013–2012, *Publicity Coordinator – International Students Club*.
- 2013–2012, *Secretary – India Association*.
- 2012–2011, *Chief Editor - International Society For Automation, VESIT Chapter*.
- 2011–2010, *Editor - International Society For Automation, VESIT Chapter*.
- 2010–2009, *Junior Editor and Coordinator – International Society For Automation, VESIT Chapter*.
- 2012-2009, *Coordination Committee*, annual symposium – 200 participants.
- 2012–2009, *Organization Committee – Praxis*

Awards

2018 Travel Award, IEEE Conference on Big-data.
2018 First Place, Intelligent System Center, Student Poster Presentation Competition.
2018 Third Place, Intelligent System Center, Student Paper Presentation Competition.
2017 Second Place, Intelligent System Center, Student Poster Presentation Competition.
2019–2015 Graduate Research Fellowship.
2019–2008 *Extra-curricular Awards*: six felicitation for outstanding contribution to India association, International students club.

References

Dr. Prasanna Balaprakash (Postdoctoral Advisor)
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Dr. Jagannathan Sarangapani (Ph.D. Advisor)
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Dr. Donald C. Wunsch
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