

Shashanka Ubaru

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Research Interests

Numerical linear and tensor algebra, machine learning, artificial intelligence, quantum computing, coding theory applications, approximation theory and algorithms.

Positions

- 2018 - present **IBM Research**, Yorktown Heights/Austin, USA.
Senior Research Scientist
Research Staff Member
Goldstine Postdoctoral Fellow
May, 2022 - present
Jan, 2020 - May, 2022
Aug, 2018 - Dec, 2019
- 2022 - present **Oden Institute**, University of Texas at Austin, TX, USA.
Lecturer
Visiting Researcher
Jan, 2024 - present
June, 2022 - present
- 2013 - 2018 **University of Minnesota**, Minneapolis, MN, USA.
Research Assistant, Department of Computer Science.
Sep, 2013 - May, 2018
- 2016 & 2017 **Lawrence Berkeley National Laboratory**, Berkeley, CA, USA.
Research Intern, Neural Systems and Data Science Lab
Research Intern, Scientific Data Management group
June - Aug, 2017
May - Aug, 2016
- 2013 **Seagate Technology**, Shakopee, MN, USA.
Signal Processing Intern
May - Aug, 2013
- 2011 - 2012 **Raman Research Institute**, Bangalore, India.
Visiting Research Student
June, 2011 - Aug, 2012

Education

- 2012-18 **University of Minnesota**, Minneapolis, MN, USA.
Ph.D. Computer Science
Advisor: Yousef Saad
Thesis: *Algorithmic advances in learning from large dimensional matrices and scientific data*
May 2018
- M.S. Computer Science*
M.S. Electrical Engineering
Advisors: Yousef Saad and Arya Mazumdar
Thesis: *Randomized techniques for matrix decomposition and estimating the approximate rank of a matrix*
October 2015
November 2014
- 2008-12 **M.S. Ramaiah Institute of Technology**, Bangalore, India.
B.Eng. Electronics and Communication

Publications

Journal articles

- [10] *Representation of the Fermionic Boundary Operator*.
I.Y. Akhalwaya, Y.H. He, L. Horesh, V. Jejjala, W. Kirby, K. Naidoo, and **S. Ubaru**
Physical Review A, volume 106, 022407, 2022.
- [9] *Dynamic graph and polynomial chaos based models for contact tracing data analysis and optimal testing prescription*.
S. Ubaru, G. Cohen, and L. Horesh
Journal of Biomedical Informatics, Novel Informatics Approaches to COVID-19 Research, 122, 103901, 2021.

- [8] *Spectrum-Adapted Polynomial Approximation for Matrix Functions with Applications in Graph Signal Processing.*
L. Fan, D. Shuman, **S. Ubaru**, and Y. Saad
Algorithms, Special Issue: Efficient Graph Algorithms in Machine Learning, 13(11), 295, 2020.
- [7] *Sampling and multilevel coarsening algorithms for fast matrix approximations.*
S. Ubaru and Y. Saad
Numerical Linear Algebra with Applications 26.3 : e2234, 2019.
- [6] *Fast estimation of $\text{tr}(f(A))$ via Stochastic Lanczos Quadrature.*
S. Ubaru, J. Chen, and Y. Saad
SIAM Journal on Matrix Analysis and Applications (SIMAX), 38(4), 1075–1099, 2017.
- [5] *Low rank approximation and decomposition of large matrices using error correcting codes.*
S. Ubaru, A. Mazumdar, and Y. Saad
IEEE Transactions on Information Theory, 63(9), 5544–5558, 2017.
- [4] *Formation enthalpies for transition metal alloys using machine learning.*
S. Ubaru, A. Miedlar, Y. Saad, and J R. Chelikowsky
Physical Review B, (Vol.95, No.21), 2017.
- [3] *Fast estimation of approximate matrix ranks using spectral densities.*
S. Ubaru, Y. Saad, and A.-K. Seghouane
Neural Computation, 29(5):1317–1351, 2017.
- [2] *Improving the Incoherence of a Learned Dictionary via Rank Shrinkage.*
S. Ubaru, A.-K. Seghouane, and Y. Saad
Neural Computation, 29(1):263–285, 2017.
- [1] *Displaying gray scales by cross pairing select and data voltages in multi-line addressed LCD.*
S. Ubaru and T.N. Ruckmongathan
IEEE Journal of Display Technology, 8(11), 669–677, 2012.

Conference proceedings

- [20] *Asynchronous Randomized Trace Estimation.*
V. Kalantzis, **S. Ubaru**, G. Kollias, C.W. Wu, and L. Horesh.
International Conference on Artificial Intelligence and Statistics (AISTATS), 2024.
- [19] *Topological Data Analysis on Noisy Quantum Computers.*
I. Akhalwaya*, **S. Ubaru***, K. Clarkson, M. Squillante, V. Jejjala, Y. He, K. Naidoo, V. Kalantzis, and L. Horesh.
International Conference on Learning Representations (ICLR), 2024. *Oral presentation, 1.2% of submissions*
- [18] *Solving Sparse Linear Systems via Flexible GMRES with In-Memory Analog Preconditioning.*
V. Kalantzis, M.S. Squillante, C. W. Wu, A. Gupta, **S. Ubaru**, T. Gokmen, and L. Horesh
IEEE High Performance Extreme Computing (HPEC), 2023.
- [17] *Quantum Graph Transformers.*
G. Kollias, V. Kalantzis, T. Salonidis, and **S. Ubaru**
International Conference on Acoustics, Speech, and Signal Processing (ICASSP), 2023.
- [16] *Accelerating matrix trace estimation by Aitken's Δ^2 process.*
V. Kalantzis, G. Kollias, **S. Ubaru**, and T. Salonidis
International Conference on Acoustics, Speech, and Signal Processing (ICASSP), 2023.
- [15] *Efficient Scaling of Dynamic Graph Neural Networks.*
V. Chakaravarthy, S. Pandian, S. Raje, Y. Sabharwal, T. Suzumura, and **S. Ubaru**
Supercomputing (SC21), 2021.
- [14] *Analysis of stochastic Lanczos quadrature for spectrum approximation.*
T. Chen, T. Trogon, and **S. Ubaru**
International Conference on Machine Learning (ICML), 2021. *Long presentation*
- [13] *Projection techniques to update the truncated SVD of evolving matrices.*
V. Kalantzis, G. Kollias, **S. Ubaru**, A. Nikolakopoulos, L. Horesh, and K.L. Clarkson
International Conference on Machine Learning (ICML), 2021.
- [12] *Sparse graph based sketching for fast numerical linear algebra.*
D. Hu, **S. Ubaru**, A. Gittens, K. Clarkson, L. Horesh, and V. Kalantzis
International Conference on Acoustics, Speech, and Signal Processing (ICASSP), 2021.
- [11] *Dynamic Graph Convolutional Networks Using the Tensor M-Product.*
O. Malik, **S. Ubaru**, L. Horesh, M. Kilmer, and H. Avron
SIAM International Conference on Data Mining (SDM), 2021.
- [10] *Multilabel Classification by Hierarchical Partitioning and Data-dependent Grouping.*
S. Ubaru, S. Dash, O. Gunluk, and A. Mazumdar
Advances in Neural Information Processing Systems (NeurIPS), 2020.

- [9] *Spectrum-Adapted Polynomial Approximation for Matrix Functions.*
L. Fan, D. Shuman, **S. Ubaru**, and Y. Saad
International Conference on Acoustics, Speech, and Signal Processing (ICASSP), 2019.
- [8] *Find the dimension that counts: Fast dimension estimation and Krylov PCA.*
S. Ubaru, A.-K. Seghouane, and Y. Saad
SIAM International Conference on Data Mining (SDM), 2019.
- [7] *Spectral Sums Beyond Fast Matrix Multiplication: Algorithms and Hardness.*
C. Musco, P. Netrapalli, A. Siffford, **S. Ubaru**, and D. P. Woodruff
Innovations in Theoretical Computer Science (ITCS), 2018.
- [6] *UoI-NMF_{cluster}: A Robust Nonnegative Matrix Factorization Algorithm for Improved Parts-Based Decomposition and Reconstruction of Noisy Data.*
S. Ubaru, K. Wu, and K. E. Bouchard
IEEE International Conference on Machine Learning and Applications (ICMLA), 2017.
Best Paper Award.
- [5] *Union of Intersections (UoI) for Interpretable Data Driven Discovery and Prediction.*
K. E. Bouchard, A. F. Bujan, F. Roosta-Khorasani, **S. Ubaru**, Prabhat, A. M. Snijders, J.-H. Mao, E. F. Chang, M. W. Mahoney, and S. Bhattacharyya
Advances in Neural Information Processing Systems (NeurIPS), 2017.
- [4] *Multilabel Classification with Group Testing and Codes.*
S. Ubaru and A. Mazumdar
International Conference on Machine Learning (ICML), 2017.
- [3] *Fast methods for estimating the Numerical rank of large matrices.*
S. Ubaru and Y. Saad
International Conference on Machine Learning (ICML), 2016.
- [2] *Group testing schemes from low-weight codewords of BCH codes.*
S. Ubaru, A. Mazumdar, and A. Barg
IEEE International Symposium on Information Theory (ISIT), 2016.
- [1] *Low rank approximation using error correcting coding matrices.*
S. Ubaru, A. Mazumdar, and Y. Saad
International Conference on Machine Learning (ICML), 2015.

Book chapters

- [2] *Quantum Computing Algorithms For Decision Making Under Uncertainty.*
L. Horesh, K. Clarkson, V. Kalantzis, M. Squillante, **S. Ubaru**, and A. Abboud
Air Force Research Lab Technical Report, AFRL-RI-RS-TR-2021-121, 2021.
- [1] *Applications of trace estimation techniques.*
S. Ubaru and Y. Saad
High Performance Computing in Science and Engineering, LNCS book series, vol. 11087, ch. 2, pp 19–33, 2018.

Workshop papers and posters

- [5] *Topological Data Analysis on Noisy Quantum Computers.*
S. Ubaru, I Akhalwaya, K. Clarkson and L. Horesh
Quantum Information Processing (QIP), 2023.
- [4] *On Quantum Algorithms for Random Walks in the Nonnegative Quarter Plane.*
V. Kalantzis, M. S. Squillante, **S. Ubaru**, and L. Horesh
Workshop on Mathematical performance Modeling and Analysis (MAMA), 2022.
- [3] *Multilabel prediction in log time and data-dependent grouping.*
S. Ubaru, S. Dash, O. Gunluk, and A. Mazumdar
NeurIPS - Workshop on Information Theory and Machine Learning, 2019.
- [2] *Tensor graph neural networks for prediction on time varying graphs.*
O. Malik, **S. Ubaru**, L. Horesh, M. Kilmer, and H. Avron
NeurIPS - Workshop on Graph Representation Learning, 2019.
- [1] *Union of Intersections (UoI) for interpretable data driven discovery and prediction in neuroscience.*
K. E. Bouchard, P. Sachdeva, S. Bhattacharyya, M. Balasubramanian, and **S. Ubaru**
Computational and Systems Neuroscience (Cosyne), 2019.

Preprints

- [9] *Combinatorial Multi-armed Bandits: Arm Selection via Group Testing.*
A. Mukherjee, **S. Ubaru**, K. Murugesan, K. Shanmugam, Ali Tajer, 2024.

- [8] *Counting Triangles of Graphs via Matrix Partitioning.*
G. Kollias, V. Kalantzis, L. Horesh, **S. Ubaru**, and P. Traganitis, 2023.
- [7] *Single-Pass Top-N Subgraph Centrality of Graphs via Subspace Projections.*
V. Kalantzis, G. Kollias, **S. Ubaru**, L. Horesh and N. Abe, 2023
- [6] *Capacity Analysis of Vector Symbolic Architectures.*
K.L. Clarkson, **S. Ubaru**, and E. Yang, 2023.
- [5] *Randomized matrix-free quadrature for spectrum and spectral sum approximation.*
T. Chen, T. Trogon, and **S. Ubaru**, 2022.
- [4] *PCENet: High Dimensional Surrogate Modeling for Learning Uncertainty.*
P.F. Shustin, **S. Ubaru**, V. Kalantzis, L. Horesh, and H. Avron, 2022.
- [3] *Quantum Topological Data Analysis with Linear Depth and Exponential Speedup.*
S. Ubaru, I. Akhalwaya, M. Squillante, K. Clarkson, and L. Horesh, 2021.
- [2] *Unsupervised Hierarchical Graph Representation Learning with Variational Bayes.*
S. Ubaru and J. Chen, 2020.
- [1] *Provably convergent acceleration in factored gradient descent with applications in matrix sensing.*
T. Ajayi, D. Mildebrath, A. Krylidis, **S. Ubaru**, G. Kollias, and K. E. Bouchard, 2019.

Patents

- [24] *P202302321 - An asynchronous modeled system for fault-tolerant environments.*
L. Horesh, V. Kalantzis, G. Kollias, **S. Ubaru**, and C. Wu. (filed)
- [23] *P202203693- Privacy-preserving graph analytics on hybrid cloud environments.*
V. Kalantzis, L. Horesh, **S. Ubaru**, and G. Kollias,. (filed)
- [22] *P202204543 - A system to update the most influential nodes of dynamic graphs.*
V. Kalantzis, G. Kollias, **S. Ubaru**, L. Horesh, and N. Abe. (filed)
- [21] *P202204563 - Quantum Graph Transformers.*
G. Kollias, V. Kalantzis, T. Salonidis, and **S. Ubaru**. (filed)
- [20] *P202203488- Aitken acceleration for estimating electronic structures of materials and the like.*
V. Kalantzis, G. Kollias, **S. Ubaru**, and T. Salonidis. (filed)
- [19] *P202105416- Processing sparse linear systems using distributed resources.*
V. Kalantzis, **S. Ubaru**, and L. Horesh. (filed)
- [18] *P202202073 - Solving systems of linear equations using mixed precision.*
T. Gokmen, V. Kalantzis, **S. Ubaru**, and L. Horesh. (filed)
- [17] *P202200441 - Polynomial Chaos Expansion Neural Network.*
P. Fink, **S. Ubaru**, H. Avron, V. Kalantzis, and L. Horesh. (filed)
- [16] *P202104622 - Linear-depth quantum system for Topological Data Analysis.*
I. Akhalwaya, **S. Ubaru**, K. Clarkson, M. Squillante, V. Kalantzis, and L. Horesh. (filed)
- [15] *P202104621 - Quantum circuit for estimating matrix spectral sums.*
S. Ubaru, I. Akhalwaya, K. Clarkson, M. Squillante, V. Kalantzis, and L. Horesh. (filed)
- [14] *P202104620 - Quantum circuits for matrix trace estimation.*
S. Ubaru, K. Clarkson, I. Akhalwaya, M. Squillante, V. Kalantzis, and L. Horesh. (filed)
- [13] *P202104619 - Quantum circuit for transformation of mixed state vectors.*
I. Akhalwaya, **S. Ubaru**, K. Clarkson, M. Squillante, V. Kalantzis, and L. Horesh. (filed)
- [12] *P202104617- Quantum circuit for pairwise testing.*
S. Ubaru, I. Akhalwaya, K. Clarkson, M. Squillante, V. Kalantzis, and L. Horesh. (filed)
- [11] *P201903947 - Quantum circuit for simulating boundary operator.*
I. Akhalwaya, Y. He, L. Horesh, V. Jejjala, W. Kirky, K. Naidoo, and **S. Ubaru** (filed)
- [10] *US20230410113A1 - Detecting network patterns using random walks.*
K.P. Onak, **S. Ubaru**, A. Abboud, and T. Suzumura. (pending)
- [9] *US20230195457A1 - Hardware acceleration with preconditioners.*
V. Kalantzis, L. Horesh, and **S. Ubaru**. (pending)
- [8] *US20220382831A1 - Projection-based techniques for updating SVD in evolving datasets.*
V. Kalantzis, G. Kollias, **S. Ubaru**, L. Horesh, and K. Clarkson. (pending)
- [7] *US20220300575A1 - Determining triangles in graph data structures using crosspoint array.*
V. Kalantzis, **S. Ubaru**, L. Horesh, and H. Avron. (pending)

- [6] *US20220107991A1 - Fast PCA of evolving data using analog crossbar array.*
S. Ubaru, V. Kalantzis, L. Horesh, M. Squillante, and H. Avron.
- [5] *US20220083623A1- Accelerated quasi-newton methods on analog crossbar hardware.*
V. Kalantzis, S. Ubaru, L. Horesh, H. Avron, and M. Onen.
- [4] *US20210357540A1 - Matrix sketching using analog crossbar architectures.*
L. Horesh, M. Onen, H. Avron, T. Gokmen, S. Ubaru, and V. Kalantzis.
- [3] *US11657312B2 - Short-depth quantum amplitude estimation without eigenstate collapse.*
I. Akhalwaya, K. Clarkson, L. Horesh, M. Squillante, S. Ubaru, and V. Kalantzis.
- [2] *US20210174242A1 - Automatic multilabel classification using machine learning.*
S. Ubaru, S. Dash, O. Gunluk, A. Mazumdar and L. Horesh.
- [1] *US20210090182A1 - Tensor-based predictions from analysis of time-varying graphs.*
O. Malik, S. Ubaru, L. Horesh, M. Kilmer, and H. Avron.

Presentations

- 2023 *Dynamic graph representation learning using tensor algebra*
 - UTD CS Colloquium, University of Texas Dallas
 - Topological data analysis on noisy quantum computers*
 - QuSoft, CWI, Amsterdam, The Netherlands
 - QIP 2023 conference, Ghent, Belgium
 - Algorithms for estimating spectral sums for large matrices*
 - Rachel Ward group, University of Texas at Austin
- 2022 *Industry Panelist*
 - SIAM Conference on Mathematics of Data Science (MDS22), San Diego
 - Towards quantum advantage on noisy computers*
 - Google Research, Bengaluru
 - Dynamic graph representation learning using tensor algebra*
 - Oden Institute Seminar Series, University of Texas at Austin
 - SIAM Conference on Mathematics of Data Science (MDS22), San Diego
 - Data Science group, University of California, San Diego.
 - Multilabel Classification by Hierarchical Partitioning and Grouping*
 - RISE workshop, Austin, TX
 - Quantum Topological Data Analysis with Linear Depth and Exponential Speedup*
 - Quantum Information Group, University of Texas at Austin
 - Quantum computing course, Columbia University, New York
- 2021 *Into another dimension - a new tensor algebra for learning on dynamic graphs*
 - Seminar at University of Albany, NY
 - Algorithms for estimating spectral sums for large matrices*
 - Oden Institute Seminar Series, University of Texas at Austin
 - Novel Tensor Framework for Data Representation and Compression*
 - SIAM Conference on Computational Science and Engineering (CSE21)
- 2020 *Multilabel Classification by Hierarchical Partitioning and Data-dependent Grouping*
 - Neural Information Processing Systems (NeurIPS) Virtually held
 - Novel tensor framework for model reduction and neural networks*
 - ICERM: Workshop on Algorithms for Dimension and Complexity Reduction, Brown University, RI
- 2019 *Tensor graph neural networks for prediction on time varying graphs*
 - NeurIPS: Workshop on Graph Representation Learning, Vancouver, Canada
 - Multilabel prediction in log time and data-dependent grouping*
 - NeurIPS: Workshop on Information Theory and Machine Learning, Vancouver, Canada
 - Spectrum approximation by Lanczos Quadrature and Preconditioned SVRG*
 - 20th International Conference On Preconditioning, Minneapolis, MN, USA
 - Find the dimension that counts: Fast dimension estimation and Krylov PCA*
 - SIAM International Conference on Data Mining (SDM), Calgary, Canada
 - Error Correcting Codes for Machine Learning.*
 - CSA Seminar, Indian Institute of Science (IISc), Bengaluru, India
- 2018 *Error Correcting Codes for Machine Learning*
 - Theory Seminar, University of Massachusetts, Amherst, MA
 - IP Seminar, IBM T.J. Watson Research Center, NY

- 2017 *UoI-NMF_{cluster}: Robust Nonnegative Matrix Factorization Algorithm for Noisy Data*
 - International Conference on Machine Learning and Applications (ICMLA), Cancun, Mexico
 - Multilabel Classification with Group Testing and Codes*
 - Neural Systems and Engineering Labs, Lawrence Berkeley National Laboratory, CA
 - International Conference on Machine Learning (ICML), Sydney, Australia
 - Error Correcting Codes for Machine Learning*
 - The University of Melbourne, Melbourne, Australia
 - UoI-NMF_{cluster} and UoI-CUR: Union of Intersections methods for matrix approximations*
 - Neural Systems and Engineering Labs, Lawrence Berkeley National Laboratory, CA
- 2016 *Error correcting codes for low rank approximation and group testing*
 - BLISS Seminar, University of California, Berkeley, CA
 - Fast methods for estimating the Numerical rank of large matrices*
 - International Conference on Machine Learning (ICML), New York, NY
- 2015 *Low rank approximation using error correcting coding matrices*
 - International Conference on Machine Learning (ICML), Lille, France

Awards

- 2023 **Master Inventor Award**, IBM Research (3-year term)
- 2023 **Outstanding Technical Achievement Award**, IBM Research
- 2022 *IBM Research Accomplishment Award*
- 2022 **Outstanding Innovation Award**, IBM Research
- 2021 *IBM Research Accomplishment Award*
- 2019 *UMN Best Dissertation Award*, Computer Science Department nominee
- 2018 **Herman Goldstine Fellowship**, IBM Research
- 2017 **Best Paper Award**, International Conference on Machine Learning and Applications (ICMLA)
- 2011 *Visiting Research Student Program*, Raman Research Institute

Teaching

University of Texas, Austin, *Instructor*

Spring 2024 CSE 392, Topics in Computer Science: Matrix and Tensor Algorithms for Data

IBM Research, *Co-instructor*

Summer 2023 Mathematics of Big Data: Sketching and (Multi-) Linear Algebra, Organized at IBM, Almaden

Summer 2021 Mathematics of Big Data: Sketching and (Multi-) Linear Algebra at MSRI Berkeley

University of Minnesota, *Teaching Assistant*

Spring 2018 CSci 2033, Elementary Computational Linear Algebra, *Recitation Instructor*

Fall 2017 CSci 5304, Computational Aspects of Matrix Theory, *Teaching Assistant*

Spring 2017 CSci 8314, Sparse Matrix Computations, *Temporary Instructor*

Mentoring

IBM Research - Interns

- 2023 Arpan Mukerjee (PhD Student - RPI), jointly with K. Murugesan
- 2022 Elizabeth Yang (PhD Student - U of California, Berkeley), jointly with K. Clarkson
- 2021 Paz F. Sustin (PhD Student - Tel Aviv University), jointly with L. Horesh, H. Avron
- 2021 Lucky Yerimah (PhD Student - RPI), jointly with P. Ram
- 2021 Emily Thompson (REU Student via. DIMACS)
- 2020 Dong Hu (PhD Student - RPI), jointly with A. Gittens
- 2019 Osman Malik (PhD Student - U of Colorado, Boulder), jointly with L. Horesh

Services

Reviewer: National Science Foundation (NSF) grant proposals, 2023.

Conferences: Neural Information Processing Systems (NeurIPS) 2016, 2019- 22 ; International Conference on Machine Learning (ICML) 2018 - 23 ; International Conference on Learning Representations (ICLR) 2021-22; AAAI conference on Artificial Intelligence 2020 - 22 ; ACM-SIAM Symposium on Discrete Algorithms (SODA) 2021; Conference on Uncertainty in Artificial Intelligence (UAI) 2019 - 22; IEEE International Conference On Machine Learning And Applications 2018 - 19; IEEE International Symposium on Information Theory (ISIT) 2017.

Journals: Acta Materialia; PLOS One; Journal of Machine Learning Research; SIAM Journal on Matrix Analysis and Applications (3 articles); IEEE Transactions on Signal Processing; IEEE Transactions on Image Porcessing; Signal Processing Letters, IEEE Transactions on Information Theory; Electronic Transactions on Numerical Analysis (2 articles); IEEE Transactions on Signal and Information Processing over Networks; BIT Numerical Mathematics; Linear Algebra and Its Applications; Journal of Mathematics and Applications, Mathematical Modeling and Analysis; Journal of Imaging.

Organizer: SIAM MDS 2024 - Member of organizing committee.

SIAM CSE 2023 - Minisymposium on Randomized Algorithms for Matrix and Tensor Analysis

ICMLA Challenge 2018 - Parts based decomposition of noisy data.

MSRIT ROBONXG-2012 - a week long robotics festival.

Programming skills

Matlab, Python, C, C++, LATEX, Basic web programming.