# Shashanka Ubaru

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☐ shashankaubaru.github.io

## 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 ScientistMay, 2022 - presentResearch Staff MemberJan, 2020 - May, 2022Goldstine Postdoctoral FellowAug, 2018 - Dec, 2019

2022 - present Oden Institute, University of Texas at Austin, TX, USA.

LecturerJan, 2024 - presentVisiting ResearcherJune, 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

June - Aug, 2017

Research Intern, Scientific Data Management group

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 May 2018

Advisor: Yousef Saad

Thesis: Algorithmic advances in learning from large dimensional matrices and scientific data

M.S. Computer Science October 2015
M.S. Electrical Engineering November 2014

Advisors: Yousef Saad and Arya Mazumdar

Thesis: Randomized techniques for matrix decomposition and estimating the approximate rank of a matrix

## 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 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  ${\bf S.\ Ubaru}$

International Conference on Acoustics, Speech, and Signal Processing (ICASSP), 2023.

- [16] Accelerating matrix trace estimation by Aitken's  $\Delta^2$  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. Trogdon, 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. Sifford, **S. Ubaru**, and D. P. Woodruff Innovations in Theoretical Computer Science (ITCS), 2018.
- [6] UoI-NMF<sub>cluster</sub>: 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. Trogdon, 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**

- [25] P202203839 Efficient look-up for vector symbolic architectures (VSA).
   T. Gokmen, V. Kalantzis, P. Ram, C. Wu, K. Clarkson, L Horesh, and S. Ubaru. (filed)
- [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] US20240028939A1 Linear-depth quantum system for Topological Data Analysis.
   I. Akhalwaya, S. Ubaru, K. Clarkson, M. Squillante, V. Kalantzis, and L. Horesh. (pending)
- [15] US20240020565A1 Quantum circuit for estimating matrix spectral sums.
   S. Ubaru, I. Akhalwaya, K. Clarkson, M. Squillante, V. Kalantzis, and L. Horesh. (pending)
- [14] US20240020564A1 Quantum circuits for matrix trace estimation.
   S. Ubaru, K. Clarkson, I. Akhalwaya, M. Squillante, V. Kalantzis, and L. Horesh.(pending)
- [13] US20240020563A1 Quantum circuit for transformation of mixed state vectors.
   I. Akhalwaya, S. Ubaru, K. Clarkson, M. Squillante, V. Kalantzis, and L. Horesh. (pending)
- [12] US20240022247A1 Quantum circuit for pairwise testing.
   S. Ubaru, I. Akhalwaya, K. Clarkson, M. Squillante, V. Kalantzis, and L. Horesh.(pending)
- [11] US20240037304A1 Quantum circuit for simulating boundary operator.

  I. Akhalwaya, Y. He, L. Horesh, V. Jejalla, W. Kirky, K. Naidoo, and S. Ubaru (pending)
- [10] US20230410113A1 Detecting network patterns using random walks. K.P. Onak, **S. Ubaru**, A. Abboud, and T. Suzumura. (pending)
- 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] US11500963B2 Fast PCA of evolving data using analog crossbar array.
   S. Ubaru, V. Kalantzis, L. Horesh, M. Squillante, and H. Avron.
- [5] *US11790033B2- Accelerated quasi-newton methods on analog crossbar hardware*. V. Kalantzis, **S. Ubaru**, L. Horesh, H. Avron, and M. Onen.
- [4] US11520855B2 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] US11379758B2 Automatic multilabel classification using machine learning. **S. Ubaru**, S. Dash, O. Gunluk, A. Mazumdar and L. Horesh.
- [1] US11386507B2 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<sub>cluster</sub>: 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
  - Uol-NMFcluster and Uol-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 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.