Haibo Li

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Current Position

Research Fellow, School of Mathematics and Statistics, The University of Melbourne, Sept. 2023 – now

Research Interest

My research interests center around utilizing mathematical modeling and computational techniques to address challenging problems in scientific computing, matrix computation and data science. The research areas mainly include:

- Inverse and ill-posed problems
- Numerical linear algebra
- Scientific machine learning

Academic Experience

Aug. 2024 – Oct. 2024	• Visiting Scholar, Department of Mathematics, Johns Hopkins Univeristy
Aug. 2021 – Sept. 2023	• Researcher, Computing System Optimization Lab, Huawei Technologies (joint with Institute of Computing Technology, Chinese Academy of Sciences)
Sept. 2015 – Jun. 2021	• Ph.D. in Computational Mathematics, Department of Mathematical Sciences, Tsinghua University, China
	• *Thesis: Joint Bidiagonalization Algorithms for the Computation of Partial GSVDs and Discrete Ill-posed Problems with General-form Regularization*
Sept. 2011 – Jun. 2015	• Bachelor in mathematics, Taishan College (talent training project), Shandong University, China

Papers

Publications:

1 • **Haibo Li**. *Characterizing GSVD by singular value expansion of linear operators and its computation*, Accepted by SIAM Journal on Matrix Analysis and Applications, 2024.

2 • **Haibo Li**. *A preconditioned Krylov subspace method for linear inverse problems with general-form Tikhonov regularization*, SIAM Journal on Scientific Computing, 46 (4), A2607-A2633, 2024.

3 • **Haibo Li**. *The joint bidiagonalization of a matrix pair with inaccurate inner iterations*, SIAM Journal on Matrix Analysis and Applications, 45 (1), 232–259, 2024.

4 • **Haibo Li**. *Double precision is not necessary for LSQR for solving discrete linear ill-posed problems*, Journal of Scientific Computing, 98 (3), 55, 2024.

5 • Yujin Yan, **Haibo Li**, Tong Zhao, Lin-Wang Wang, Lin Shi, Tao Liu, Guangming Tan, Weile Jia, Ninghui Sun. *10-million atoms simulation of first-principle package LS3DF on Sugon supercomputer*, Journal of Computer Science and Technology, 39 (1), 45-62, 2024.

6 • Zhongxiao Jia, **Haibo Li**. *The joint bidiagonalization method for large GSVD computations in finite precision*, SIAM Journal on Matrix Analysis and Applications, 44 (1), 382–407, 2023.

7 • Zhongxiao Jia, **Haibo Li**. *The joint bidiagonalization process with partial reorthogonalization*, Numerical Algorithms (88), 965–992, 2021.

Preprints:

Papers (continued)

8 • **Haibo Li**, Fei Lu. *Automatic kernel regression and regularization for learning convolution kernels*, 2024, manuscript.

9 • Rongrong Liu, Zhuoqiang Guo, Qiuchen Sha, Tong Zhao, **Haibo Li**, Wei Hu, Lijun Liu, Guangming Tan, Weile Jia. *Large scale finite-temperature rt-TDDFT simulation with hybrid functional*, 2024, submitted.

10 • **Haibo Li**. *A new interpretation of the weighted pseudoinverse and its applications*, 2024, submitted.

11 • **Haibo Li**. *Projected Newton method for large-scale Bayesian linear inverse problems*, 2024, submitted to SIAM Journal on Optimization (major revision).

12 • **Haibo Li**, Jinchao Feng, Fei Lu. *Scalable iterative data-adaptive RKHS regularization*, 2024, submitted.

13 • **Haibo Li**. *Generalizing the SVD of a matrix under non-standard inner product and its applications to linear ill-posed problems*, 2023, submitted.

14 • **Haibo Li**. *Subspace projection regularization for large-scale Bayesian linear inverse problems*, 2023, submitted.

15 • **Haibo Li**, Xingxing Wu, Liping Liu, Long Wang, Lin-Wang Wang, Guangming Tan, Weile Jia, *ALKPU: an active learning method for the DeePMD model with Kalman filtering*, 2023, submitted.

16 • **Haibo Li**, Guangming Tan, Tong Zhao. *Backward error analysis of the Lanczos bidiagonalization with reorthogonalization*, 2022, submitted (Minor revision).

Presentations

- Talk: *Scalable iterative data-adaptive RKHS regularization*, Applied Math Seminar at Lehigh University, Oct. 24, 2024.
- Talk: *A preconditioned Krylov subspace method for regularizing linear inverse problems*, Data Science Seminar at Johns Hopkins University, Oct. 02, 2024.
- Talk: *Subspace projection regularization for high-dimensional Bayesian inverse problems*, MATRIX research program: Multivariate Dependence Modeling: Theory and Applications, Jul. 30, 2024.
- Talk: *Scalable iterative data-adaptive RKHS regularization*, International Conference on Scientific Computation and Differential Equations (SciCADE 2024), Jul. 16, 2024.
- Talk: *Subspace Projection Regularization: preconditioned Golub-Kahan bidiagonalization methods for regularizing linear inverse problems*, The 67th Annual Meeting of the Australian Mathematical Society (AustMS 2023), Dec. 2023.
- Talk: *A mixed precision variant of LSQR for solving discrete linear ill-posed problems*, Research Center for Mathematics and Interdisciplinary Sciences, Shandong University, Mar. 2023.
- Talk: *A Kalman filter based optimizer for training the neural network force field with first-principles accuracy*, Forum for High Performance Computing and Industrial Material Simulations, CCF HPC China, Dec. 2022.
- Talk: *The joint bidiagonalization process with reorthogonalization*, Forum for Doctoral Students, Tsinghua University, May 2020.
- Talk: *Introduction to iterative algorithms for solving large scale ill-posed problems*, Forum in Mathematics and Interdisciplinary Sciences, Research Center for Mathematics and Interdisciplinary Sciences, Shandong University, Nov. 2019.
- Technical report: *Preconditioned MINRES algorithm: basic theory and implementation*, CAEP Software Center for High Performance Numerical Simulation, Sep. 2019

Academic service

Reviewer of journals:

- Reviewer for Mathematical Reviews (No. 161348)
- SIAM Journal on Matrix Analysis and Applications
- BIT Numerical Mathematics

Academic service (continued)

Reviewer of conferences:

- The International Conference for High Performance Computing, Networking, Storage, and Analysis (SC22), 2022
- The 13th International Conference on Electronics, Communications and Networks (CECNet 2023), 2023

Reviewer of grants:

- International reviewer for Czech Science Foundation (Czech Republic).

Teaching Experience

- Stochastic Mathematical Methods (for undergraduates), teaching assistant, Tsinghua University. 2015.9-2016.1
- Stochastic Mathematical Methods (for undergraduates), teaching assistant, Tsinghua University. 2016.2-2016.6
- Linear Algebra (for undergraduates), teaching assistant, Tsinghua University. 2016.9-2017.1
- Calculus (for undergraduates), teaching assistant, Tsinghua University. 2017.2-2017.6
- Advanced Numerical Analysis (for postgraduates), teaching assistant, Tsinghua University. 2017.9-2018.1
- Calculus (for undergraduates), teaching assistant, Tsinghua University. 2018.2-2018.6
- Numerical Analysis (for postgraduates), teaching assistant, Tsinghua University. 2018.9-2019.1

Supervision of students

Co-supervised with Dr. Hailong Guo:

Master students
- Jiayue Ma, The University of Melbourne, 2024 – now

Co-supervised with Prof. Weile Jia:

Ph.D. candidates
- Yujin Yan, Chinese Academy of Sciences (Co-supervised in 2021–2023)

Master students
- Xingxing Wu, Chinese Academy of Sciences (Co-supervised in 2022–2023)

Undergraduates
- Weijian Liu, Wuhan University of Technology (Co-supervised in 2021–2022 at Chinese Academy of Sciences)
- Qiuchen Sha, Beijing Forestry University (Co-supervised in 2021–2022 at Chinese Academy of Sciences)

Skills

Programming
- Advanced: MATLAB, Python
  Basic: C/C++, Linux, JAX

Language
- English, Chinese

Awards

- Small Grant Proposal for *Research Project: Data-driven methods for learning dynamics from observations*, funded by School of Mathematics and Statistics, University of Melbourne, 2024
- Professor Maurice H. Belz Fund, funded by School of Mathematics and Statistics, University of Melbourne, 2024