CV of Yuan YAO

CONTACT INFORMATION

Hong Kong University of Science and Technology
Department of Mathematics
3430 Academic Building, Clear Water Bay, Kowloon
Hong Kong SAR, P.R. China

Phone: (852) 2358-7461
Fax: (852) 2358-1643
E-mail: yuany@ust.hk
WWW: yao-lab.github.io

RESEARCH INTERESTS

Mathematics of data science (esp. topological and geometric methods), statistical machine learning, with applications in computer science, biomedical engineering, and life sciences etc.

ACADEMIC QUALIFICATIONS

University of California at Berkeley, USA

Ph.D. Mathematics, December 2006

- Dissertation: A dynamic theory of learning: online learning and stochastic algorithms in Reproducing Kernel Hilbert Spaces
- Committee: Stephen Smale (chair), Peter Bartlett, and Steve Evans.

City University of Hong Kong, Hong Kong SAR, China

M.Phil. Mathematics, June 2002

Harbin Institute of Technology, Harbin, China

M.S. Control Engineering, July 1998
B.S. Control Engineering, July 1996

ACADEMIC POSITIONS

Hong Kong University of Science and Technology, China
Department of Mathematics
Department of Chemical and Biological Engineering
(by courtesy) Department of Computer Science and Engineering
Associate Professor with Substantiation (Tenure) — Aug 2016 - June 2022
Professor with Substantiation (Tenure) — July 2022 -

Peking (Beijing) University, China
School of Mathematical Sciences
Department of Probability and Statistics
Associate Professor with Tenure — July 2015 - 2016
Professor of Statistics in the Hundred Talents Program[1] — July 2009 - 2016

Stanford University, USA
Department of Mathematics and Computer Science
Postdoctoral Fellow — August 2006 – August 2009

AWARDS AND GRANTS

Hong Kong Research Grants Council NSFC/RGC Joint Research Scheme, N_HKUST635/20
Principal investigator — HKD 1,083,932.000, Jan 2022 - Dec 2024
Establishing a Novel Platform Tightly Coupling Single-Molecule Experiments with Molecular Dy-

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[1]The Program was introduced 10 years ago by Peking University to attract overseas talents, in which I was appointed as Professor in the traditional Chinese academic ranking system. Recently Peking University introduced tenure-track and tenured positions following the US practice. After an internationally wide evaluation, I was appointed as Associate Professor with tenure in 2015.

namics Simulations to Reveal Molecular Mechanisms behind Glycosylasess Efficient Search for Damaged Nucleotides among an Enormous Pool of Genomic DNAs

Hong Kong Innovation and Technology Fund, grant UIM/390
Principal investigator   HKD 5,031,089.630, Sep 2019 - Aug 2022
Advanced Data Analytics for Abnormal Detection of Semiconductor Devices

Hong Kong RGC Collaborative Research Fund
Co-PI   HKD 3,719,654, Mar 2020 - Feb 2023
X-GPU: An Extreme GPU Cluster for Interdisciplinary Research on Molecular Dynamics Simulations and Genomics Studies

Hong Kong Innovation and Technology Fund, Project ID: P0316
Co-PI   HKD 5,426,707.41, Jun 2020 - May 2022
Development of Statistical and Machine Learning Methods for Large Scale Genomic Data Analysis

Hong Kong RGC General Research Fund, Project 16308321
Principal investigator   HKD 598,015, 2021 - 2024
Robust Statistical Learning via Generative Adversarial Networks

Hong Kong RGC General Research Fund, Project 16303817
Principal investigator   HKD 472,351, Aug 2017 - Jul 2020
Social Choice, Crowdsourced Ranking, and Hodge Theory

Tencent AI Lab, collaborative research award
Principal investigator   HKD 160K, 2017 -
Moreau-Yosida Regularization in Deep Learning

Si Family Foundation, research donation
Principal investigator   HKD 217,257.75, 2017 -
Mathematics for Data Science

Microsoft Research Asia, collaborative research award
Principal investigator   2015 -
Active Sampling Strategy (Optimal Budget Plan) for Crowdsourced Pairwise Ranking Aggregation

Baidu, collaborative research award
Principal investigator   2015 - 2020
Statistical Machine Learning Algorithms and Applications for Internet Technology

National Science Foundation of China, award 61370004
Principal investigator   2014 - 2017
Applied Geometric and Topological Methods in Multimedia Data Analysis

National Science Foundation of China, award 61071157
Principal investigator   2011 - 2013
Statistical Theory and Algorithms in Information Fusion for Multimodal Molecular Imaging

National Science Foundation of China (joint China-Japan-Korea (A3)), award 11421110001
co-PI   2014 - 2017
Modeling and Simulation of Hierarchical and Heterogeneous Flow Systems with Applications to Materials Science

National Basic Research Program of China, 973 Program 2015CB856000
co-PI   2015 - 2019

Statistical Learning of Unstructured Data: Mathematical Foundation and Algorithms

National Basic Research Program of China, 973 Program 2012CB825501
co-PI   2012 - 2016
Fundamental Units of Cognation

National Basic Research Program of China, 973 Program 2011CB809105
co-PI   2011 - 2013
Studies of Frontiers and Key Technology in Dynamic Cellullar Signaling

Peking University, Beijing, China
Professorship in the Hundred Talents Program   2009 -

NCSA, USA
co-PI   2009 - 2010
Computational Studies to Elucidate the Fundamental Mechanism of Transcription

PUBLICATIONS   Books:

1. **Yao, Yuan**, *A Dynamic Theory of Learning – Online Learning and Stochastic Algorithms in Reproducing Kernel Hilbert Spaces*, Verlag Dr. Müller, ISBN: 978-3-639-09390-2. 2008.

2. **Yao, Yuan**, *A Mathematical Introduction to Data Analysis*, Lecture Notes, AMS, preprint.

Book chapters:

1. Jiechao Xiong[2], Feng Ruan, and **Yuan Yao**, A Tutorial on Libra: R package for the Linearized Bregman Algorithm in High Dimensional Statistics, *Handbook of Big Data Analytics*, ed. by Wolfgang Härdle, Henry Horng-Shing Lu, and Xiaotong Shen, Springer, page 425 - 453, 2018, `arXiv:1604.05910`; Cran R-package `https://cran.r-project.org/web/packages/Libra/`.

2. Hanlin Gu, Yin Xian, Ilona Christy Unarta, and **Yuan Yao**, Generative Adversarial Networks for Robust Cryo-EM Image Denoising, *Handbook of Mathematical Models and Algorithms in Computer Vision and Imaging*, ed. by Ke Chen, Carola-Bibiane Schönlieb, Xue-Cheng Tai, and Laurent Younes, Springer, 2022, `arXiv:2008.07307`; Source codes: `https://github.com/ghl1995/denoise-gan-in-cryo-em`.

Journal publications:

1. Yang Cao, Xinwei Sun, and **Yuan Yao**. Split Knockoffs for Multiple Comparisons: Controlling the Directional False Discovery Rate. *Journal of the American Statistical Association*, preprint, 2023. `arXiv:2310.07605`

2. Yang Cao, Xinwei Sun and **Yuan Yao**. Controlling the False Discovery Rate in Transformational Sparsity: Split Knockoffs. *Journal of Royal Statistical Society: Series B (Statistical Methodology)*, preprint, 2023. `arXiv:2103.16159`.

3. Yanwei Fu, Chen Liu, Donghao Li, Zuyuan Zhong, Xinwei Sun, Jinshan Zeng, and **Yuan Yao**. Exploring Structural Sparsity of Deep Networks via Inverse Scale Spaces. *IEEE Transactions on Pattern Analysis and Machine Intelligence (TPAMI)*, 45(2): 1749-1765, 2023, `DOI:10.1109/TPAMI.2022.3168881`. `arXiv:1905.09449`.

4. Xiaowei Wang, **Yuan Yao**, Xin Gao, and Lu Zhang. SARS-CoV-2 RdRp Follows Asynchronous Translocation Pathway for Viral Transcription and Replication. *The Journal of Physical Chemistry Letters*. 2023. `DOI:10.26434/chemrxiv-2022-7t1jg`

5. Weizhi Zhu, Yifei Huang, **Yuan Yao**. On Breiman's Dilemma in Neural Networks: Phase Transitions of Margin Dynamics. *Annals of Mathematical Sciences and Applications*, Volume 7,

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[2]Note: stands for the co-correspondence authors,   stands for co-first authors,   indicates current students/postdocs/visitors,   indicates former students/postdocs/visitors,   indicates former supervisors.

Number 2, pages: 221-258, 2022. DOI: https://dx.doi.org/10.4310/AMSA.2022.v7.n2.a4.
This work was presented at ICCM'2019 in Beijing.

6. Luo, Xueying, Xiaowei Wang, **Yuan Yao**, Xin Gao, and Lu Zhang. Unveiling the "Template-dependent" Inhibition on the Viral Transcription of SARS-CoV-2. *The Journal of Physical Chemistry Letters*. July 30, 2022, 13: 7197–7205. DOI:10.1021/acs.jpclett.2c01314

7. Yikai Wang, Li Zhang, **Yuan Yao**, Yanwei Fu. How to trust unlabeled data? Instance Credibility Inference for Few-Shot Learning. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 44(10): 6240-6253, 01 October 2022. DOI: 10.1109/TPAMI.2021.3086140. arXiv:2007.08461.

8. Xu, Qianqian; Yang, Zhiyong; Jiang, Yangbangyan; Cao, Xiaochun; **Yao, Yuan**; Huang, Qingming. Not All Samples are Trustworthy: Towards Deep Robust SVP Prediction. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 44(6): 3154 - 3169, 01 June 2022. DOI: 10.1109/TPAMI.2020.3047817.

9. Hanlin Gu, Wei Wang, Siqin Cao, Ilona Christy Unarta, **Yuan Yao**, Fu Kit Sheong, and Xuhui Huang. RPnet: A Reverse Projection Based Neural Network for Coarse-graining Metastable Conformational States for Protein Dynamics. *Physical Chemistry Chemical Physics*, 2022, 24, 1462-1474, DOI: 10.1039/D1CP03622J. bioRxiv: https://doi.org/10.1101/2021.08.04.455071.

10. Jinshan Zeng, Shao-Bo Lin, **Yuan Yao**, Ding-Xuan Zhou. On ADMM in Deep Learning: Convergence and Saturation-Avoidance. *Journal of Machine Learning Research*, 22(199): 1-67, 2021. arXiv:1902.02060.

11. Qianqian Xu, Jiechao Xiong, Xiaochun Cao, Qingming Huang and **Yuan Yao**. Evaluating Visual Properties via Robust HodgeRank. *International Journal of Computer Vision*, 129: 1732–1753, 2021. DOI: 10.1007/s11263-021-01438-y, arXiv:1408.3467.

12. Jiefu Zhang, Leonardo Zepeda-Núñez, **Yuan Yao**, Lin Lin. Learning the mapping $x \mapsto \sum_{i=1}^{d} x_i^2$: the cost of finding the needle in a haystack. *Communications on Applied Mathematics and Computation*, 3: 313-335, 2021. https://doi.org/10.1007/s42967-020-00078-2, arXiv:2002.10561.

13. Chao Gao, **Yuan Yao**, Weizhi Zhu. Generative Adversarial Nets for Robust Scatter Estimation: A Proper Scoring Rule Perspective. *Journal of Machine Learning Research*, 21(160):1-48, 2020. arXiv:1903.01944.

14. Weizhi Zhu, Yifei Huang, **Yuan Yao**. Rethinking Breiman's Dilemma in Neural Networks: Phase Transitions of Margin Dynamics. *Frontiers in Applied Mathematics and Statistics*, special section on Mathematical Fundamentals of Machine Learning, October 2020. doi: 10.3389/fams.2020.575073, arXiv:1810.03389.

15. Chendi Huang, Xinwei Sun, Jiechao Xiong, and **Yuan Yao**, Boosting with Structural Sparsity: A Differential Inclusion Approach, *Applied and Computational Harmonic Analysis*, 48(1):1-45, January 2020, https://doi.org/10.1016/j.acha.2017.12.004, arXiv:1704.04833

16. Jinshan Zeng, Ke Ma, **Yuan Yao**, On Global Linear Convergence in Stochastic Nonconvex Optimization for Semidefinite Programming. *IEEE Transactions on Signal Processing*, Vol. 67, No. 16, Page: 4261 - 4275, August 15, 2019. ICCM-2020_Distinguished_Paper_Award.

17. Ke Ma, Jinshan Zeng, Jiechao Xiong, Qianqian Xu, Xiaochun Cao, Wei Liu, and **Yuan Yao**, Fast Stochastic Ordinal Embedding with Variance Reduction and Adaptive Step Size, *IEEE Transactions on Knowledge and Data Engineering* (TKDE), Nov. 29, 2019, DOI: 10.1109/TKDE.2019.2956700, arXiv:1912.00362.

18. Qianqian Xu, Jiechao Xiong, Xiaochun Cao, Qingming Huang, and **Yuan Yao**, From Social to Individuals: a Parsimonious Path of Multi-level Models for Crowdsourced Preference Aggregation, *IEEE Transactions on Pattern Analysis and Machine Intelligence* (TPAMI), 41(4): 844-856, 2019, DOI: 10.1109/TPAMI.2018.2817205, arXiv:1804.11177.

19. Eriksson, Nick and **Yuan Yao**. Metric Learning for Phylogenetic Invariants: An Algebraic Approach to Evolutionary Tree Construction. *Journal of Chinese Linguistics*, special issue on New Horizons in Evolutionary Linguistics, ed. by PENG Gang and WANG Feng, Monograph No. 27, page: 67-85, 2017. `arxiv.org/abs/q-bio/0703034`.

20. Ting Hu and **Yuan Yao**, Learning Rates of Regression with q-norm Loss and Thresholds, *Analysis and Applications*, special issue on Learning Theory, 14(6): 809-827, November 2016, DOI: `http://dx.doi.org/10.1142/S0219530516400030`, `arXiv:1701.01956`.

21. Braxton Osting, Jiechao Xiong, Qianqian Xu, and **Yuan Yao**, Analysis of crowdsourced sampling strategies for hodgerank with sparse random graphs, *Applied and Computational Harmonic Analysis*, 41(2), 540-560. 2016, `http://dx.doi.org/10.1016/j.acha.2016.03.007`, `arXiv:1503.00164`.

22. Stanley Osher, Feng Ruan, Jiechao Xiong, **Yuan Yao**, and Wotao Yin, Sparse Recovery via Differential Inclusions, *Applied and Computational Harmonic Analysis*, 41(2), 436-469, 2016, DOI: `http://dx.doi.org/10.1016/j.acha.2016.01.002`. `arXiv:1406.7728`, with cran R-package `https://cran.r-project.org/web/packages/Libra/`.

23. Liu, Haixia, Raymond H. Chan, and **Yuan Yao**, *Geometric Tight Frame based Stylometry for Art Authentication of van Gogh Paintings*, *Applied and Computational Harmonic Analysis*, 41(2): 590-602, 2016, doi:10.1016/j.acha.2015.11.005, `arXiv:1407.0439`.

24. Yanwei Fu, Timothy M. Hospedales, Tao Xiang, Jiechao Xiong, Shaogang Gong, Yizhou Wang, and **Yuan Yao**, *Robust subjective visual property prediction from crowdsourced pairwise labels*, *IEEE Transactions on Pattern Analysis and Machine Intelligence*, vol.38, no.3, pp. 563-577, March 2016, `arXiv:1501.06202`.

25. Jiang, Xiaoye, **Yuan Yao**, Han Liu, and Leonidas Guibas. Compressive Network Analysis, *IEEE Transactions on Automatic Control*, special issue on Convex Relaxation Methods, 59(11): 2946 - 2961, 2014. `arXiv:1104.4605`.

26. Tarrès, Pierre and **Yuan Yao**. Online Learning as Stochastic Approximations of Regularization Paths: Optimality and Almost-sure Convergence. *IEEE Transactions on Information Theory*, 60(9):5716-5735, 2014. `arXiv.org:1103.5538`.

27. Qianqian Xu, Jiechao Xiong, Qingming Huang, and **Yuan Yao**, Online HodgeRank on Random Graphs for Crowdsourceable QoE Evaluation. *IEEE Transactions on Multimedia*, 16(2): 373-386, Feb 2014.

28. Weinan E, Jianfeng Lu, and **Yuan Yao**, The Landscape of Complex Networks, *Methods and Applications of Analysis*, special issue in honor of Professor Stanley Osher on his 70th birthday, 20(4):383-404, 2013. `arXiv:1204.6376`.

29. Jiang, Xiaoye, Mo Li, **Yuan Yao**, and Leonidas Guibas, Property Management in Wireless Sensor Networks with Overcomplete Radon Bases. *ACM Transactions on Sensor Networks*, 9(3):36, May 2013.

30. **Yuan Yao**, Raymond Z. Cui, Gregory R. Bowman, Daniel Silva, Jian Sun, and Xuhui Huang, Hierarchical Nystrom method for Markov Models in Biomolecular Folding. *Journal of Chemical Physics*. 138 (17):174106, 2013. `arXiv:1301.0974`.

31. Qianqian Xu, Qingming Huang, Tingting Jiang, Bowei Yan, **Yuan Yao**, and Weisi Lin, HodgeRank on Random Graphs for Subjective Video Quality Assessment, *IEEE Transactions on Multimedia*, 14(3): 844-857, 2012.

32. Jiang, Xiaoye, Lek-Heng Lim, **Yuan Yao**, and Yinyu Ye. Statistical Ranking and Combinatorial Hodge Theory. *Mathematical Programming*, Ser. B, Volume 127, Number 1, Pages 203-244, 2011, (online first) 27 November, 2010. `arXiv:0811.1067`.

33. **Yuan Yao**. On Complexity Issue of Online Learning Algorithms. *IEEE Transactions on Information Theory*, 56 (12): 6470-6481, 2010.

34. Caponnetto, Andrea and **Yuan Yao**. Adaption for Regularization Operators in Learning Theory, *CBCL Paper #265/AI Technical Report #063*, Massachusetts Institute of Technology, Cambridge, MA, September, 2006. *Analysis and Applications*, 8(2): 185-197, 2010.

35. **Yuan Yao**, Jian Sun, Xuhui Huang, Gregory Bowman, Vijay Pande, Leonidas Guibas and Gunnar Carlsson. Topological Methods for Exploring Low-density States in Biomolecular Folding Pathways. *J. Chem. Phys.* 130, 144115, 2009.

36. Bowman, Gregory, Xuhui Huang, **Yuan Yao**, Jian Sun, Gunnar Carlsson, Leonidas Guibas and Vijay Pande. Structural insight into RNA hairpin folding intermediates. *Journal of American Chemistry Society*, 130(30): 9676-8, 2008.

37. **Yuan Yao**, Lorenzo Rosasco and Andrea Caponnetto. On Early Stopping in Gradient Descent Learning. *Constructive Approximation*, Special Issue: Learning Theory, 26(2): 289-315, 2007.

38. Smale, Steve and **Yuan Yao**. Online Learning Algorithms. *Foundation of Computational Mathematics*, 6(2): 145-170, 2006.

39. **Yuan Yao**, Gian Luca Marcialis, Massimiliano Pontil, Paolo Frasconi, and Fabio Roli. Combining Flat and Structured Representations for Fingerprint Classification with Recursive Neural Networks and Support Vector Machines. *Pattern Recognition*, 36(2): 397-406, 2003.

40. Li, Lian-Feng, Guang-Xiong Wang and **Yuan Yao**. Global Optimal Robust Controller Design. *Journal of Control Theory and Applications* (in Chinese), 18(2): 266-269, 2001.

41. **Yuan Yao**, Guang-Xiong Wang and Tian-Wen Zhang. Morphological Reconstruction for Color Images Implemented by Fuzzy Cellular Neural Networks. *Chinese Journal of Computers* (in Chinese), 22(7): 727-732, 1999.

42. **Yuan Yao**, Guang-Xiong Wang and Tian-Wen Zhang. Application of Fuzzy Cellular Neural Networks to Stone Inscription Reconstruction in Chinese Calligraphy. *Journal of Computer Research and Development* (in Chinese), 36(3): 282-286, 1999.

43. **Yuan Yao**, Lian-Feng Li and Ge-Jun Bao. On the Application Problem of the Gap Metric for SISO Systems. *Journal of Harbin Institute of Technology* (in Chinese), 31(6): 19-21, 1999.

44. **Yuan Yao** and Jing Luo. FEM-Based Modeling in Servo Design. *Electric Machine and Control* (in Chinese), 2(2): 108-111, 1998.

Conference publications:

1. Xuantong Liu, Jianfeng Zhang, Tianyang Hu, He Cao, Lujia Pan, Yuan Yao. Inducing Neural Collapse in Deep Long-tailed Learning. *Proceedings of the 26th International Conference on Artificial Intelligence and Statistics (AISTATS)*, Valencia, Spain, PMLR: Volume 206. April 25-27, 2023. `arXiv:2302.12453`.

2. Yuxuan Han, Zhicong Liang, Zhipeng Liang, Yang Wang, Yuan Yao, and Jiheng Zhang. Optimal Private Streaming SCO in ℓ_p-geometry with Applications in High Dimensional Online Decision Making. *Proceedings of the 39th International Conference on Machine Learning (ICML)*, Baltimore, Maryland, USA, PMLR 162, July 17-23, 2022. `arXiv:2206.08111`.

3. Yifei Huang, Yaodong Yu, Hongyang Zhang, Yi Ma, **Yuan Yao**. Adversarial Robustness of Stabilized Neural ODEs Might be from Obfuscated Gradients. *Mathematical and Scientific Machine Learning (MSML)*, August 16-19, 2021. `arXiv:2009.13145`.

4. Jinshan Zeng, Qi Chen, Yunxin Liu, Mingwen Wang, **Yuan Yao**. StrokeGAN: Reducing Mode Collapse in Chinese Font Generation via Stroke Encoding. *AAAI Conference on Artificial Intelligence (AAAI)*, Feb 2-9, 2021. `arXiv:2012.08687`.

5. Qianqian Xu, Zhiyong Yang, Zuyao Chen, Yangbangyan Jiang, Xiaochun Cao, **Yuan Yao** and Qingming Huang. Deep Partial Rank Aggregation for Personalized Attributes. *AAAI Conference on Artificial Intelligence (AAAI)*, Feb 2-9, 2021.

6. Yanwei Fu, Chen Liu, Donghao Li, Xinwei Sun, Jinshan Zeng, **Yuan Yao**. DessiLBI: Exploring Structural Sparsity of Deep Networks via Differential Inclusion Paths. *The Thirty-seventh International Conference on Machine Learning (ICML)*, July 12-18, 2020.

7. Qianqian Xu, Jiechao Xiong, Zhiyong Yang, Xiaochun Cao, Qingming Huang and **Yuan Yao**. Who Likes What? – SplitLBI in Exploring Preferential Diversity of Ratings. *The Thirty-fourth AAAI Conference on Artificial Intelligence (AAAI)*, New York, February 7-12, 2020.

8. Bingzhe Wu, Chaochao Chen, Shiwan Zhao, Cen Chen, **Yuan Yao**, Guangyu Sun, Li Wang, Xiaolu Zhang, and Jun Zhou, Characterizing Membership Privacy in Stochastic Gradient Langevin Dynamics, *The Thirty-fourth AAAI Conference on Artificial Intelligence (AAAI)*, New York, February 7-12, 2020. `arXiv:1910.02249`.

9. Qianqian Xu, Xinwei Su, Zhiyong Yang, Xiaochun Cao, Qingming Huang, **Yuan Yao**. iSplit LBI: Individualized Partial Ranking with Ties via Split LBI. *the 33rd Conference on Neural Information Processing Systems (NeurIPS 2019)*, Vancouver, Canada, December 7-14, 2019. `arXiv:1910.05905`.

10. Zhicong Liang, Bao Wang, Quanquan Gu, Stanley Osher, **Yuan Yao**. Exploring Private Federated Learning with Laplacian Smoothing. *the 33rd Conference on Neural Information Processing Systems (NeurIPS 2019)*, Workshop on Federated Learning for Data Privacy and Confidentiality, Vancouver, Canada, Dec. 8-14, 2019. `arXiv:2005.00218`.

11. Qianqian Xu, Zhiyong Yang, Yangbangyan Jiang, Xiaochun Cao, Qingming Huang, **Yuan Yao**. Deep Robust Subjective Visual Property Prediction in Crowdsourcing. *Conference on Computer Vision and Pattern Recognition (CVPR)*, Long Beach, CA, June 16-20, 2019. `arXiv:1903.03956`.

12. Jinshan Zeng, Tim Tsz-Kit Lau, Shaobo Lin, and **Yuan Yao**. Global Convergence of Block Coordinate Descent in Deep Learning. `arXiv:1803.00225`, *The 36th International Conference on Machine Learning (ICML)*, Long Beach, CA, June 9-15, 2019.

13. Chao Gao, Jiyi Liu, **Yuan Yao**, Weizhi Zhu. Robust Estimation and Generative Adversarial Networks. *International Conference on Learning Representations (ICLR)*, New Orleans, LA. May 6-9, 2019. `arXiv:1810.02030`.

14. Bo Zhao, Xinwei Sun, Xiaopeng Hong, **Yuan Yao**, and Yizhou Wang. Zero-Shot Learning via Recurrent Knowledge Transfer. *IEEE Winter Conference on Applications of Computer Vision (WACV)*, Waikoloa Village, HI, USA, 7-11 Jan. 2019.

15. Yin Xian, Hanlin Gu, Wei Wang, Xuhui Huang, **Yuan Yao**, Yang Wang, Jian-Feng Cai. Data-Driven Tight Frame for Cryo-EM Image Denoising and Conformational Classification. *The 6th IEEE Global Conference on Signal and Information Processing*, Anaheim, California, Nov 26-29, 2018. `arXiv:1810.08829`.

16. Qianqian Xu, Jiechao Xiong, Xinwei Sun, Zhiyong Yang, Xiaochun Cao, Qingming Huang, **Yuan Yao**. A Margin-based MLE for Crowdsourced Partial Ranking. *In 2018 ACM Multimedia Conference (MM-18)*, October 22-26, 2018, Seoul, Republic of Korea. `arXiv:1807.11014`

17. Xinwei Sun, Lingjing Hu, Fandong Zhang, **Yuan Yao**, Yizhou Wang. FDR-HS: An Empirical Bayesian Identification of Heterogenous Features in Neuroimage Analysis. *The 21st International Conference on Medical Image Computing and Computer Assisted Intervention (MICCAI)*, Granada, Spain, Sep 16 - 20, 2018. `arXiv:1807.08125`.

18. Bo Zhao, Xinwei Sun, Yanwei Fu, **Yuan Yao**, Yizhou Wang. MSplit LBI: Realizing Feature Selection and Dense Estimation Simultaneously in Few-shot and Zero-shot Learning. *The 35th International Conference on Machine Learning (ICML)*, Stockholm, Sweden, 2018. `arXiv:1806.04360`.

19. Tim Tsz-Kit Lau, Jinshan Zeng, Baoyuan Wu, and **Yuan Yao**. A Proximal Block Coordinate Descent Algorithm for Deep Neural Network Training *The 6th International Conference on Learning Representations (ICLR)*, 2018, Workshop Track. `arXiv:1803.09082`.

20. Jinshan Zeng, Ke Ma, and **Yuan Yao**, Finding Global Optima in Nonconvex Stochastic Semidefinite Optimization with Variance Reduction. *Proceedings of the 21st International Conference on Artificial Intelligence and Statistics (AISTATS)*, Lanzarote, Spain, 2018. `arXiv: 1802.06232`.

21. Chendi Huang and **Yuan Yao**, A Unified Dynamic Approach to Sparse Model Selection. *Proceedings of the 21st International Conference on Artificial Intelligence and Statistics (AIS-TATS)*, Lanzarote, Spain, 2018.

22. Ke Ma, Jinshan Zeng, Jiechao Xiong, Qianqian Xu, Xiaochun Cao, Wei Liu, and **Yuan Yao**. Stochastic Non-Convex Ordinal Embedding with Stabilized Barzilai-Borwein Step Size. *The Thirty-Second AAAI Conference on Artificial Intelligence (AAAI-18)*, New Orleans, Louisiana, Feb 2-7, 2018. `arXiv:1711.06446`

23. Qianqian Xu, Jiechao Xiong, Xi Chen, Qingming Huang, and **Yuan Yao**. HodgeRank with Information Maximization for Crowdsourced Pairwise Ranking Aggregation. *The Thirty-Second AAAI Conference on Artificial Intelligence (AAAI-18)*, New Orleans, Louisiana, Feb 2-7, 2018. `arXiv:1711.05957`.

24. Tsz-Kit Lau and **Yuan Yao**. Accelerated Block Coordinate Proximal Gradients with Applications in High Dimensional Statistics. *The 10th NIPS Workshop on Optimization for Machine Learning (NIPS 2017)*, Long Beach, California, Dec 3-8, 2017. `arXiv:1710.05338`.

25. Qianqian Xu, Ming Yan, Chendi Huang, Jiechao Xiong, Qingming Huang, and **Yuan Yao**. Exploring Outliers in Crowdsourced Ranking for QoE. *ACM Conference on Multimedia (ACMMM)* (Oral presentation), Mountain View, California, Oct 23-27, 2017. `arXiv:1707.07539`.

26. Xinwei Sun, Lingjing Hu, **Yuan Yao**, and Yizhou Wang. GSplit LBI: Taming the Procedural Bias in Neuroimaging for Disease Prediction. *Medical Image Computing and Computer Assisted Interventions Conference (MICCAI)*, Quebec City, Canada, Sept 10-14, 2017. `arXiv:1705.09249`.

27. Lijing Wang, Yangzhong Tang, Stevan Djakovic, Julie Rice, Tony Wu, Daniel J. Anderson, and **Yuan Yao**, A Statistical Learning Approach for Drug Sensitivity Prediction with Cancer Cell Line Data, *Dahshu 2017: Data Science and Computational Precision Health*, San Francisco, Feb 20-22, 2017.

28. Chendi Huang, Xinwei Sun, Jiechao Xiong, and **Yuan Yao**, Split LBI: an Iterative Regularization Path with Structural Sparsity, *Advances in Neural Information Processing Systems 29 (NIPS)*, Barcelona, Spain, December 5-10, 2016.

29. Qianqian Xu, Jiechao Xiong, and **Yuan Yao**, Parsimonious Mixed-Effects HodgeRank for Crowdsourced Preference Aggregation, *ACM Conference on Multimedia (ACMMM)*, Netherland, Oct 2016. `arXiv:1607.03401`.

30. Qianqian Xu, Jiechao Xiong, Xiaochun Cao, and **Yuan Yao**, False Discovery Rate Control and Statistical Quality Assessment of Annotators in Crowdsourced Ranking, *International Conference on Machine Learning (ICML)*, New York, June 18- 25, 2016, `arXiv:1605.05860`.

31. Qing Wang, Hengshu Zhu, Wei Hu, Zhiyong Shen, and **Yuan Yao**, *Discerning Tactical Patterns for Professional Soccer Teams: An Enhanced Topic Model with Applications*, *Proceedings of the 21th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining (KDD)*, Sydney, Australia, Aug 10-13, 2015.

32. Yanwei Fu, Timothy M. Hospedales, Tao Xiang, Shaogang Gong, and **Yuan Yao**. Interestingness Prediction by Robust Learning to Rank. *13th European Conference on Computer Vision (ECCV)*, Zurich, Switzerland, Sep 8-12, 2014.

33. Qianqian Xu, Jiechao Xiong, Qingming Huang, and **Yuan Yao**. Robust Evaluation for Quality of Experience in Crowdsourcing. *ACM Conference on Multimedia (ACMMM)*, Barcelona, Catalunya, Spain, 2013.

34. Qianqian Xu, Qingming Huang, and **Yuan Yao**, Online Crowdsourcing Subjective Image Quality Assessment. *ACM Conference on Multimedia (ACMMM)*, Nara, Japan, 2012.

35. Xiuyuan Cheng, Jiechao Xiong, and **Yuan Yao**, Phase Transitions in Robust Ranking, preprint, short version appeared in Challenges in Geometry, Analysis and Computation: High Dimensional Synthesis. *A Conference in Honor of Ronald R. Coifman, Peter W. Jones and Vladimir Rokhlin, Yale University*, June 4- 6, 2012.

36. Jiang, Xiaoye, **Yuan Yao**, Han Liu and Leonidas Guibas, Detecting Network Cliques with Radon Basis Pursuit, *The Fifteenth International Conference on Artificial Intelligence and Statistics (AISTATS)*. La Palma, Canary Islands, Spain, April 2012.

37. Wei Wang, Cheng Chen, Yizhou Wang, Tingting Jiang, Fang Fang, and **Yuan Yao**. Simulating Human Saccadic Scanpaths on Natural Images. *IEEE Computer Vision and Pattern Recognition (CVPR)*, 2011.

38. Qianqian Xu, Tingting Jiang, **Yuan Yao**, Qingming Huang, Bowei Yan, Weisi Lin. Random Partial Paired Comparison for Subjective Video Quality Assessment via HodgeRank. *ACM Conference on Multimedia (ACMMM)*, Scottsdale, Arizona, USA, 2011.

39. Jiang, Xiaoye, Mo Li, **Yuan Yao**, and Leonidas Guibas, Overcomplete Radon Bases for Target Property Management in Sensor Networks, *Information Processing in Sensor Networks (IPSN), the 10th International Conference on*, 2011.

40. Zhanglong Ji, Yang An, Ying Chen, **Yuan Yao**, Jun Xu, and Hang Li, Hodge Decomposition of Paired Comparison Flows in Click-through Data. Oral presentation, in *6th Joint Workshop on Machine Perception and Robotics (MPR)*, Fukuoka, Japan, 2010.

41. Huang, Xuhui, **Yuan Yao**, Jian Sun, Leonidas Guibas, Gunnar Carlsson and Vijay Pande. Constructing Multi-Resolution Markov State Models (MSMS) to Elucidate RNA Hairpin Folding Mechanisms. in *Proceedings of the Pacific Symposium on Biocomputing*, 15, 228-239, 2010.

42. Sun, Jian, **Yuan Yao**, Xuhui Huang, Vijay Pande, Gunnar Carlsson, and Leonidas Guibas. A Fast Geometric Clustering Method on Conformation Space of Biomolecules. *Technical report, Stanford University*, 2009

43. **Yuan Yao**, Jian Sun, Xuhui Huang, Vijay Pande, Leonidas Guibas and Gunnar Carlsson. Topological Methods for Exploring Biomolecular Folding Pathways. *Biomedical Computation at Stanford (BCATS)*, spotlight poster presentation, October 26, 2008, Stanford, CA.

44. Sun, Jian, Xuhui Huang, **Yuan Yao**, Gunnar Carlsson, Vijay Pande and Leonidas Guibas. A Well-controlled Fast Clustering Method on Conformation Space of Biomolecules. *Biomedical Computation at Stanford (BCATS)*, poster presentation, October 26, 2008, Stanford, CA.

45. Bowman, Gregory, Xuhui Huang, **Yuan Yao**, Jian Sun and Vijay Pande. Adaptive Seeding: A New Method for Simulating Biologically Relevant Timescales. *Biomedical Computation at Stanford (BCATS)*, poster presentation, October 26, 2008, Stanford, CA.

46. Scheler, G. and **Yuan Yao**. Equilibria in neuroadaptive pathways. *RECOMB Systems Biology*, poster presentation, Dec 1-2, 2007, La Jolla, CA.

47. Minh, Ha Quang, Partha Niyogi and **Yuan Yao**. Mercer's Theorem, Feature Maps, and Smoothing. In: *Proc. of Computational Learning Theory (COLT)*, 2006.

48. **Yuan Yao**, Gian Luca Marcialis, Massimiliano Pontil, Paolo Frasconi, and Fabio Roli. A New Machine Learning Approach to Fingerprint Classification. *Congress of the Italian Association for Artificial Intelligence (AI*IA)*, LNCS, vol.2175: pp. 57-63, 2001.

49. **Yuan Yao**, Fabio Roli, Massimiliano Pontil. Fingerprint Classification with Combinations of Support Vector Machines. In: *Proceedings of Audio- and Video-Based Biometric Person Authentication, Third International Conference, AVBPA 2001*: Halmstad, Sweden, 2001.

50. **Yuan Yao** and Jin-Yun Ke (2000). Exploring Semantic Complexity by Computational Learning Theory. *Evolutionary Computation and Cognitive Science Workshop (ECCS)*, poster presentation, January, 2000, Melbourne, Australia, 2000.

51. **Yuan Yao**, Xiao-Feng Zhang, Tian-Wen Zhang and Guang-Xiong Wang. Multiscale Morphology for Color Images Implemented by Fuzzy Cellular Neural Network. In: *Proceedings of IEEE Hong Kong Symposium on Robotics and Control*, July 1999, Hong Kong, pp. 459-462.

52. **Yuan Yao**, Jing-Bo Wang, Lian-Feng Li and Guang-Xiong Wang. Optimal Robust Performance in Constantly Scaled $\mathscr{H}_\infty$ control. *Korea-China Process System Engineering Workshop*. Korea, August 1999.

53. **Yuan Yao**, Lian-Feng Li, Guang-Xiong Wang and Jing-Bo Wang. Robust Gain-scheduled $\mathscr{H}_\infty$ control with Constant Diagonal Scaling. In: *Proceedings of IEEE Hong Kong Symposium on Robotics and Control*, July 1999, Hong Kong, pp. 628-632, 1999.

54. Xiao-Feng Wang, **Yuan Yao**, Guang-Xiong Wang and Jing-Bo Wang. Application of Quadratic Stabilization, Constantly Scaled $\mathscr{H}_\infty$ control and μ-Synthesis. In: *Proceedings of IEEE Hong Kong Symposium on Robotics and Control*, July 1999, Hong Kong, pp. 633-637, 1999.

55. Jingbo Wang, Jibril Jiya, Xiaoping Liu, **Yuan Yao**, Guang-Xiong Wang and Shijie Xu. Identifying Noise Model in Closed-Loop Using Subspace Method. In: *Proceedings of the IEEE International Vehicle Electronics Conference (IVEC '99)*, Changchun, China, pp. 349-351, September 6-9, 1999.

Technical Reports:

1. Optimal Sample Selection Through Uncertainty Estimation and Its Application in Deep Learning. Yong Lin, Chen Liu, Chenlu Ye, Qing Lian, Yuan Yao, Tong Zhang. `arXiv:2309.02476`

2. Liang Ding, Tianyang Hu, Jiahang Jiang, Donghao Li, Wenjia Wang, Yuan Yao. Random Smoothing Regularization in Kernel Gradient Descent Learning. `arXiv:2305.03531`

3. Donghao Li, Yang Cao, Yuan Yao. Optimizing Random Mixup with Gaussian Differential Privacy. `arXiv:2202.06467`

4. Hanlin Gu, Lixin Fan, Bowen Li, Yan Kang, Yuan Yao, and Qiang Yang. Federated Deep Learning with Bayesian Privacy. `arXiv:2109.13012`

5. Wenqi Zeng, Siqin Cao, Xuhui Huang, and Yuan Yao. A Note on Learning Rare Events in Molecular Dynamics using LSTM and Transformer. `arXiv:2107.06573`.

6. Hanlin Gu, Wei Wang, Ilona Christy Unarta, Wenqi Zeng, Fu Kit Sheong, Peter Cheung, Song Liu, Yuan Yao, and Xuhui Huang. An Efficient Method to Quantify Structural Distributions in Heterogeneous cryo-EM Datasets. `bioRxiv:10.1101/2021.05.27.446075`.

7. Jinshan Zeng, Yixuan Zha, Ke Ma, Yuan Yao. On Stochastic Variance Reduced Gradient Method for Semidefinite Optimization. `arXiv:2101.00236`.

8. Yanwei Fu, Donghao Li, Xinwei Sun, Shun Zhang, Yizhou Wang, and Yuan Yao. S^2-LBI: Stochastic Split Linearized Bregman Iterations for Parsimonious Deep Learning. `arXiv:1904.10873`.

9. Xiao Li, Jinzhu Jia, and Yuan Yao, *Mixed and missing data: a unified treatment with latent graphical models*, `arXiv:1511.04656`.

STUDENTS SUPERVISED

Postdoctoral or Visiting scholars:

- Xiaowei Wang, Postdoc, Department of Chemical and Biological Engineering, Hong Kong University of Science and Technology, 2021-2023
- Yingqiao Yang, Postdoc, Department of Mathematics, Hong Kong University of Science and Technology, 2020-2022, now at Huawei.
- Kaiyi Huang, Research Associate, Department of Mathematics, Hong Kong University of Science and Technology, 2020-2021, now at University of Wisconsin at Madison
- Jinshan Zeng, Visiting scholar, Department of Mathematics, Hong Kong University of Science and Technology, 2017-2018, now at Jiangxi Normal University

- Zhen Li, Postdoc, Department of Mathematics, Hong Kong University of Science and Technology, 2016-2018, now at Huawei Theory Lab
- Qianqian Xu, Postdoc, BICMR Peking University, 2013-2015, PhD in Computer Science and Engineering, Chinese Academy of Sciences (CAS), now Associate Professor at Institute of Computing Technology, Chinese Academy of Sciences (CAS)
- Yanwei Fu, Visiting scholar, Peking University, 2013, PhD in EECS, University of London, Queen Mary, now Assistant Professor at Fudan University, Young Thousand Talent Program

Ph.D. students:
- Ruihe WANG, Department of Mathematics, HKUST, 2024-present
- Yuxuan CHEN, Department of Mathematics, HKUST, 2023-present
- Hangyu LIN, Department of Mathematics, HKUST, 2022-present
- Chen LIU, Department of Mathematics, HKUST, 2021-present
- Zhe WANG, Department of CSE, HKUST, 2020-present
- He Cao, HKUST (GZ-AI), 2020-present
- Ruoxue Liu, HKUST (GZ-DSA), 2020-present
- Xuantong Liu, HKUST (GZ-DSA), 2020-present
- Xiasi Wang, HKUST (GZ-DSA), 2020-present
- Yang Cao, Department of Mathematics, HKUST, 2019-present
- Donghao Li, Department of Mathematics, HKUST, 2019-present
- Jiamin Wu, Department of Mathematics, HKUST, 2019-present
- Wenqi Zeng, Department of Mathematics, HKUST, 2019-present
- Congmin Yuan, Program of Biological Engineering, HKUST, 2019-2022.
- Zhicong Liang, Department of Mathematics, HKUST, 2018-2022, now at Citadel.
- Yifei Huang, Department of Mathematics, HKUST, 2017-2021.
- Hanlin Gu, Department of Mathematics, HKUST, 2017-2021, now at Tencent Webank.
- Zhen Li, Department of Probability and Statistics, Peking University, 2015-present
- Weizhi Zhu, Department of Probability and Statistics, Peking University, 2014-2017; Department of Mathematics, HKUST, 2017-2020, now at Jane Street
- Xinwei Sun, Department of Probability and Statistics, Peking University, 2013-2018, now Assistant Professor at Fudan University
- Chendi Huang, Department of Probability and Statistics, Peking University, 2012-2017
- Jiechao Xiong, BICMR, Peking University, 2012-2017, now at Tencent AI Lab

Master students:
- Ying Chen, M.S., Statistics, Peking University, 2012, now at AIbee.
- Bowei Yan, M.S., Statistics, Peking University, 2014, now at Citadel
- Qing Wang, M.S., Statistics, Peking University, 2015, now at Tencent AI Lab.
- Yuan Lv, M.S., Statistics, Peking University, 2015, now at Shanghai bank
- Tim Lau, M.Phil., Data Science, HKUST, 2018-2019, now at Northwestern University
- Min Fan, M.Phil., Department of Mathematics, HKUST, 2017-2021
- Wing Kin Wong, M.Phil., Department of Mathematics, HKUST, 2021-present

Undergraduate (selected) and Visiting students:
- Xiuyuan Cheng, PhD in PACM, Princeton University, 2013, now at Duke University
- Xiaoye Jiang, PhD in ICME, Stanford University, 2010, now at 2-Sigma Co. Ltd.
- Jingshu Wang, B.S. Statistics, Peking University 2010, now at Stanford University
- An Yang, B.S. Statistics, Peking University 2010, now at Chinese University of Hong Kong
- Yuting Wei, B.S. Statistics, Peking University 2013, now at CMU
- Yu Lu, B.S. Statistics, Peking University, 2013, now at Yale University
- Feng Ruan, B.S. Statistics, Peking University 2014, now at UC Berkeley
- Jiyue Wang, B.S. Math, Shanghai Jiaotong University, 2014, now at Stanford University
- Tian Wang, B.S. Math, Shanghai Jiaotong University, 2014, now at NYU Courant Institute
- Kaizheng Wang, B.S. Statistics, Peking University, 2015, now at Columbia University

- Yao Yao, Oxford University, 2016.

COURSES	Graduate courses and undergraduate courses. Most course materials are published online in English (https://yao-lab.github.io/course.html).

- Advanced Topics in Deep Learning, Fall 2018, Fall 2020
- Capstone Project in Data Science, Fall 2020, Fall 2021
- Topological and Geometric Data Reduction and Visualization, Fall 2017, Spring 2019, Spring 2020
- Artificial Intelligence in Finance/Fintech, Spring 2019, Spring 2020, Fall 2021
- Statistical Machine Learning, Spring 2018, Spring 2022
- Statistical Prediction, Spring 2022
- Deep Learning: Towards Deeper Understanding, Spring 2018, Fall 2019
- A Mathematical Introduction to Data Science with R, Spring 2015 (planned)
- A Mathematical Introduction to Data Science, Fall 2011, Fall 2012, Fall 2013, Fall 2014, Spring 2017
- Statistical Learning, Spring 2013, Spring 2014, Fall 2015
- Probability and Statistics, Spring 2015
- Stochastic Dynamical Models in Life Sciences, Spring 2011
- Calculus for undergraduates in Economics and Yuan-Pei College, Fall 2010
- B.S. Statistics Thesis Seminar, Spring 2010
- Selected Topics in Advanced Statistics, Fall 2009

PROFESSIONAL SERVICE	Conference program committee or Journal editorship

- AAAI 2020 Area Chair
- IJCAI 2020, 2021 Senior Program Committee
- NIPS/NeurIPS 2011, 2021, 2022, 2023 Area Chair
- ICLR 2019, 2020, 2021, 2022 Area Chair
- ICML 2021 Area Chair
- CVPR 2022, Tutorial session on Sparsity Learning in Neural Networks and Robust Statistical Analysis
- HKUST IAS, The Mathematics of Deep Learning, 2018
- ICML, workshop on Topological Methods for Machine Learning, 2014
- IMA, workshop on Modern Applications of Homology and Cohomology, 2013
- ICIAM, Minisymposium of Applied Hodge Theory, 2011
- Frontiers in Applied Mathematics and Statistics (EPFL, Switzerland), Associate Editor
- SIAM Journal Applied Algebra and Geometry, Associate Editor, 2022 -
- Chinese Society of Cognitive Science, Scientific Committee, 2019 -

Journal or conference referee:
- ICML 2013, 2015, 2016, 2017, 2019
- NIPS 2003, 2005, 2014, 2016, 2018, 2019, 2020, and Area Chair 2011, 2021-2023
- ICLR 2018 and Area Chair 2019, 2020, 2022
- AISTATS 2011
- Annals of Statistics
- Applied and Computational Harmonic Analysis
- Frontiers in Applied Mathematics and Statistics (EPFL, Switzerland), Associate Editor
- Foundations of Computational Mathematics
- IEEE Transactions on Information Theory
- Journal of Approximation Theory
- Journal of Machine Learning Research
- Neural Computation
- Proceedings of National Academy of Sciences (PNAS)
- PLOS One

University committee
- Data Science cluster hiring search committee, University, 2016 - 2017
- The Taskforce on CryoEM, University, 2017 -

Department committee
- Substantiation and Promotion Committee, Department of Mathematics, 2023 -
- Search committee, AI Thrust of HKUST-GZ, 2020 -
- Search committee, Department of Mathematics, 2017 - 2018
- Executive committee, Department of Mathematics, 2020 - 2022