

Zheng Shi

Curriculum Vitae

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Machine Learning \simeq Optimization $_{f,w} \{f(w) \mid f \in \mathcal{F}\}$

Summary

full-time $\stackrel{\text{def}}{=}$ **Scientist Developer**, ≥ 7 yrs of experiences in AI & optimization application development.
part-time $\stackrel{\text{def}}{=}$ **PhD Candidate**, \subseteq advancing theory & practice of machine learning algorithms.

Education

2016–Present **Ph.D., Industrial and Systems Engineering**, GPA: 4.0, Lehigh Univ., US.
Exp. 01/2022 · Advisor: [Martin Takáč - Lab](#) 🔗
· Focus: **Deep Learning, Reinforcement Learning, Optimization for Machine Learning.**

2010–2013 **M.S., Industrial and Systems Engineering**, GPA: 3.9, Lehigh Univ., US.
· Focus: **Operations Research**

2005–2009 **B.A., English Literature**, Tianjin Univ., China.
B.Econ., Finance, Nankai Univ., China.

Professional Experiences

2020–Present **Senior Data Scientist & Scientist Developer**, *IBM Systems*, United States.
◦ Work closely with *Systems* executives to drive AI transformation of worldwide supply chain business.
◦ Conceptualize and formulate business problems as mathematical models and design solution architect.
◦ Lead a team and collaborate within IBM to develop & deploy ML and optimization applications.
◦ Lead algorithm development in AI products, e.g. *IBM Test Advisor*.
◦ Mentor junior data scientists & algorithm engineers and Co-create education programs.

2013–2020 **Staff, Advisory Data Scientist & Scientist Developer**, *IBM Global Services*, US.
◦ Work closely with *Services* executives to support decision-making in global service business.
◦ Define business problems and collaborate with academia to conduct research & produce solutions.
◦ Lead AI application development for global service supply chain management and revenue management, e.g. *IBM Network Neighborhood Service Parts Optimization*.
◦ Collaborate with IBM manufacturing, finance, research, etc on Operations Research projects.

2012–2013 **Operations Research Intern**, *IBM Global Technology Services*, US.
◦ Develop machine learning algorithms for service parts demand forecasting.
◦ Build optimization models for service parts inventory planning.

2009–2010 **Customer Manager**, *Agricultural Bank of China*, China.
◦ Conduct feasibility study of railway & real estate construction loan projects.

Technical Skills

ML & DS Pytorch, Tensorflow, PySpark, SQL, SPSS, SAS, R
Programming & Computing Python, Matlab, Java, C++, MPI, GPU computing
Math Programming CPLEX, Gurobi, AMPL, Mosek

Research Experiences

Deep Learning **Dynamical Systems and Quantum Chemistry.**

Design deep neural networks to solve & discover partial differential equations, predict behaviors & properties of large-scale molecular systems, and develop algorithms to boost training & inference efficiency.

- [1] Finite Difference Neural Networks: Fast Prediction of Partial Differential Equations
Shi, Z., Gulgec, N.S., Berahas, A., Pakzad, S. and Takáč, M. 19th IEEE International Conference on Machine Learning and Applications, 2020 [🔗](#) [📄](#)
- [2] Improved Training of Graph-Embedding Based Neural Network Energy Functions for Catalysis
Shi, Z., Rangarajan, S. and Takáč, M. AIChE Annual Meeting, 2020 [🔗](#) [📄](#)
- [3] FD-Net with Auxiliary Time Steps: Fast Predictions of PDEs using Hessian-free Trust-Region Methods
Gulgec, N.S., Shi, Z., Deshmukh, N., Pakzad, S. and Takáč, M. NeurIPS 2019 Workshop (Beyond First Order Methods in ML), 2019 [🔗](#)
- [4] Finite Difference Neural Networks: Discovering Hidden PDEs of Dynamical Systems
Shi, Z., Gulgec, N.S., Berahas, A., Pakzad, S. and Takáč, M. Working paper, 2021
- [5] Coupling Deep Learning with Hessian-Free Optimization on Predicting Potential Energy Function of Periodic Molecular Systems
Shi, Z., Rangarajan, S. and Takáč, M. Working paper, 2021

ML Algorithms **Advanced, Adaptive, and Distributed Optimization Algorithms.**

Develop novel algorithms and improve existing algorithms to solve large-scale ML problems. Develop adaptive (tune-free) gradient based algorithms, second-order algorithms, and distributed/HPC algorithms.

- [6] AI-SARAH: Adaptive and Implicit Stochastic Recursive Gradient Methods
Shi, Z., Loizou, N., Richtárik, P. and Takáč, M. Preprint & Under review, 2021 [🔗](#)
- [7] Doubly Adaptive Scaled Algorithm for Machine Learning Using Second-Order Information
Jahani, M., Rusakov, S., Shi, Z., Richtárik, P., Mahoney, M. and Takáč, M. Under review, 2021
- [8] Stochastic Variance Reduced Methods for Distributed and Federated Learning
Shi, Z., Richtárik, P. and Takáč, M. Working paper, 2021
- [9] Stochastic Trust-Region Conjugate Gradient Methods for Deep Learning
Shi, Z. and Takáč, M. Working paper, 2021

Reinforcement Learning **Combinatorial Optimization.**

Propose deep reinforcement learning approach to solve large-scale, NP-hard and stochastic combinatorial optimizations, e.g. job shop scheduling.

- [10] Asynchronous DRL for Stochastic Job Shop Scheduling Problem
Li, T., Shi, Z., Snyder, L. and Takáč, M. Working paper, 2021

Reviewers for Conferences and Workshops

2021 **38th International Conference on Machine Learning.**

2020 **34th Conference on Neural Information Processing Systems.**

2020 **12th OPT Workshop on Optimization for Machine Learning @ NeurIPS 2020.**

Awards & Recognitions

2020 **IBM Special Equity Award.**

2017–2019 **IBM Merit Award.**

2016–2022 **IBM Scholarship for Ph.D. Study.**

2015 **IBM Eminence & Excellence Award.**

2014–2020 **IBM Top Contributor.**

2013–2015 **IBM Manager's Choice Award.**