

# Tianfan Fu

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CONTACT INFORMATION	Computational Science and Engineering Atlanta, US Voice: +1 4706013173	Georgia Institute of Technology Email: futianfan@gmail.com & tfu42@gatech.edu Homepage: <a href="https://futianfan.github.io/">https://futianfan.github.io/</a>
RESEARCH INTERESTS	AI for Drug Discovery and Development, Machine Learning for Healthcare, AI for Science.	
EDUCATION	<b>Georgia Institute of Technology</b> , Atlanta, US. Ph.D. candidate, Advisor: <b>Jimeng Sun</b> , Computer Science Program in Department of Computational Science and Engineering, August 2018 - Present. <b>Shanghai Jiao Tong University (SJTU)</b> , Shanghai, CHINA M.S., Advisor: <b>Zhihua Zhang</b> , Computer Science and Technology, Sept 2015 - March 2018. <b>Shanghai Jiao Tong University (SJTU)</b> , Shanghai, CHINA B.E., Electronics and Electric Engineering (IEEE Honor Class), Computer Science, Sept 2011 - June 2015.	
RESEARCH EXPERIENCE	<b>Research Assistant</b> , Speech Lab, Shanghai Jiao Tong University (SJTU) Advisor: <b>Kai Yu</b> , June 2013 - Jan 2015. Research topic: application of deep learning on speech recognition and speaker verification. <b>Research Assistant</b> , Learning and Optimization Group, Shanghai Jiao Tong University (SJTU) Advisor: <b>Zhihua Zhang</b> , Feb 2015 - May 2017. Research topic: Bayesian computation and inference. <b>Research Assistant</b> , SunLab, Georgia Institute of Technology Advisor: <b>Jimeng Sun</b> , Sept 2018 - Present. Research topic: Drug Discovery and Development.	
INDUSTRY EXPERIENCE	<b>Research Intern</b> , Machine Learning Group, IQVIA, Boston Advisor: <b>Cao Xiao</b> , May 2021 - Aug 2021. Research topic: clinical trial outcome prediction <b>Research Intern</b> , Machine Learning Group, IQVIA, Boston Advisor: <b>Cao Xiao</b> , May 2020 - Aug 2020. Research topic: clinical trial outcome prediction	
TEXTBOOK	<b>Tianfan Fu</b> , Cao Xiao, Jimeng Sun: Machine learning for drug discovery and development. Expect to appear in May 2023 by Springer. <a href="https://ml4drug-book.github.io/">https://ml4drug-book.github.io/</a> Shenjian Zhao, Yujun Li, <b>Tianfan Fu</b> , Kai Li, Zhihua Zhang: <b>Chinese Translation of “Deep Learning (Goodfellow et al)”</b> . Sales volume: receiving <b>200K+</b> comments in <a href="https://jd.com">jd.com</a> .	
PUBLICATIONS	<b>Tianfan Fu*</b> , Wenhao Gao*, Connor W. Coley, Jimeng Sun. Reinforced Genetic Algorithm for Structure-based Drug Design. Neural Information Processing Systems ( <b>NeurIPS</b> ) 2022. Wenhao Gao*, <b>Tianfan Fu*</b> , Jimeng Sun, Connor W. Coley: Sample Efficiency Matters: A Benchmark for Practical Molecular Optimization. Neural Information Processing Systems ( <b>NeurIPS</b> 2022) Track on Datasets and Benchmarks.	

Kexin Huang\*, **Tianfan Fu\***, Wenhao Gao\*, Yue Zhao, Yusuf Roohani, Jure Leskovec, Connor W. Coley, Cao Xiao, Jimeng Sun, Marinka Zitnik: Artificial Intelligence Foundation for Therapeutic Science. **Nature Chemical Biology**, 2022.

**Tianfan Fu**, Jimeng Sun: SIPF: Sampling Method for Inverse Protein Folding. The 28th ACM **SIGKDD** Conference on Knowledge Discovery and Data Mining (2022).

**Tianfan Fu**, Jimeng Sun: Antibody Complementarity Determining Regions (CDRs) design using Constrained Energy Model. The 28th ACM **SIGKDD** Conference on Knowledge Discovery and Data Mining (2022).

**Tianfan Fu\***, Wenhao Gao\*, Cao Xiao, Jacob Yasonik, Connor W. Coley, Jimeng Sun. Differentiable Scaffolding Tree for Molecular Optimization. International Conference on Learning Representation (**ICLR**), 2022.

**Tianfan Fu**, Kexin Huang, Cao Xiao, Lucas M. Glass, Jimeng Sun. HINT: Hierarchical Interaction Network for Clinical Trial Outcome Prediction. Cell Patterns, 2022. **cover paper of Cell Patterns**, [https://www.cell.com/patterns/issue?pii=S2666-3899\(21\)X0005-0](https://www.cell.com/patterns/issue?pii=S2666-3899(21)X0005-0)

Kexin Huang\*, **Tianfan Fu\***, Wenhao Gao\*, Yue Zhao, Yusuf Roohani, Jure Leskovec, Connor W. Coley, Cao Xiao, Jimeng Sun, Marinka Zitnik: Therapeutics Data Commons: Machine Learning Datasets and Tasks for Drug Discovery and Development. Neural Information Processing Systems (**NeurIPS** 2021) Track on Datasets and Benchmarks.

**Tianfan Fu**, Cao Xiao, Lucas Glass, Jimeng Sun: MOLER: Incorporate Molecule-Level Reward to Enhance Deep Generative Model for Molecule Optimization. IEEE Transactions on Knowledge and Data Engineering (**TKDE**) 2021.

**Tianfan Fu**, Cao Xiao, Cheng Qian, Lucas Glass, Jimeng Sun: Probabilistic and Dynamic Molecule-Disease Interaction Modeling for Drug Discovery. The 27th ACM **SIGKDD** Conference on Knowledge Discovery and Data Mining (2021).

**Tianfan Fu**, Cao Xiao, Xinhao Li, Lucas Glass, Jimeng Sun: MIMOSA: Multi-constraint Molecule Sampling for Molecule Optimization. Association for the Advancement of Artificial Intelligence (**AAAI**) 2021.

Kexin Huang, **Tianfan Fu**, Lucas Glass, Marinka Zitnik, Cao Xiao, Jimeng Sun: DeepPurpose: a Deep Learning Library for Drug-Target Interaction Prediction. **Bioinformatics** 2020.

**Tianfan Fu**, Cao Xiao, Jimeng Sun: CORE: Automatic Molecule Optimization using Copy & Refine Strategy. Association for the Advancement of Artificial Intelligence (**AAAI**) 2020, New York, NY, USA. (**Oral**)

**Tianfan Fu\***, Tian Gao\*, Cao Xiao, Tengfei Ma, Jimeng Sun: PEARL: Prototype Learning via Rule Learning. ACM Conference on Bioinformatics, Computational Biology, and Health Informatics (**ACM BCB**) 2019, Niagara Fall, NY, USA. (**Oral**)

**Tianfan Fu\***, Trong Nghia Hoang\*, Cao Xiao, Jimeng Sun: DDL: Deep Dictionary Learning for Predictive Phenotyping. International Joint Conferences on Artificial Intelligence (**IJCAI** 2019), Macau, China. (**Oral**)

**Tianfan Fu**, Cheng Zhang, Stephan Mandt: Continuous Word Embedding Fusion via Spectral Decomposition. SIGNLL Conference on Natural Language Learning (**CoNLL** 2018), Brussels, Belgium. (**Oral**)

**Tianfan Fu**, Zhihua Zhang: CPSG-MCMC: Clustering-Based Preprocessing method for Stochastic Gradient MCMC. **AISTATS** 2017: 841-850, Lauderdale, FL, USA. (**Poster**)

**Tianfan Fu**, Luo Luo, Zhihua Zhang: Quasi-Newton Hamiltonian Monte Carlo. Conference on Uncertainty in Artificial Intelligence, **UAI** 2016, New York, NY, USA. (**Poster**)

Wei Li, **Tianfan Fu**, Hanxu You, Jie Zhu, Ning Chen: Feature sparsity analysis for i-vector based speaker verification. **Speech Communication** 80: 60-70, 2016.

Yuan Liu, Yanmin Qian, Nanxin Chen, **Tianfan Fu**, Ya Zhang, Kai Yu: Deep feature for text-dependent speaker verification. **Speech Communication** 73: 1-13, 2015. (**2019 EURASIP award for the best paper published in Speech Communication (2014-2017)**)

Wei Li, **Tianfan Fu**, Jie Zhu: An improved i-vector extraction algorithm for speaker verification. **EURASIP J. Audio, Speech and Music Processing** 2015: 18, 2015.

Wei Deng, Yanmin Qian, Yuchen Fan, **Tianfan Fu**, Kai Yu: Stochastic data sweeping for fast DNN training. IEEE International Conference on Acoustics, Speech and Signal Processing, **ICASSP** 2014: 240-244.

Yuan Liu, **Tianfan Fu**, Yuchen Fan, Yanmin Qian, Kai Yu: Speaker verification with deep features. International Joint Conference on Neural Networks, **IJCNN** 2014: 747-753, Beijing, China (**Oral**)

**Tianfan Fu**, Yanmin Qian, Yuan Liu, Kai Yu: Tandem deep features for text-dependent speaker verification. **INTERSPEECH** 2014: 1327-1331, Singapore. (**Oral**)

#### RELATED SKILLS

- Programming Skills: Python, C++, Bash(awk, sed, etc.), LaTeX, git, Pytorch, Tensorflow

#### AWARDS

- 2016 SJTU Academic Excellence Scholarship Class-A (Top 15%)
- 2017 CS Graduates Education & Development Fund and Yang Yuanqing Education Fund (Top-3 in all graduate students in CS Department).

#### ACADEMIC INVOLVEMENT

- 2016 UAI Travel Award & Volunteer
- 2016 NIPS (Neural Information Processing Systems) Reviewer (5 papers)
- 2017 AAI sub-reviewer (2 papers)
- 2017 AISTATS Travel Award
- 2018 AAI Reviewer (1 paper)
- 2019 Frontiers in Genetics (1 paper)
- Frontiers Bioengineering (1 paper)
- 2020 IEEE Journal of Biomedical and Health Informatics (JBHI) Reviewer (1 paper)
- 2020 IEEE Transactions on Cybernetics reviewer (1 paper)
- 2020 ICCCN (The 29th International Conference on Computer Communications and Networks) reviewer (1 paper).
- 2020 PLOS Computational Biology (1 paper)
- 2020 NeurIPS (6 papers)
- 2021 AAI (3 papers)
- 2021 IJCAI (Senior Program Committee (SPC) members, 2 papers).
- 2021 ICML (5 papers).
- 2021 IEEE Transactions on Neural Networks and Learning Systems (TNNLS) (1 paper).
- 2021 KDD DLG (Deep Learning on Graphs) Workshop (2 papers).
- 2021 NeurIPS (1 paper).
- 2021 Mathematical Biosciences and Engineering (1 paper).
- 2022 ICLR (1 paper).

- **Organizer of NeurIPS 2021 “1st AI for Science: Mind the Gaps” Workshop**
- 2022 CHIL (Conference on Health, Inference, and Learning) (3 papers).
- 2022 ICML (1 paper).
- **Organizer of ICML 2022 “2nd AI for Science” Workshop.**
- **Organizer of NeurIPS 2022 “3rd AI for Science: Progress and Promises” Workshop.**  
(<https://ai4sciencecommunity.github.io/>)
- 2022 ICML AI for Science Workshop (18 paper).
- 2022 KDD Travel Award

#### TEACHING

- 2016 Spring Prof. Zhihua Zhang’s course “Statistical Machine Learning” TA
- 2018 Spring Prof. Bo Yuan’s course “Artificial Intelligence” TA
- 2019 Fall Prof. Jimeng Sun’s course “Big Data Analytics for Healthcare” TA
- 2020 Spring Prof. Jimeng Sun’s course “Big Data Analytics for Healthcare” TA
- 2020 Fall Prof. Jimeng Sun’s course “Big Data Analytics for Healthcare” TA