

YU BAO

Research Scientist · ByteDance

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EDUCATION

Nanjing University

Nanjing, China

PH. D. IN COMPUTER SCIENCE

Mar. 2022

- Dissertation: *Research on Deep Text Generation Models with Structure Modeling*
- Advisor: Prof. [Jiajun Chen](#) and Prof. [Shujian Huang](#)

Northeast Forestry University

Harbin, China

B. SC. IN MATHEMATICS

Jul. 2015

- Thesis: *Stock Selection by Clustering and Dynamic Programming*

RESEARCH INTERESTS

My research is in natural language processing and deep learning, focusing on DEEP GENERATIVE MODELS and their application in structure or sequence modeling. Recently, my responsibility transferred to research on AI FOR SCIENCE, especially in small molecular drug design, and aimed to advance using diffusion models to (1) generate molecules and (2) molecular optimization.

EMPLOYMENTS

ByteDance Research

Shanghai, China

RESEARCH INTERN & RESEARCH SCIENTIST

Apr. 2021 - Present

- Research on AI FOR SCIENCE (STRUCTURE-BASED DRUG DESIGN)

Goal: Explore and develop the best methodology for molecular design

We design a better protein-ligand binding priori for the diffusion model, significantly improving the success rate of structure-based drug design[2][3]. Then, we propose a controllable and decomposed diffusion model for structure-based molecular optimization and open a new paradigm that combines molecular generation and optimization for structure-based drug design[1].

- Research on NON-AUTOREGRESSIVE GENERATION

Addressing Multi-modality Problem[11][12]: We first discuss the risk of knowledge distillation to non-autoregressive Transformer (NAT) and propose selectively using distillation data or using latent variables to alleviate the *multi-modality problem*, which successfully supports parallel decoding in more scenarios, even without the need for knowledge distillation.

Word Dependency Modeling[13]: We develop Glancing Transformer[13]. It achieves success in [WMT-2021](#) and *won first place in the German↔English translation task*. It can also be the first deployed parallel translation system [ByteDance VolcTrans](#), achieving 10X speedups.

AWARDS

Excellent Doctoral Dissertation Award, Jiangsu Association of Artificial Intelligence, 2022

Outstanding PhD candidate, Nanjing University, 2020

Artificial Intelligence Scholarship, Nanjing University, 2019

Outstanding Graduate Student, Nanjing University, 2019

First-Class Academic Scholarship of Graduate Student, Nanjing University, 2016

Second Prize of the Heilongjiang Province Division in National University Student Mathematical Modeling Competition, 2013

PUBLICATIONS

(Note: * indicates equal contributions, † indicates interns I mentored at ByteDance/NJU.)

AI FOR SCIENCE (STRUCTURE-BASED DRUG DESIGN)

1. Xiangxin Zhou[†], Xiwei Cheng[†], Yuwei Yang, Yu Bao, Liang Wang, Quanquan Gu, [DecompOpt: Controllable and Decomposed Diffusion Models for Structure-based Molecular Optimization](#), in **ICLR 2024**
2. Zhilin Huang, Ling Yang[†], Zaixi Zhang, Xiangxin Zhou[†], Yu Bao, Xiwu Zheng, Yuwei Yang, Yu Wang, Wenming Yang, [Binding-Adaptive Diffusion Models for Structure-Based Drug Design](#), in **AAAI 2024**
3. Jiaqi Guan[†], Xiangxin Zhou[†], Yuwei Yang, Yu Bao, Jian Peng, Jianzhu Ma, Qiang Liu, Liang Wang, Quanquan Gu, [DecompDiff: Diffusion Models with Decomposed Priors for Structure-Based Drug Design](#), in **ICML 2023**

DEEP GENERATIVE MODELS, LLMs, ETC

4. Shimao Zhang[†], Yu Bao, Shujian Huang, [EDT: Improving Large Language Models by Entropy-based Dynamic Temperature Sampling](#), *Arxiv Preprint*
5. Jiasheng Ye, Zaixiang Zheng, Yu Bao, Lihua Qian, Quanquan Gu, [Diffusion Language Models Can Perform Many Tasks with Scaling and Instruction-Finetuning](#), *Arxiv Preprint*
6. Jiasheng Ye, Zaixiang Zheng, Yu Bao, Lihua Qian, Mingxuan Wang, [DiNoISer: Diffused Conditional Sequence Learning by Manipulating Noises](#), **Transaction of ACL, 2024**
7. Yawen Ouyang, Yuan Gao, Shi Zong, Yu Bao, Xinyu Dai, [Pobe: Generative Model-based Out-of-distribution Text Detection Method](#), **Journal of Software, 2023**
8. Yu Bao, Shujian Huang, Hao Zhou, Lei Li, Xinyu Dai, Jiajun Chen, [Unsupervised Paraphrasing via Syntactic Template Sampling](#), **SCIENTIA SINICA Informationis, 2022**
9. Jiahuan Li*, Yu Bao*, Shujian Huang, Xinyu Dai, Jiajun Chen, [Explicit Semantic Decomposition for Definition Generation](#), in **ACL 2020**
10. Yu Bao*, Hao Zhou*, Shujian Huang, Lei Li, Lili Mou, Olga Vechtomova, Xinyu Dai, Jiajun Chen, [Generating Sentences from Disentangled Syntactic and Semantic Spaces](#), in **ACL 2019**

NON-AUTOREGRESSIVE GENERATION

11. Min Liu[†], Yu Bao, Chengqi Zhao, Shujian Huang, [Selective Knowledge Distillation for Non-Autoregressive Neural Machine Translation](#), in **AAAI 2023**
12. Yu Bao, Hao Zhou, Shujian Huang, Dongqi Wang, Lihua Qian, Xinyu Dai, Jiajun Chen, Lei Li, [latent-GLAT: Glancing at Latent Variables for Parallel Text Generation](#), in **ACL 2022**
13. Lihua Qian, Hao Zhou, Yu Bao, Mingxuan Wang, Lin Qiu, Weinan Zhang, Yong Yu, Lei Li, [Glancing Transformer for Non-Autoregressive Neural Machine Translation](#), in **ACL 2021**
14. Yu Bao, Shujian Huang, Tong Xiao, Dongqi Wang, Xinyu Dai, Jiajun Chen, [Non-Autoregressive Translation by Learning Target Categorical Codes](#), in **NAACL-HLT 2021**
15. Yu Bao, Hao Zhou, Jiangtao Feng, Mingxuan Wang, Shujian Huang, Jiajun Chen, Lei Li, [PNAT: Non-Autoregressive Transformer by Position Learning](#), *Preprint 2019*

TALKS

1. Grammar Learning and Its Application for Molecular Design, Tsinghua University AIR, Oct. 2022.
2. *latent-GLAT: Glancing at Latent Variables for Parallel Text Generation*, CIPSC & PaperWeekly & MLNLP, ACL-IJCAI-SIGIR, Apr. — May. 2022.
3. Research and Development of Parallel Text Generation, ByteDance AI Lab, Oct. 2021.
4. Advice for Undergraduate Students, Northeast Forestry University, Nov. 2020.

PROFESSIONAL SERVICES

- AREA CHAIR of
 - The 1st GenBio Workshop on New Frontiers of Generative AI and Biology at NeurIPS 2023
- JOURNAL REVIEWER of
 - IEEE Transaction on Pattern Analysis and Machine Intelligence (TPAMI)
 - IEEE Transactions on Neural Networks and Learning Systems (TNNLS)
 - Journal of Artificial Intelligence Research (JAIR)
- PC MEMBER/REVIEWER of
 - International Conference on Machine Learning (ICML) 2023-
 - Annual Conference on Neural Information Processing Systems (NeurIPS) 2022-
 - International Conference on Learning Representations(ICLR) 2022-
 - Annual Meeting of the Association for Computational Linguistics (ACL) 2021-
 - Conference on Empirical Methods in Natural Language Processing (EMNLP) 2021-
 - North American Chapter of the Association for Computational Linguistics (NAACL) 2022-
 - ACM SIGKDD International Conference on Knowledge Discovery and Data Mining (KDD) 2022-
 - AAAI Conference on Artificial Intelligence (AAAI) 2022-
 - International Joint Conferences on Artificial Intelligence (IJCAI) 2020
 - The Chinese National Conference on Computational Linguistics (CCL) 2022
 - The CCF Conference on Natural Language Processing and Chinese Computing (NLPCC) 2022

TEACHING EXPERIENCES

1. TA: Natural Language Generation and Machine Translation, Nanjing University, 2021
2. TA: Advanced Programming in C++, Nanjing University, 2018 & 2020
3. TA: Introduction to Software Industry, Nanjing University, 2018