

# S-Data Science Lab



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# Overview

- **Our Mission**

- New AI Paradigms
  - Model Architectures, Optimization Methods, etc.
- AI-Empowered Scientific Discovery
  - AI4Science, *AI4Health*, *AI4Math*

- **Tech Questions**

- Structured Data (e.g., Graphs and Sequences) Inference, Analysis, Generation, and ***Control***

- **Applications**

- Drug design
- Network analysis
- **3D Graphics**
- **Mathematical Problem Solver**

# Your Missions (Our Goals)

- **Strong Mathematical Modeling Skill**
  - Abstract Ability: Describe Real-World Problems in Math
  - Association Ability: Connect Knowledge/Tech in Different Fields
  - Problem Solver: Learn Optimization Methods and Theory
- **Outstanding Communication Skill**
  - Listening, Writing, Presentation, English Skill
- **Terrific Coding Skill**
  - Fluent on Python, Build and Maintain Toolboxes and Libs (Your Research Fruits)
  - If you would like, teach me other things (e.g., CUDA)
- **A Honest Person THE MOST IMPORTANT!**
  - Fight to Academic Misconduct
- **If our goals are inconsistent, we need to talk in person...**

# Target Publications

- **Conferences**

- **CCF-A:** ICML, NeurIPS, ICLR, COLT, KDD, WWW, AAI, IJCAI, CVPR, ICCV, SIGIR, ACMMM
- **CCF-B:** ECCV, WSDM, CIKM, UAI, AISTATS, ICASSP, SDM, ICDM, ICME...

- **Journals**

- JMLR, TPAMI, TIT, SIAM Optimization, Nature Machine Intelligence, ...
- TMLR, TSP, TNNLS, TKDE, TSIPN, ...

- **1. Let me know when you have other targets.**
- **2. Show me your COMPLETE draft two weeks before ddl.**
- **3. Don't abuse coauthorship.**
- **4. Be careful, make your work systematic.**

# Workload and Payment

- **Payment Strategy**

- Time: <10 months
- Amount: Depend on funding status

- **Internship and visiting scholarship**

- For summer internships, no restrictions.
  - Be responsible for yourselves.
- For the internships in other time periods
  - Let me know in advance. Correlated with your research.
- Open to international exchange and visiting projects.
  - Let me know in advance. Correlated with your research.

- **Flexibility of Workload**

- Do not absent group/project meetings without notices
- No more rules

# Project Management

- **<https://github.com/SDS-Lab>**
  - Release our code through this organization and fork to yourself.
  - Maintain your works on your own.
- Generally, each work is associated with **papers, codes, and patents.**

# What We Did Last Year?

- **Accepted Works (Let us cheer up:))**

- My work: TPAMI + 2, ACMMM 2023, IJCAI 2023 + 2
- Team work: AAAI 2023 + 2, CIKM 2023 + 1
- Every PhD has at least one submission/accepted paper.

- **Projects:**

- CAAI-Huawei Mindspore (9w, Nov 2023)
- NSFC重大研究计划培育项目 (80w, Dec 2025)
- MOOC Funding (2w, Done)
- NSFC青基 (30w, Dec 2024)
- RUC Startup Funding (15w, Dec 2024)
- NSFC海外优青 (300w, Dec 2025)

# What Will We Do This Year?

- **Projects:**

- 中央引导地方人工智能专项 (1800w, 申请中)
- 302 Hospital Project (推进中)
- CAAI-Huawei Mindspore (9w, Nov. 2023)
- **Prepare for writing and applying other proposals**

- **Research work:**

- 1st-year PhD: at least submit one paper.
- 2nd-year PhD: one accepted work + at least submit one more paper.
- 3rd-year PhD: at least submit one paper **based on your own idea.**
- **Sharpen your reading, talking and writing skills.**



# What Will We Do This Year?

- **Research**

- **More reading workloads.** Improve your reading and investigation efficiency.
  - Try to compress your preparation time for reading groups
  - Push me with papers, rather than let me push you
- **More informative group meeting report.**
  - It is a good chance to share your research and interact with others.
- After reading sufficiently, more brain storms
  - Try to propose research ideas by yourselves
- **Coding and math**
  - **Be familiar with basic concepts, knowledge and tools in your field**

# What Will We Do This Year?

- **AI4Science**

- New Model Architectures for AlphaFold and Others (Shen)
- **LLM for Molecular Retrosynthesis/Synthesis (Shen, Fanmeng)**
- **Shape-based Molecular Generation (Fanmeng)**
- Toxicology Prediction (Fanmeng)
- OT-based GNN Learning (Minjie)
- Quaternion-based Conformation Analysis (Angxiao)
- Self-supervised Learning for **Single-cell Analysis** (Fengjiao, Angxiao)

# What Will We Do This Year?

- **Point Process for Healthcare**
  - EOT-based TPP Learning (Qingmei)
  - NTPP Clustering (Qingmei)
  - **LLM for TPP** (Yuxin)
  - Granger Causality for NTPP (Ke, Yuxin)
- **Toolboxes and Benchmarks (Dec. 2023)**
  - PoPPy2 (Yuxin, Qingmei)
  - OT Package, developing POT API + Mindspore version (Minjie, Angxiao)
- **Write ML Book (Hongteng, Jan. 2024)**

Thanks & QA!