XIAO WANG

✉ wang3702@purdue.edu · in Xiao Wang · ○ GitHub · Website · Google Scholar

EDUCATION

Purdue University, West Lafayette, U.S   Aug, 2018 – Present
PhD student in Computer Science GPA:**3.91/4.0**

Xi'an JiaoTong University, Xi'an, China   Aug, 2014 – June, 2018
B.S. in Computer Science GPA: 90.57/100; Rank: **1/170**

EXPERIENCE

Kihara Bioinformatics Lab,West Lafayette, U.S   Aug, 2018 – Present
Research Assistant   Advisor: Prof. Daisuke Kihara

Deep learning for 3D protein structure modeling and function prediction.
- 1) DOVE:Apply 3D CNN to evaluate the quality of protein docking models.
- 2) Emap2sec+: Apply 3D ResNet to detect protein and DNA structures in Cryo-EM maps of intermediate resolution.
- 3) MAINMAST_Seg: Apply MST and LDP to extract reliable protein fragments from Cryo-EM map.
- 4) GNN_DOVE : Apply Graph neural network to evaluate protein docking models.
- 5) Deep MAINMAST: Build a graph based on deep-learning based structure prediction in Cryo-EM maps and then trace the main chain of protein from the graph.
- 6) DAQ: Utilize deep learning to evaluate the deposited structures and yield promising information for experimental scientists to revise their structures.

Facebook AI Research, Menlo Park, U.S   May, 2021 – Aug, 2021
Research Intern   Advisor: Dr. Xinlei Chen, Haoqi Fan

Self-supervised learning for Image Classification without labels
- Proposed novel asymmetrical self-supervised learning methods
- Extend asymmetrical design to several existing methods and verified its generalization
- Investigated the BatchNorm (BN) importance in self-supervised learning with asymmetrical design.
- Achieved state-of-the-art performance of self-supervised ResNet-50 on ImageNet with less computation.

JD AI Research, Mountain View, U.S   May, 2020 – Dec, 2020
Research Intern   Advisor: Dr. Jingen Liu

Temporal contrastive learning for video event segmentation
- Proposed self-supervised learning framework for event segmentation in videos
- Integrated Transformer and contrastive learning to detect event boundary
- Achieved state-of-the-art performance on video segmentation dataset with much higher MOF and IOU.
- Proposed our own evaluation metrics F1@5% that is more general for event segmentation

Futurewei AI Lab, Bellevue, U.S   May, 2019 – August, 2019
Computer Vision Research Intern   Mentor: Dr. Lin Chen, Supervisor: Prof. Guojun Qi, Prof. Jiebo Luo

Pre-task representation learning for self-supervised and semi-supervised learning.
- 1) EnAET: Proposed novel idea based on Auto-Encoding Transformation, which achieved SOTA performance on semi- and fully- supervised benchmarks.
- 2) CLSA: Introduced stronger augmentation to contrastive learning as an auxiliary task, which greatly boosted the performance.
- 3) AdCo: Adversarial contrastive learning methods by building an adversarial trainable memory bank.
- 4) CaCo: Cooperative and Adversarial contrastive learning methods by building a trainable memory bank with cooperative positive and adversarial negative training.

Institute of Automation, Chinese Academy of Sciences,Beijing, China   June, 2016 – June, 2018

Machine Learning Intern Mentor: Dr. Yilun Lin, Supervisor: Prof. Li-Li, Prof. Fei-Yue Wang

Deep learning for car-following trajectory prediction and traffic simulation.

- Proposed GRU-based car-following model, which greatly improved performance on NGSIM dataset.
- Built the traffic flow simulation platform with our car-following model and reproduced the classical traffic congestion pattern.
- Proposed a novel way based on DQN(A2C) and ARS to adjust GAN's hyper-parameters.
- Tests are carried on MNIST, CIFAR and CelebA but without stable and extraordinary performance.
- Codes available in ARS GAN.

SELECTED PUBLICATIONS

1 **Xiao Wang***, Genki Terashi* , Sai Raghavendra Maddhuri Venkata Subramaniya, John J. G. Tesmer Daisuke Kihara. Residue-Wise Local Quality Estimation for Protein Models from Cryo-EM Maps. **Nature Methods**. (2021). (minor revision). [GitHub]. [Colab]

2 **Xiao Wang**, Eman Alnabati, Tunde W Aderinwale, Sai Raghavendra Maddhuri Venkata Subramaniya, Genki Terashi & Daisuke Kihara. Emap2sec+: Structure Detection in Intermediate Resolution Cryo-EM Maps Using Deep Learning. **Nature Communications**. (2021). [Paper] [GitHub]

3 **Xiao Wang**, Guo-Jun Qi. Contrastive Learning with Stronger Augmentations. IEEE Transactions on pattern analysis and machine intelligence (**IEEE T-PAMI**).(2021). (2nd round review) [Paper] [GitHub]

4 **Xiao Wang**, Yuhang Huang, Dan Zeng, Guo-Jun Qi. CaCo: Both Positive and Negative Samples are Directly Learnable via Cooperative-adversarial Contrastive Learning. IEEE Transactions on pattern analysis and machine intelligence (**IEEE T-PAMI**).(2022). (Submitted).[Paper] [GitHub]

5 Guo-Jun Qi, Liheng Zhang, Feng Lin, **Xiao Wang**. Learning Generalized Transformation Equivariant Representations via Autoencoding Transformations. IEEE Transactions on pattern analysis and machine intelligence (**IEEE T-PAMI**). (2020). [Paper] [GitHub]

6 **Xiao Wang***, Haoqi Fan*, Yuandong Tian, Daisuke Kihara, Xinlei Chen. On the Importance of Asymmetry for Siamese Representation Learning. IEEE/CVF Conference on Computer Vision and Pattern Recognition (**CVPR 2022**).[Paper] [GitHub]

7 **Xiao Wang***, Qianjiang Hu*, Wei Hu, Guo-Jun Qi. AdCo: Adversarial Contrast for Efficient Learning of Unsupervised Representations from Self-Trained Negative Adversaries. IEEE/CVF Conference on Computer Vision and Pattern Recognition (**CVPR 2021**). [Paper] [GitHub]

8 **Xiao Wang**, Daisuke Kihara, Jiebo Luo, Guo-Jun Qi. Enaet: Self-trained ensemble autoencoding transformations for semi-supervised learning. IEEE Transactions on Image Processing (**IEEE TIP**). (2020). [Paper] [GitHub]

9 **Xiao Wang**, Jingen Liu, Tao Mei, Jiebo Luo. CoSeg: Cognitively Inspired Unsupervised Generic Event Segmentation. IEEE Transactions on Neural Networks and Learning Systems (**IEEE TNNLS**). (Submitted) [Paper]

10 **Xiao Wang**, Sean T, Flannery, Daisuke Kihara. Protein Docking Model Evaluation by Graph Neural Networks. Frontiers in Molecular Biosciences (**FMOLB**).(2021). [Paper] [GitHub]

11 **Xiao Wang**,Genki Terashi, Charles W. Christoffer, Mengmeng Zhu, and Daisuke Kihara, Protein Docking Model Evaluation by 3D Deep Convolutional Neural Networks. **Bioinformatics** 36: 2113-2118 (2020). [Paper] [GitHub]

12 **Xiao Wang**, Rui Jiang, Li Li, Yi-Lun Lin, and Fei-Yue Wang. Long memory is important: A test study on deep-learning based car-following model. Physica A: Statistical Mechanics and its Applications,514: 786-795, (2019) [Paper]

13 **Xiao Wang**, Rui Jiang, Li Li, Yilun Lin, Xinhu Zheng, and Fei-Yue Wang. Capturing car-following behaviors by deep learning. IEEE Transactions on Intelligent Transportation Systems (**IEEE T-ITS**), PP(99):1–11, (2018). [Paper]

OTHER PUBLICATIONS

1 Broyles, Bradley K., Andrew T. Gutierrez, Theodore P. Maris, Daniel A. Coil, Thomas M. Wagner, **Xiao Wang**, Daisuke Kihara, Caleb A. Class, and Alexandre M. Erkine. "Activation of gene expression by detergent-like protein domains." **Iscience** 24, no. 9 (2021): 103017. [Paper] [GitHub]

2 M.F. Lensink, ..., Charles Christoffer, Genki Terashi, Jacob Verburgt, Daipayan Sarkar, Tunde Aderinwale, **Xiao Wang**, Daisuke Kihara, ..., & S.J. Wodak (108 authors), Prediction of protein assemblies, the next frontier: The CASP14-CAPRI experiment. Proteins, in press, (2021) [Paper]

3 Zhang, Mei, Zhicheng Zhang, **Xiao Wang**, Hui Yu, Yifan Xia, Kanran Tan, and Fei-Yue Wang. "From AR to AI: Augmentation Technology for Intelligent Surgery and Medical Treatments." IFAC-PapersOnLine 53, no. 5 (2020): 792-796. [Paper]

4 **Xiao Wang**, Mizu Kittaka, Yilin He, Yiwei Zhang, YYasuyoshi Ueki, and Daisuke Kihara. OC_Finder: A deep learning-based software for osteoclast segmentation, counting, and classification. Frontiers in Bioinformatics. (2021). [Paper] [GitHub] [Colab]

5 Ilja Gubins, Marten L. Chaillet, Gijs van der Schot, Remco C. Veltkamp, Friedrich Förster, Yu Hao, Xiaohua Wan, Xuefeng Cui, Fa Zhang, Emmanuel Moebel, **Xiao Wang**, Daisuke Kihara, Xiangrui Zeng, Min Xu, Nguyen P. Nguyen, Tommi White, Filiz Bunyak, SHREC'20 Benchmark: Classification in cryo-electron tomograms, Computers & Graphics, (2020). [Paper]

6 **Xiao Wang**, Yuanyuan Zhang, Shengnan Yu, Xiwei Liu, Yong Yuan, and Fei-Yue Wang. E-learning recommendation framework based on deep learning. In SYSTEMS,MAN,AND CYBERNETICS, 2017 IEEE International Conference on (**IEEE SMC**). pp. 455-460, IEEE, (2017). [Paper]

7 **Xiao Wang**, Yuanyuan Zhang, Shengnan Yu, Xiwei Liu, and Fei-Yue Wang. Computerized adaptive English ability assessment based on deep learning. In Pacific-Rim Symposium on Image and Video Technology. pp. 158-171. Springer, (2017). [Paper]

8 Xiaoyan Gong, Xiwei Liu, Sifeng Jing, and **Xiao Wang**. Parallel education systems under perspective of system construction for new IT era. In Pacific-Rim Symposium on Image and Video Technology. pp. 131-143. Springer, (2017). [Paper]

PROFESSIONAL SERVICES

Reviewer of IEEE Transactions on Pattern Analysis and Machine Intelligence

Reviewer of IEEE Transactions on Image Processing

Reviewer of Pattern Recognition

Reviewer of Bioinformatics

Reviewer of IEEE Transactions on Intelligent Transportation Systems

Reviewer of IEEE Transactions on Multimedia

Reviewer of ACM Transactions on Knowledge Discovery from Data

Reviewer of IEEE Intelligent Systems

Reviewer of Frontiers in Bioinformatics

Reviewer of Conference on Neural Information Processing Systems (NurIPS)

Reviewer of Conference on Computer Vision and Pattern Recognition (CVPR)

Reviewer of International Conference on Computer Vision (ICCV)

Reviewer of European Conference on Computer Vision (ECCV)

PRESENTATIONS

1 "The OC_Finder: A deep learning-based software for in vitro osteoclast counting", **Xiao Wang**,Mizuho Kittaka, Yilin He, Yiwei Zhang, Daisuke Kihara, Yasuyoshi Ueki, 2021 Annual Meeting of The American Society for Bone and Mineral Research, October 1-4, 2021

2 "Emap2sec+: Decting protein and DNA/RNA stru tures in cryo-EM maps of intermediate resolution using deep learning." **Xiao Wang**, Eman Alnabati, Tunde W. Aderinwale, Sai Raghavendra Maddhuri Venkata Subramaniya, Genki Terashi, Daisuke Kihara, 71st Annual Meeting of the American Crystallographic Association, July 30 - Aug 5, 2021.

3 "Detecting protein and DNA/RNA structures in cryo-EM maps of intermediate reosolution using deep learning", **Xiao Wang**, Eman Alnabati, Tunde W. Aderinwale, Sai Raghavendra Maddhuri Venkata Subramaniya, Genki Terashi, Daisuke Kihara, The Hitchhiker's Guide to the Biomolecular Glaxy 2021, May 12-13, 2021.

4 "Detecting protein and DNA/RNA structures in cryo-EM maps of intermediate reosolution using deep learning", **Xiao Wang**, Eman Alnabati, Tunde W. Aderinwale, Sai Raghavendra Maddhuri Venkata Subramaniya, Genki Terashi, Daisuke Kihara, 2021 65th Biophysical Society Annual Meeting, February 22-26, 2021.

5 "Emap2sec+: Detecting protein and DNA/RNA structures in cryo-EM maps of intermediate resolution using deep learning", **Xiao Wang**, Eman Alnabati, Tunde Aderinwale, Sai Raghavendra Maddhuri Venkata Subramaniya, Genki Terashi, Daisuke Kihara, Frontiers in Cryo-Electron Microscopy, Keystone Symposia, Feb. 3-4, 2021.

6 "Protein Docking Model Evaluation by Graph Neural Networks", **Xiao Wang**, Sean T. Flannery, Daisuke Kihara, Structural and Computational Biology and Biophysics (SCBB) Graduate Student Symposium of Purdue, Dec 16, 2020.

7 "Emap2sec+: Detecting protein and DNA/RNA structures in cryo-EM maps of intermediate resolution using deep learning", **Xiao Wang**, Eman Alnabati, Tunde Aderinwale, Sai Raghavendra Maddhuri Venkata Subramaniya, Genki Terashi, Daisuke Kihara,5th Annual Southern California Cryo-EM Symposium, Oct 30, 2020.

8 "Protein docking model evaluation by 3D convolutional neural networks", **Xiao Wang**, Genki Terashi, Charles W Christoffer, Mengmeng Zhu, Daisuke Kihara, invited talk by Aggregate Intellect - AI.SCIENCE, Mar 24. [Video].

OPEN SOURCE PROJECT

Asym-Siam

Asym-Siam experimentally verified the importance of asymmetry for Siamese Representation Learning with obvious improvement.
Available at: `https://github.com/facebookresearch/asym-siam`.

DAQ

DAQ is a software accesses the quality of protein models built from cryo-Electron Microscopy (EM) maps, which uses local map density features captured by deep learning.
Available at: `https://github.com/kiharalab/DAQ` and `https://bit.ly/daq-score`.

CaCo

CaCo is a state-of-the-art cooperative-adversarial contrastive learning method where both positive and negative samples are directly learnable.
Available at: `https://github.com/maple-research-lab/caco`.

OC_Finder

OC_Finder is a computational tool using deep learning for fully automated osteoclast segmentation, classification, and counting.
Available at: `https://github.com/kiharalab/OC_Finder`.

CLSA

CLSA is a general contrastive learning framework by introducing the information from stronger augmentation.
Available at: `https://github.com/maple-research-research-lab/CLSA`.

GNN_DOVE

GNN_DOVE is a software can evaluate the quality of protein-docking models using graph neural networks by reformulating protein structures as graphs.
Available at: `https://github.com/kiharalab/GNN_DOVE`.

GNN_Pocket

GNN_Pocket is a software that can detect protein pockets with graph neural network.
Available at: `https://github.com/kiharalab/GNN_Pocket`.

AdCo

AdCo is an algorithm for effective self-supervised learning through adversarial training of negative examples.
Available at: `https://github.com/maple-research-lab/AdCo`.

Emap2sec+

Emap2sec+ is a software detects local structure information of proteins and DNA/RNA in cryo-EM maps using deep learning.
Available at: `https://github.com/kiharalab/Emap2secPlus`.

Attention_AD

Attention_AD is a software that can distinguish active and inactive peptides for gene expression using Long Short Term Memory (LSTM).
Available at: `https://github.com/kiharalab/Attention_AD`.

EnAET

EnAET is a software that benefits semi-supervised learning via self-trained ensemble auto-encoding transformations.
Available at: `https://github.com/maple-research-lab/EnAET`.

DOVE

DOVE is a software can evaluate the quality of protein-docking models using 3D neural networks.
Available at: `https://github.com/kiharalab/DOVE` and `https://kiharalab.org/dove`.

HONORS AND AWARDS

Google Fellowship Nomination of Purdue (5 across Purdue), West Lafayette, IN, U.S.A.	Sep,2021
Microsoft Fellowship Nomination of Purdue (5 across Purdue), West Lafayette, IN, U.S.A.	Sep,2020
Chiang Chen Overseas Fellowship (10 across China, $50,000), Shenzhen, China.	Jan,2018
HIWIN Outstanding Student Scholarship (Top 0.3%), Xi'an China	Oct,2018
Excellent Student Pacesetter (Top 10 across university), Xi'an, China	Nov,2017
National Scholarship, Xi'an, China	Oct,2016

SKILLS

- Expertise: Pytorch, Python,Tensorflow, Matlab, Java
- Capable: SQL, C, C++, Fortran, Java Web, Latex, Android