## Contact

# Yue Song

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# Biography

I am a Computing & Mathematical Sciences postdoctoral research associate at Caltech, supervised by Yisong Yue, Pietro Perona, and Max Welling. I pursued doctoral studies under European Laboratory for Learning and Intelligent Systems (ELLIS), where I was affiliated with Multimedia and Human Understanding Group (MHUG) at the University of Trento, Italy and Amsterdam Machine Learning Lab (AMLab) at University of Amsterdam, the Netherlands, advised by Nicu Sebe and Max Welling. Prior to my Ph.D. studies, I received the B.Sc. cum laude from KU Leuven, Belgium and the joint M.Sc. summa cum laude from the University of Trento, Itally and KTH Royal Institute of Technology, Sweden, co-advised by Nicu Sebe. Besides the technical master's degree, I received an Innovation & Entrepreneurship minor degree from European Institute of Innovation and Technology (EIT Digital).

### Research Interests

I research Structured Representation Learning at the Science-Al Interface. Scientific data are inherently structured – shaped by geometric, temporal, and topological regularities rooted in the laws of physics, biology, and chemistry. My research focuses on developing deep learning models that uncover and encode these structures, enabling more interpretable, generalizable, and data-efficient solutions across scientific domains. Central to this agenda is a reciprocal philosophy: I leverage beneficial inductive biases from scientific disciplines such as physics and neuroscience to inform the design of machine learning models (Science4AI), and in turn, use these structured models to deepen our understanding of complex scientific phenomena (Al4Science). My current research is not task-oriented; instead, I am interested in developing structured methods and finding appropriate applications in the broad scientific domain.

# 🔛 Appointment

#### California Institute of Technology

Position: Post-doctoral Research Associate

Adviser: Yisong Yue, Pietro Perona, & Max Welling

Education

University of Amsterdam

Amsterdam, the Netherlands 2022-2024 ELLIS Ph.D. student

Pasadena, California

2024-2026

2020-2024

2018-2020

2014-2018

Adviser: Max Welling

University of Trento Trento, Italy

Ph.D. student in Information Communication and Engineering

Dissertation: Numerical Methods in Deep Learning and Computer Vision

Thesis Committee: Yisong Yue, Vitorrio Murino, & Paolo Rota Adviser: Nicu Sebe,

University of Trento & KTH Royal Institute of Technology Trento, Italy & Stockholm, Sweden

M.Sc. summa cum laude in Electrical Engineering Adviser: Nicu Sebe & Kevin Smith, Examiner: Prof. Danica Kragic

**KU** Leuven Leuven, Belgium

B.Sc. cum laude in Electrical Engineering

### Selected Publications

My research in structured representation learning drives three core research directions:

- Matrix Manifold Learning for Scientific Perception:
  - Yue Song, Nicu Sebe, and Wei Wang. "Why Approximate Matrix Square Root Outperforms Accurate SVD in Global Covariance Pooling?" ICCV 2021.
  - Yue Song, Nicu Sebe, and Wei Wang. "Fast Differentiable Matrix Square Root." ICLR 2022.
  - Yue Song, Nicu Sebe, and Wei Wang. "Fast Differentiable Matrix Square Root and Inverse Square Root." IEEE

T-PAMI 2022.

- **Yue Song**, Nicu Sebe, and Wei Wang. Batch-efficient Eigendecomposition for Small and Medium Matrices." ECCV 2022.
- Yue Song, Nicu Sebe, and Wei Wang. "Improving Covariance Conditioning of the SVD Meta-layer by Orthogonality." ECCV 2022.
- **Yue Song**, Nicu Sebe, Wei Wang. "RankFeat: Rank-1 Feature Removal for Out-of-distribution Detection." NeurIPS 2022.
- Ziheng Chen, **Yue Song**, Gaowen Liu, Ramana Rao Kompella, Xiaojun Wu, Nicu Sebe. "Riemannian Multinomial Logistics Regression for SPD Neural Networks." CVPR 2024.
- Ziheng Chen, **Yue Song**, Yunmei Liu, Nicu Sebe. "A Lie Group Approach to Riemannian Batch Normalization." ICLR 2024.
- Ziheng Chen, **Yue Song**, Rui Wang, Xiaojun Wu, Nicu Sebe. "RMLR: Extending Multinomial Logistic Regression into General Geometries." NeurIPS 2024.
- **Yue Song**, Wei Wang, Nicu Sebe. "RankFeat&RankWeight: Rank-1 Feature/Weight Removal for Out-of-Distribution Detection." T-PAMI 2024.
- Ziheng Chen, **Yue Song**, Yunmei Liu, Nicu Sebe. "A Lie Group Approach to Riemannian Batch Normalization." ICLR 2024.
- Ziheng Chen, **Yue Song**, Xiaojun Wu, Gaowen Liu, Nicu Sebe. "Understanding Matrix Function Normalizations in Covariance Pooling from the Lens of Riemannian Geometry." ICLR 2025.
- Ziheng Chen, Yue Song, Xiaojun Wu, Nicu Sebe. "Gyrogroup Batch Normalization." ICLR 2025.
- Disentanglement and Equivariance for Temporal Scientific Data:
  - **Yue Song**, Nicu Sebe, and Wei Wang. "Orthogonal SVD Covariance Conditioning and Latent Disentanglement." IEEE T-PAMI 2022.
  - **Yue Song**, Jichao Zhang, Nicu Sebe, Wei Wang. "Householder Projector for Unsupervised Latent Semantics Discovery." ICCV 2023.
  - **Yue Song**, T. Anderson Keller, Nicu Sebe, Max Welling. "Latent Traversals in Generative Models as Potential Flows." ICML 2023.
  - **Yue Song**, T. Anderson Keller, Nicu Sebe, Max Welling. "Flow Factorized Representation Learning." NeurIPS 2023.
  - Guanghao Wei, Yining Huang, Chenru Duan, **Yue Song\***, Yuanqi Du\*. "Navigating Chemical Space with Latent Flows." NeurIPS 2024. (\* denotes equal supervision)
  - Lingkai Kong, Haorui Wang, Wenhao Mu, Yuanqi Du, Yuchen Zhuang, Yifei Zhou, **Yue Song**, Rongzhi Zhang, Kai Wang, Chao Zhang. "Aligning Large Language Models with Representation Editing: A Control Perspective." NeurIPS 2024.
  - -Fengze Xie, Sizhe Wei, **Yue Song**, Yisong Yue, Lu Gan. "Morphological-Symmetry-Equivariant Heterogeneous Graph Neural Network for Robotic Dynamics Learning." L4DC 2024.
  - Raphi Kang, Yue Song, Georgia Gkioxari, Pietro Perona. "Is CLIP ideal? No. Can we fix it? Yes!." ICCV 2025.
- Orientation Diffusion Models for Scientific Vector Field Modeling:
  - **Yue Song**, T. Anderson Keller, Sevan Brodjian, Takeru Miyato, Yisong Yue, Pietro Perona, Max Welling. "Kuramoto Orientation Diffusion Models." NeurIPS 2025 Submission.
  - **Yue Song**, Yisong Yue, Pietro Perona, Max Welling. "Polar Diffusion Model for Modeling Scientific Vector Fields." Ongoing work.

## **Books**

**Yue Song**, T. Anderson Keller, Nicu Sebe, Max Welling. "Structured Representation Learning: From Homomorphisms and Disentanglement to Equivariance and Topography". Springer Nature.

## Professional Activity and Lectures

Regularly serve as reviewers for T-PAMI, NeurIPS, ICLR, ICML, CVPR, ICCV, and ECCV.

Serve as Area Chair for NeurIPS 2025.

CVPR 2024 Tutorial: Disentanglement and Compositionality in Computer Vision

ECCV 2024 Tutorial: Emerging Trends in Disentanglement and Compositionality

ICCV 2025 Workshop: Workshop and Challenge on Disentangled Representation Learning for Controllable Generation