## Xue Gong

## **Education and Professional Experience**

#### **Nanyang Technological University**

Singapore

Presidential Postdoctoral Fellowship

Dec 2023 - Now

- Supervisor: Xia Kelin
- Developed topological deep learning tools for machine learning tasks on molecular data, with applications in protein and material design
- Designed algorithms to extract topological features from the shape of molecules, utilizing mathematical toolkits such as algebraic topology, and tested the methods on learning tasks with chemical and biological molecular data

#### The University of Edinburgh, Heriot-Watt University

Edinburgh, UK

PhD in Applied Mathematics

Sep 2019 - Nov 2023

- MAC-MIGS CDT scholarship, a joint Doctoral Training Programme with Integrated Study in Mathematical Modelling, Analysis and Computation between The University of Edinburgh and Heriot-Watt University
- **Supervisors**: Des Higham, Kostas Zygalakis
- Thesis: Laplacians for Structure Recovery on Directed and Higher-order Graphs
- Research interests: Graph-based algorithms, Graph models, Node embedding, Spectral clustering, Graph mining, Learning on graphs

#### **National University of Singapore**

Singapore

M.Sc in Statistics (Honours with Distinction)

2017 - 2019

#### Nanyang Technological University

Singapore

BSc (Hons) in Physics (First Class Honours)

2011 - 2015

- Dean's List (top 5% of cohort)
- Singapore Government Merit Undergraduate Scholarship

#### Awards\_

#### **Turing Enrichment Award**

London, UK

Alan Turing Institute Oct 2022

Offer PhD students the opportunity to enrich and enhance their current research by accessing the facilities and opportunities available at The Alan Turing Institute and its partners as well as a grant to undertake research activity.

#### **Associate Fellowship**

UK

Advanced Higher Education

Sep 2022

In recognition of attainment against the UK Professional Standards Framework for teaching and learning support in higher education

Outstanding	ialk Award
SIAM Workshop	on Network Science (NS22)

Online Sep 2022

# **Teaching Award**The University of Edinburgh

UK Sep 2022

## Laura Wisewell Travel Scholarship

UK

## The University of Edinburgh MATH+ Thematic Firstein Semester Summer School Trav

Jun 2022

## MATH+ Thematic Einstein Semester Summer School Travel Award Zuse Institute Berlin

Germany
Jun 2022

# MAC-MIGS Travel Fund EPSRC

UK 2019 - 2023

## MAC-MIGS CDT Scholarship (Fully Funded)

UK 2019

## Dean's List (top 5% of cohort)

**EPSRC** 

Singapore

## Nanyang Technological University Singapore Government Merit Undergraduate Scholarship (Fully Funde

2014

# Singapore Government Merit Undergraduate Scholarship (Fully Funded) Ministry of Education of Singapore

Singapore 2011

## **Publications**

- **Gong, X.**, Higham, D.J., Zygalakis, K., and Bianconi, G. Higher-order Connection Laplacians for Directed Simplicial Complexes. *Journal of Physics: Complexity*. 2024 Feb 12
- **Gong, X.**, Higham, D.J. and Zygalakis, K. Generative hypergraph models and spectral embedding. *Scientific Report* 13, 540 (2023). https://doi.org/10.1038/s41598-023-27565-9

- **Gong, X.**, Higham, D.J. and Zygalakis, K., 2021. Directed network Laplacians and random graph models. *Royal Society open science*, 8(10), p.211144.
- Lu, X., Utama, M.I.B., Lin, J., **Gong, X.**, Zhang, J., Zhao, Y., Pantelides, S.T., Wang, J., Dong, Z., Liu, Z. and Zhou, W., 2014. Large-area synthesis of monolayer and few-layer MoSe2 films on SiO2 substrates. *Nano letters*, 14(5), pp.2419-2425.

### Manuscript \_\_\_\_\_

- Tan, J., Wee, J.J., **Gong, X.**, and Xia, K. Mathematics-assisted Peptide-based Machine Learning Model (MAP-ML) for anticancer peptide prediction.
- Wee, J.J., **Gong, X.**, Tuschmann, W., and Xia, K. Cohomology-based ultrametric Gromov-Hausdorff distance for quantifying structural similarity.

### Talks & Presentations

Sunbelt Conference 2024  Oral Presentation, "Generative hypergraph models and spectral embedding"  Conference on Complex Systems 2022 (CCC 2022)	Edinburgh, UK Jun 2024
Conference on Complex Systems 2022 (CCS 2022)  Poster Presentation, "Spectral Embedding and Associated Generative Models for Hypergraphs"	Palma de Mallorca, Spain Oct 2022
SIAM Workshop on Network Science	Online
Outstanding Talk Award, Lightning Talk, "Generative Hypergraph Models and Spectral Embedding"	Sep 2022
4th IMA Conference on The Mathematical Challenges of Big Data	Oxford, UK
Contributed Talk, "Hypergraph Generative Models and Associated Spectral Embedding Algorithms"	Sep 2022
Conference on Network Science (NetSci)	Online
Contributed Talk, "Hypergraph Generative Models and Associated Laplacians"	Jul 2022
AAAI 2022 Workshop on Graphs and More Complex Structures for Learning and Reasoning	UK
Short Paper, "Visualizing and Quantifying Linear and Periodic Structures in Directed Networks"	Feb 2022
Oxford Network Seminar	Online
Seminar Talk, "Random Graph Interpretation of Directed Graph Laplacians"	Dec 2021
<b>10th International Conference on Complex Networks &amp; Their Applications</b> Contributed Talk, "Random Graph Interpretation of Directed Graph Laplacians"	Online Nov 2021
Conference on Complex Systems	Online
Contributed Talk, "Directed Random Graph Models and Their Associated Laplacians"	Oct 2021
Oxford-Warwick-Edinburgh Network Science Workshop	Online
Contributed Talk, "Mapping Directed Networks Using the Magnetic Laplacian"	Mar 2021
Cambridge Joint CDT Student Conference	Online
Contributed Talk, "Mapping Directed Networks Using the Magnetic Laplacian"	Dec 2020

## Events Participation \_\_\_\_\_

Jun 2022 Mathematics of Complex Social Systems Summer School, Participant	Berlin, Germany
Jul 2021 Networks 2021 (Joint Sunbelt and NetSci Conference), Participant	Online
Jun 2021 SIAM-IMA Edinburgh - Study Group with Industry, Participant in the project "Generating Irregular Sequences for Seismic Imaging Problems"	Online
"Generating Irregular Sequences for Seismic Imaging Problems"	
Dec 2020 Conference on Complex Systems 2020 (CCS 2020) online, Participant	Online
Sep 2020 Agrifood Data Study Group: Evaluating the UK's resilience to supply chain shocks, Participant	Online
May 2020 ICMS and MAC-MIGS Modelling Camp 2020, Participant	Edinburgh, UK

## Teaching Experience \_\_\_\_

#### **MATH08058 Calculus and its Applications**

The University of Edinburgh

Spring 2022

Tutor and Marker
An undergraduate course offered to College of Science and Engineering students to develop calculus skills

• Facilitated weekly problem-solving tutorials, marked assignments and final exams

#### MATH11197 Research Skills for Computational and Applied Mathematics

The University of Edinburgh

Fall 2020

A Master's level course to develop research skills through a set of programming exercises, workshops and group projects

Facilitated programming workshops, soft-skill workshops; marked programming assignments and final reports

#### School of Physical and Mathematical Sciences Learning Centre

Nanyang Technological

University

Peer Tutor

2014

 One-to-one tutoring with undergraduate students on Fluid Mechanics, Classical Mechanics, Quantum Mechanics, and experiment modules

### **Research Projects**

#### **Directed Laplacian on Simplicial Complexes**

Edinburgh, UK

Turing Enrichment Scheme

Aug 2022 - Now

- Collaborators: Ginestra Bianconi, Desmond Higham, Konstantinos Zygalakis
- Developed theories for directed simplicial complexes
- Extended directed graph Laplacian such as the Magnetic Laplacian to higher-order graphs

#### **Spectral Embedding and Generative Hypergraph Models**

Edinburgh, UK Aug 2021 - Aug 2022

The University of Edinburgh

• **Supervisors**: Desmond Higham ,Konstantinos Zygalakis

- Studied spectral algorithms for hypergraphs that captures higher-order interactions
- Established the connection between novel random graph models and spectral algorithms
- · Performed numerical experiments on synthetic and real hypergraph from social sciences for node embedding, clustering, and link prediction

#### **Visualizing and Quantifying Structures in Directed Networks**

Edinburgh, UK May 2020 - Aug 2021

The University of Edinburgh

• Supervisors: Desmond Higham ,Konstantinos Zygalakis

- Analyzed spectral algorithms for clustering and mapping directed graphs
- Derive associated random graph models and proposed workflow for comparing structures based on the models
- · Ran experiments on synthetic and real networks from ecology, biology and social sciences for graph visualization and structure recovery

#### **Efficient Approximation of Pricing Functions**

Edinburgh, UK Jan - Mar 2020

The University of Edinburgh

• Supervisors: Aretha Teckentrup, Abdul-Lateef Haji-Ali

• Enhanced the efficiency of option price estimation by by generating training data using multi-level Monte Carlo, and estimating price function using Gaussian process regression

**Opinion Dynamics** The University of Edinburgh Edinburgh, UK Oct - Dec 2019

- Supervisor: Ben Goddard
- Simulated and studied the behaviors of opinion dynamics models including the voter model, the Deffuant model and the HK model

#### **Modified Dealer's Model for the Electricity Market**

Singapore

Nanyang Technological University

Aug 2014- May 2015

• **Supervisor**: Cheong Siew Ann

 Modelled the spiking behaviour of the electricity market using modified dealer's model; studied the spike statistics and the impact of model parameters

#### The Minority Game Model

Singapore

Nanyang Technological University

Jun 2012 - Aug 2012

• **Supervisor**: Chew Lock Yue

· Simulated the dynamics of a system using the Minority Game Model and studied the influence of agent memory and strategy pool on the volatility of the system

#### **EVENTS CO-ORGANIZED**

#### NTU-NUS Joint Workshop on Applied Topology and Geometry for AI

Singapore

Nanyang Technological University

Feb 2024

Organized workshop to present recent advancements in both the theories of algebraic topology and geometry, as well as their applications within AI and data science.

#### MAC-MIGS Research Afternoon on Learning Complex Structures on Graphs

Edinburgh, UK

MAC-MIGS CDT

Jul 2022

Invited speakers to present recent advances in the research on learning graph structures, such as clustering and structure recovery on graphs and hypergraphs

#### **Networks Book Club**

Online 2021-2022

Held regular online meetings to discuss books and topics on network science, such as graph representation learning, dynamics and modularity on graphs, and natural language processing

#### **Networks Reading Group**

Edinburgh, UK 2022 - Now

The University of Edinburgh

Ran regular face-to-face meetings in Edinburgh to discuss papers on graphs and networks covering topics such as graph neural networks, community detection, and spectral clustering

**Reviewer** 

Neurocomputing

### **PROFESSIONAL SOCIETIES**

Society for Industrial and Applied Mathematics

The Institute of Mathematics and its Applications

### Other Experience\_

#### **Quantiative Market Analyst**

Singapore

Rio Tinto

Built statistical models such as time series forecasting; designed optimization model for planning and scheduling

**Geophysicist**CGG
Singapore
Jul 2015 - Apr 2017

Performed seismic image processing using techniques such as inversion algorithm, wave equation, and signal processing

### Skills

**Programming** Python, Matlab R, C/C++, HTML/CSS, SQL **Miscellaneous** Linux, Shell, ŁTEX, Tableau, Power BI, Git

**Languages** English, Chinese

### **Languages**

**English** Professional proficiency **Chinese** Native proficiency