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B.S. Applied Math & Computational Science; Computer Science Track
Class of 2026

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📍 Kunshan, CN • Durham, USA

Bridging AI, mathematics, and biomedical modeling through computational design and visualization.

“The impediment to action advances action.

What stands in the way becomes the way.”

— Marcus Aurelius, Meditations 5.20

*Turning obstacles into methods across AI,
math, and biomedicine.*



WEBSITE

About This Portfolio

This portfolio showcases my work at the intersection of artificial intelligence, applied mathematics, and computational science. It includes research contributions under peer review at top-tier conferences (ICLR, BICS), open-source software tools with 600+ GitHub stars, teaching experience, and computational modeling projects.

Each project demonstrates technical depth, practical impact, and creative problem-solving across machine learning, systems design, and computational modeling.

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Research Projects

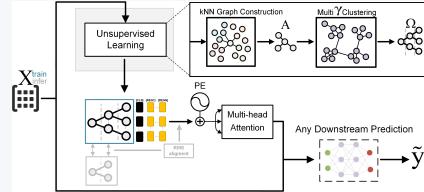
Mixing Configurations for Downstream Prediction

First Author, Research Assistant with Prof. Shixin Xu PyTorch, Unsupervised Learning

- Proposed GraMixC: a configuration – mixing module that fuses unsupervised “configurations” with task predictors for label – efficient downstream performance.
- Defined configuration extraction and mixing objectives, and integrated them with linear probing / 3LP predictors without changing the backbone.
- Validated on DSNI regression (pH/temperature) and image benchmarks; figures show attention maps, lineage diagrams, and quantitative gains.
- Ablation demonstrates incremental mixing (GMC) outperforms static concatenation (GC).
- Co-authored with Hao Wu, Runkun Guo, Yihan Wang, Dongmian Zou, and Prof. Shixin Xu; under ICLR 2026 review.

Links: [arXiv preprint](#)

Highlights: [Unsupervised Learning](#) [ICLR under review](#)



Technical Highlights: This project tackles the challenge of learning meaningful representations from unlabeled data by mixing configurations in a learned latent space. The key innovation is a training objective that encourages the model to predict properties of mixed configurations based on the mixing coefficients and component configurations.

Key Results:

- Regression (DSNI): 3LP+GC improves over the 3LP baseline; 3LP+GMC further raises R^2 (up to > 0.9), see Fig. 2a.
- Ablation: Incrementally mixing configurations (GMC) consistently outperforms static train/test pairing (GC), Fig. 2b.
- Interpretability: Attention maps and lineage diagrams indicate configurations capture semantically meaningful structure (Fig. 1).
- Design: GraMixC fuses configuration features with task predictors without modifying the backbone.

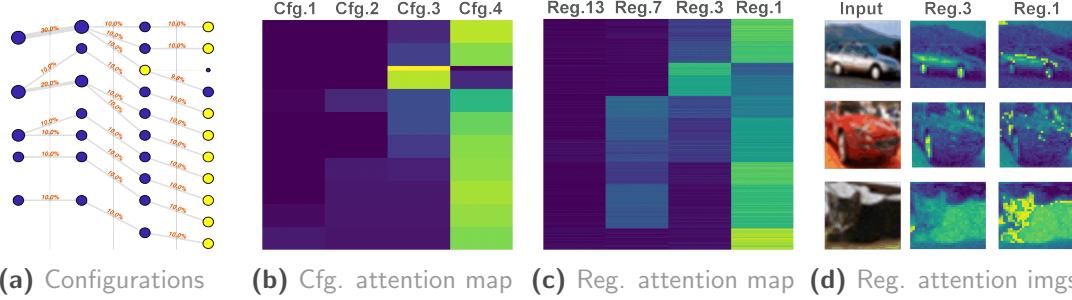


Figure 1: Comparison of attention maps obtained from configurations and registers, rows for samples.

(a): Lineage diagram for configurations, near GT balls are marked yellow. **(b):** Attention map of configuration tokens in an attention-based linear probing. **(c):** Attention map of DINOv2-reg register tokens, mean of all patch norms is used. **(d):** Attention maps over the register tokens, as images.

Impact: This work contributes to the growing field of self-supervised and unsupervised representation learning, with potential applications in materials science, molecular design, and any domain with configurable systems. Part of signature work research at Duke Kunshan University under Prof. Shixin Xu, focusing on unsupervised/semi-supervised methods for biomedical tasks.

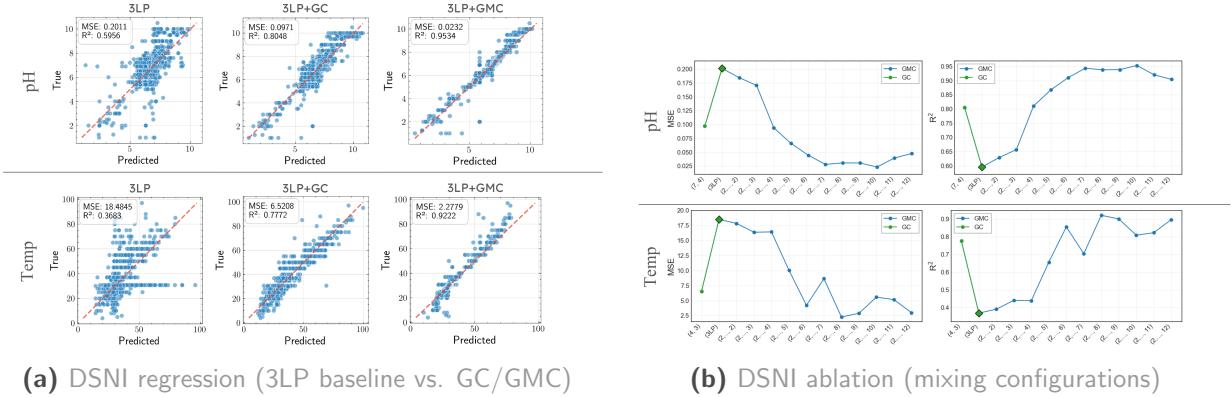


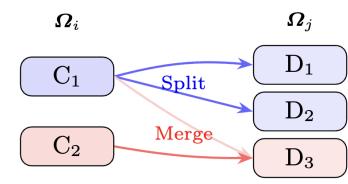
Figure 2: Quantitative results on DSNI. (Left) Predicted vs. actual pH/temperature: 3LP+GC improves over 3LP; 3LP+GMC further increases R^2 (up to > 0.9). (Right) Ablation: Incremental mixing (GMC) outperforms static train/test pairing (GC).

Brain-Inspired Perspective on Configurations: Unsupervised Similarity and Early Cognition

First Author Theory, Unsupervised Learning, Brain-Inspired Computation

- Studies configurations from a cognitive perspective, relating unsupervised similarity and early cognition.

- Provides theoretical motivation for why configuration structure supports downstream prediction (complementary to GraMixC).
- Connects lineage diagrams, attention structure, and similarity to emergent representation geometry.



Links: [arXiv preprint](#)

Highlights: [Brain-Inspired Computation](#) [BICS 2025](#)

Technical Highlights: This work formalizes configurations as organizing structures that emerge from unsupervised similarity, offering a brain-inspired account of early category formation. We analyze how a lineage parameter γ controls hierarchical granularity and how energy components (attraction h_a , repulsion h_r) shape stable configuration landscapes that support downstream learning.

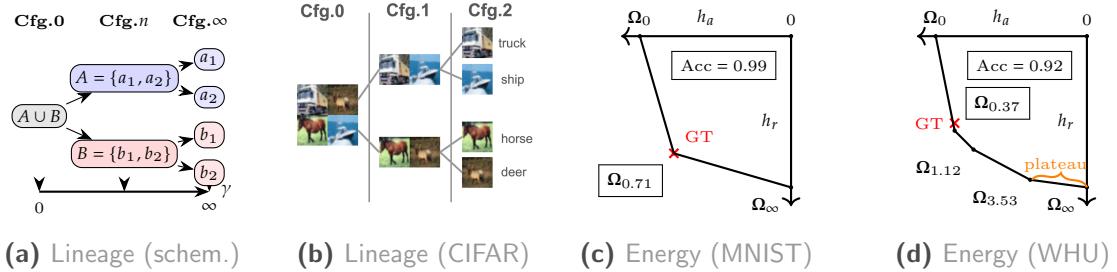


Figure 3: Configuration lineage and energy landscapes. **(a)&(b)** Configuration lineages: γ controls hierarchical granularity from coarse to fine. **(c)&(d)** Energy landscapes: Axes show attraction h_a and repulsion h_r .

Key Results:

- Hierarchical selectivity: superordinate categories stabilize at low γ , basic-level categories at higher γ , reflecting scale-dependent organization (Fig. 4a).
- Novelty detection: energy distributions separate familiar vs. novel inputs ($AUC \approx 0.87$), echoing infant habituation paradigms (Fig. 4b).
- Dynamic evolution: configurations achieve consistently lower 1/ARI than baselines during category evolution, indicating more stable organization (Fig. 4c).
- Geometry: lineage diagrams and energy contours reveal interpretable structure that aligns with emergent representation geometry (Fig. 3).

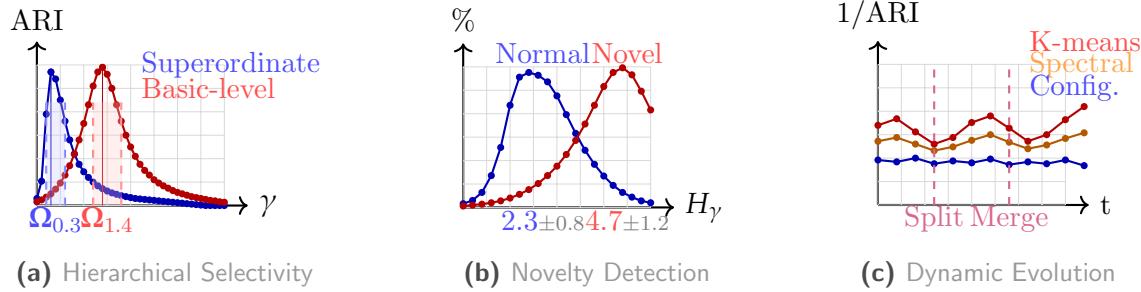


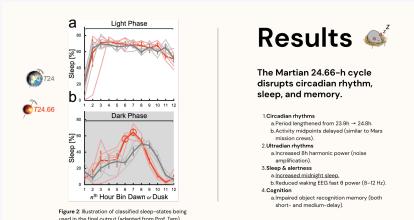
Figure 4: Brain-inspired capabilities of configurations. **(a)** Superordinate categories emerge at low γ (0.2–0.6), basic-level at high γ (1.2–1.8). Plateaus show stable organizational scales. **(b)** Energy distributions distinguish novel from familiar stimuli (87% AUC), paralleling infant habituation. **(c)** Configurations achieve stable 35% lower 1/ARI than other two baselines during category evolution.

Impact: By linking unsupervised similarity, hierarchical lineage, and energy-based organization, this project offers a principled, cognitively motivated view of how early concepts can form without labels. The framework complements GraMixC by explaining why configuration structure is predictive, and it suggests broader applications in domains where category structure and novelty signals emerge from unlabeled data.

EEG/EMG Vigilance Classification under Martian Photoperiod (T24.66)

First Student Author EEG/EMG, FFT/Wavelet, Sleep & Memory, CNN

- Tested whether mammals adapt to Mars-like 12.33h light:12.33h dark cycles (T24.66).
- Found circadian realignment without free-running; ultradian noise increased under T24.66.
- Observed advanced siesta peak and increased midnight sleep; waking theta (8–12 Hz) attenuated at night.
- Night-time short-term object memory attenuated due to altered response to familiar objects; novelty response intact.
- Implemented a CNN for EEG/EMG vigilance-state classification achieving $\geq 90\%$ accuracy; compared 10+ existing methods.
- Publications: CNS 2025 (conference) and PNAS Nexus (journal, under review).



Links: [CNS 2025 paper](#) [Slides](#)

Highlights: [PNAS Nexus under review](#) [CNS 2025](#)

Technical Highlights: We investigate mammalian adaptation to a Martian-length day (T24.66) using laboratory mice. The regime lengthens intrinsic period (τ) enabling realignment to the slightly longer photoperiod without free running. Spectral analyses reveal preserved circadian power but amplified ultradian components; sleep architecture shifts and night-time waking theta decreases.

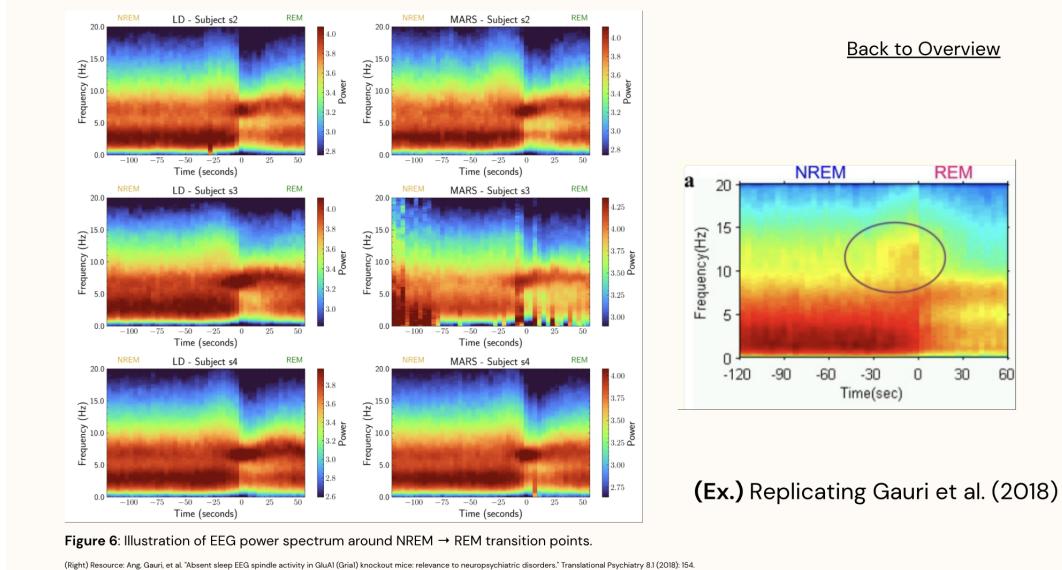


Figure 6: Illustration of EEG power spectrum around NREM → REM transition points.

(Right) Resource: Ang, Gauri, et al. "Absent sleep EEG spindle activity in GluA1 (Gria1) knockout mice: relevance to neuropsychiatric disorders." *Translational Psychiatry* 8(1) (2018): 154.

Figure 5: EEG spectral analyses around state transitions under T24.66. Wavelet/FFT-based spectra highlight attenuated waking theta (8–12 Hz) at night and altered sleep timing relative to T24.

Methodology:

- Entrainment protocol: 12.33h light : 12.33h dark (T24.66) vs. T24 controls
- EEG/EMG recording; spectral analyses via fast Fourier transform (FFT) and wavelets
- Behavioral assessments: rest–activity rhythm, sleep timing, object memory assays

Key Findings:

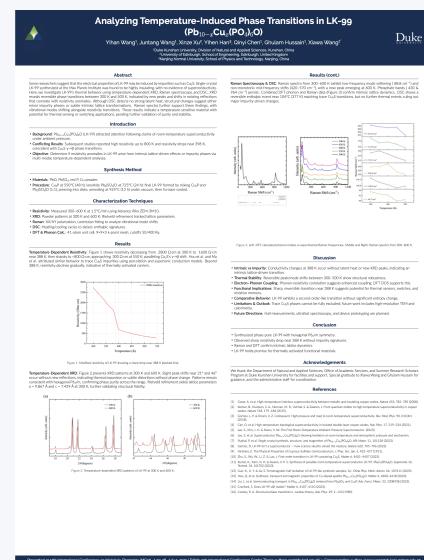
- Circadian: τ lengthened; rhythms realigned with T24.66 without free running; circadian power not damped
- Ultradian: Increased ultradian spectral power (FFT/wavelet)
- Sleep: Advanced siesta peak; increased midnight sleep; time-of-day dependent changes
- EEG: Night-time waking theta (8–12 Hz) attenuated
- Memory: Night-time short-term object memory attenuated due to altered response to familiar objects; novelty response spared

Impact: Findings suggest that adapting to a slightly non-24h photoperiod (T24.66) is feasible but entails neurophysiological trade-offs in sleep, alertness, and memory—relevant for space mission planning.

Analyzing Temperature-Induced Phase Transitions in $\text{Pb}_{10-x}\text{Cu}_x(\text{PO}_4)_6\text{O}$

Research Independent Study with Prof. Xiawa Wang Phonon/exciton dynamics

- Investigated LK-99 thermal behavior (300–500 K) via temperature-dependent XRD, Raman spectroscopy, and DSC.
- Observed reversible structural transitions in XRD (new/shifted peaks) correlating with resistivity jumps.
- Conducted density functional theory (DFT) analysis to interpret observed transitions and spectra.
- Raman modes shift in tandem with resistivity transition; DSC shows no pronounced latent heat.
- Results suggest either minor impurity (e.g., Cu₂S) contribution or subtle intrinsic lattice transformation.



Links: [🔗 MC17 paper](#) [🔗 Poster](#)

Highlights: [Materials Chemistry](#) [DFT](#) [MC17](#)

Technical Highlights: We examine temperature-sensitive structural responses in LK-99 that align with electrical resistivity changes. Reversible XRD peak evolution between 300–500 K and concomitant Raman shifts indicate a repeatable transition regime, while DSC lacks strong latent heat signatures.

Methodology:

- Variable-temperature XRD to identify reversible phase/structure evolution
- Raman spectroscopy to track vibrational mode shifts across the transition
- Differential scanning calorimetry (DSC) to probe latent heat signatures
- Resistivity measurements correlated with structural/spectral changes
- Density functional theory (DFT) analysis to interpret observed transitions and spectra

Key Findings:

- Reversible structural transition correlates with resistivity jumps (300–500 K)
- Raman modes shift coherently with structural/electrical changes
- Absence of strong DSC peak suggests subtle transformation or low-fraction impurity phase
- Thermal/electrical repeatability indicates potential for sensing/switching applications

Impact: The coupling between structure and electrical response highlights LK-99 as a temperature-sensitive material of interest for functional electronics. Disentangling impurity effects from intrinsic copper-doped lattice behavior requires further microstructural analysis.

Unsupervised Segmentation in Hyperspectral Imaging

Summer Research & Independent Study with Prof. Xiaobai Sun, Prof. Nikos Pitsianis, Dimitrios Floros Python, SG-t-SNE-II, Spectral Methods, Community Detection

- Studied precursor clustering and community detection methods, collecting over 5 methods and more than 10 datasets for hyperspectral imaging segmentation.
- Implemented and optimized SG-t-SNE-II algorithm for dimensionality reduction preserving local and global structure.
- Utilized k-nearest neighbor graphs, Stochastic Graph t-SNE, and Parallel Clustering with Resolution Variation for unsupervised segmentation.
- Developed Python packages mheatmap and pysgtsnepi for HSI data processing, achieving 600+ GitHub stars community adoption.
- Worked with Python (scikit-learn), MATLAB, and Julia for implementation and validation.

Links:  Poster

Highlights: HSI Graph Unsupervised Learning

Technical Highlights: Hyperspectral images contain hundreds of spectral bands per pixel, creating extremely high-dimensional data that is challenging to segment without labels. This project leverages spectral graph theory to build a similarity graph where pixels are nodes and edges encode spectral similarity.

Methodology:

- Construct k-nearest neighbor graph in spectral space using efficient approximate nearest neighbor search
 - Apply SG-t-SNE-II to embed the graph structure into 2D/3D space while preserving cluster structure
 - Use community detection to identify coherent spectral regions corresponding to materials or land cover types
 - Validate segmentations against ground truth using metrics like adjusted Rand index and normalized mutual information

Key Findings:

- BlueRed consistently outperforms traditional baselines on HSI clustering
 - Robust to spectral noise and spatial variability; produces coherent segments

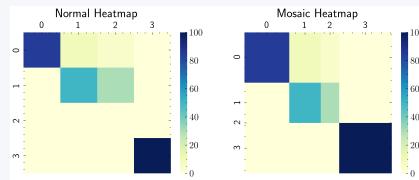
Impact: The approach sets a stronger baseline for unsupervised HSI analysis with practical implications in agriculture, climate, remote sensing, and medical diagnostics. Future work: improve computational efficiency and extend to more HSI scenarios.

Software Tools & Open Source Contributions

mheatmap: Proportional Heatmaps with Spectral Reordering

Creator & Maintainer Python, NumPy, Matplotlib, Spectral Graph Theory

- Developed Python package for creating proportional heatmaps where cell sizes reflect data magnitude.
- Implemented spectral reordering algorithms (Fiedler vector, spectral seriation) to reveal hidden structure.
- Achieved 600+ GitHub stars and widespread adoption in bioinformatics, systems biology, and network analysis.
- Package has been cited in peer-reviewed publications and used in production data analysis pipelines.
- Maintained comprehensive documentation with tutorials, examples, and API reference.



Links: [GitHub repository](#) [Documentation](#)

Highlights: [Data Visualization](#) [600+ Stars](#)

Technical Highlights: Traditional heatmaps use fixed-size cells regardless of data magnitude, making it difficult to compare values across orders of magnitude. `mheatmap` solves this by making cell areas proportional to values, creating a more intuitive visualization of hierarchical or networked data.

RMS alignment (optional) helps align permutation-invariant clusters to labels, improving interpretability and evaluation fairness (Fig. 6).

Key Features:

- Proportional sizing: Cell areas scale with data magnitude, preserving quantitative relationships
- Spectral reordering: Automatically reorders rows/columns to reveal clusters and patterns using graph Laplacian eigenvectors
- Flexible color mapping: Supports custom colormaps, logarithmic scaling, and diverging color schemes

- High-quality output: Vector graphics export (PDF, SVG) suitable for publication
- Easy integration: Works seamlessly with pandas DataFrames and NumPy arrays

Use Cases:

- Gene expression matrices in systems biology
- Correlation matrices in financial data analysis
- Adjacency matrices for network visualization
- Confusion matrices in machine learning evaluation
- Any tabular data with hierarchical or network structure

Example Code:

```
import numpy as np
import mheatmap as mh

conf_mat = np.array([
    [85, 10, 5],
    [15, 70, 15],
    [5, 20, 75]
])

mh.mosaic_heatmap(conf_mat)
```

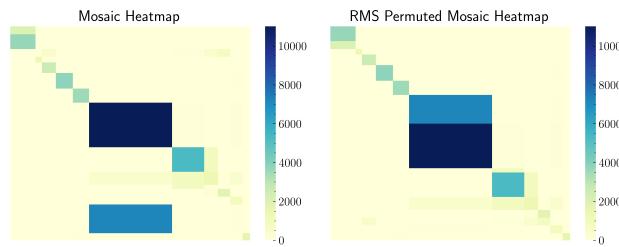


Figure 6: Salinas example: after RMS alignment, a diagonal emerges in the mosaic heatmap, improving cluster–category correspondence.

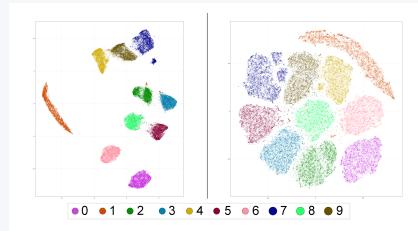
Impact: `mheatmap` has been adopted by research groups worldwide and cited in publications spanning biology, computer science, and data science. The tool fills a gap in the Python visualization ecosystem and has become a standard tool for exploratory data analysis.

pysgtsnepi: Stochastic Graph t-SNE- Π Implementation

Creator & Maintainer Python, NumPy, SciPy, scikit-learn, Julia

- Implemented \textcircled{S} SG-t-SNE-II from scratch in Python, making state-of-the-art graph-aware DR accessible.
- Delivered clean, well-documented APIs (scikit-learn compatible) for seamless pipeline integration.
- Optimized performance-critical paths with Cython; 10x speedup over pure Python baselines.
- Provided examples and docs to foster efficient use by researchers and practitioners.

- Enables embeddings that preserve communities and global topology in high-dimensional graphs.



Links: [GitHub repository](#) [Documentation](#)

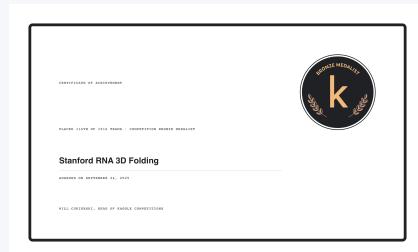
Highlights: Dimensionality Reduction, Python/Julia

Academic Achievements & Teaching

Stanford RNA 3D Folding (Kaggle Competition)

Bronze Medal (Top 8%, 1500+ teams) Python, Boltz-1, Protenix, TM-score, US-align

- Parsed CSV-format sequence and label data, generated YAML-format inputs, and handled data preprocessing including sequence redundancy and multi-conformation reference structures.
- Integrated and deployed a dual-model prediction pipeline combining Boltz-1 and Protenix for RNA 3D structure prediction.
- Configured cache and advanced diffusion parameters for optimal inference performance.
- Calculated TM-score using US-align, fused model outputs, corrected invalid coordinates, and generated compliant submissions.
- Achieved top 8% finish among 1500+ teams in highly competitive international competition.



Links: [Kaggle Competition](#) [Certificate](#)

Highlights: Bronze, RNA Folding, DL/AI

Technical Highlights: RNA 3D structure prediction is a critical challenge in computational biology, with applications in drug discovery and understanding RNA function. This

competition required predicting 3D atomic coordinates from RNA sequences.

Methodology:

- Data preprocessing: Handled complex multi-conformation reference structures and sequence redundancy
- Model ensemble: Combined predictions from Boltz-1 (Google DeepMind) and Protenix models
- Structure alignment: Used US-align for computing TM-scores to evaluate prediction quality
- Coordinate correction: Implemented validation and correction for physically invalid atomic coordinates
- Optimization: Tuned diffusion parameters and caching strategies for computational efficiency

Key Results:

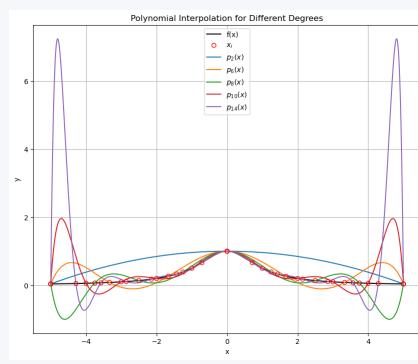
- Bronze medal finish (top 8% out of 1500+ international teams)
- Successfully deployed production-ready prediction pipeline
- Achieved competitive TM-scores on validation and test sets
- Demonstrated ability to integrate state-of-the-art AI models for scientific applications

Impact: This competition showcased the application of cutting-edge deep learning models to fundamental problems in structural biology. The techniques developed here have broad applicability to protein and RNA structure prediction tasks.

Teaching Assistant: Numerical Analysis (MATH 302)

TA to Prof. Dangxing Chen Numerical Methods, Python/MATLAB, Teaching

- Supported instruction across root finding, interpolation, numerical differentiation and integration.
- Led weekly recitations with Python/MATLAB implementations of numerical methods.
- Brought in supplementary CS 521 material to deepen understanding.
- Received positive feedback for making abstract methods accessible via coding demos.
- Topics: Newton's method, interpolation, quadrature, finite differences, numerical ODE solvers.



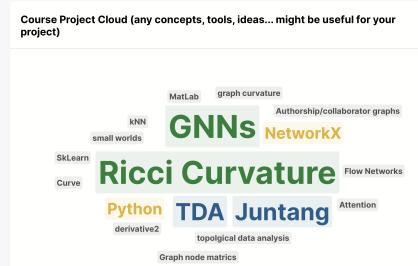
Links: [🔗 GitHub repository](#)

Highlights: [TA](#) [Numerical Analysis](#)

Teaching Assistant: Matrix, Graph, and Network Analysis (CS 521)

TA to Prof. Xiaobai Sun Spectral/Graph, Python/MATLAB, Teaching

- Assisted in teaching graduate course covering Perron–Frobenius Theorem (PageRank), Graph Laplacian (Fiedler Vector), and spectral embedding.
- Led recitations and office hours to review assignments and clarify concepts; managed course Canvas site and code base.
- Provided Python implementations in addition to instructor's MATLAB code for improved accessibility.
- Graded homework and delivered guest lecture comparing embedding spaces and clustering methods.
- Received positive feedback from instructor and students for making course administration efficient and concepts accessible.



Links: [🔗 Course website](#) [🔗 GitLab repository](#)

Highlights: [TA](#) [Spectral Methods](#) [Graph Theory](#)

Technical Highlights:

- PageRank & Perron-Frobenius: Eigenvalue analysis for ranking and importance measures

- Graph Laplacian: Fiedler vector, spectral partitioning, and community detection
- Spectral Embedding: Dimensionality reduction preserving graph structure
- Matrix Factorization: SVD, NMF, and applications to data analysis
- Network Analysis: Centrality measures, clustering coefficients, graph metrics

Methodology:

- Created Python implementations of key algorithms (complementing MATLAB originals)
- Delivered guest lecture on "Comparing Embedding Spaces and Clustering Methods"
- Developed supplementary materials connecting theory to practical applications
- Provided one-on-one mentoring during office hours for complex mathematical concepts
- Managed course logistics including Canvas site, assignments, and grading

Teaching Assistant: Calculus (MATH 101)

TA to Prof. Dangxing Chen Calculus, Teaching

- Supported a class of 40+ students covering derivatives, integrals, and applications.
- Led weekly recitations: reinforced lecture concepts and guided problem-solving and discussions.
- Received positive feedback for strengthening foundations and fostering interest in mathematics.
- Topics: Limits, derivatives, integration techniques, applications to physics and optimization.

Math 101
Calculus
Session 1, 2023

Dates: Aug 21 – October 12
 Course meeting time: Mo-Th 1:15 pm – 2:30 pm (Beijing Time), AB 1046
 Recitation 001R: Tu 2:45 pm – 4:00 pm (Beijing Time), AB 1079
 Th 6:00 pm – 7:15 pm (Beijing Time), AB 1079
 Academic credit: 4 DUKE credits

Instructor's information
 Dangxing (Dan) Chen, Assistant Professor of Mathematics
 Email: dangxing.chen@dukekunshan.edu.cn
 Research interests: My research focuses on quantitative finance and efficient numerical methods in science and engineering.

Office hours: Monday, 2:30 pm – 3:30 pm, Wednesday and Thursday, 2:30 – 3:00 pm
 Office: WDR2113

TAs
 Yihao Wang: yihao.wang@dukekunshan.edu.cn
 Office hours: 7:15 pm – 8:15 pm (Beijing Time) Thursday, AB 1079 (AB 1087 for the first week)
 Junting Wang: junting.wang@dukekunshan.edu.cn
 Office hours: 7:15 pm – 8:15 pm (Beijing Time) Thursday, AB 1079
 Yuanxuan Feng: yuanxuan.feng@dukekunshan.edu.cn
 Tutors:
 Yiqi Zhang: yiqi.zhang@duke.edu.cn
 Jiaqi Zheng: jiaqi.zheng@dukekunshan.edu.cn

What is this course about?
 Calculus is the foundation for a large part of modern mathematics and has countless application across the sciences and engineering.

This course covers the elements of basic calculus concepts (limits, continuity, differentiation, integration) and explores related applications. The treatment of these topics is relatively rigorous, and it involves basic principles of mathematical logic.

The course begins with an introduction to the concept of a limit. The derivative function is then introduced, which lead to a unit on ordinary differential equations and their numerical solutions. This is followed by a unit on integration concepts and techniques. Throughout the course, classroom activities and homework reinforce understanding by requiring the formulation of and solution of mathematical problems using analytical and computational approaches. Recitation sessions allow for small group learning activities, including collaborative work to solve calculus problems. If applicable, the relation between these problems and physics or other science areas are discussed.



昆山杜克
UNIVERSITY

Links: [GitHub repository](#)

Highlights: [TA](#) [Calculus](#)

Personal & Creative Projects

Beyond formal research and coursework, I enjoy building tools that blend automation, creativity, and data visualization. These projects showcase practical problem-solving and exploratory programming.

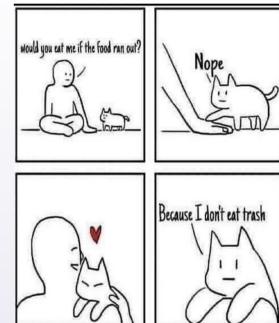
Resident Assistant Automation Suite

Resident Assistant — Res Life, DKU Python, Automation, Scraping

- Assisted student residents with academic/personal issues; built community; handled 50+ incidents across 3 years.
- Developed Python script to scrape Reddit images and resident roster for automatic door decoration creation; used by fellow RAs.
- Automated routine RA workflows (duty rotations, maintenance tracking, monthly reporting) to save hours per month.

Juntang

F-3116a



Links: [GitHub repository](#)

Highlights: [RA](#) [Automation](#) [Scraping](#)

Creative Tools & Experiments (Deprecated Services)

Personal Projects Web UI, HSI Clustering, LLM UI

- c4h.qqgjyx.com: Clustering 4 hyperspectral images (HSI) to analyze/visualize spectral data.

- sd-webui.qqgjyx.com: Fork of Stable Diffusion Web UI with customized UX/performance.
- llama.qqgjyx.com: Open web UI running a pre-tuned language model as an AI chatbot.

The screenshot shows Junlang Wang's GitHub profile page. At the top, it displays a heatmap visualization titled "qqgjyx.com/mheatmap" which is described as a Python package for advanced heatmap visualization and matrix analysis, featuring mosaic/proportional heatmaps, confusion matrix post-processing, and spectral rendering capabilities. Below this is a line graph titled "Star history" showing the number of stars over time from March 2022 to May 2023. The graph shows a significant increase in star count starting in April 2022, reaching approximately 450 stars by May 2023. Further down, there is another project entry for "qqgjyx.com/pysgtsnepl", described as a Python wrapper for the t-SNE algorithm for dimensionality reduction and visualization. This project is marked as deprecated. A sidebar on the left lists Junlang Wang's GitHub activity, including contributions to Intel, DCCD, GHUB, and LinkedIn. The bottom of the page includes links to the GitHub repository and a note that the page is on version 1.0.1.

Links: Personal projects website

Highlights: [Web Tools](#) [Deprecated](#)

I am grateful to my advisors, collaborators, and peers who have supported and challenged me throughout these projects. Special thanks to Prof. Shixin Xu, Prof. Xiaobai Sun, Prof. Shu Kit Eric Tam, Prof. Sze Chai Kwok, Prof. Nikos Pitsianis, Prof. Xiawa Wang, and the teams at Duke Kunshan University and Duke University.

Contact & Additional Materials

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- /github: github.com/qqgjyx
- 🌐 Website: www.qqgjyx.com
- 📞 Phone: +86 137 0626 7747 / +1 919-201-4521



Website



GitHub

Additional materials, demo videos, and interactive visualizations are available via embedded links throughout this portfolio.

Last updated: October 2025