HIL Research Seminars

by

Health Informatics Lab

Friday, 27 March 2026

1.00 pm – 2.30 pm

LT3, North Spine

PROGRAMME OVERVIEW

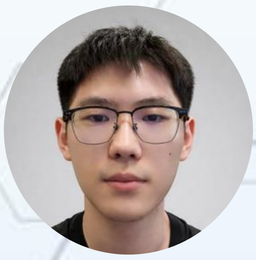
1:00 pm	Single-cell trajectory analysis of direct dell reprogramming using computational biology and artificial intelligence approaches by **Liu Chen**
1:15 pm	Missing-aware evolving fuzzy learning for MASLD risk prediction from irregular time series by **Zhan Zhuoxuan**
1:30 pm	Target-aware latent diffusion model for design of apoptosis-inducing anticancer peptides by **Tiara Natasha Binte Sayuti**
1.45pm	Q&A
1:55 pm	Enhancing risk awareness in LLM agents via probing safety boundaries by **Jiang Yu**
2:10 pm	Can LLMs reason over non-text modalities without training? A case study of in-context representation learning by **Zhang Tianle**
2.25pm	Q&A


Liu Chen


Zhan Zhuoxuan


Tiara Natasha Binte Sayuti


Jiang Yu


Zhang Tianle

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College of Computing and Data Science

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Single-Cell Trajectory Analysis Of Direct Cell Reprogramming Using Computational Biology And Artificial Intelligence Approaches

27 MAR 2026, FRIDAY

1.00PM - 1.15PM

LT3, North Spine

ABSTRACT

Direct cell reprogramming has significant potential for regenerative medicine, yet identifying effective transcription factor combinations remains a major challenge. A key limitation of existing computational approaches is their reliance on static ranking, which often fails to capture the dynamic, stage-specific nature of cell fate transition. This talk presents an integrative computational framework that combines single-cell trajectory analysis with artificial intelligence to investigate direct cell reprogramming in a dynamic and interpretable manner. By incorporating pseudotime-based temporal modeling, transcription factor role assignment, and network-level analysis, the framework characterizes how regulatory factors act across distinct stages of reprogramming and identifies stable transcription factor cores associated with lineage conversion.

ABOUT THE SPEAKER

Liu Chen is a fourth-year PhD student supervised by Professor Kwoh Chee Keong. His research lies at the intersection of computational biology and artificial intelligence, with a focus on single-cell trajectory analysis, gene regulatory network modeling, and transcription factor discovery for direct cell reprogramming. He is particularly interested in developing interpretable AI-driven methods to understand dynamic cell fate transitions and to advance computational strategies for regenerative medicine.

Liu Chen

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Missing-Aware Evolving Fuzzy Learning For MASLD Risk Prediction From Irregular Time Series

27 MAR 2026, FRIDAY **1.15PM - 1.30PM**

LT3, North Spine

ABSTRACT

Metabolic dysfunction-associated steatotic liver disease (MASLD) affects a large and growing population worldwide, and a subset of patients progress to clinically significant liver outcomes, creating a need for longitudinal risk monitoring from routinely collected follow-up data. In this work, we study a monitoring-style prediction problem: given an irregular history of follow-up laboratory measurements for a MASLD patient, predict whether the patient will develop severe liver outcomes in the near future.

We study a previously underexplored monitoring-style risk prediction formulation for MASLD progression risk prediction using irregular follow-up laboratory records, and show that a missing-aware evolving neuro-fuzzy classifier (MEF-Classifier) is well suited to this setting.

MEF-Classifier explicitly encodes both observed and missing states without ad hoc imputation, activates interpretable fuzzy rules that accumulate positive and negative evidence, and aggregates evidence into probabilistic risk estimates using imbalance-aware class weighting to stabilize learning under rare outcomes. Evaluated on a large public cohort and a local Singapore cohort, MEF-Classifier demonstrates improved performance over diverse baseline models while providing transparent explanations in the form of if--then rules that support clinical inspection and hypothesis generation.

ABOUT THE SPEAKER

Zhan Zhuoxuan is a PhD student at Nanyang Technological University, Singapore. His research focuses on medical AI, particularly irregular clinical time-series modeling, missing data handling, and interpretable machine learning. He is currently working on predictive modeling with electronic health record data, with a focus on missing-aware and interpretable methods.

Zhan Zhuoxuan

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Target-Aware Latent Diffusion Model For Design Of Apoptosis-inducing Anticancer Peptides

27 MAR 2026, FRIDAY **1.30PM – 1.45PM**

LT3, North Spine

ABSTRACT

Anticancer peptides (ACPs) are promising therapeutic candidates due to their high specificity and lower toxicity compared with conventional small-molecule drugs. However, designing peptides with strong binding affinity and biological activity remains challenging due to the vast sequence space and the complex relationship between peptide sequence, structure, and their ability to bind and inhibit target proteins.

In this work, we present a structure-aware generative framework for designing apoptosis-inducing anticancer peptides targeting the anti-apoptotic protein BCL-xL, a key regulator of tumor survival. The approach integrates protein language models with graph neural networks and a target-aware latent diffusion model to generate peptide sequences guided by receptor structural information. By conditioning the generative process on binding-pocket representations, the model produces peptides that are both biologically plausible and structurally compatible with the target interface.

Comprehensive evaluation shows that the generated peptides demonstrate strong physicochemical realism, high sequence fluency, and favorable docking scores compared with existing generative approaches. This work highlights how combining advances in deep learning with structural biology can enable more efficient discovery of peptide therapeutics and illustrates the potential of generative AI in computational drug design.

ABOUT THE SPEAKER

Tiara is a third-year PhD student, advised by Professor Jagath C. Rajapakse. She earned her Bachelor of Engineering in Pharmaceutical Engineering from the Singapore Institute of Technology and previously worked in the pharmaceutical industry at Amgen Singapore Manufacturing and Tessa Therapeutics.

Motivated by the potential of AI in drug discovery, she later joined the Singapore University of Technology and Design as a Research Assistant. Her current research focuses on integrating deep learning, protein language models, and generative AI with structural biology to design functional peptides and study protein–protein interactions for therapeutic development.

Tiara Natasha Binte Sayuti

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Enhancing Risk Awareness in LLM Agents via Probing Safety Boundaries

27 MAR 2026, FRIDAY

1.55PM - 2.10PM

LT3, North Spine

ABSTRACT

Large Language Models (LLMs) have evolved to function as autonomous agents capable of real-world tasks, including multi-step reasoning, tool use, and decision-making. While promising for complex task execution, such capabilities introduce unpredictable risks, highlighting the need for LLM agents to maintain internal risk awareness throughout task processes.

In this talk, we introduce a judgment mechanism that evaluates LLM agent behavior in terms of harmfulness and response consistency across multiple interactions. Using information-theoretic analysis, we identify safety boundaries that separate distinct behavioral patterns without relying on manual annotation or binary classification. Building on these boundaries, we propose a dual-objective training strategy for safety alignment that combines supervised fine-tuning to reinforce consistently safe responses with unlearning techniques to reduce harmful behaviors.

ABOUT THE SPEAKER

Jiang Yu is a PhD candidate in the College of Computing and Data Science at Nanyang Technological University, Singapore. Her research interests include AI safety, LLM agents, and distributed systems.

Jiang Yu

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Can LLMs Reason Over Non-Text Modalities Without Training? A Case Study of In-Context Representation Learning

27 MAR 2026, FRIDAY **2.10PM - 2.25PM**

LT3, North Spine

ABSTRACT

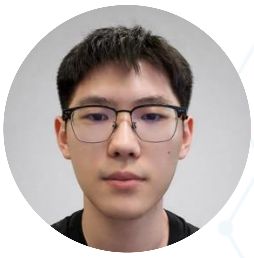
Large Language Models (LLMs) have demonstrated strong in-context learning capabilities, enabling them to adapt to new tasks without parameter updates. However, extending this ability to non-text modalities (e.g., molecular structures, images, or sensor data) typically requires additional supervised training and modality-specific alignment.

In this talk, we present In-Context Representation Learning (ICRL), a training-free framework that allows LLMs to directly leverage representations from external foundation models (FMs) during inference. Instead of using textual inputs, ICRL injects modality representations into the LLM either as prompt-level tokens or embedding-level features, enabling multi-modal reasoning without fine-tuning.

This work provides the first systematic study of training-free multimodal integration into LLMs, highlighting a promising direction for efficient and scalable multimodal reasoning.

ABOUT THE SPEAKER

Zhang Tianle is a Ph.D. student at Nanyang Technological University (NTU), Singapore, supervised by Prof. Alvin Chan. His research focuses on large language models, multimodal learning, and exploring effective integration strategies between foundation models and LLMs.



Zhang Tianle

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