NANYANG TECHNOLOGICAL UNIVERSITY SINGAPORE

School of Physical and Mathematical Sciences



Final Presentation Topics in Scientific Computation II

5 & 12 November 2026

Organizer

Zhongjian Wang

DAY 1 / THURSDAY, 5 NOVEMBER 2026

Presentation Programme

10:30 am–12:30 pm | All times Singapore time (SGT)

SESSION 1 **10:30–11:30 am**

Mathematical foundations: spectral methods, approximation, and geometry

10:30–10:50 am	**Zhu Haoran** Card Shuffling with Adjacent Swaps and Fill's Gap Problem
10:50–11:10 am	**Shi Yanhao** Explicit Construction of Approximate Kolmogorov Superpositions with C^2-Smoothness
11:10–11:30 am	**Bharadwaj Shreyas Narendra** Geometric Learning with Positively Decomposable Kernels

SESSION 2 **11:30 am–12:30 pm**

Stochastic models, inverse problems, and neural solvers

11:30–11:50 am	**Omori Shu** Generative Models for High-Dimensional Option Pricing: Toward Arbitrage-Free Market Paths
11:50 am–12:10 pm	**Huang Liangcai** Wasserstein Bounds for Generative Diffusion Models with Gaussian Tail Targets
12:10–12:30 pm	**Wang Weiqian** Bayesian Inverse Problems for Obstacle Variational Inequalities

Each presentation is allocated 20 minutes, including questions and transitions.

DAY 2 / THURSDAY, 12 NOVEMBER 2026

Presentation Programme

10:30 am–12:30 pm | All times Singapore time (SGT)

SESSION 3 **10:30–11:30 am**

Learning from structured data: limitations and forecasting

10:30–10:50 am	**Chen Xiyao** Learning-Based Cryptanalysis of Lattice Problems: Neural Approaches to LWE and Their Theoretical Limits
10:50–11:10 am	**Toerngren Lukas** N-BEATS and Beyond: Residual learning, Meta-learning and Zero-shot forecasting
11:10–11:30 am	**Chen Canbin** Multi-View Stock Correlation Learning with LSTM-GCN for Price Prediction

SESSION 4 **11:30 am–12:10 pm**

AI for scientific and behavioral applications

11:30–11:50 am	**Chen Qing Yang** 3D-Enhanced Machine Learning for Macrocyclic Peptide Permeability Prediction
11:50 am–12:10 pm	**Liu Jiayi** A Survey of Consumers' Willingness to Pay for Paid Micro-Dramas

Each presentation is allocated 20 minutes, including questions and transitions.

THURSDAY, 5 NOVEMBER 2026

Presentation Abstracts

Abstracts from NTULearn submissions and the cited papers, updated 5 November 2026.

SESSION 1 | Mathematical foundations

Zhu Haoran

Card Shuffling with Adjacent Swaps and Fill's Gap Problem

Certain biased card shuffles can be modeled by Markov chains on the symmetric group, where neighboring elements are swapped with prescribed probabilities. This talk presents a sharp lower bound on the spectral gap for a broad class of these chains and explains how it resolves a conjecture of Fill. The key idea decomposes the transition matrix into an average of elementary transition matrices interpreted as orthogonal projections in a suitable inner-product space. The talk also discusses the multiplicity of the second-largest eigenvalue when the spectral gap is minimized.

Shi Yanhao

Explicit Construction of Approximate Kolmogorov Superpositions with C^2-Smoothness

We explicitly construct an approximate version of the Kolmogorov superpositions, which is composed of C^2-inner and outer functions, and can approximate an arbitrary α-Hölder continuous function $f \in \mathcal{H}^\alpha([0,1]^d)$, $\alpha \in (0,1]$ with accuracy $O(N^{-\alpha})$, where N denotes the number of outer summations. The inner functions are generated by applying suitable translations and dilations to a piecewise C^2, strictly-increasing function, while the outer functions are constructed row-wise through piecewise C^2-interpolation using newly designed shape functions. This novel variant of Kolmogorov superpositions overcomes the "wild" and "pathological" behaviors of the inherent single variable functions, but retains the essence of Kolmogorov's strategy of exact representation—an objective that Sprecher (Neural Netw. 144 (2021) 438–442) has actively pursued. We also discuss the implications of this new construction and demonstrate its applicability to related neural networks.

Paper abstract: Lunji Song, Zilan Cheng, Juan Diego Toscano, and Li-Lian Wang, arXiv:2508.04392v2 (2026), CC BY 4.0.

Bharadwaj Shreyas Narendra

Geometric Learning with Positively Decomposable Kernels

Kernel methods traditionally use positive definite kernels to learn in reproducing kernel Hilbert spaces, but such kernels can be difficult to construct for non-Euclidean data. This talk introduces methods based on reproducing kernel Krein spaces, which require only kernels admitting a positive decomposition. Learning does not require access to that decomposition. The talk investigates conditions for positive decomposability and shows that invariant kernels on homogeneous spaces admit positive decompositions under tractable regularity assumptions, providing theoretical foundations and a practical route for kernel learning on non-Euclidean data.

THURSDAY, 5 NOVEMBER 2026

Presentation Abstracts

SESSION 2 | Stochastic models, inverse problems, and neural solvers

Omori Shu

Generative Models for High-Dimensional Option Pricing: Toward Arbitrage-Free Market Paths

This presentation explores generative modeling for high-dimensional option pricing. Classical models such as Black–Scholes can deviate from real market behavior, while grid-based methods suffer from the curse of dimensionality. Deep BSDE methods make high-dimensional pricing and hedging computationally tractable but still rely on assumed market models. Score-based generative models offer a way to learn market-path distributions directly from data. The presentation highlights open challenges, particularly enforcing no-arbitrage constraints and ensuring the explainability of generated paths.

Huang Liangcai

Wasserstein Bounds for Generative Diffusion Models with Gaussian Tail Targets

We present an estimate of the Wasserstein distance between the data distribution and the generation of score-based generative models. The sampling complexity with respect to dimension is $O(\sqrt{d})$, with a logarithmic constant. In the analysis, we assume a Gaussian-type tail behavior of the data distribution and an ϵ-accurate approximation of the score. Such a Gaussian tail assumption is general, as it accommodates a practical target - the distribution from early stopping techniques with bounded support.

The crux of the analysis lies in the global Lipschitz bound of the score, which is shown from the Gaussian tail assumption by a dimension-independent estimate of the heat kernel. Consequently, our complexity bound scales linearly (up to a logarithmic constant) with the square root of the trace of the covariance operator, which relates to the invariant distribution of the forward process.

Paper abstract: Xixian Wang and Zhongjian Wang, arXiv:2412.11251v2 (2025); TMLR (2026).

Wang Weiqian

Bayesian Inverse Problems for Obstacle Variational Inequalities

This presentation discusses Bayesian recovery of unknown obstacles from noisy state observations, including theoretical and experimental results. It then reviews preconditioned one-step generative modeling for posterior sampling in function spaces and considers its potential to accelerate uncertainty quantification in obstacle inverse problems.

THURSDAY, 12 NOVEMBER 2026

Presentation Abstracts

SESSION 3 | Learning from structured data

Chen Xiyao

Learning-Based Cryptanalysis of Lattice Problems: Neural Approaches to LWE and Their Theoretical Limits

This project studies SALSA, the first transformer-based attack on the Learning With Errors problem. SALSA recovers sparse binary secrets up to dimension 128, but only with Hamming weight at most 4. Controlled experiments indicate that architecture, data, noise, and encoding mainly affect data requirements, while secret weight and input size relative to the modulus determine what can be learned. Through the course's error decomposition, the limitation is interpreted in terms of optimization and estimation rather than approximation. Uniform inputs produce sparse-parity-like behavior, while small inputs make the problem linear. A toy model confirms the threshold, suggesting that learnability depends on input representation.

Toerngren Lukas

N-BEATS and Beyond: Residual learning, Meta-learning and Zero-shot forecasting

This project examines N-BEATS, a deep learning architecture for time-series forecasting that outperforms domain-specific statistical and hybrid methods in the reported studies. Its doubly residual structure iteratively removes components of the input signal while contributing to the forecast. The architecture can be made interpretable and generalizes across heterogeneous datasets. The project explores a proposed meta-learning interpretation of the residual architecture and its potential to explain zero-shot forecasting on unseen datasets. It also places N-BEATS within the broader development of neural forecasting, including N-HiTS and time-series foundation models.

Chen Canbin

Multi-View Stock Correlation Learning with LSTM-GCN for Price Prediction

This project combines stock trading similarities and industry relationships to predict stock prices. Dynamic Time Warping captures similarities in trading data, while Latent Dirichlet Allocation extracts industry relationships from company business descriptions. These relationships are integrated through three fusion methods (equal weighting, principal component analysis, and Laplacian eigenmaps) into an LSTM-GCN model. Experiments use 84 representative Chinese stocks, with four selected for detailed evaluation. Although predicted price levels can be biased, predictions in the reported examples broadly follow the direction of actual price movements.

THURSDAY, 12 NOVEMBER 2026

Presentation Abstracts

SESSION 4 | AI for scientific and behavioral applications

Chen Qing Yang

3D-Enhanced Machine Learning for Macrocyclic Peptide Permeability Prediction

This proposed project investigates whether explicit three-dimensional structural information improves predictions of macrocyclic peptide membrane permeability. The approach combines Transformer representations of molecular sequences, graph neural networks for molecular topology, and geometry-aware networks such as SchNet for 3D structures. Model comparisons and ablation studies will assess the contribution of 3D information beyond conventional 1D and 2D representations, addressing the influence of flexible conformations on membrane permeation.

Liu Jiayi

A Survey of Consumers' Willingness to Pay for Paid Micro-Dramas

This study investigates willingness to pay for micro-dramas using the Technology Acceptance Model, LLM-generated data, and real-user survey data. Structural Equation Modeling and Random Forest analysis reveal different payment mechanisms: simulated data suggest an experience–satisfaction–payment pathway, whereas real-user data indicate an experience–value–payment mechanism. Emotional value, including stress relief and emotional resonance, motivates viewing. Sufficient free content is a major barrier to payment, while particular intellectual properties and actors can trigger paid conversion.