HDDA-XIII
Schedule and abstracts

Schedule

- **Day 1: August 27 (Tuesday), 2024.** Room 1C4, 1st floor.

    - **17:00–19:00**: registration.

- **Day 2: August 28 (Wednesday), 2024.** Room 1C4, 1st floor.

    - **09:20–10:30**: coffee and registration.
    - **10:30–11:00**: **opening session**. Welcome speeches by Prof. Ejaz Ahmed (founder of HDDA) and Prof. Reetika Gupta (Deputy Dean of ESSEC Asia-Pacific).
    - **11:00–12:45**: **session**: High-dimensional matrices: theory and applications.
    - **12:45–14:00**: lunch. Room 5C1, 5th floor.
    - **14:00–15:45**: **session**: Cutting-edge machine learning methods for complex biological problems.
    - **15:45–16:15**: coffee break.
    - **16:15–18:00**: **session**: High-dimensional models I: grouping and aggregating predictors.

- **Day 3: August 29 (Thursday), 2024.** Room 1C1, 1st floor.

    - **09:20–10:30**: **session**: Mean field and variational approximations.
    - **10:30–11:00**: coffee break.
    - **11:00–12:45**: **session**: Bayesian methods in statistics and machine learning.
    - **12:45–14:00**: lunch. Room 5C1, 5th floor.
    - **14:00–15:45**: **session**: Disease modelling and epidemiology.
    - **15:45–16:15**: coffee break.
    - **16:15–18:00**: **session**: High-dimensional models II: robustness & overparametrization.
    - **18:00–20:00**: **poster session** & light buffet. Room 5C1, 5th floor.

- **Day 4: August 30 (Friday), 2024.** Room 1C1, 1st floor.

    - **09:20–10:30**: **session**: Data science, AI, and high-dimensional spatiotemporal dynamics.
    - **10:30–11:00**: coffee break.
    - **11:00–12:45**: **session**: Recent advances in the theory of machine learning.
    - **13:20-. . .** : lunch. Room 5C1, 5th floor.

Invited Session 1 – High-dimensional matrices: theory and applications

Chair: Ejaz Ahmed (Brock University).

Guangming Pan (Nanyang Technological University).

Asymptotic of eigenvectors of large sample covariance matrices. *The talk is about asymptotics of eigenvectors of large sample covariance matrices when the dimension and sample size both tend to infinity with their ratio being a positive constant. The eigenvectors are not limited to those corresponding to the spiked sample eigenvalues. We also explore its application in nonlinear shringage estimators for population covariance matrices.*

Wanjie Wang (National University of Singapore).

Recovery of Timestamps on Noisy High-Dimensional Data . *The analysis of proteins and biological macromolecules is of great interest today, with the development of single-particle cryo-electron microscopy (cryo-EM). The observation Y_i follows $X_{t_i} + Noise$ because of the motions of the molecule. Since the motions repeated a hidden pattern, the ordering of t_i does not have the same ordering with i. Hence, a proper ordering of Y_i will largely improve the recovery of the functional $X(t)$.*
In our work, we present a spectral method on the Laplacian matrix to order Y_i. We first reduce the noise in Y by taking the top eigenvectors of Y. Let Z be the matrix formed by these eigenvectors and we find the ordering of rows in Z. To do it, we first build the Gaussian kernel matrix on Z and then set L_Z to be the Laplacian of the kernel matrix. Ordering the second smallest eigenvector of Z will give the correct ordering of Y. We have set up the theoretical results to show consistency.

Antoine Ledent (Singapore Management University).

On approximate recovery in deep non-linear matrix completion with Schatten-p quasi-norm constraints. *Matrix Completion has a rich history of research from several angles. In the approximate recovery literature, it is known that regardless of the sampling distribution, $\widetilde{O}(n^{3/2}r^{1/2})$ entries are sufficient to approximate the ground truth matrix to a desired degree of accuracy by employing trace norm constraints, where n is the size of the matrix and r is a constraint of a similar scaling to the ground truth rank. In this talk, we extend those results to the case of Schatten p quasi norm constraints, which is known to be equivalent to the popular Deep Matrix Factorization framework. Our distribution-free generalization bound corresponds to a sample complexity of $\widetilde{O}(n^{1+\frac{p}{2}}r^{1-\frac{p}{2}})$. This demonstrates the power of increasing depth in terms of stable rank restriction, and to the best of our knowledge, this is the first non-vacuous result for this setting. Furthermore, we provide a weighted analogue of the Schatten p quasi norm which brings the rate down to $\widetilde{O}(nr)$ in a phenomenon similar to the effect of the weighting on the trace norm regularizer in existing literature. Next, we consider extensions of the model which include nonlinearities and show how to combine our results with neural network bounds in such scenarios. Lastly, we briefly touch upon earlier work on the question of incorporating side information in the form of linear constraints and discuss future avenues of research.*

Invited Session 2 – Cutting-edge machine learning methods for complex biological problems

Chair: Yi Li (University of Michigan).

Yuedong Wang (University of California - Santa Barbara).

A Nonparametric Mixed-Effects Mixture Model for Patterns of Clinical Measurements Associated with COVID-19. *Some patients with COVID-19 show changes in signs and symptoms, such as temperature and oxygen saturation, days before being positively tested for SARS-CoV-2, while others remain asymptomatic. It is important to identify these subgroups and to understand what biological and clinical predictors are related to these subgroups. This information will provide insights into how the immune system may respond differently to infection and can further be used to identify infected individuals. We propose a flexible nonparametric mixed-effects mixture model that identifies risk factors and classifies patients with biological changes. We model the latent probability of biological changes using a logistic regression model and trajectories in the latent groups using smoothing splines. We developed an EM algorithm to maximize the penalized likelihood for estimating all parameters and mean functions. We evaluate our methods by simulations and apply the proposed model to investigate changes in temperature in a cohort of COVID-19-infected hemodialysis patients.*

Kin Yau Wong (The Hong Kong Polytechnic University).

Robust score tests with incomplete covariates and high-dimensional auxiliary variables for genomic studies. *Analyses of modern genomic data are often complicated by missing data. When variables of interest are missing for some subjects, it is desirable to use observed auxiliary variables, which are sometimes high dimensional, to impute or predict the missing values in order to improve statistical efficiency. Although many methods have been developed for prediction using high-dimensional variables, it is challenging to perform valid inference based on such predicted values. In this study, we develop a general association test for an outcome variable, which may be continuous, discrete, or censored, and a potentially missing covariate. The missing covariate values can be predicted using variables selected from a set of high-dimensional auxiliary variables. The test is flexible and robust against model misspecification. We establish the validity of the test under data-driven model-selection procedures. We also demonstrate the validity of the proposed method and its advantages over existing methods using extensive simulation studies and applications to major cancer genomic studies.*

Yi Li (University of Michigan).

Penalized Deep Partially Linear Cox Models: Error Rate and Selection Consistency. *Partially linear Cox models have gained popularity for survival analysis by dissecting the hazard function into parametric and nonparametric components, allowing for the effective incorporation of both well-established risk factors (such as age and clinical variables) and emerging risk factors (e.g., image features) within a unified framework. However, when the dimension of parametric components exceeds the sample size, the task of model fitting becomes formidable, while nonparametric modeling grapples with the curse of dimensionality. We propose a novel Penalized Deep Partially Linear Cox Model (Penalized DPLC), which incorporates the SCAD penalty to select important texture features and employs a deep neural network to estimate the nonparametric component of the model. We prove the convergence and asymptotic properties of the estimator and compare it to other methods through extensive simulation studies, evaluating its performance in risk prediction and feature selection.*

Invited Session 3 – High-dimensional models I: grouping and aggregating predictors

Chair: Kamélia Daudel   (ESSEC Business School, Paris campus).

Anand N. Vidyashankar   (George Mason University).

Grouping Predictors using network-wide metrics and divergences. *When multitudes of features can plausibly be associated with a response, privacy considerations and model parsimony suggest grouping them to increase the predictive power of a regression model. If the set of predictors possesses common characteristics, methods such as group LASSO integrated with tools that account for model selection uncertainty can be used for downstream data analysis. However, if little is known about the features, ad hoc grouping can lead to erroneous inference. In these situations, grouping the predictors using alternate metrics is convenient. We describe a new weighted implicit network approach to group variables where the weights represent the relative association of the variables to the response. Specifically, we describe a new algorithm (supervised learning algorithm) that utilizes network-wide metrics and a sequential testing procedure to find groups of variables that have significant association with the response. For this reason, we describe asymptotic distributional results concerning the network-wide metrics and a novel bootstrap approach for uncertainty assessment. We illustrate the performance of the results using numerical experiments and data from sports analytics.*

Ha (Van) Hoang   (University of Science, Vietnam National University).

Functional mixtures-of-experts. *We consider the statistical analysis of heterogeneous data for prediction in situations where the observations include functions, typically time series. We extend the modeling with Mixtures-of-Experts (ME), as a framework of choice in modeling heterogeneity in data for prediction with vectorial observations, to this functional data analysis context. We first present a new family of ME models, named functional ME (FME) in which the predictors are potentially noisy observations, from entire functions. Furthermore, the data generating process of the predictor and the real response, is governed by a hidden discrete variable representing an unknown partition. Second, by imposing sparsity on derivatives of the underlying functional parameters via Lasso-like regularizations, we provide sparse and interpretable functional representations of the FME models called iFME. We develop dedicated expectation–maximization algorithms for Lasso-like (EM-Lasso) regularized maximum-likelihood parameter estimation strategies to fit the models. The proposed models and algorithms are studied in simulated scenarios and in applications to two real data sets, and the obtained results demonstrate their performance in accurately capturing complex nonlinear relationships and in clustering the heterogeneous regression data.*
Joint work with F. Chamroukhi, N. T. Pham and G. J. McLachlan.

Chiung-Yu Huang   (University of California, San Francisco).

Synthesizing external aggregated information in the presence of population heterogeneity: A penalized empirical likelihood approach. *With the increasing availability of data in the public domain, there has been a growing interest in exploiting information from external sources to improve the analysis of smaller-scale studies. An emerging challenge in the era of big data is that the subject-level data are high dimensional, but the external information is at an aggregate level and of a lower dimension. Moreover, heterogeneity and uncertainty in the auxiliary information are often not accounted for in information synthesis. We propose a unified framework to summarize various forms of aggregated information via estimating equations and develop a penalized empirical likelihood approach to incorporate such information in logistic regression. When the homogeneity assumption is violated, we extend the method to account for population heterogeneity among different sources of information. When the uncertainty in the external information is not negligible, we propose a variance estimator adjusting for the uncertainty. The proposed estimators are asymptotically more efficient than the conventional penalized maximum likelihood estimator and enjoy the oracle property even with a diverging number of predictors. Simulation studies show that the proposed approaches yield higher accuracy in variable selection compared with competitors. We illustrate the proposed methodologies with a pediatric kidney transplant study.*

Invited Session 4 – Mean-field and variational approximations

Chair: Badr-Eddine Chérief-Abdellatif   (CNRS & Sorbonne Université).

Kamélia Daudel   (ESSEC Business School, Paris campus).

Alpha-divergence Variational Inference Meets Importance Weighted Auto-Encoders: Methodology and Asymptotics. *Variational Inference methods are optimization-based methods that have generated a lot of attention in Bayesian Statistics due to their applicability to high-dimensional machine learning problems. In particular, several algorithms involving the Variational Rényi (VR) bound have been proposed to optimize an alpha-divergence between a target posterior distribution and a variational distribution. Despite promising empirical results, those algorithms resort to biased stochastic gradient descent procedures and thus lack theoretical guarantees. In this paper, we formalize and study the VR-IWAE bound, a generalization of the Importance Weighted Auto-Encoder (IWAE) bound. We show that the VR-IWAE bound enjoys several desirable properties and notably leads to the same stochastic gradient descent procedure as the VR bound in the reparameterized case, but this time by relying on unbiased gradient estimators. We then provide two complementary theoretical analyses of the VR-IWAE bound and thus of the standard IWAE bound. Those analyses shed light on the benefits or lack thereof of these bounds. Lastly, we illustrate our theoretical claims over toy and real-data examples.*
Reference: K. Daudel, J. Benton, Y. Shi and A. Doucet (2023). Alpha-divergence Variational Inference Meets Importance Weighted Auto-Encoders: Methodology and Asymptotics. Journal of Machine Learning Research, 24(243):1–83.

Atsushi Nitanda   (A*STAR CFAR, Singapore).

Improved Particle Approximation Error for Mean Field Neural Networks. *Mean-field Langevin dynamics (MFLD) minimizes an entropy-regularized nonlinear convex functional defined over the space of probability distributions. MFLD has gained attention due to its connection with noisy gradient descent for mean-field two-layer neural networks. Unlike standard Langevin dynamics, the nonlinearity of the objective functional induces particle interactions, necessitating multiple particles to approximate the dynamics in a finite-particle setting. Recent works have demonstrated the uniform-in-time propagation of chaos for MFLD, showing that the gap between the particle system and its mean-field limit uniformly shrinks over time as the number of particles increases. In this work, we improve the dependence on logarithmic Sobolev inequality (LSI) constants in their particle approximation errors which can exponentially deteriorate with the regularization coefficient. Specifically, we establish an LSI-constant-free particle approximation error concerning the objective gap by leveraging the problem structure in risk minimization. As the application, we demonstrate improved convergence of MFLD, sampling guarantee for the mean-field stationary distribution, and uniform-in-time Wasserstein propagation of chaos in terms of particle complexity.*

Invited Session 5 – Bayesian methods in statistics and machine learning

Chair: David Kepplinger   (George Mason University).

Linda S. L. Tan   (National University of Singapore).

Variational inference based on a subclass of closed skew normals. *Gaussian distributions are widely used in Bayesian variational inference to approximate intractable posterior densities, but the ability to accommodate skewness can improve approximation accuracy significantly, especially when data or prior information is scarce. We study the properties of a subclass of closed skew normals constructed using affine transformation of independent standardized univariate skew normals as the variational density, and illustrate how this subclass provides increased flexibility and accuracy in approximating the joint posterior density in a variety of applications by overcoming limitations in existing skew normal variational approximations. The evidence lower bound is optimized using stochastic gradient ascent, where analytic natural gradient updates are derived. We also demonstrate how problems in maximum likelihood estimation of skew normal parameters occur similarly in stochastic variational inference and can be resolved using the centered parametrization.*

David Tyler Frazier   (Monash University).

Generalized Bayesian Inference with Intractable Discrepancies. *Generalized or Gibbs posteriors are currently limited to situations where the loss function used in the analysis is analytically tractable. This limitation ensures that many interesting classes of loss functions, such as those based on robust measures of distance, e.g., maximum mean discrepancy, cannot be used within Generalized Bayesian inference. We show that so long as one can obtain a reasonable estimate of the analytically intractable loss function, then it is feasible to construct a novel type of Gibbs posterior that is nearly as accurate as if one had access to the intractable loss function. We demonstrate that the price to pay for replacing the intractable loss with an estimated version is a (possible) reduction in the rate of posterior concentration, with the speed of concentration ultimately depending on the quality of the estimated loss. We demonstrate these issues through several examples including generalized Bayesian inference based on maximum mean discrepancy, and likelihoods estimated using kernel densities.*

Cheng Li   (National University of Singapore).

Bayesian fixed-domain asymptotics for covariance parameters in spatial Gaussian process models. *Gaussian process models typically contain finite dimensional parameters in the covariance function that need to be estimated from the data. We study the Bayesian fixed-domain asymptotics for the covariance parameters in spatial Gaussian process regression models with an isotropic Matern covariance function, which has many applications in spatial statistics. For the model without nugget, we show that when the dimension of the domain is less than or equal to three, the microergodic parameter and the range parameter are asymptotically independent in the posterior. While the posterior of the microergodic parameter is asymptotically close in total variation distance to a normal distribution with shrinking variance, the posterior distribution of the range parameter does not converge to any point mass distribution in general. For the model with nugget, we derive new evidence lower bound and consistent higher-order quadratic variation estimators, which lead to explicit posterior contraction rates for both the microergodic parameter and the nugget parameter. We further study the asymptotic efficiency and convergence rates of Bayesian kriging prediction. All the new theoretical results are verified in numerical experiments and real data analysis.*

Invited Session 6 – Disease modelling and epidemiology

Chair: Linda S. L. Tan   (National University of Singapore).

Shuangge Ma   (Yale University).

Heterogeneous Network Analysis of Disease Clinical Treatment Measures via Mining Electronic Medical Record Data. *The analysis of clinical treatment measures has been extensively conducted and can facilitate more effective resource management and planning and also assist better understanding diseases. Most of the existing analyses have been focused on a single disease or a large number of diseases combined. Partly motivated by the successes of gene-centric and phenotypic human disease network (HDN) research, there has been growing interest in the network analysis of clinical treatment measures. However, the existing studies have been limited by a lack of attention to heterogeneity and relevant covariates, ineffectiveness of methods, and low data quality. In this study, our goal is to mine the Taiwan National Health Insurance Research Database (NHIRD), a large population-level electronic medical record (EMR) database, and construct HDNs for number of outpatient visits and medical cost. Significantly advancing from the existing literature, the proposed analysis accommodates heterogeneity and effects of covariates (for example, demographics). Additionally, the proposed method effectively accommodates the zero-inflation nature of data, Poisson distribution, high-dimensionality, and network sparsity. Computational and theoretical properties are carefully examined. Simulation demonstrates competitive performance of the proposed approach. In the analysis of NHIRD data, two and five subject groups are identified for outpatient visit and medical cost, respectively. The identified interconnections, hubs, and network modules are found to have sound implications.*

Yaqing Xu   (Shanghai Jiao Tong University School of Medicine).

Hierarchical Multi-Label Classification with Gene-Environment Interactions in Disease Modeling. *In biomedical studies, gene-environment (G–E) interactions have been demonstrated to have important implications for disease prognosis beyond the main G and main E effects. Many approaches have been developed for G-E interaction analysis, yielding important findings. However, hierarchical multi-label classification, which provides insightful information on disease outcomes, remains unexplored in G-E analysis literature. Moreover, unlabeled data is commonly observed in practical settings but omitted by many existing methods of hierarchical multi-label classification. In this study, we consider a semi-supervised scenario and develop a novel approach for the two-layer hierarchical response with G-E interactions. A two-step penalized estimation is then proposed using an efficient expectation-maximization (EM) algorithm. Simulation shows that it has superior accuracy in classification and feature selection performance. The analysis of The Cancer Genome Atlas (TCGA) data on lung cancer demonstrates the practical utility of the proposed approach. Overall, this study can fill the important knowledge gap in G-E interaction analysis by providing a widely applicable framework for hierarchical multi-label classification for complex disease outcomes.*

Hao Mei   (Renmin University of China).

A Variance Reduction Approach for the Inverse Probability-of-Treatment Weighted Estimator of Average Treatment Effects in Observational Studies. *The inverse probability-of-treatment weighted (IPTW) estimator is widely used for estimating average treatment effects (ATE) in observational studies. Although the IPTW method eliminates confounding by creating a pseudo-population where treatment assignment is independent of observed covariates, increased variance due to variability in propensity score estimation is often a major concern. In this study, we propose a machine learning predictor-adjusted IPTW (MLPA-IPTW) estimator, where the weighted least squares estimator of ATE is derived from a linear model that adjusts for machine learning predictors of the outcome. Advanced from the traditional covariate-adjusted regression, machine learning techniques are employed to handle high-dimensionality and non-linearity. We establish the consistency and asymptotic normality of the proposed estimator. Additionally, we demonstrate that the MLPA-IPTW estimator remains robust even when the machine learning step yields poor predictions, performing asymptotically no worse than the standard IPTW estimator. Our simulations and data analysis show that the proposed method achieves substantial variance reduction in the unbiased estimation of ATE.*

Invited Session 7 – High-dimensional models II: robustness & overparametrization

Chair: David Tyler Frazier   (Monash University).

David Kepplinger   (George Mason University).

Robust Variable Selection Under Adversarial Contamination in High-Dimensional Data. *Outliers and adversarial contamination are common issues when dealing with high-dimensional data. Including a large number of variables in an analysis opens the door for adversarial contamination to render variable selection and statistical inference unreliable. Most often such adversarial values are present in only a few entries of the data table, but we demonstrate that these values can completely distort variable selection and estimation if not handled appropriately. We further highlight that common pre-processing strategies to deal with these outliers poses the risk of removing valuable information, thereby lowering the efficiency of classical variable selection methods, and simultaneously instilling unwarranted confidence in the results. In this talk we present a robust and reliable alternative to classical penalized regression estimators. We show the superior stability of variable selection in the presence of a wide range of adversarial contamination settings and discuss in detail how these properties are achieved.*

Badr-Eddine Chérief-Abdellatif   (CNRS, Paris).

Label Shift Quantification via Distribution Feature Matching. *Quantification learning deals with the task of estimating the target label distribution under label shift. In this talk, we present a unifying framework, distribution feature matching (DFM), that recovers as particular instances various estimators introduced in previous literature. We derive a general performance bound for DFM procedures and extend this analysis to study robustness of DFM procedures in the misspecified setting under departure from the exact label shift hypothesis, in particular in the case of contamination of the target by an unknown distribution.*

Masaaki Imaizumi   (The University of Tokyo / RIKEN AIP).

Statistical Analysis on Overparameterized Models and In-Context Learning. *Deep learning and artificial intelligence technologies, one of the modern data science technologies, have made great progress, and their mathematical understanding is required to efficiently control and develop these technologies. In this talk, we present two types of research related to this topic. (I) The first is high-dimensional statistics for excess parameter models as typified by large-scale neural networks. Traditional high-dimensional statistics havs developed a methodology to reduce excess dimension. However, since recent large-degree-of-freedom models do not have explicit excess dimension, another theoretical approach has been developed in recent years. We present several results on the application of this approach to more practical statistical models. (II) The second is a statistical analysis of a scheme called in-context learning, which explains foundation models for artificial intelligence such as ChatGPT. We argue that in-context learning can achieve efficient learning under certain conditions, owing to the property of the transformer, which can handle the entire property of empirical distributions.*

Invited Session 8 – Data science, artificial intelligence, and high-dimensional spatiotemporal dynamics

Chair: Ivo D. Dinov   (University of Michigan).

Ivo D. Dinov   (University of Michigan).

AI and Spacekime Analytics in Health Research and Biomedical Inference. *This talk will present a direct connection between quantum mechanical principles, data science foundations, AI, and statistical inference on repeated longitudinal data. By extending the concepts of time, events, particles, and wavefunctions to complex-time (kime), complex-events, data, and inference-functions, spacekime analytics provides a new foundation for representation, modeling, analyzing, and interpreting dynamic high-dimensional data. We will show the effects of kime-magnitude (longitudinal time order) and kime-phase (related to repeated random sampling) on the induced predictive AI analytics, forecasting, regression, and classification.*
The mathematical foundation of spacekime analytics also provides mechanisms to introduce spacekime calculus, expand Heisenberg's uncertainty principle to reveal statistical implications of inferential uncertainty, and a develop a Bayesian formulation of spacekime inference. Lifting the dimension of time opens a number of challenging theoretical, experimental, and computational data science problems. It leads to a new representation of commonly observed processes from the classical 4D Minkowski spacetime to a 5D spacekime manifold. Using simulated data and clinical observations (e.g., structural and functional MRI), we will demonstrate alternative strategies to transform time-varying processes (time-series) to kime-surfaces and show examples of spacekime analytics.

Eric (Tatt Wei) Ho   (Universiti Teknologi PETRONAS).

A survey of opportunities through case studies of Generative AI, adaptation of Large Foundation Models and Physics Informed Neural Networks for high dimensional data analysis. *Deep neural networks have demonstrable ability to learn effective feature representations for state-of-art classifiers and regressors from data. From the perspective of data analytics, the task of extracting salient features from data shares similarities with the signal processing task of learning parsimonious and descriptive feature representations. When paired with sensitivity analysis methods from the explainable AI community, these form a powerful new toolbox to explore the complex associations embedded in high dimensional data. However, training deep neural networks on high dimensional data remains challenging with no guarantee of convergence to a good solution, presumably stymied by the curse of dimensionality. Deep neural network models tend to be overparameterized to facilitate convergence towards a good solution via gradient descent optimization. Often, it is also challenging practically to acquire sufficient high-quality labeled training data. This results in a sparse sampling of the high dimensional data space which introduces challenges to generalization. Training deep neural networks via supervised learning can be conceived as solving an under-determined system of nonlinear equations so model overparameterization and paucity of constraints from training data can be understood as limitations to converging the training of an accurate neural network model. In linear algebra, under-determined systems are solved by imposing additional constraints via regularization. Drawing inspiration from this, I discuss how recent advances in generative AI, adaptation of large foundation models and physics informed neural networks can be conceptualized as imposing additional constraints to ameliorate the challenge of sparse sampling in high dimensional data space. While generative AI attempts to learn additional constraints directly from the training data, transfer learning from large foundation models such as Low Rank Adaptation of Large Models attempt to borrow generalizable constraints from a different data domain whereas physics-informed neural networks impose constraints expressed as differential equations directly in the gradient descent training. Through case studies, I propose some practical approaches to apply these concepts and conclude with brief sharing on a method to reduce overparameterization of deep neural networks.*

Invited Session 9 – Recent advances in the theory of machine learning

Chair: Pierre Alquier   (ESSEC Business School, Singapore campus).

Makoto Yamada   (Okinawa Institute of Science and Technology).

Approximating 1-Wasserstein distance with Trees and its application to KNN and self-supervised learning. *The Wasserstein distance, which measures the discrepancy between distributions, shows efficacy in various types of natural language processing and computer vision applications. One of the challenges in estimating the Wasserstein distance is that it is computationally expensive and does not scale well for many distribution-comparison tasks. In this study, we propose a regression-based approach for approximating the 1-Wasserstein distance by the tree-Wasserstein distance (TWD), where the TWD is a 1-Wasserstein distance with tree-based embedding that can be computed in linear time with respect to the number of nodes on a tree. We first apply the proposed method for nearest neighbor search problems in NLP tasks and then introduce to use TWD for self-supervised learning.*

Jonathan Scarlett   (National University of Singapore).

Recent Developments in High-Dimensional Estimation with Generative Priors.   *The problem of estimating an unknown vector (or image) from linear or non-linear measurements has a long history in statistics, machine learning, and signal processing. Classical studies focus on the "$n \gg p$" regime (#measurements $\gg$ #parameters), and more recent studies handle the "$n \ll p$" regime by exploiting low-dimensional structure such as sparsity or low-rankness. Such variants are commonly known as compressive sensing. In this talk, I will overview recent methods that move beyond these explicit notions of structure, and instead assume that the underlying vector is well-modeled by a data-driven generative model (e.g., produced by deep learning methods). I will focus primarily on theoretical developments, including upper and lower bounds on the sample complexity in terms of various properties of the generative model, such as its number of latent (input) parameters, its Lipschitz constant, and its width and depth in the special case of neural network models.*

Jeremy Heng   (ESSEC Business School, Singapore campus).

Diffusion Schrödinger Bridges.   *Denoising diffusion models are a novel class of generative models that have recently become extremely popular in machine learning. The key idea is to consider a forward "noising" diffusion initialized at the target distribution which "transports" this latter to a normal distribution for long diffusion times. The time-reversal of this process, the "denoising" diffusion, thus "transports" the normal distribution to the target distribution and can be approximated so as to sample from the target. To accelerate simulation, we show how one can introduce and approximate a Schrödinger bridge between these two distributions, i.e. a diffusion which transports the normal to the target in finite time.*

Poster session

Sota Nishiyama   (University of Tokyo).

Analysis of feature learning dynamics of two-layer neural networks using Tensor Programs. *Feature learning in neural networks (NN) forms the foundation of modern deep learning successes. However, its analysis is challenging due to the nonlinearity with respect to its parameters, and understanding the mechanisms underlying feature learning is still a developing problem. In this study, we analyze the learning dynamics of NNs trained by stochastic gradient descent (SGD) to investigate the number of gradient update steps required to learn a certain function, and find NNs that learn features need fewer update steps compared to those that do not. We employ Tensor Programs, a theory for describing the infinite-width limit of neural networks, and approximate the SGD dynamics using differential equations.*

Luca Attolico   (University of Macerata and ESSEC Business School).

Nowcasting Singapore's GDP growth: a Machine Learning approach. *Economic policymaking requires assessing the state of the economy in real-time rather than relying solely on data from earlier periods. This has led to the emergence of nowcasting, the practice of predicting the contemporaneous state of the economy. Most nowcasting efforts within economics have focused on GDP growth and rely on one of two variants: an "adding up" model—where high-frequency data that comprise output are incrementally included into the model as they are released—and dynamic factor models (DFM), which reduces the dimensionality of large datasets by summarizing information available into a small number of latent factors that evolve over time. While DFMs are a popular approach, they suffer from two significant shortcomings: selecting factors through explained variance does not guarantee that those chosen ones exhibit optimal forecasting ability, and the forecasting model may also lose interpretability. Machine learning (ML) techniques are powerful tools that offer the ability to approximate nonlinear relationships with a high degree of robustness. The literature has shown that such models tend to outperform traditional forecasting models across many applications. This paper investigates the effectiveness of ML algorithms in improving the accuracy of real-time forecasts, using the example of Singapore's GDP growth. We analyze a set of up to eighty variables, encompassing economic fundamentals (such as prices, industrial production, investment, and population) collected between 1990Q1 and 2023Q4 from the Department of Statistics and other sources. We perform one-step forecasting for quarter-on-quarter GDP growth by implementing various ML models, including Ridge and Lasso, Elastic Nets, Partial Least Squares regression, Support Vector Machines, K-Nearest Neighbor, Random Forest, AdaBoost and XGBoost, and Neural Networks. To mitigate look-ahead bias, we employ expanding window nested cross-validation to estimate the ML models and apply a Bayesian optimization search algorithm to select the optimal hyperparameters via cross-validation in each iteration. Such Bayesian algorithms provide computationally efficient, adaptable, and robust hyperparameter selection. Our findings reveal that all ML-augmented models outperform not only a naïve autoregressive benchmark but also a standard dynamic factor model, among others. Our research contributes to the growing body of literature exploring the application of ML algorithms in macroeconomic forecasting for a small open economy. Beyond our academic contributions, our approach also enhances the accuracy of real-time GDP growth predictions, which in turn offers valuable insights for policymakers as they make real-time decisions on policy interventions.*

Niharika Bhootna   (Indian Institute of Technology Madras).

GARTFIMA Process and its Empirical Spectral Density Based Estimation. *We introduce a Gegenbauer autoregressive tempered fractionally integrated moving average (GARTFIMA) process. We work on the spectral density and autocovariance function for the introduced process. The parameter estimation is done using the empirical spectral density with the help of the nonlinear least square technique and the Whittle likelihood estimation technique. The performance of the proposed estimation techniques is assessed on simulated data. Further, the introduced process is shown to better model the real-world data in comparison to other time series models.*

Qing Wang   (Ca'Foscari University of Venice).

Markov Switching Tensor Regression. *A Markov Switching tensor regression model is proposed, which allows for model instability and accounts for multi-dimensional array data. Regarding model instability, the parameters are assumed to be time-varying and are driven by latent processes to address structural breaks in the data. Regarding high dimensionality, the Soft PARAFAC strategy is followed to achieve dimensionality reduction while preserving the structural information between the covariates. Modified multi-way shrinkage prior is further imposed to address over-parametrization issues. An efficient MCMC algorithm that adopts random scan Gibbs within a back-fitting strategy is developed to achieve better scalability of the posterior approximation. The performance of the MCMC algorithm is demonstrated using synthetic datasets in simulation studies. Real-world applications are used to test the proposed model against the benchmark Lasso regression, where the model delivers superior performance.*

Ye Yuan   (Chonnam National University, Department of Mathematics and Statistics).

Masculinity level predicts the risk of eating disorders among adolescents in China: a study based on a Bayesian network. *Gender differences exist in eating disorders. This study hypothesizes that anxiety, depression, self-esteem, and body image mediate the relationship between masculinity and eating disorders. 789 college students completed the Self-Rating Anxiety Scale (SAS), Body Image States Scale (BISS), Eating Disorder Scale (EDS-19), Self-Esteem Scale (SES), Revised Bem Sex Role Inventory, and Self-Rating Depression Scale (SDS). Descriptive statistical correlations, circular and multidimensional scaling (MDS) networks, and Bayesian network analysis were conducted. Also, network centrality and the stability of centrality indices were calculated. The correlations between anxiety, depression, self-esteem, body image, eating disorders, masculinity, and feminization are all statistically signiffcant. Anxiety and depression mediate the relationship between masculinity and EDS. Self-esteem plays an intermediary role between masculinity and feminization. Masculinity directly affects eating disorders by inhibiting feminization. The results indicate that anxiety and depression mediate the relationship between masculinity and EDS, while self-esteem moderates the relationship between masculinity and feminization. This provides a new approach to understanding the mechanisms of eating disorders and offers a fresh perspective for clinical intervention from the viewpoint of gender roles, particularly masculinity*

Tuobang Li   (University of California, Berkeley).

Matrix dissimilarity based on differences in moments and sparsity. *Generating a dissimilarity matrix is typically the first step in big data analysis. Although numerous methods exist, such as Euclidean distance, Minkowski distance, Manhattan distance, Bray–Curtis dissimilarity, Jaccard similarity and Dice dissimilarity, it remains unclear which factors drive dissimilarity between groups. In this paper, we introduce an approach based on differences in moments and sparsity. We show that this method can delineate the key factors underlying group differences. For example, in biology, mean dissimilarity indicates differences driven by up/down-regulated gene expressions, standard deviation dissimilarity reflects the heterogeneity of response to treatment, and sparsity dissimilarity corresponds to differences prompted by the activation/silence of genes. Through extensive reanalysis of genome, transcriptome, proteome, metabolome, immune profiling, microbiome, and social science datasets, we demonstrate insights not captured in previous studies. For instance, it shows that the sparsity dissimilarity is as effective as the mean dissimilarity in predicting the alleviation effects of a COVID-19 drug, suggesting that sparsity dissimilarity is highly meaningful.*

Lindani Dube   (North-West University).

Interpretability of random forest model under class imbalance. *In predictive modelling, addressing class imbalance is a critical concern, particularly in applications where certain classes are disproportionately represented. This study delves into the implications of class imbalance on the interpretability of random forest model. Class imbalance is a common challenge in machine learning, particularly in domains where certain classes are under-represented. This study investigated the impact of class imbalance on random forest model performance in churn and fraud detection scenarios. We trained and evaluated random forest models on churn datasets with class imbalances*

ranging from 20% to 50% and fraud datasets with imbalances from 1% to 15%. The results revealed consistent improvements in precision, recall, F1-score, and accuracy as class imbalance decreases, indicating that models become more precise and accurate in identifying rare events with balanced datasets. Additionally, we employed interpretability techniques such as Shapley values, partial dependence plots (PDPs), and breakdown plots to elucidate the effect of class imbalance on model interpretability. Shapley values showed varying feature importance across different class distributions, with a general decrease as datasets became more balanced. PDPs illustrated a consistent upward trend in estimated values as datasets approached balance, indicating consistent relationships between input variables and predicted outcomes. Breakdown plots highlighted significant changes in individual predictions as class imbalance varied, underscoring the importance of considering class distribution in interpreting model outputs. These findings contribute to our understanding of the complex interplay between class balance, model performance, and interpretability, offering insights for developing more robust and reliable predictive models in real-world applications.