

 $\frac{Ollscoil NAGAILLIMHE}{UNIVERSITY OF GALWAY}$ 

# School of Mathematical and Statistical Sciences 14th Annual Research Day

# 10 April 2024

# Programme

|             | Talks take place in the Orbsen building seminar room                                |
|-------------|---|
|             | Coffee, lunch, posters, and reception take place in the Orbsen building atrium      |
| 9:30-9:35   | Welcome by Aisling McCluskey, Head of School  |
| 9:35-9:50   | Rachel Quinlan (University of Galway)   |
|             | Building an inclusive research community  |
| 9:50-10:10  | John Ferguson (University of Galway)  |
|             | Approximate propagation of imprecision: a new method to derive confidence intervals |
| 10:10-10:30 | Nina Snigireva (University of Galway)   |
|             | Contractivity in the theory of Iterated Function Systems                            |
| 10:30-10:50 | Quan Zhang (University of Galway)   |
|             | Nonlinear elastic vector solitons in hard-magnetic soft mechanical metamaterials    |
| 10:50-11:20 | Viktor Senderov (Institut de Biologie de l'École Normale Supérieure,                |
|             | Paris)  |
|             | How Universal Probabilistic Programming Languages Democratize Modeling in Com-      |
|             | putational Biology  |
| 11:20-12:00 | Tea and coffee  |
| 12:00-12:20 | Sinéad Beacom (University of Galway)  |
|             | The Researcher Development Centre   |
| 12:20-13:20 | Lightning talks   |
|             | Harrison Anthony • Michael Flattery • Amanda Forde • Thomas Hayes • Sophie          |
|             | Matthews • Deirdre Ní Chonchubhair • Vikrant Pratap                                 |
| 13:20-14:30 | Lunch, poster session, reception, and prizes  |

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# 1 Introduction

Fáilte chuig Lá Taighde Scoil na nEolaíochtaí Matamaitice agus Staitistice 2024, ceiliúradh speisialta cursaí taighde inár scoil.

Welcome to our 2024 annual School Research Day, a celebration of our research progress and prowess over the past year. As for previous years, this year's event is no less distinctive in reflecting the steady and powerful pulse of our research outputs and achievements. This booklet demonstrates the continuing creativity, strength and resilience of our community in an ongoing challenging environment. Our researchfocused School Board meeting in February allowed us the opportunity to share our research strategy, vision and ambition with the Executive Dean, Director of Strategic Development and Vice-Dean for Research and Innovation, whilst reinforcing the need for action to improve our research infrastructure in pursuit of that ambition. Our continuing excellence in research performance must be underpinned and supported by sustainability and we will continue to seek urgent action in this regard.

Today's programme of talks and poster exhibition highlight the quality, the breadth, and the international significance of the research activities in each of our disciplinary clusters: the de Brún Centre for Mathematics, the Stokes Cluster for Applied Mathematics and the Sonraí Health Data Science Research Cluster. Our research clusters encapsulate and extend from core blue sky research to very targeted and focused applications. Our research covers a wide variety of subject areas including algebra and combinatorics, analysis, geometry and topology, mathematics education, quantum information theory, modelling of soft solids/tissues and drug delivery applications, and mathematical, statistical and genomics data science; our applications range from clinical research, sports and exercise science, traumatic brain injury, cancer, immunology to neuroscience.

The research-teaching nexus is at the heart of our activity. As we seek to discover and push frontiers in our research, we also inevitably teach, mentor, connect with and inspire others: our colleagues, our postdoctoral researchers, our graduate and our undergraduate students. As acclaimed author C.S. Lewis would have it, *if we are any good, we must always be working towards the moment when our pupils are fit to become our critics and rivals.* The research ecosystem in our School reflects very well such a pulse as we note below some highlights since the last Research Day:

- We welcomed to the School new lecturers Matthew Dorman, John Ferguson, Fintan Hegarty, Lars Jermiin, Joshua Maglione, Pouyan Nejadi and Nina Snigireva.
- We welcomed research staff Jair Andre, Omid Khazaei, Nastaran Sharifian, Yeuyen Zhu (working with Andrew); Devesh Haseja, Seyed Aghil Hooshmand, Noor Kherreh (working with Pilib); Suhib Abu Qbeitah (working with Stephan); Shaima Dsouza, Chethana Rao, Pratyush Kumar, Nirupama Sharma (working with Bharat).
- The ebb and flow of our PhD programmes continued unabated. We were proud to celebrate the successful PhD defences in our School of Declan Bennett, Siobhán Cleary, Sarah Ennis, Noor Kherreh, Lydia King, Shane O'Connell, Brian O'Sullivan, Koushik Paul and Victoria Sánchez Muñoz. Sincere congratulations to all our graduates we wish them every success in the next phase and we will surely miss their force for good in our community. We extend a warm céad míle fáilte to our new students who commenced their PhD studies with us in the same period.
- In this vein, let us also recognize the research development of our MSc students across all four programmes as they progress their Masters projects, and also of our undergraduate students who recently completed their final-year projects.
- We continued to publish extensively in world-class journals, to be awarded distinguished visiting positions and other key research leadership roles, to undertake high-profile editorial positions, to host

seminar series and workshops with international participation, to organise international conferences, and to participate and progress significantly in prestigious funding schemes.

- Notable amongst the foregoing is the recent news of significant funding in pure mathematics led by Angela and Tobias. Research awards over the past year accrue to more than €2M, including grants from Enterprise Ireland (Disruptive Technologies Innovation Fund, led by Andrew), Irish Research Council (Postdoctoral Fellowship scheme, Shaima and Bharat) and the China Scholarship Council (Doctoral scheme, Angela). Also notable is the upcoming secondment of Michel as national expert to the executive agency of the European Research Commission.
- We established 10 adjunct appointments in the School, reinforcing in particular our Athena SWAN commitment to action in terms of gender representation.
- We opened a new postdoctoral office on the ground floor, paving the way for the refurbishment of offices to accommodate recently arrived colleagues. We continue to work tirelessly to address ongoing pressing physical space limitations in Áras de Brún.

Today's event showcases the indefatigable spirit and impressive reach of our research community. The energy and ambition of our research success is aptly matched by the energetic and dedicated School Research and Graduate Studies team who have organised today – tá muid buíoch díobh (we are grateful to you). We note also their hard work in leading the special February research meeting and towards the upcoming IRRP in 2025/26. Particular thanks go to Tobias for the production of this booklet, to Mark for running the Lightning Talks session, and to Harold for organising the poster session and for preparing the monthly School Research News digest. We also acknowledge the unstinting support of our administrative and technical staff throughout.

Falling as it does just after the end of a busy second semester, let today mark the recharging and restoration of a newly productive and fulfilling research drive over the coming months.

Bainigí sult as, agus bígí bródúil as, Lá Taighde na Scoile 2024! Enjoy, and be proud of, the 2024 School Research Day!

Aisling McCluskey Head of School

# 2 Abstracts of invited talks

John Ferguson (University of Galway): Approximate propagation of imprecision: a new method to derive confidence intervals

Abstract: A common task is to calculate a confidence interval for a derived parameter that is a function, f, of K other parameters. For instance the population attributable fraction can be sometimes expressed as a function of relative risk and risk factor prevalence, both of which might be independently estimated. In these settings both the delta method and parametric bootstrap may be used to generate confidence intervals, but both have drawbacks. For instance, delta method intervals require the derived estimator to be approximately normally distributed, and may have poor coverage when this is not the case. In contrast, bootstrap confidence intervals have the disadvantage that they are non-deterministic unless a seed for the random number generator is set to a pre-specified value.

Propagation of imprecision (propimp), as defined by [1], is an alternative method to construct confidence intervals in this setting, that has advantages over the bootstrap, in that it is deterministically calculated, and over the delta method, since it does not require the derived estimator to be normally distributed. However [1] gave no general justification that propimp confidence intervals had correct asymptotic coverage, apart from in the trivial case of a difference in normally distributed means. Furthermore, if the derived parameter is a function of K other parameters, application of the original algorithm requires grid search over a K-1 dimensional hypersphere, rendering the algorithm computationally infeasible for large K.

Here, we show a close asymptotic connection between propimp and delta method intervals, thereby justifying propimp in the settings where Newcombe recommended its use: f monotonic in all its arguments, and the K estimators that are 'plugged' into f are independent. In fact, this connection justifies the algorithm in more generality; for instance when the K estimators are correlated. To alleviate computational issues, we also present a new algorithm: approximate propimp (apropimp) that produces confidence intervals that closely replicate propimp intervals, without the grid search. We conclude by comparing apropimp intervals and associated coverage to intervals produced by the delta method and the bootstrap in a range of practical settings.

[1] Newcombe, Robert G. "Propagating imprecision: combining confidence intervals from independent sources." Communications in Statistics-Theory and Methods 40, no. 17 (2011): 3154–3180

Nina Snigireva (University of Galway): Contractivity in the theory of Iterated Function Systems Abstract: "Fractal sets" are often described as attractors of Iterated Functions Systems (IFSs). The maps which comprise an IFSs determine its properties. In particular, if an IFS consists of maps which are contractions then it is well know that such an IFS has a unique attractor. Much less is known in the case of noncontractive IFSs. In this talk we will explore some noncontractive IFSs.

This is joint work with K. Lesniak, F. Strobin and A. Vince.

# **Quan Zhang (University of Galway):** Nonlinear elastic vector solitons in hard-magnetic soft mechanical metamaterials

**Abstract:** We present a design for metamaterials capable of magnetically tunable propagation of nonlinear vector solitary waves. The metamaterial is composed of a periodic array of units comprising hard-magnetic inclusions embedded within a soft matrix, interconnected by thin and highly deformable ligaments. Our theoretical and numerical modeling results demonstrate that the metamaterial undergoes significant transformations when activated by a magnetic field. These controllable microstructural changes profoundly influence the propagation of vector solitary waves within the metamaterial system. Specifically, we observe the magnetic field-enabled propagation of solitary waves, showcasing the ability of the proposed soft magnetoactive metamaterial to tune key characteristics of the supported nonlinear solitary waves, including pulse width and amplitude. Our findings underscore the potential of magneto-mechanical coupling in advancing unterhered mechanical metamaterial systems, with implications for applications in nondestructive testing, energy harvesting, and smart soft wave devices.

# 3 Abstracts of lightning talks

# Performance assessment of computational tools to detect microsatellite instability Harrison Anthony Supervisor: Prof. Cathal Seoighe

Microsatellite instability (MSI) is a phenomenon seen in several cancer types where repeating regions of the genome accumulate many insertion and deletion mutations [1]. The identification of MSI is important because cancers with high microsatellite instability can be good candidates for immune checkpoint inhibitor treatment [2]. To facilitate this, researchers have developed computational tools that categorize samples as having high microsatellite instability, or as being microsatellite stable using next-generation sequencing data [3]. While the majority of these tools were published with high performance metrics, nearly all were evaluated on a single dataset comprised of a single sequencing method. Moreover, they have not yet been independently benchmarked. To address these issues, we assessed the performance of five leading MSI tools across several unique datasets that encompass a wide variety of sequencing methods. While we were able to replicate the original findings of each tool on whole exome sequencing data, most tools performed worse on whole genome sequencing data. We also found that they lacked agreement with one another and with commercial MSI software on gene panel data, and lastly, that optimal threshold cut-offs vary by tool and sequencing type. Two MSI tools (MSI-sensor 2, MANTIS) performed well across nearly all datasets, but they each have their own drawbacks. Notably, MSI-sensor 2 provided unrealistic results on a 161-marker panel dataset, and MANTIS cannot be used with datasets lacking paired-normal samples. Taken together, these results caution that MSI tools can have much lower performance on datasets other than those on which they were originally evaluated.

Supported in part by a research grant from Science Foundation Ireland (SFI) under Grant number 18/CRT/6214.

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# Computing General Degree Casimir Operator Eigenvalues for Semisimple Lie Algebras

### Michael Flattery Supervisor: Michael Tuite

Lie Algebras are of use throughout physics and mathematics from quantum mechanics to the classification of finite simple groups. There is a strong basis of existing work which describes semisimple Lie Algebras and their irreducible representations [1] which this presentation will serve as a brief overview of. Casimir Operators are central invariants in the study of Lie Algebras and this presentation will display a new approach to calculating their eigenvalues which bypasses the need to work with computationally complex Weyl transformations, building on the work of Okubo [2] and Klimyk [3][4]. This is summarised in a generating function for the eigenvalues of Casimir Operators of every degree which is the sum of reciprocals of linear terms.

### References

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- [4] D. Snow. Computing Tensor Product Decompositions ACM Transactions on Mathematical Software, Vol. 19, Issue 1, 95, 1993.

# Breaking the Winner's Curse: Methods to eliminate selection bias in Two-Sample Mendelian Randomization

## Amanda Forde Supervisor: Dr. John Ferguson

Genome-wide association studies (GWAS) are commonly used to identify genomic variants that are associated with complex traits, and estimate the magnitude of this association for each variant. However, it has been widely observed that the association estimates of variants tend to be lower in a replication study than in the study that discovered those associations. This observation is due to the phenomenon known as Winner's Curse [1]. Winner's Curse bias can have many practical consequences, especially with respect to techniques which are reliant on variant-trait association estimates obtained from GWASs. One such example is Mendelian randomization (MR), a statistical framework which uses genetic variants as instrumental variables to estimate the magnitude of the casual effect of an exposure on an outcome [2]. In the case of two-sample MR, if the same GWAS is used to identify instrument variants and estimate their effects relative to the exposure, Winner's Curse will result in the overestimation of these variant-exposure associations. This bias will then propagate into the causal estimate, resulting in a deflation of this estimate [3].

In our work, we first look at potential further developments in statistical corrections for *Winner's Curse* using summary statistics from a discovery study [4]. Following this, we propose an approach, namely MR-SimSS (MR Simulated Sample Splitting), which combats *Winner's Curse* in MR. The method works via simulated splitting of the full dataset into two fractions. Conditional on the estimated variant-exposure and variant-outcome associations obtained in the full dataset, values for the estimated associations in the first fraction are simulated. Using these simulated values, the estimated associations in the second fraction are obtained. This permits the removal of *Winner's Curse* using repeated randomisation and selection of variants based on the estimated variant-exposure associations from the first fraction. The Inverse-Variance Weighted (IVW) method (or indeed, any suitable MR method of the analyst's choosing) is then fitted using estimated associations from the second fraction and these estimators are averaged over different repeated runs.

We illustrate and evaluate the method by both applying it to simulated datasets with varying degrees of sample overlap and confounding, and by performing same-trait analyses using the UK Biobank BMI data set [6]. Results demonstrate that the implementation of MR-SimSS, combined with the Robust Adjusted Profile Score (RAPS) method [5], has great potential in successfully providing a causal estimate void of both *Winner's Curse* and weak instrument bias, especially in the case of full sample overlap.

This work is supported by Science Foundation Ireland under Grant number [18/CRT/6214].

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# Multi-scale modelling of musclular atrophy

### Thomas Hayes Supervisors: Giuseppe Zurlo, Eoin McEvoy

The growth of contractile tissue depends on a complex interplay between active cell tension, mass transport, and assembly/disassembly processes. Complex shape changes arising during morphogenesis can be explored through advanced bioprinting platforms, facilitating the precise positioning of cells and extracellular matrix [1] to analyse subsequent remodelling. To understand the biomechanisms underlying dynamic morphological evolution of contractile tissues more deeply, we propose a novel computational model that considers the thermodynamics of cytoskeletal growth and force generation that guide tissue-level remodelling. .

### Methods

Muscle and non-muscle cells generate active forces through the remodelling and force generation of contractile actomyosin fibers. These processes are, in turn, highly sensitive to cytoskeletal stress ( $\sigma_f$ ), stretch ( $\lambda$ ), and strain rate [2]. Radial growth ( $\lambda_{rr}^g$ ) of these contractile fibers can be described by:

$$\lambda_{rr}^{g} = \left[\frac{(1 - \lambda_{rr}^{g} \lambda_{zz}^{g})}{\pi \lambda_{zz}^{g}}\right] \exp\left\{-\frac{\lambda_{zz}^{g}(\mu_{b} - \mu_{u})}{k_{B}T}\right\}, \quad (1)$$

where  $\mu_b(\sigma_f)$  and  $\mu_u(C)$  are the enthalpies of the assembled and unassembled fiber proteins, respec-

tively. The rate of axial fiber growth  $(\dot{\lambda}_{zz}^g)$  is further given as:

$$\dot{\lambda}_{zz}^{g} = \underbrace{\left[\lambda_{zz}^{g}\psi - \frac{d\psi}{d\lambda_{zz}^{g}}\lambda\right]}_{\text{Eshelby stress}} \left(\frac{\left(1 - \lambda_{rr}^{g}\lambda_{zz}^{g}\right)}{\lambda_{rr}^{g}\lambda_{zz}^{g}}\right)^{2}\beta, \quad (2)$$

where the internal energy  $\psi$  depends both on active and passive fiber constituents and  $\beta$  is a constant. Active tension is then computed as  $\sigma_{act} = \sigma_f \lambda_{rr}^g f_0 \lambda$ , where  $f_0$  is the volume fraction of contractile cells in the tissue.

The active framework is combined in parallel with a passive anisotropic hyperelastic model [3, 4]. The combined active and passive framework was implemented using user-defined material subroutines within the Finite Element (FE) software Abaqus. The developed computational model was applied to predict the biomechanical behaviour of contractile cells and tissue. The framework is validated by bioprinting contractile tissues using a fibroblastcollagen bioink, with construct evolution analysed over 14 days.

Supported by College of science and Engineering

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Nature Communications, 2021.

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Journal of Biomechanical Engineering (JBME), 2018.

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Journal of the Mechanical Behavior of Biomedical Materials, 2017.

# Evidence that gene copy number plays a role in the evolution of life history traits across mammals

### Sophie Matthews Supervisor: Marc Tollis, Cathal Seoighe

Cancer is a disease of multicellularity, observed across the tree of life. In principle, animals with larger body sizes and longer lifespans should be at increased risk of developing cancer. However, cancer risk is not found to increase with body size or lifespan across mammals. Previous studies have proposed the duplication of cancer-related genes as an explanation of this phenomenon, whereby an increased number of cancer genes enhances the robustness of cancer suppression pathways. However, these studies have not extended beyond genes that are already deemed to be cancer related. In this study, we conducted a phylogenetic generalized least squares (PGLS) analysis for association between copy number of all protein-coding genes and longevity, body size and cancer prevalence, in 94 mammalian species. Applying gene set analysis methods to these results, several processes showed evidence of enrichment for genes that show an association between their copy number and these traits. Notably, we found associations between copy number and cancer for gene sets relating to transforming growth factor-beta (TGF- $\beta$ ), a cytokine shown to play a role in cancer progression. These results provide a more comprehensive picture of processes and pathways that are likely to be important in the evolution of key life history traits, helping to shed light on long-standing questions relating to the mechanisms of adaptation to changes in life history traits that have decoupled these traits from cancer risk.

# Flare Star: EQ Pegasi Deirdre Ní Chonchubhair Supervisor: Prof. Aaron Golden

Flaring is common in magnetically active stars and can be observed across the electromagnetic spectrum, with the Sun being no exception. The most interesting solar flares are those extreme events that also produce coronal mass ejections (CME) that can result in potentially debilitating space

weather events here on Earth. Hundreds of 'habitable zone' exoplanets have been to date, discovered around nearby stars, many of which are more active then our Sun - could these planets survive more powerful CMEs? EQ Peg is a nearby red dwarf flare star binary system with a period of  $\sim 180$  years. We present results of a 6 hour observation of the EQ Peg system with the I:IO photometer on the Liverpool Telescope. Both components, EQ Peg A and EQ Peg B, were found to produce flares. EQ Peg A was found to be particularly active with a complex pattern of flare events occurring towards the end of the optical observations. We speculate on the likely association of this flare event with a CME, particularly in light of the recently discovered 2.3 Jupiter mass size planet orbiting EQ Peg Α.

# Physics Informed Neural Networks for hyperelasticty in soft solids

# Vikrant Pratap Supervisor: Dr Bharat B Tripathi

Millions of people suffer from traumatic brain injury (TBI) every year globally [1]. Event like mechanical falls, contact sports like American football, Rugby, etc., could lead to TBI. A real-time estimate of brain deformation in the event of an head impact can provide a quantitative insight towards development of TBI injury metrics. Inspired by Raissi et al.'s Physics Informed Neural Networks (PINNs) concept in 2019, our goal was to create a real-time, fully connected dense multi-layer perceptron to model homogeneous deformation in soft solids, such as the brain [2].

This work presents a mesh-free causal-marching physics-informed neural network (CMPINN) model for fourth-order hyperelastic material model. Our CMPINN was trained without labeled data, employing an innovative incremental-training algorithm that captures the causality of the physical phenomenon, specifically homogeneous deformation. Our approach involves formulating nondimensionalized governing equations to efficiently train the CMPINN, minimizing residuals [3]. The developed CMPINN model accurately captures three-dimensional hyperelasticity, focusing on high order hyperelastic models for different homogeneous deformations. Once trained, the model swiftly responds to any spatial coordinate within the physical domain for the specified homogeneous deformation.

The data-free CMPINN solution for the fourthorder Landau hyperelastic model demonstrated low RMSE values of 0.04%, 0.08%, 0.16%, 0.18%, 0.07%, and 0.10% for uniaxial tension (UT), uniaxial compression (UC), biaxial tension (BT), biaxial compression (BC), pure shear (PS), and simple shear (SS), respectively. These results affirm the effectiveness of the proposed approach across different deformation cases for Landau hyperelastic model. The success encourages the natural extension of CMPINN to capture viscoelasticity in soft solids.

Supported by College of Science and Engineering, University of Galway.

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# 4 Abstracts of posters

# Modelling Composition Response Data with Application to Clot Composition Observed for Acute Ischemic Stroke (AIS) Patients Malak Almutairi

# Supervisors: Dr. Emma Holian & Prof. Karen Doyle

Modelling composition response data presents challenges due to the nature of multivariate proportions for multiple elements making up the whole composition of an individual's sample. This poster investigates the modelling of composition response data, focusing on thrombotic material extracted from Acute Ischemic Stroke (AIS) patients using mechanical thrombectomy, which measures five components making up the clot composition. The aim is to model composition response considering the effects of factors that may influence changes in clot composition.

The challenges of modelling composition response data include bounded responses, continuous scale bounded between 0 and 1, correlation between multivariate responses, and multivariate responses within the sample constrained to sum to 1, as proportions of the composition of the whole sample. Using a traditional statistical analysis which assumes a normal error structure, for continuous univariate response data bounded between 0 and 1, can lead to biased and incorrect estimates. Therefore, an appropriate model like beta regression should be used for reliable parameter estimates rather than normal linear regression. Similarly, expanding to the multivariate response setting, Dirichlet regression is an appropriate modelling approach. We present results in application to the AIS patient cohort to cluster and model clot composition with candidate predictors, such as type of extraction device, hospital of procedure, etiology categorisation, and use of drug treatment tPA.

Multivariate longitudinal functional data analysis with applications in biomechanics John Andrew Supervisor: Dr. Andrew J Simpkin Fatigue, defined as a decline in muscular force due to exercise, affects athletes' performance and monitoring it is vital in sports. Assessing fatigue helps to optimise athletes' performance and their readiness to train. Objective assessment of fatigue is usually done in specialised laboratories that are expensive (facilities, personnel, etc.) and environmentally constrained. Low-cost lightweight sensors offer a compelling alternative, but the highthroughput data they collect are complex and functional in nature. This research aims to identify and characterise the difference between fatigued and non-fatigued running and clustering athletes using data from wearable sensors.

We explored the data from 19 athletes running 400M under normal condition (healthy) and again under fatigued condition with a sensor mounted on their lumbar spine. The running involved three segments, running under healthy condition followed by fatiguing protocol, and later finished by running when fatigued. In all three segments, the sensor captured six signals 256 times per second: the accelerometer in three directions (X, Y, Z) and the gyroscope in three directions (X, Y, Z). The long record of any of the six signals can be broken into individual strides forming a series of functional strides arising longitudinally, combining all six signals together bring a multivariate data structure. In this study, we make use of a multivariate longitudinal functional data analysis framework to identify and quantify the difference between fatigued and unfatigued running. In particular, we use multivariate functional principal components analysis to derive univariate components of variation and scores and then combine these scores across the signals. This modelling approach enables us to use all the collected data and captures the changes arising over the run when fatigued and when not.

We analysed acceleration in X, Y, and Z directions, and with our modelling framework, we demonstrate, (1) how all collected data can be fully utilised adding the statistical/predictive advantage over simple approaches, (2) an appropriate way of summarising data from multiple signals into a better representation that captures details from all signals considered, (3) using these generated representations to identify and characterise fatigue throughout running among athletes, and (4) segment athletes into different groups. These findings serve as a foundation for understanding fatigue and how it differs from athlete to athlete. This will help in developing an effective personalised fatigue monitoring and assessment tool for personalised training.

Supported by Science Foundation Ireland, grants SFI/19/FFP/7002 and SFI/12/RC/2289

# INTRAGRAFT GENE EXPRESSION PROFILES OF TRANSPLANT GLOMERULOPATHY WITHOUT DONOR-SPECIFIC ANTIBODIES, C4d OR MICROVASCULAR INFLAMMATION Marial Barbachan e Silva Supervisors: Pilib Ó Broin

Background: Transplant glomerulopathy (TGP) with donor-specific anti-HLA antibodies (DSA) with C4d or microvascular inflammation (MVI) is classified as chronic active antibody-mediated rejection (CAMR). We aimed to analyze intragraft gene expression profiles of TGP without any DSA or C4d or MVI.

Methods: One transplant kidney biopsy core was collected into a vial containing 1 mL of RNALater and analyzed by Affymetrix Human Gene 1.0 ST Array hybridization (28 869 gene probe sets). A support vector machine (SVM) with recursive feature elimination (RFE) was used to identify gene signatures capable of classifying TGP samples from normal transplant kidney biopsies without any acute or chronic Banff Allograft injury scores. Selected genes werethen used as input to the Enrichr pathway enrichment analysis tool. DSAs were studied by Luminex single antigen beads and mean fluorescence intensity value more than 1000 were accepted as positive.

Results: Twenty-two TGP samples with DSA and C4d or MVI,10 TGP samples without any DSA or C4d or MVI, and 22 normal transplant kidney biopsy samples were included in analysis. Biopsies were done at a median 6.4 years (IQR, 3.3-9.8) after transplantation. Median serum creatinine level was 2.2 mg/dl (IQR, 1.7-3.1) and spot urine protein/creatinine 1.7 g/g (IQR, 0.6-3.0). 59Conclusion: TGP samples without DSA or C4d, or MVI

showed significantly different intragraft gene expression profiles not related to immune activity or CAMR. These results indicated that TGP could develop through different mechanisms and not all related to CAMR.

This work was carried out in collaboration with Prof. Enver Akalin's research group at Einstein-Montefiore Kidney Transplant program and has been accepted for presentation in a Poster Abstract Session at the American Transplant Congress 2024 being held June 1 – June 5, 2024 at the Philadelphia Convention Center in Philadelphia, PA

# Instability pattern transformations in soft magnetoactive materials: the Bloch-Floquet analysis

#### Andrei Cherkasov

#### Supervisor: Stephan Rudykh

This study is dedicated to exploring the stability of soft magnetoactive materials, with a specific focus on investigating the microscopic instability transformations within a material system consisting of periodically distributed magnetic inclusions embedded in a soft matrix. Utilizing numerical simulations through COMSOL Multiphysics, the research analyzes the transition between mechanically dominant and magnetically dominant instability patterns. Two types of numerical analyses are carried out: firstly, the full-scale model is examined during nonlinear buckling and post-buckling process, yielding insights into the deformed configuration and critical loading values. Secondly, employing the Bloch theorem, a linearized eigenfrequency analysis is conducted for the minimal periodic unit cell of the system, facilitating precise computation of critical wavenumbers and strains. These two approaches align well, providing a comprehensive understanding of the transformation in instability patterns.

Based on the research article of Arora et al. [1].

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# Base Extension to Dual Numbers of Algebraic Zeta Functions

### David Cormican Supervisor: Dr. Tobias Rossmann

In this poster, we outline our work towards characterising the effect on algebraic zeta functions of extending rings, modules, and algebras to their corresponding dual structure by adjoining an element  $\varepsilon$  with  $\varepsilon^2 = 0$ . We present the first new result of this PhD project, whereby we obtain an explicit formula for the ideal zeta function of the dual extension of the Heisenberg Lie algebra of strictly upper triangular  $3 \times 3$  matrices over the *p*-adic integers. This finding is significant for both the computational and theoretical aspects of our research.

Computationally, the derivation of the formula uses techniques for the simplification of certain p-adic integrals [1, 2]. We are seeking to automate these using the Zeta package [3] in SageMath [4]. This will allow similar techniques to be applied to other algebraic structures where the challenge of computing an explicit formula for associated subobject zeta functions has thus far proved intractable.

In a more theoretical direction, the abscissa of convergence is unchanged for our formula compared to that of the ideal zeta function for the Heisenberg Lie algebra over the *p*-adic integers. This provides a new point of evidence in favour of the Persistence Conjecture for Subobject Zeta Functions, as formulated by Tobias Rossmann (project supervisor). Informally, this conjecture postulates that the abscissa of convergence of a subobject function over the ring of integers of a number field never changes when passing to a power series ring over the base ring.

Supported by a University of Galway Hardiman PhD Research Scholarship.

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# Differences between bipolar patients and healthy participants across the structure-function coupling gradient

# Shir Dahan Supervisor: Dr Pilib Ó Broin, Prof Dara Cannon

Bipolar disorder (BD) is a psychiatric disorder characterized by recurring episodes of depression and mania [1]. Structural MRI and diffusion MRI studies suggest structural differences in BD patients compared to healthy controls [2], [3]. In addition, findings from fMRI studies show aberrant functional connectivity in known resting-state networks in BD patients [4]. More recent studies look at the coupling of structural connectivity (i.e., physical connection between brain regions) and functional connectivity (i.e., statistical dependency in activation between brain regions). This coupling reflects the relationship between a structural connection and a functional connection. Structure-function coupling has been found to differ in BD patients, although results from different studies point to different coupling strengths and involved brain regions [5]. In healthy participants, the coupling was found to vary between brain region across a gradient, whereby unimodal regions (e.g., primary motor cortex) show strong structurefunction coupling, and transmodal cortex regions (e.g., resting state networks), show weaker coupling [6]. This study aims to look at regional differences in coupling between BD patients and controls.

The study includes 162 healthy controls and 163 BD patients from the UK Biobank. For each participant, a functional region-based connectivity matrix was calculated from the regional time series of 554 brain parcels, obtained from the Schaefer 7 network atlas, and the Melbourne Subcortex Atlas. The same parcellation was used to obtain the structural connectivity matrix for each participant. For each region, a multilinear regression was performed with structural connectivity properties (path length, communicability, Euclidean distance, and original edge) of all the edges for a given region as the predictors and the functional edges connecting the region to all other regions were predicted. The goodness of fit for each region was calculated as the R2 between the observed and the predicted functional connectivity. Then an independent Ttest for each region was conducted between the BD group and controls.

After Bonferroni correction for multiple testing, out of 554 regions, one region showed a statistically significant difference in the regional structurefunction coupling between the BD group and the controls. The significant region is in the prefrontal cortex and is involved in the executive control network, which has been linked to BD in previous studies.

The findings of this study are in line with previous findings in the literature that relate functional and structural connectivity of the executive control network to bipolar disorder [7]. However, the study has low power due to the low sample size in comparison to the number of parcellations.

Supported by The SFI Centre for Research Training in Genomics Data Science

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# Mapping Genetic Determinants of DNA Methylation Across Early Development Anna Großbach

# AA Lussier, EC Dunn, AJ Simpkin

Epigenetic mechanisms, such as DNA methylation (DNAm), play a key role in genomic regulation, thereby shaping various complex phenotypic outcomes. DNAm patterns are influenced by both genetic predisposition as well as environmental exposures. Understanding how genetics and epigenetics interact is crucial for unravelling geneenvironment interactions, particularly during early childhood - a period marked by rapid developmental changes and heightened susceptibility to environmental influences. Methylation quantitative trait loci (mQTLs) represent genetic loci that influence DNAm sites, either locally (cis-mQTL) or genomically more distant (trans-mQTL). Although large cohort studies have shown that mQTLs act dynamically across different life stages, our understanding of mQTL influences in early development remains limited.

In this study, we investigate the temporal dynamics of mQTLs during early childhood within a South African cohort, the Drakenstein Child Health Study (DCHS; n=1,143). DCHS provides genotypes for over 6 million genetic loci as well as DNAm data across 850k sites from whole blood samples for each participant. Using linear regression, we identify genetic determinants of DNAm at ages 1, 3, and 5. Moreover, we explore the genetic impact on longitudinal DNAm trajectories using individual-level slopes and intercepts, known as best linear unbiased predictors (BLUPs), derived from linear mixed effect models.

Our findings will illuminate how genetic variation influences the epigenome throughout early childhood, characterizing effects that persist across developmental stages, emerge in later childhood, or manifest exclusively during sensitive periods.

# Predicting Muscle Age and Identifying Aging-Related Genes from Gene Expression Data Karen Guerrero-Vazquez Supervisor: Pilib O Broin, Katarzyna Goljanek-Whysall

Understanding the molecular mechanisms underlying aging is essential for developing targeted interventions to mitigate age-related diseases. While recent advancements have employed omics analyses to identify signature genes of various age-related conditions, skeletal muscle aging remains relatively underexplored.

We present a deep learning approach to predict the age of individuals based on gene expression data from human vastus lateralis, while identifying key genes associated with muscle aging. We identified genes implicated in well-known aging mechanisms such as inflammation, cell proliferation, and autophagy, intersecting with genes previously published as differentially expressed in sarcopenia.

Our data collection integrates expression data from 19 microarray projects and 12 RNAseq experiments, totaling more than 900 samples from different countries. The datasets were rigorously curated through pseudoalignment, sequence ID analysis, batch correction, and two-point normalization. Datasets were binned across three age groups: young (18-35 years old), middle-aged (35-65), and old (older than 65).

Our results show that a set of 300 genes is sufficient to predict an individual's muscle age with a mean absolute error of 8.6. Our study represents the first comprehensive effort to predict age based on muscle tissue gene expression profiles at this scale that can be used to predict the biological age of the muscle.

Our methodology extends existing approaches by effectively generalizing across diverse data sources, ensuring independence from project-specific biases and ethnicities, enhancing applicability in realworld scenarios.

The genes identified in our study hold potential implications for understanding the molecular basis of aging-related processes in muscle. Furthermore, these findings provide a foundation for future research to develop targeted interventions for sarcopenia. In ongoing work, we plan to integrate these genes into a microRNA regulatory network model to identify potential therapeutic targets for sarcopenia, underscoring the translational relevance of our findings.

Supported by Science Foundation Ireland under Grant number [18/CRT/6214].

# Every odd diagram class is poset isomorphic to an upper interval of some Young subgroup.

### Michael Joyce Maher Supervisor: Dr. Angela Carnevale

Odd analogues of Rothe diagrams for permutations in type A Coxeter groups, called odd diagrams, were introduced and studied in [1]. Permutations in a group can be partitioned by their odd diagrams, resulting in what we call odd diagram classes. Odd diagram classes were studied in [2] and a particularly surprising result from that paper is that odd diagram classes are Bruhat intervals. It has also been shown in [3] that these odd diagram classes are rank symmetric. In that paper the authors conjectured that the Kazhdan-Lusztig polynomial associated to any odd diagram class is equal to 1.

Inspired by this conjecture, I carried out a further analysis of the structure of odd diagram classes. In this poster we will describe a mapping  $\mathcal{M}$  on an odd diagram class then introduce a new object called an *Index Set*. Using some elementary properties of these index sets and the mapping  $\mathcal{M}$  we will then show that every odd diagram class is poset isomorphic to an upper interval in some Young subgroup. Supported by the College of Science and Engineering, University of Galway

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# Commognitive Investigation on the Development of Undergraduates' Comprehension of Proof by Mathematical Induction

### Latifah Mustofa Lestyanto Supervisor: Dr. Kirsten Pfeiffer

Commognition is a relatively new approach in mathematics education and has been used by many researchers as a framework in recent years. It is formed by two words: *Cognition* and *Communication*. In this framework, thinking is seen as a form of communication, and learning mathematics means participating in this particular form of communication[1]. In the poster, the idea of commognition will be explained in more detail.

Mathematical proof is seen as a natural discourse in mathematics. Teaching and learning mathematical proof require communicative activity and are an initiation into the mathematical community's discursive practice. Hence, the commognitive framework is a considerably suitable approach for exploring learning of mathematical proof. Despite many studies related to teaching and learning of mathematical proof, the area of proof and proving using mathematical induction remains relatively unexplored, especially in research using the commognitive framework. In this study, we will use this framework to investigate how undergraduates may develop comprehension of proof by mathematical induction. We will also develop teaching and learning activities that may help students in developing their comprehension of proof by mathematical induction.

Supported by Indonesia Endowment Fund for Education (LPDP)

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Quantum Stabilizer Codes Obtained Via Codes Over GF(4)Aisling Mac Aree

# Supervisor: Dr. Mark Howard

The main objective of this poster is to explore a method in which certain types of classical codes over GF(4) can be used to represent quantum *stabilizer codes*.

Stabilizer codes can be achieved using a mathematical formalism that exploits structures in group theory. Such codes are generated by commutative elements of the stabilizer group S which do not affect the codespace. It also turns out that these generators can be built from the parity check matrix of classical codes.

These stabilizer generators consist of *n*-fold tensor products of elements from the single qubit Pauli group. Critically, the multiplication of these Pauli elements (with the phases "thrown out") has a *one*to-one correspondence with addition of elements over GF(4). In this poster, we exploit both the previously established correspondence between Pauli elements and elements in GF(4) as well as the relationship between the stabilizer generators and the classical parity check matrix to construct a quantum code from a classical code.

Supported by Royal Society/Science Foundation Ireland

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# Strand-specific oxidative damage artefacts in TCGA whole-exome sequencing samples

# Tyler Medina Supervisor: Cathal Seoighe

Oxidative damage to DNA can produce 8oxoguanine (8-oxo-G), leading to  $G \rightarrow T$  mutations upon DNA replication. Such oxidative mutations can occur in DNA samples during library preparation for sequencing, leading to artefacts in alignment results and possibly causing false variant calls. These oxidative artefacts can be distinguished from biological mutations by their orientation specificity in paired-end sequencing: replication of a DNA fragment and its palindromic Illumina sequencing adapter during PCR leads mechanistically to  $G \rightarrow T$  mutations on forward or reverse read pairs, but not on both[1]. This has led to the introduction of methods to filter 8-oxo-G artefacts such as the FoxoG filter calculated by Mutect2 for somatic variant calling [2]. While this phenomenon has been recognized and addressed, biases influencing which strand is mutated have not.

Following on our finding in the UK Biobank that whole-exome sequencing (WES) capture kits skew 8-oxo-G mutations towards the captured strand, we investigated this bias in cancer data from The Cancer Genome Atlas (TCGA). We analyzed 706 WES samples from 9 TCGA cohorts that were each sequenced using the same capture kit. We first calculated the ratio of reference strand versus nonreference strand alignment mismatches, per single base substitution (SBS) type, per sample. We then calculated similar ratios for each sample's variant calls per SBS type to identify any evidence of similar biases influencing somatic genotyping.

Out of the 6 SBS types and their reverse strand complements,  $G \rightarrow T$  alignment mismatches exhibited the greatest strand-specific bias by far, occurring more than twice as often on the reference strand overall. Similarly,  $G \rightarrow T$  genotype calls occurred twice as often as their reverse strand complement calls on average, though this imbalance is only reflected in the calls that fail filtering. Nevertheless, even when restricting only to variants that pass all filters, including FoxoG, we found a significant correlation (Pearson coeff. = 0.21) between the  $G \rightarrow T$  mismatch and variant call ratios, suggesting the presence of residual artefacts in tumour genotypes. This work highlights the need to account for strand-specific biases introduced by capture kits, particularly for applications reliant on low-frequency mutations, such as tumour sequencing.

This research was funded by Science Foundation Ireland through the SFI Centre for Research Training in Genomics Data Science under Grant number 18/CRT/6214. This research was supported in part by the EU's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie grant H2020-MSCA-COFUND2019-945385.

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# Mean Residual Function as A Translational Tool in Survival Analysis

# Parastoo Niloofar Supervisors: Shirin Moghaddam, Amirhossein Jalali, Alberto Alvarez-Iglesias, John Newell

The Mean Residual Life (MRL) function gives an attractive summary of time to event data as it can provide a clear and simple translation of the expected time remaining.

Estimating the MRL is difficult due to the presence of administrative censoring. A hybrid estimator for the MRL has been suggested [1] combining a non-parametric Kaplan-Meier estimator with a parametric component. Methods to calculate the variance estimate for such a hybrid estimator at the start of follow-up time t=0 have been proposed [2]. As no closed form for the variance of this hybrid estimator is available, the bootstrap approach can be used to assess the variability in the MRL function at any arbitrary time point. Moghaddam et al [3] proposed a Bayesian approach to impute the censored observations which allows a simple parametric approach to be used to estimate the MRL as censoring is no longer an issue.

The hybrid and Bayesian approaches are discussed and compared using data from clinical trials and observational studies. Covariate-adjusted MRL plots including plots of the between group differences and their ratios along with their confidence envelopes will be presented. In addition, the application of these plots will be illustrated in Health Economy field to mention the importance of a good translational tool and how it can facilitate the health decision making process.

The concept of Translational Statistics [4] was proposed to facilitate the integration of biostatistics within clinical research to enhance communication of statistical research findings in an accurate and accessible manner to diverse audiences. The use of appropriate visualisation is central to all areas of statistical research. An advantage of the MRL function over plots of the estimated survival curves and hazard rates is that the MRL is presented in units of time rather than probabilities or rates making it a potentially useful translational tool.

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Comparative Assessment of Copy Number Alteration Calling Tools for the Identification of Malignant Cells in an Acute Myeloid Leukaemia Single-Cell RNA Sequencing Dataset

# Micheál Ó Dálaigh Supervisors: Eva Szegezdi, Simone Coughlan, Pilib Ó Broin

**Background:** Acute myeloid leukaemia (AML) is an aggressive malignancy, resulting in the accumulation of poorly differentiated white blood cells in the bone marrow (BM). In AML, normal and malignant blood production take place simultaneously and the malignant cells share features with normal haematopoietic cells which makes identifying the malignant cells a challenging task. Single cell transcriptomics (scRNA-seq) data have been used in recent years to infer the presence of copy number alterations (CNAs). We hypothesised that AML cells may differ from normal haematopoietic cells in the complement of expressed CNAs which could be used to demarcate the malignant cells from their normal counterparts.

Methods: We previously performed scRNA-seq on 28 longitudinal samples (diagnosis, n=10; remission, n=7; relapse, n=11) from BM aspirates of 10 AML patients [1]. In the current project, we evaluated the ability of three different CNA profiling tools (inferCNV [2], CopyKAT [3], Numbat [4]) to identify the leukemic cell populations based on altered CNA profiles. InferCNV and CopyKAT use expression levels of adjacent genes to infer genomic copy numbers, while Numbat integrates additional allelic ratio and haplotype data to identify CNAs present.

**Results:** CopyKAT and Numbat differed in their malignant predictions with only 41% of cells sharing a malignant prediction from both tools with the concordance of these predictions showing variability between individual samples. InferCNV does not provide malignant annotations. In an effort to extract these annotations, we first tested for the presence of multiple clusters (tumour vs normal) in the inferCNV-generated data with methods proposed for scRNA-seq data [5]. Only 1 sample had evidence of multiple clusters. Clustering these cells into 2 clusters with hierarchical clustering generated annotations which were more similar to Copy-KAT than to Numbat (Adjusted Rand Index of 0.56 and 0.13 respectively).

**Conclusions:** Numbat was deemed to be the most promising tool for identifying malignant cells in our AML dataset due to its ability to produce malignant cell labels as well as to identify loss of heterozygosity CNA events which would be invisible to CopyKAT and Numbat which rely solely on gene expression.

Supported by Science Foundation I reland under grant number  $18/\mathrm{CRT}/6214$ 

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Identification of potential neoantigens in cancer-associated fibroblasts isolated from breast cancer patients

# Kevin Ryan Supervisor: Dr Pilib Ó Broin, Dr Laura Barkley (Lambe Institute for Translational Research)

#### Background:

Cancer-associated fibroblasts (CAFs) are a heterogeneous cell type found in the tumour microenvironment (TME). CAFs support tumour growth and metastasis and contribute to therapeutic resistance. CAFs also impact immune infiltration and immune responses in the TME. Therefore, therapeutic targeting of CAFs is a viable strategy to treat cancer. In this study, we aim to identify somatic mutations in CAFs, which may potentially give rise to neoantigens. Ultimately, we aim to elucidate the therapeutic potential of targeting CAFs by exploiting CAF-specific neoantigens.

#### Methods:

CAFs and corresponding tumour-associated normal fibroblasts (TANs) were cultured from tissue of 12 breast cancer patients (11 Luminal A and one triple-negative). Bulk RNA-sequencing was carried out on all samples. Leveraging both bulk-sorted [1] and single-cell RNA-sequencing [2] reference datasets, CIBERSORTx [3] was used to characterise CAFs and TANs into fibroblast subpopulations. Whole-exome sequencing (WES) was carried out on CAFs and TANs from six patients. Landscape of Effective Neoantigens Software (LENS) was used to identify CAF-specific neoantigens [4].

#### **Results and Discussions:**

Our studies confirm the heterogeneity of our patient-derived CAFs and TANs, with the immunosuppressive-myofibroblastic subpopulation being the most prevalent in our samples. This is important as for the effective design of CAF-targeting therapies, it is necessary to target pro-tumourigenic CAF subpopulations. We also observed differences in the inferred proportion of several CAF subpopulations, including antigen-presenting CAFs and vascular CAFs, between CAFs and TANs. WES identified 13 private missense mutations, with five of the six patients exhibiting one or more such variants. Interestingly, genes with these mutations included previously reported CAF markers and genes implicated in tumour metabolism, specifically lipid metabolic pathways. CAFs contribute to lipid metabolism within the TME, thus playing a vital role in cancer progression and tumour immunogenicity.

### **Conclusions:**

In this study, we have identified candidate neoantigens in breast cancer CAFs. The next step is their validation using T-cell immunogenicity assays. These studies may help to unravel the potential of targeting CAF neoantigens to enhance the efficacy of anti-cancer therapy. This publication has emanted from research supported in part by a research grant from Science Foundation Ireland (SFI) under Grant number 18/CRT/6214

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# ZX-Calculus in Fault-Tolerant Quantum Computation

# Mark Ryder Supervisor: Dr. Mark Howard

The ZX-Calculus is a graphical language for reasoning about quantum computations and circuits. Since it can describe any linear map, it can be considered a diagrammatically complete generalization of the usual quantum circuit representation.[1] The ZX-Calculus is based on category theory, an approach to mathematics which studies objects in terms of their relations rather than in isolation. Thus, the ZX-Calculus provides a rigorous way to understand the structure underlying quantum problems.

Within a fault-tolerant quantum computing framework, the ZX-Calculus demonstrates promise as a tool for simplifying complex quantum circuits and aiding in error analysis. Its ability to streamline error correction protocols, optimize resource utilisation,[2] and facilitate the design of robust quantum algorithms, demonstrates how the utilisation of the ZX-Calculus can contribute to the development of fault-tolerant quantum computing. In this poster, we explore these applications of ZX-Calculus within a fault-tolerant framework, utilising the powerful rewrite tools to optimise resources, refine error correction codes, and visually show properties of these quantum circuits.

Supported by the Irish Research Council Postgraduate Scholarship.

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Rank distributions of matrix representations of graphs over  $\mathbb{F}_2$ 

# Badriah Safarji Supervisors: Rachel Quinlan and Cian O'Brien

Over a finite field  $\mathbb{F}$ , the number of  $n \times n$  matrices of rank r typically increases as r increases,  $0 \leq r \leq n$ . However, over the field of two elements  $\mathbb{F}_2$ , the most frequently occurring rank in  $M_n(\mathbb{F}_2)$  is not n but n-1. The numbers of symmetric  $\mathbb{F}_2$ -matrices of rank n and n-1 coincide if n is odd, and differ marginally if n is even. This opens the door to a more thorough investigation of the distribution of the matrix ranks over the field of two elements.

Let  $\Gamma$  be a simple undirected graph. A symmetric matrix  $M(\Gamma)$  with entries in a field  $\mathbb{F}$  represents  $\Gamma$  if the off-diagonal entries of  $M(\Gamma)$  correspond to edges of  $\Gamma$  in the sense that  $M_{ij}(\Gamma) \neq 0_{\mathbb{F}}$  if and only if  $x_i$  and  $x_j$  are adjacent in  $\Gamma$ . The diagonal entries of  $M(\Gamma)$  are not subject to any conditions, and therefore there are many matrices representing  $\Gamma$  over  $\mathbb{F}$ . This project aims to identify and characterise simple graphs of order n with more  $\mathbb{F}_2$ -matrix representations of rank n-1 than rank n, a property rare over other finite fields.

We restrict our attention to graphs of order  $n \geq 3$  with an induced sub-graph isomorphic to  $P_{n-1}$  or  $C_{n-1}$ . This poster presents results on the rank distributions of matrix representations of such graphs over  $\mathbb{F}_2$ .

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## Griffen Small Supervisor: Valentina Balbi

Brain tissue accommodates nonlinear deformations, and its mechanical response is markedly viscoelastic. To investigate its viscoelastic behaviour, we performed ramp-and-hold torsion tests on four fresh cylindrical ovine brain samples (25 mm diameter and 10mm height). The tests were conducted using a commercial rheometer at a strain level of 80% and a strain rate of  $3s^{-1}$ , generating two independent data sets for the torque and normal force. The complete set of viscoelastic material parameters was estimated by performing a least squares regression fit to the analytical solutions predicted by the quasilinear viscoelastic (QLV) model [1, 2]. The average values of the instantaneous shear modulus  $\mu_0 = 748 \pm 237 \,\mathrm{Pa}$  and second Mooney–Rivlin parameter  $c_2 = 1062 \pm 308 \,\mathrm{Pa}$  are indicative of an extremely soft solid. These results show that the QLV model—criticised in the past for not always yielding physically reasonable behaviour but recently reappraised and, until now, unexploited—has huge potential vis-à-vis data fitting and material parameter estimation. Such estimates, when combined with bespoke finite element models like the University College Dublin Brain Trauma Model [3], could potentially lead to a more accurate quantification of the role forces and deformations developed in the brain during rotational head impacts play in traumatic brain injury and contribute to the design of improved headgear for boxing and motorsports.

Supported by the College of Science and Engineering at University of Galway.

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# DeepONet: A Framework for Learning Differential Operators

### Sean Tobin Supervisor: Dr. Bharat Tripathi

Artificial Neural Networks have been instrumental to the field of predictive modelling, proving to be a popular alternative to conventional numerical methods, which require solving the equations at each discrete point in a given domain. This becomes far more computationally expensive and time-consuming when the geometry in question becomes more complex, so the neural network approach of not only predicting values based on given data, but approximating functions, has become a more appealing one. A loss function determines model performance, within which physical equations can be encoded, an advancement known as PINNs (physics-informed neural networks).

However, a neural network is only as good as the input data provided, and often directly depends on the grid from which the inputs are sampled. This is where we introduce a generalisation, known as neural operators; mappings between infinitedimensional function spaces, which are resolutioninvariant. In essence, we move from traditional numerical discretization to something closer to a continuous solution. In this poster, we outline a particular architecture, known as "DeepONet", first proposed by Lu et. al [1]. We look at the setup, the performance, and some current applications. Supported by CURAM

### References

[1] L. Lu DeepONet: Learning nonlinear operators for identifying differential equations based on the universal approximation theorem of operators. Nature Machine Intelligence, 2021.

# TargetRank – A novel Nextflow pipeline for the identification of target genes from scRNA-Seq data

Jacopo Umberto Verga Supervisors: Eva Szegezdi, Pilib O'Broin, Michael O'Dwyer

### Introduction:

Multiple myeloma (MM) is a blood cancer resulting from excess plasma cells in bone marrow, linked to immune suppression [1]. Natural killer (NK) cells are vital for antitumor defence [2]. To understand whether or not, and how the NK cells may be impacted by MM, we analyzed NK cell transcriptomic changes at the single-cell level.

#### Methods:

We integrated six scRNA-Seq studies covering all disease stages (MGUS, SMM, PMM and RRMM). NK cells were classified as resident (rNK) or exhausted (eNK) using an algorithm we developed that scores the cell state based on a gene expression signature [3]. This classification score has been validated with GSEA and MSigDB gene sets. To characterize eNK cells and rank those genes involved in immune suppression, we developed a Nextflow pipeline. Starting from the annotated scRNA-Seq object it runs Differential Gene Expression (DGE), Gene Ontology (GO) enrichment, active ligandreceptor pairs (LIANA), and transcription factors (TF) analyses. The active ligands from the interaction analysis and the active regulons from the TF activity analysis are used as inputs to build an immune checkpoint receptor (ICR) signalling network (NicheNet).

### **Results:**

The dataset had 14,103 MM and 7,596 healthy NK cells. eNK cells increased in number in all disease stages compared to the healthy baseline (p.value<0.01). They up-regulated ICRs, and

malignancy-associated genes, and altered the immune microenvironment. A minority of DEGs, enriched Biological Processes (BPs), and TFs were shared by eNK cells in MM and healthy samples, suggesting disease-specific pathways driving NK cell exhaustion in MM. Cell-cell interactions suggest the tumour microenvironment actively supports immune exhaustion via ICRs. The expression of top-ranked genes from the network analyses showed a significant correlation with exhaustion scores. In vitro experiments are planned for gene validation.

### **Conclusions:**

Our study revealed myeloma-specific pathways driving NK exhaustion, even early in disease progression. By delineating the exhaustion signalling cascade, we have pinpointed potential therapeutic targets. These targets will be submitted to experimental evaluation, to design NK cells resistant to the debilitating influences of the tumor microenvironment. The pipeline is being actively developed and, after in vitro validation of the identified targets, may provide a novel tool for the identification of target genes for the development of cell-based therapies.

Supported by CRT Genomics Data Science - SFI.

#### References

- A. Díaz-Tejedor et al. Immune System Alterations in Multiple Myeloma: Molecular Mechanisms and Therapeutic Strategies to Reverse Immunosuppression. Cancers 2021, 13, 1353. https://doi.org/10.3390/cancers13061353.
- Wu, SY., Fu, T., Jiang, YZ. et al. Natural killer cells in cancer biology and therapy.. Mol Cancer 19, 120 (2020). https://doi.org/10.1186/s12943-020-01238-x.
- [3] JU. Verga Function to score the expression of positive and negative markers in single cell RNA seq data.. https://github.com/VergaJU/ScoreMarkers.

# Identification and analysis of transcriptomic changes of MSC cells from people with Type 2 Diabetes Mellitus

#### Jingyan Wang

### Cynthia Coleman,Katarzyna Whysall, Pilib Ó Broin

Type 2 Diabetes Mellitus(T2DM) is a chronic disease, characterized by elevated blood sugar levels. It has emerged as a significant global health concern, ranking among the leading causes of death and disability worldwide [1]. Notably, diabetes mellitus (DM) is now recognized for its association with osteoporosis, a condition marked by increased bone fragility, contributing to elevated morbidity, mortality, and healthcare expenditures [1]. Studies have elucidated that the diabetic milieu negatively impacts the healing process, leading to a reduction in callus size, diminished bone formation, and a decline in the mechanical strength of the mended fracture site. This, in turn, significantly heightens the vulnerability to fractures across various skeletal locations [2].

A prominent characteristic of osteoporosis is the compromised functionality of bone marrow mesenchymal stem cells (BM-MSCs), highlighting their pivotal role in bone health [3]. Traditionally, the differentiation ability of MSCs has been broadly categorized into three main lineages: osteogenesis (formation of bone tissue), adipogenesis (generation of fat cells), and chondrogenesis (development of cartilage) [4]. These distinct differentiation pathways enabling them to give rise to diverse cell lineages essential for tissue regeneration and maintenance and underscore the versatility and regenerative potential of MSCs, making them invaluable candidates for therapeutic applications in tissue engineering and regenerative medicine [5, 6, 7].

Recent advancements in high-throughput sequencing technologies, particularly single-cell RNA sequencing (scRNA seq), have revolutionized our understanding of MSC biology [8, 9]. By dissecting the transcriptomic landscape of individual MSCs, sc-RNA seq has unravelled previously hidden complexities within MSC populations, revealing diverse cellular clusters and directional differentiation trajectories at unprecedented resolution [8]. , However, sc-RNA seq remains relatively costly and noisy compared to bulk RNA-seq leading to the development of deconvolution methods to infer individual cell type proportions and gene expression profiles from bulk RNA seq data.

In response to these challenges, our study aims to leverage existing knowledge of gene regulatory mechanisms from the literature to develop a novel strategy for subpopulation identification within MSC populations. By integrating transcriptomic data from scRNA-seq datasets derived from public databases, we seek to identify robust marker genes that serve as reliable indicators of cellular identity and differentiation potential. Subsequently, we plan to conduct comprehensive comparative analyses between T2DM and non-T2DM cohorts to identify significant transcriptomic changes and potential associations especially in osteoprogenitors and other subpopulations. Ultimately, this study aims to provide valuable insights into the complex regulatory mechanisms governing MSC behaviour and pave the way for targeted therapeutic interventions for individuals with T2DM who are living with osteoporosis.

Supported by Chinese Scholarship Council

### References

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- [2] Murray and Coleman. Impact of diabetes mellitus on bone health. 20(19):4873.
- [3] Klemen Camernik, Anze Mihelic, Rene Mihalic, et al. Comprehensive analysis of skeletal muscle- and bonederived mesenchymal stem/stromal cells in patients with osteoarthritis and femoral neck fracture. 11(1):146. Place: England.
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- [5] June Seok Heo, Youjeong Choi, Han-Soo Kim, and Hyun Ok Kim. Comparison of molecular profiles of human mesenchymal stem cells derived from bone marrow, umbilical cord blood, placenta and adipose tissue. 37(1):115–125.
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- [8] Zun Wang, Xiaohua Li, Junxiao Yang, et al. Single-cell RNA sequencing deconvolutes the in vivo heterogeneity of human bone marrow-derived mesenchymal stem cells. 17(15):4192–4206.
- [9] Yuchen Gao, Ying Chi, Yunfei Chen, et al. Multiomics analysis of human mesenchymal stem cells shows cell aging that alters immunomodulatory activity through the downregulation of PD-l1. 14(1):4373.

## Undergraduate Research

### Undergraduate students

in the School of Mathematical and Statistical Sciences

This poster presents a small selection of the images created by undergraduate students in the School of Mathematical and Statistical Sciences, as part of their final year projects. They show the diversity of topics our students are researching, covering numerous areas of pure and applied mathematics, statistics, bioinformatics, and computing.

The contributors are: Thomas O'Connor (The Duffing Equation); Dara Kelly & Cronan Ward (Modelling Extremes in Finance and Investigating Asymptotic Dependence); Sean Janson & Dmytro Lyubka (Unveiling Emergent Patterns and Euclidean Approximations using Physarum Polycephalum); Lise Wall & Emma Meaney (Predicting the US president election using network approaches); Ailbhe Keane, Karen Gillooly & Paulina Krungleviciute (Analysis of Expected Goals in La Liga 2019/2020); Katelyn McMahon & Matthew Talbot (The Impact of County Demographics and Major Events on Votes for the Demo-Cian Hughes & Conal O'Mahony cratic Party); (Investigating the evolution of tactics in soccer through data analysis); Julia Kompanowska & Maeve Samali (Brain Mechanics); Ciarán Campbell (The Windkessel Model); Niall Cahalan & Daire Elberse (Statistical Modelling of Fantasy Premier League Data) Claire Nolan & Leah Wyse (Analysing Risk Factors in Automobile Insurance Policies); Eli Sheedy (Finite Difference Meth-James Nohilly & Caoimhe Doods for PDEs); herty McLaughlin (Group Theoretic Analysis of Music); Paul Cassidy (Probability distribution for discrete time alternating lazy quantum walk after 100 steps).

# 5 Abstracts of PhD theses

# Analysis of putative somatic mutations in 200,000 human exomes Declan Bennett Supervisor: Prof. Cathal Seoighe

Somatic mutations accumulate throughout life and contribute significantly to disease risk. While research into somatic mutation is well established in cancer, it is only in recent years that investigations into the implications of somatic mutations in healthy tissues have begun to be feasible, due to advances in sequencing technologies and protocols. The requirement of specialist techniques has, however, limited the study of somatic mutations in healthy tissues to small sample sizes, which do not allow for assessment of the impact of somatic mutations on human health on a population scale. We posited that it may be possible to study variation in the somatic mutation rate between individuals and across the genome through analysis of low-depth sequencing data, by developing strategies to distinguish the contribution of somatic mutations to the mismatches (relative to the reference genome) observed in these data from sequencing errors, DNA damage and other artefacts.

Using somatic mutation rates obtained from the literature, we estimated that 0.4 of the mismatches between the UK Biobank exome sequencing reads and the reference genome were due to somatic mu-We demonstrated that this proportion tations. was sufficient to induce a relationship between the abundance of mismatches and age, when individuals were grouped by integer age. We then searched for additional sample properties that are correlated with the mismatch burden and found positive correlations with cancer diagnosis and smoking status. However, by carefully examining the UK Biobank exome sequencing data, we uncovered previously unreported batch effects relating to sequencing run. The observed associations with cancer diagnosis and smoking status were lost when we corrected for this batch effect. However, the batch correction improved the correlation between age and mismatch load.

Individuals diagnosed with Lynch syndrome have increased somatic mutation loads due to deficiencies in mismatch repair genes and we investigated whether this effect could be detected in the exome sequencing data. In the UK Biobank, we identified 160 individuals with pathogenic variants associated with Lynch syndrome. Using the COSMIC signatures associated with mismatch repair, we compared the contribution of mismatch repair mutational signatures between the Lynch syndrome samples and the remaining samples. We detected a marginally statistically significant difference between the contribution of SBS18 between the two sample groups; however, this result did not survive multiple testing correction.

Somatic and germline mutations show transcription-strand asymmetry, arising from transcription-associated DNA damage and repair. We postulated that the strength of transcriptionstrand asymmetry could provide insights into the contribution of somatic mutations to the exome sequencing data, because technical sources of mismatches, such as DNA damage and sequencing error, should not be directly affected by transcription. We indeed observed substantial transcription-strand asymmetry; however, this was far stronger than we expected, given the inferred proportion of somatic mutations in the data. This result led us to identify a technical effect that resulted in transcription-strand asymmetry, arising from the use of single-stranded probes targeting the coding strand in the exome capture kit used by the UK Biobank. Surprisingly, this has not previously been published and it has important implications for NGS quality control and rare variant analyses.

The large sample size of the UK Biobank also raised the possibility of testing for genetic variation affecting the somatic mutation rate. Treating the normalized number of mismatches per sample as a quantitative phenotype, we performed a GWAS and discovered a genome-wide significant hit in linkage with an eQTL for ERCC8, an integral component of the transcription-coupled repair machinery. Although promising, this candidate GWAS locus turned out to be a false-positive association, resulting from an unusual genetic variant that our germline filter had not removed. In the course of this work, we also proposed a methodological innovation in GWAS that consists of including background genetic variation as a fixed effect in the linear mixed models used in GWAS. We demonstrated that this can improve the power of GWAS when combined with state-of-the-art polygenic scoring methodologies. Our method substantially improved the estimation of effect sizes and power. However, the improvement depended on heritability and polygenicity and consequently, the mismatch data, which showed low heritability, did not benefit from our method.

We then pivoted our focus from understanding the variation in mismatch load acting across samples to understanding variation across the genome. We again found evidence that variation in the somatic mutation rate across the genome can be detected in the exome sequencing data, observing correlations in the expected directions for known mutation rate modifiers, such as gene expression, replication timing and chromatin structure. Interestingly, we recovered a complex relationship between mismatch recurrence and gene expression, consistent with the literature. The recurrence of potentially functional mismatches also provides a means to infer positive selection acting on somatic mutations and we found that several genes associated with clonal haematopoiesis of indeterminate potential showed strong evidence of positive selection.

# Analysis of clonal mutations in cancer as a means of studying variation in somatic mutation processes

### Siobhán Cleary Supervisor: Prof. Cathal Seoighe

Somatic mutations are mutations that arise throughout a person's lifetime. They contribute to ageing, cancer and other age-related disorders. Recent technological advances led to many studies investigating somatic mutations in normal tissues. However, somatic mutations are hard to identify in normal tissues due to their low frequency and the difficulty distinguishing between real mutations and errors incorporated during the experimental processes. Studies of somatic mutations in normal tissues suggest that there is still much unknown about how somatic mutations contribute to cancer. Somatic mutations can be studied by analysing cancer samples. Generally, somatic mutations in cancer samples are studied to understand cancer progression and response to treatment. This thesis aimed to investigate somatic mutations present in

all cancer cells of a sample (clonal mutations) as a means to understand what is happening in normal tissue.

Chapter 2 describes a method to predict the total clonal mutation load of a cancer sample and the use of this approach to investigate the relationship between variation in clonal somatic mutation load and differences between tissues in the risk of developing cancer. Before predicting the total clonal load, we first needed to distinguish between clonal mutations and mutations present in only a subset of cells (subclonal). We adjusted variant frequency for tumour purity and local copy number variation to classify variants as clonal or subclonal. We used the linear relationship between clonal variants and age to predict the total clonal burden for each tissue type. Under the assumption that subclonal mutation accumulation does not correlate with age, we determined what proportion of true clonal variants were classified as clonal. By adjusting various thresholds for classifying variants as clonal variants, we could classify, at best, 45% of the true clonal variants. We then used the relationship between clonal mutation burden and age to estimate the true clonal load for our samples. To investigate whether the estimated clonal mutation burden could be used as a proxy for the number of somatic mutations in healthy cells, we compared our results to somatic mutation burdens that have been measured directly in normal tissues (matched for age and tissue type with the cancer samples). We also found that the predicted clonal load was correlated with lifetime cancer risk. Our findings suggest that we can use predicted clonal load from cancer samples to investigate somatic mutations in the normal tissue and has the advantage of being able to use the large volume of cancer genomics data that has already been generated to extend our understanding of the accumulation of somatic mutations in normal tissues. The major histocompatibility complex (MHC) can present neoantigens resulting from somatic mutations on the cell surface, potentially directing an immune response against it. In Chapter 3, we investigated whether gene expression explains the lack of signal of immunoediting observed among clonal passenger mutations. This hypothesis stemmed from two publications that reported that driver mutations arise in gaps in the capacity of the immune system to recognize them.

We investigated whether passenger mutations capable of eliciting an immune response occur preferentially on lowly expressed genes or if the mutant allele has a lower expression than the reference allele through a process termed allele-specific expression (ASE). The neoantigen must be expressed to be presented by the MHC on the cell surface, so a reduction in expression could be a means by which the immunogenic mutations are tolerated. After accounting for gene length and sequence context, we found no difference in the expression of genes harbouring immunogenic mutations compared to nonimmunogenic or synonymous mutations. Additionally, there was no evidence that the mutant allele exhibited ASE more often for immunogenic mutations than nonimmunogenic mutations. Using simulations, we also estimated an upper bound for the impact of immunoediting on the mutational landscape in cancer, showing that at most 5could be removed by this process. To our knowledge, this was the first attempt to quantify the proportion of missense mutations removed through immunoediting.

Finally, in Chapter 4, we extended our analysis on the relationship between gene expression and somatic mutation accumulation by investigating the relationship between germline ASE and cancer risk. Here, we investigated the hypothesis that a single score representing germline ASE in all TSGs for an individual would be associated with an increased cancer risk because only mutations on the expressed copy would be required to disrupt the function of the gene. To assess this, we first tested the ability of two methods to predict ASE using genotype data. We modified a tool called PrediXcan which predicts overall gene expression to predict the expression of each haplotype and generated a ratio with the predicted values. We also applied logistic regression models using heterozygous SNP status as predictors and ASE status as the outcome. Although the performance of ASE predictions was poor for many genes using both methods, our results indicate that it may be possible to generate more accurate predictions using genotype data as input as more data becomes available. As a pilot study, we generated a single TSG ASE score using the genes for which the predictions worked well and assessed the relationship with breast cancer risk. We found no statistically significant relationship between TSG ASE and cancer risk, which is likely due to our inability to predict ASE in the TSGs that contribute to cancer risk in this tissue type, as assessed using cancer data.

In conclusion, this thesis presented a novel approach to predict the true clonal load of cancer samples and demonstrated its similarity to the observed somatic mutation load in normal tissue. We also provided further insight into the role of the immune system in shaping the mutational landscape of cancer samples and, using a novel method, generated an estimate for the proportion of missense mutations removed through immunoediting. Finally, we also presented a novel approach to predict germline ASE using genotype data showing it is feasible for some genes and performance

Single-cell characterisation of the bone marrow microenvironment and its contribution to acute myeloid leukemia

# Sarah Ennis Supervisors: Pilib Ó Broin and Eva Szegezdi

The human bone marrow is a complex tissue, responsible for replenishing the entire blood system. It comprises many types of hematopoietic as well as non-hematopoietic cells that together coordinate the production of billions of blood cells everyday. In the case of acute myeloid leukemia (AML), this process is damaged and abnormal myeloid-lineage blood cell progenitors accumulate in the bone marrow, impairing the production of healthy blood cells and leading to disease. AML is an aggressive cancer with a poor survival rate owing to the propensity of leukemic cells to develop resistance to chemotherapy and a lack of alternative treatment strategies. It is well-known that cell-cell interactions between AML cells and other cell types in the bone marrow are a major driver of drug resistance and these interactions could represent viable therapeutic targets. However, the exact signalling molecules and cell types involved in these interactions are not well-characterised. Thus, the central aim of this thesis was to characterise the roles played by different bone marrow cell types in the initiation and progression of AML. As the

bone marrow is an intricate and heterogenous microenvironment, efforts to profile this tissue using traditional bulk-sequencing methods that require the dissociation of tissues, have left gaps in our understanding. Newer technologies such as single-cell RNA-sequencing (scRNA-seq) allow gene expression to be traced back to individual cells and provide a higher-resolution and more granular view of complex tissues and therefore, we have used scRNA-seq to achieve our aim of characterising the human bone marrow.

# Differences in immunogenicity between cancer mutation signatures shed light on immunoediting

## Noor Khehrah Supervisor: Prof. Cathal Seoighe

Neoantigens are mutated peptides that have the potential to initiate immune responses against tumors. These immunogenic mutations are reportedly removed by selection in a process referred to as immunoediting. Although it has been studied extensively, the influence of patient MHC-I genotype on the extent of immunoediting has not been quantified precisely and remains controversial. We reanalyzed two recent high-profile studies and found no evidence to support their reports of MHC molecules restricting the oncogenic mutational landscape. Considering these findings and recent research indicating a connection between background mutational signatures and immunoediting in cancer, we conducted a comprehensive characterization of COSMIC signatures. Additionally, we developed a method to detect and quantify the immunoediting signal within tumors by comparing the observed and expected proportions of immunogenic mutations, considering patient-specific mutation signature activity profiles and HLA-I genotype. We implemented this method using data from TCGA. We found that mutated peptides resulting from specific mutation signatures were more likely to be presented by certain HLA alleles compared to peptides originating from other mutation signatures. In most tumor types, the signal of immunoediting was weak or absent. In a pan-cancer analysis we found slightly

stronger evidence of immunoediting in the subclonal compared to clonal mutations, in line with previous reports. Overall, our results are consistent with at most 1% of mutations having been removed through immunoediting, suggesting that the effect of immunoediting on the cancer mutational landscape is, at most, marginal. Indeed, a weak signal of immunoediting persisted even when HLA alleles were shuffled randomly between patients, casting doubt on the existence of an HLA-I dependent immunoediting signal in the data. Overall, there was no evidence that HLA-I dependent immunoediting makes a substantial contribution to the somatic mutations observed in cancer samples.

# Investigating the genetics of deep learning-derived neuroimaging phenotypes of brain disorders

# Shane O'Connell Supervisors: Pilib Ó Broin and Dara Cannon

Brain disorders are collections of debilitating phenotypes that can affect cognition and general life quality via a myriad of symptoms, including mood swings, memory loss, altered thought processes, and psychosis. Despite their common area of action in the brain, few biomarkers have been characterised. Furthermore, the causal relationship between neuroimaging measures and brain disorders remains largely un- explored. Understanding the biological manifestations of these conditions could help to inform improved diagnostic, prognostic, and treatment systems. To this end, we identified neuroimaging biomarkers of Alzheimer's disease using a convolutional neural network, finding 7 significant genome-wide loci. These findings were consistent with previously observed genetic results of Alzheimer's disease and further implicated impaired cellular homeostasis as a molecular association of Alzheimer's disease-related neuroanatom-We also trained an autoencoder ical variation. on participant tabular neuroimaging data from the same dataset and highlighted a latent space node significantly associated with Alzheimer's participants, finding three genome-wide significant loci associated with its value. These three variants mapped to non-coding RNA transcripts, suggesting that intronic and intergenic regulatory elements could be influential in Alzheimer's disease neuroanatomical differences. Across both studies, we also demonstrate evidence of tissue-specific expression in clinically relevant brain regions, such as the substantia nigra. Finally. we explored the causal relationship between neuroimaging measures and bipolar disorder using graph-based Mendelian randomization methods, finding that white matter microstructural phenotypes exert greater effects in a network context than gray matter structural phenotypes. Specifically, we find evidence of bidirectional causality between bipolar disorder and the area of the lateral orbitofrontal cortex and several components of the limbic system involved in emotional regulation.

# Computational approaches to identify and explain sources of error in cancer somatic mutation data Brian O'Sullivan Supervisor: Prof. Cathal Seoighe

Errors in identifying somatic mutations in cancer samples can have critical implications, leading to missed treatment opportunities or misleading research findings. We developed vcfView, an interactive Rshiny application, to reevaluate variants excluded from analysis, allowing us to incorporate biological context into our assessment and identify overlooked putative somatic variants. Additionally, we developed a simulation framework to generate comprehensive and realistic tumour genomic sequencing data, accurately representing the frequency profile observed in real sequencing data and documenting the true source of each nonreference base. The framework not only identifies variant caller errors but also enables us to explain the reasons behind erroneous calls. Using the GATK Mutect2 variant calling pipeline, we apply this framework to highlight and explain sources of error in somatic mutation data and biases in somatic allele frequency estimation. Finally, we apply these methods to low-depth, heavily DNAdamaged, tumour-only sequencing data from an unpublished cohort of 60 pancreatic cancer patients and recover clinically and research-relevant information.

# Boolean games played in a triangle using bi-partite and tri-partite entanglement

# Victoria Sánchez Muñoz Supervisor: Michael Mc Gettrick

This dissertation analyses the Nash equilibrium points in a triangle network when the three nodes/players are playing pairwise boolean games using bi-partite and tripartite entanglement. The players are given one bit as input and must output another bit; the boolean games are defined by choosing two boolean functions of two variables, one function for the input bits and another for the outputs. The players win jointly each of the games if the function of the inputs matches the function of the outputs. The players also share a 6-qubit quantum state, each owning two qubits, which will be used to play the games, i.e. to decide on their outputs given their inputs by measuring locally their two qubits. This 6-qubit state corresponds either to two GHZ-like quantum states (tri-partite entanglement) or three Bell-like quantum states (bi-partite entanglement). The aim is to compare the performance in terms of the (new) Nash equilibrium points of these two types of quantum resources in the described triangle-network situation for any choice of the two boolean functions defining the game. This research, that mixes quantum games, quantum networks, and quantum resources, presents an interesting and rather rich situation, with potential applications in quantum information, for example, in the quantum internet.

# 6 Staff profiles

### Balbi, V.

#### Current research interests

My research field is in soft tissues mechanics, I am interested in both experimental and theoretical aspects. Due to their complexity, soft tissues are difficult to test. From the experimental viewpoint, I am interested in developing robust and reliable testing protocols suitable for different tissues. Theoretically, I develop new mathematical models to capture the non-linear mechanical behaviour of soft tissues. I am also interested in modelling wrinkling instabilities is soft meta-materials and biological tissues. Continuum mechanics, non-linear elasticity and visco-elasticity are my everyday tools.

#### **Recent** publications

- SP. Venkata, V. Balbi, M. Destrade, G. Zurlo. Designing necks and wrinkles in inflated auxetic membranes. *Int J Mech Sciences*, 268, 109031, 2024.
- [2] G. Small, H. Berjamin, V. Balbi. Programmable wrinkling for functionally-graded auxetic circular membranes. Int J Non-Linear Mech, 159, 104601, 2024.
- [3] SP. Venkata, V. Balbi, M. Destrade, D. Accoto, G. Zurlo. Programmable wrinkling for functionally-graded auxetic circular membranes. *Extreme Mech Letters*, 63, 102045, 2023.
- [4] M. Destrade, Y. Du, J. Blackwell, N. Colgan, V. Balbi. Canceling the elastic Poynting effect with geometry. *Phys Rev E*, 107 (5), L053001, 2023.

#### **Research** activities

- *Invited talks*: Euromech Colloqium (Edinburgh): Nonlinear Elasticity: Modelling of multi-physics and applications; European Solid Mechanics Conference 2022 (Galway).
- Organised conferences: mini-symposium on "Stability of Soft Materials" at the ESMC 2022 (Galway).

- Supervision: I am currently supervising two PhD students on the following projects: (1) modelling the nonlinear viscoelastic behaviour of the brain and (2) modelling the instabilities of auxetic metamaterials.
- *Grants*: Millenium Fund (CSE).
- I am a member of the International Society for Interaction of Mechanics and Mathematics.

# Berjamin, Harold Current research interests

My current research deals with the mechanical modelling of soft magneto-active composite materials. Applications of these works are found in material science and soft robotics.

#### **Recent** publications

- H. Berjamin, M. Destrade, G. Saccomandi. Singular travelling waves in soft viscoelastic solids of rate type. *Eur. J. Mech. A Solids*, 103, 2024. (link)
- [2] G. Small, H. Berjamin, V. Balbi. Poynting effect in fluid-saturated poroelastic soft materials in torsion. *Int. J. Non-Linear Mech.*, 159, 2024. (link)
- [3] H. Berjamin, A. L. Gower. Universality of the angled shear wave identity in soft viscous solids. *Extreme Mech. Lett.*, 68, 2024. (link)
- [4] H. Berjamin, M. Destrade. Models of fractional viscous stresses for incompressible materials. *Math. Mech. Solids*, 2024. (link)

#### **Research** activities

- Conferences: 2. 10<sup>th</sup> International Congress on Industrial and Applied Mathematics, Tokyo (Japan); RAM3 - Recent Advances in Mechanics and Mathematics of Materials, Rome (Italy).
- *Invited talks:* 3. Irmar, Rennes (France); Cermics, Marne-la-Vallée (France); LAUM, Le Mans (France).

- Papers refereed: 10.
- *Memberships:* SIAM, AFM-Euromech.

#### Carnevale, Angela

#### Current research interests

My research is mostly in the field of algebraic and enumerative combinatorics. Recently, I have been especially interested in posets and permutation statistics and their applications to problems related to zeta functions in algebra.

#### **Recent** publications

- A. Carnevale and T. Rossmann, Linear relations with disjoint supports and average sizes of kernels, J. Lond. Math. Soc. (2) 106 (2022), no. 3, 1759–1809.
- [2] A. Carnevale, M. Dyer and P. Sentinelli, *The intermediate orders of a Coxeter group*, Proc. Amer. Math. Soc. 151 (2023), 1433–1443.
- [3] A. Carnevale, M. M. Schein and C. Voll, Generalized Igusa functions and ideal growth in nilpotent Lie rings, Algebra and Number Theory, 18 (2024), no. 3, 537–582.
- [4] A. Carnevale, V. D. Moustakas, T. Rossmann, From coloured permutations to Hadamard products and zeta functions, FPSAC 2024 extended abstract, to appear.

### **Research** activities

- I was awarded funding under the CSE Strategic Research Fund scheme to work on the project "Ask zeta functions, shufflecompatibility and Hadamard products".
- Recent invited talks: Oberseminar of the Institute for Algebra and Geometry, Magdeburg, Germany, July 2023. ♦ Counting Problems in Groups, Lincoln, UK, August 2023. ♦ Congress of the Italian Mathematical Union, Combinatorics section, Pisa, Italy, September 2023.
- Conference organised: *Groups in Galway* 2023 (with G. Pfeiffer).

- I am co-organising the two-week research programme Combinatorial Methods in Enumerative Algebra (with U. Onn, A. Prasad, P. Singla, C. Voll) at the ICTS Bangalore (India) from 2–13 December 2024.
- I am currently supervising a PhD student (Michael Joyce Maher) since September 2022.

#### Cruickshank, James

#### Current research interests

- Geometric and combinatorial rigidity theory.
- Face numbers of simplicial complexes.
- Finite groups of deficiency zero.
- More generally geometric/algebraic combinatorics and group theory.

#### **Research** outputs

2 papers appeared and 2 papers submitted since April 2023. Currently 5 papers under review at various journals.

#### **Recent** publications

- Bryan Gin-ge Chen, James Cruickshank, and Derek Kitson. Block-and-hole graphs: Constructibility and (3,0)-sparsity, 2023. https://arxiv.org/abs/2309.06804
- [2] James Cruickshank, Fatemeh Mohammadi, Anthony Nixon, and Shin ichi Tanigawa. Identifiability of points and rigidity of hypergraphs under algebraic constraints, 2024. https://arxiv.org/abs/2305.18990
- [3] James Cruickshank, Fatemeh Mohammadi, Harshit J. Motwani, Anthony Nixon, and Shinichi Tanigawa. Global rigidity of line constrained frameworks. *SIAM J. Discrete Math.*, 38(1):743–763, 2024.
- [4] James Cruickshank, Eleftherios Kastis, Derek Kitson, and Bernd Schulze. Braced triangulations and rigidity. *Discrete & Computational Geometry*, Aug 2023.

#### **Research** activities

I have been on sabbatical since January 1, 2024.

- Invited talks:
  - Landscapes of Rigidity Workshop, RI-CAM, Austria, March 2024.
  - IMS Annual Meeting, Limerick, September 2023.
  - Alberta Topology Colloquium, Kananaskis, Canada, July 2024.
- Contributed talks:
  - Workshop on Geometric and Algebraic Combinatorics, Universidad de Cantabria, Spain, January 2024.
  - Workshop on Geometric Constraints: Materials, Graphs and Matroids, Rigidity and Packings, Fields Institute, Canada, July 2023.
  - Graph rigidity and applications, Lancaster University, UK, April 2023
- Research visits to Lancaster University, University of Tokyo, MIC Thurles, RICAM.
- Hosted research visit from Prof Fernando Szechtman, University of Regina.

#### Das, Kishor

#### Current research interests

My research is focused on analysing highdimensional data using Mixed-effects Modelling framework and Functional Data Analysis. In addition to that I am also interested in analysing data arising in clinical research, public health research and sport science.

### **Recent** publications

 Das, K., de Paula Oliveira, T., and Newell, J. Comparison of markerless and markerbased motion capture systems using 95% functional limits of agreement in a linear mixedeffects modelling framework. *Scientific Reports*, 13(1):22880, 2023.

- [2] Arnold, B.F., Rerolle, F., Tedijanto, C., Njenga, S.M., Rahman, M., Ercumen, A., Mertens, A., Pickering, A.J., Lin, A., Arnold, C.D. and Das, K. Geographic pair matching in large-scale cluster randomized trials. *Nature Communications*, 15(1):1069, 2024.
- [3] Butzin-Dozier, Z., Mertens, A. N., Tan, S. T., Granger, D. A., Pitchik, H. O., Il'yasova, D., Das, K., ... and Lin, A. Stress Biomarkers and Child Development in Young Children in Bangladesh. *Psychoneuroendocrinology*, 107023, 2024.

#### **Research** activities

- Five manuscripts submitted.
- Attended 43rd Conference on Applied Statistics in Ireland.
- Co-organised 4th Young-ISA, a network of career-young statisticians in Ireland, meeting.

### Destrade, Michel Current research interests

I work on the modelling of dielectric and magnetoelastic elastomers, on elastic waves travelling in soft tissues and in stressed solids, on the imaging of soft solids, and on the wrinkling of auxetic materials.

### **Recent** publications

- F. Zhu, B. Wu, M. Destrade, H. Wang, R. Bao, W. Chen. Voltage-controlled non-axisymmetric vibrations of soft electro-active tubes with strain-stiffening effect. International Journal of Solids and Structures. 290 (2024) 112671.
- [2] A. Alibakhshi, S. Rahmanian, M. Destrade, G. Zurlo. Local and global dynamics of a functionally graded dielectric elastomer plate. International Journal of Engineering Science. 195 (2024) 103987.
- [3] H. Berjamin, M. Destrade, G. Saccomandi. Singular travelling waves in soft viscoelastic solids of rate type European Journal of Mechanics / A Solids. 103 (2024) 105144.

- [4] S.P. Venkata, V. Balbi, M. Destrade, D. Accoto, G. Zurlo. Programmable wrinkling for functionally-graded auxetic circular membranes. Extreme Mechanics Letters. 63 (2023) 102045.
- [5] M. Destrade, Y. Du, J. Blackwell, N. Colgan, V. Balbi. Canceling the elastic Poynting effect with geometry. Physical Review E. 1007 (2023).

#### **Research** activities

- Current research grants: 2 Marie Sklodowska Curie Fellowships (one pre-, one postdoctoral); 1 Chinese Research Council fellowship.
- *PhD Examiner*: Besancon, France and Madrid, Spain.
- Conferences/Seminars: Bari, Besancon, Cambridge, Edinburgh, Hangzhou, Madrid, Ningbo, Tianjin, Zhuji.
- *Graduate Course*: Zhejiang University, Hangzhou, China.
- Appointments: Academic Promotion Committee; Reviews Editor at Proceedings of the Royal Society A; Associate Editor at Mechanics of Soft Solids, Adjunct Professor at University College Dublin and Zhejiang University; Directeur de Recherche at Institut d'Alembert, CNRS, Paris, France (on leave); Member of the International Brain Mechanics and Trauma Lab (Oxford).

# Dorman, Matthew J. Current research interests

My research interests focus on microbial genomics, particularly on Gram-negative human pathogens. Areas of interest and of previous research include: using genomic data to contextualise experimental microbiology into bacterial species and their population structures; gene regulation and regulatory networks in single pathogens and across species; pathogen genomic epidemiology, including in lower-middle income settings; long-read sequencing and the production of high-quality microbial genome assemblies.

#### **Recent** publications

- F. Lassalle, et al. Genomic epidemiology reveals multidrug resistant plasmid spread between Vibrio cholerae lineages in Yemen. Nat Microbiol, 8:1787-1798, 2023.
- [2] M. J. Dorman, N. R. Thomson. Vibrio cholerae O37: one of the exceptions that prove the rule. *Microbiol Genom*, 9(4):mgen000980, 2023.
- [3] R. Soontarach, et al. Isolation and characterisation of bacteriophage selective for key Acinetobacter baumannii capsule chemotypes. Pharmaceuticals, 15(4):443, 2022.
- [4] T. G. Fennell, et al. gbpA and chiA genes are not uniformly distributed amongst diverse Vibrio cholerae. Microbiol Genom, 7(6):mgen.0.000594, 2021.
- [5] M. J. Dorman, et al. Genomics of the Argentinian cholera epidemic elucidate the contrasting dynamics of epidemic and endemic Vibrio cholerae. Nat Commun, 11(1):4918, 2020.

### **Research** activities

- Co-organising and co-chairing of two sessions at Microbiology Society Annual Conference; Edinburgh, UK, Apr 2024.
- Instructor, Genomics and Epidemiological Surveillance of Bacterial Pathogens. Wellcome Global Training course; Asunción, Paraguay, Apr 2023.
- Member and Prokaryotic Division Member (2022-2024); Microbiology Society.

#### Ferguson, John

#### Current research interests

Automatic methods to produce confidence intervals in high-dimensional settings. Causal inference, especially as applied to estimating impacts of population-level health interventions through analysis of observational data. Bayesian statistical modeling. Statistical bioinformatics, including the correction of selection bias in genome wide association studies (GWAS), methods to correct for ensuing bias propagating into 2-sample estimates from Mendelian Randomisation, and Empirical Bayes methods to simultaneously analyse GWAS data over several diseases or traits.

#### **Recent** publications

- Ferguson, John, Alberto Alvarez, Martin Mulligan, Conor Judge, and Martin O'Donnell. "Bias assessment and correction for Levin's population attributable fraction in the presence of confounding", *European Journal of Epidemi*ology, (2024): 1-9.
- [2] Forde, Amanda, Gibran Hemani, and John Ferguson. "Review and further developments in statistical corrections for Winner's Curse in genetic association studies", *PLoS Genetics*, 19, no. 9 (2023).
- [3] Reddin, Catriona, John Ferguson, Robert Murphy, Aoibhin Clarke, Conor Judge, Vincent Griffith, Alberto Alvarez et al. "Global mean potassium intake: a systematic review and Bayesian meta-analysis", *European Journal of Nutrition*, 62, no. 5 (2023): 2027-2037.
- [4] O'Connell, Maurice M., and John Ferguson.
   "Pathway-specific population attributable fractions", *International Journal of epidemiology*, 51, no. 6 (2022): 1957-1969.
- [5] Ferguson, John. "Bayesian interpretation of p values in clinical trials", *BMJ Evidence-Based Medicine*, 27, no. 5 (2022): 313-316.

#### **Research** activities

- PhD supervision: Amanda Forde, "Statistical Correction of Selection Bias in Genome Wide Association Studies, with applications to Mendelian Randomisation".
- Conference presentations at the International Society for Clinical Biostatistics (ISCB) Meeting (August, 2023) and the European Meeting for Causal Inference (April, 2023).
- Poster presentation at the Conference for Applied Statistics in Ireland (May, 2023).

- Invited talk at the Mendelian Randomisation Methods Seminar, Integrative Epidemiology Unit, University of Bristol (January, 2024).
- Assessment of ISCB Conference Awards for Scientists (for ISCB 2024 in Greece) for the ISCB National Groups Committee.
- Referee reports for several journals during 2023/2024 including Statistical Modeling, European Journal of Epidemiology, American Journal of Epidemiology and BMC Medical Research Methdology.

# Fitz-Simon, Nicola. Current research interests

My main research interests concern the estimation of causal effects using observational and experimental data. My primary application areas are biostatistics/medical statistics, especially in the areas of neonatal, paediatric, cardiovascular, and environmental health. I also have research interests in the intersection between infectious disease modelling and causal inference.

#### **Recent** publications

- Kamiya T; Alvarez-Iglesias A; Ferguson J; Murphy S; Sofonea MT; Fitz-Simon N. Estimating time-dependent contact: a multi-strain epidemiological model of SARS-CoV-2 on the island of Ireland. *Global Epidemiology*, 5:100111, 2023.
- [2] Fitz-Simon N; Ferguson J; Alvarez-Iglesias A; Sofonea MT; Kamiya T. Understanding the role of mask-wearing during COVID-19 on the island of Ireland. *Royal Society Open Science*, 10(7), 2023.

#### **Research** activities

- Reviewer for International Journal of Epidemiology
- Fellow of the Royal Statistical Society, member of the Irish Statistical Association and the International Society for Clinical Biostatistics.

#### Flannery, Dane L.

#### Current research interests

Linear groups and computation; combinatorial design theory.

#### **Recent** publications

- J. A. Armario, R. Egan, and D. L. Flannery, Generalized partially bent functions, generalized perfect arrays, and cocyclic Butson matrices, Cryptogr. Commun. 16 (2024), no. 2, 323–337.
- [2] A. S. Detinko, D. L. Flannery, and A. Hulpke, Zariski density and computing with S-integral groups, J. Algebra 624 (2023), 93–105.
- [3] A. S. Detinko, D. L. Flannery, and A. Hulpke, Freeness and S-arithmeticity of rational Möbius groups, Computational Aspects of Discrete Subgroups of Lie Groups, Contemp. Math., vol. 783, Amer. Math. Soc., [Providence], RI, [2023] ©2023, pp. 47–56.

#### **Research** activities

- Research in Groups, International Centre for Mathematical Sciences, Edinburgh, UK, 5-16 June, 2023.
- Oberwolfach Research Fellowship, Mathematisches Forschungsinstitut Oberwolfach, 2-15 July, 2023

# Haseja, Devesh

#### Current research interests

In recent years, there has been increased interest in the generation of synthetic data for use in biomedical research and precision medicine. This interest has partially been driven by the EU GDPR directive for health data anonymization and pseudonymization, based on the draft European Health Data Space (EHDS) Regulation[1], which focuses on securing sensitive personal information, in particular confidential healthcare data[2]. Generating synthetic data which can sufficiently recapitulate the underlying characteristics of the real datasets from which they are created can allow researchers to overcome some of the limitations of sharing restrictions on real data, such as providing sufficient power for statistical models or ensuring adequate training dataset sizes for machine learning algorithms. In the field of transcriptomic research, simulation of artificial RNA-Seq and scRNA-seq data can be used especially for the purpose of genetic expression analysis, isoform expression analysis and enrichment analysis[3]. This can have wide ranging applications in the field of biomarker identification, novel therapeutic discovery and functional pathway research[4]. The main objective of this study is to review the underlying statistical models and/or generative algorithms used to create some of these datasets, and to survey the evaluation metrics commonly used to benchmark their similarity to the underlying real data. This project is part of an initiative by the ELIXIR machine learning focus group [5] to assess the usage and utility of a wide range of synthetic data types across the biomedical research community.

### References:

1. He, Z., From Privacy-Enhancing to Health Data Utilisation: The Traces of Anonymisation and Pseudonymisation in EU Data Protection Law. Digital Society, 2023. 2(2): p. 17.

2. Alloza, C., et al., A Case for Synthetic Data in Regulatory Decision-Making in Europe. Clinical Pharmacology and Therapeutics, 2023. 114(4 3. Shakola, F., D. Palejev, and I. Ivanov, A Framework for Comparison and Assessment of Synthetic RNA-Seq Data. Genes, 2022. 13(12): p. 2362.

4. Thind, A.S., et al., Demystifying emerging bulk RNA-Seq applications: the application and utility of bioinformatic methodology. Briefings in Bioinformatics, 2021. 22(6): p. bbab259.

5. Queralt-Rosinach, N., et al., Infrastructure for synthetic health data. 2023, BioHackrXiv.

# Holian, Emma Current research interests

Prognostic models in Breast Cancer, modelling treatment outcome on longitudinal biomarkers,

variable selection in survival models for data with various missingness mechanisms. Statistical methods in Genomics Data Science, change point status multi-response modelling in Copy Number Alterations. Statistical challenges in environmental impact studies and climate data, challenges of leftcensored distributions in groundwater data. Classification and cluster analysis of longitudinal data profiles via mixture modelling, Regression Cluster Model (RCM). Modelling Composition Response data, influencing factors in blood clot composition via Dirichlet Regression.

### **Recent** publications

- M. Davey, et al. Evaluating the Role of Circulating MicroRNAs in Predicting Long-Term Survival Outcomes in Breast Cancer: A Prospective, Multicenter Clinical Trial. Journal of the American College of Surgeons, 2023. 236(2), 317-327.
- [2] M. Davey, et al. MicroRNA Expression Profiling Predicts Nodal Status and Disease Recurrence in Patients Treated with Curative Intent for Colorectal Cancer. Cancers, 14(9), 2022.
- [3] L. King, A. Flaus, S. Coughlan, E. Holian, A. Golden. GNOSIS: an R Shiny app supporting cancer genomics survival analysis with cBio-Portal *HRB Open Research*, 2022.
- [4] L. King, A. Flaus, E. Holian, A.Golden. Survival Outcomes are Associated with Genomic Instability in Luminal Breast Cancers. *Plos One*, 2021.
- [5] E. McGrory, E. Holian, L. Morrison. Assessment of groundwater processes using censored data analysis incorporating non-detect chemical, physical, and biological data. *Journal Of Contaminant Hydrology*, 2020.

#### **Research** activities

- Director of Outreach and Research initiative: *Figuring out Y (FOY)*. Collaborators: Dr Mairead Greene, CELT.
- Ph.D Student Supervision: (1) Lydia King
  SFI CRT Genomics Data Science, *The*

Role of Genomic Data in Stratifying Patients within Predictive Models for Breast Cancer Survival Outcome, successful Viva Jan 2024. (2) Malak Almutairi - Modeling composition response data with application to clot composition observed for Acute Ischemic Stroke (AIS) patients.

#### Seyed Aghil Hooshmand

#### Current research interests

My research focuses on the integration and management of liquid biopsy data for improved cancer diagnosis and prognosis. As part of the Cancer Liquid Biopsies Consortium (CLuB), I am streamlining the processing and storage of clinical and genomic data from breast, ovarian, lung, and pancreatic cancers. This involves extending and deploying the cBioPortal web application on AWS for improved accessibility and functionality for the liquid biopsy research community, while ensuring data security with frameworks like Keycloak, and developing user-friendly web tools for seamless data management. Once our datahas been integrated with public datasets, we will employ advanced computational methods such as machine learning, deep learning, and network analysis to helps uncover novel insights into cancer biology. Through these endeavors, CLuB accelerates diagnostic innovation and professional training in cancer research.

#### **Research** activities

• Grants :

This research was supported by the North-South Research Programme administered by the Higher Education Authority on behalf of the Department of Further and Higher Education, Research, Innovation and Science and the Shared Island Fund (CLuB: The All-Ireland Cancer Liquid Biopsies Consortium https://www.clubcancer.ie).

### • Conferences :

Irish Computational Biology and Genomics Symposium, December 2023, Galway; All-Ireland Cancer Liquid Biopsies Consortium (CLuB) Symposium, October 2023, Dublin • Memberships: EACR

### Howard, Mark Current research interests

I'm primarily interested in quantum information theory, specifically:

- Stabilizer formalism (generalization to d-level systems, quantum error-correcting codes, Gottesman-Knill theorem)
- Clifford group and classical simulability of restricted quantum circuits
- Discrete Wigner functions (negative quasiprobabilities, relationship with GK theorem)
- Magic state distillation and quantum fault tolerance more generally
- Nonlocality & Contextuality, Mutually unbiased bases, SIC-POVMs, foundations of quantum theory

### **Recent** publications

- Pierre-Emmanuel Emeriau, Mark Howard, and Shane Mansfield. Quantum advantage in information retrieval. *PRX Quantum*, 3(2):020307, 2022.
- [2] Michael Beverland, Earl Campbell, Mark Howard, and Vadym Kliuchnikov. Lower bounds on the non-clifford resources for quantum computations. *Quantum Science and Technology*, 5(3):035009, 2020.
- [3] Sergey Bravyi, Dan Browne, Padraic Calpin, Earl Campbell, David Gosset, and Mark Howard. Simulation of quantum circuits by low-rank stabilizer decompositions. *Quantum*, 3:181, 2019.

### **Research** activities

• Supervising 2 PhD students since Sept 2022: Aisling MacAree (Royal Society and COSE funded) and Mark Ryder (IRC funded) working on Quantum Error Correction & Fault Tolerance.

- Seminar Series Co-organizer: School of Mathematical & Statistical Sciences, Galway.
- Member of National Advisory Forum for Quantum Technologies

### Kherreh, Noor.

Postdoctoral Researcher in Bioinformatics at O'Broin lab.

I am a researcher in the field of bioinformatics with a strong background in computer sciences. I recently completed my PhD in bioinformatics, specializing in onco-immunology, where I investigated the influence of adaptive immune system on the mutational landscape of cancer. During my Ph.D., I had the privilege of being a Marie Curie fellow and working as an early-stage researcher for the multi-disciplinary consortium QUANTII. Prior to my involvement with QUANTII, I pursued an M.Phil and an undergraduate degree in Computer Sciences. During my M.Phil research, I developed a computer-aided device employing machine learning and image processing techniques for detecting nodules in lung CT scan images.

### Current research interests

In recent years, immunotherapy has revolutionized cancer treatment by harnessing the body's immune system to combat cancer, marking a significant departure from traditional cytotoxic methods. HEALED, an Irish-based multi-disciplinary consortium, seeks to advance cancer immunotherapy by leveraging revolutionary nanoreactor technology and expertise in data science to enhance productivity and cost-effectiveness. Neoantigens, mutated peptides resulting from somatic mutations in cancer cells and presented on cell surfaces by MHC molecules, are key targets for immunotherapy. Our goal is to provide a thorough review of existing neoantigen prediction tools, highlighting their methodologies, strengths, and limitations. Through systematic benchmarking, we aim to ensure the reliability and reproducibility of neoantigen prediction results, thereby propelling the field of cancer immunotherapy forward. Additionally, we plan to develop an integrated, cloud-based pipeline that may incorporate novel approaches or

combinations of top-performing existing neoantigen prediction tools identified through comprehensive benchmarking analysis.

### **Recent** publications

 Noor Kherreh, Siobhán Cleary, and Cathal Seoighe, "No evidence that HLA genotype influences the driver mutations that occur in cancer patients," *Cancer Immunology, Immunotherapy*, vol. 71, no. 4, pp. 819–827, 2022, Springer.

### Madden, Niall

#### Current research interests

My research is in the field of numerical analysis: numerical solution of partial differential equations, particularly those that arise in the investigation of boundary layer phenomena, and computational linear algebra. My recent interest has been in finite element methods, adaptive meshing, and fast linear solvers. I'm also interested in research relating to gender equality in higher education, including the Gender Pay Gap.

#### **Research outputs**

- G. Saha, N. Poddar, K.K. Mondal and N. Madden Hydrodynamic dispersion of volatile contaminant in an open channel flow using a fitted operator approach. *Proc IC-NDA 2024.* Springer Proceedings in Physics. Feb 2024.
- [2] R. Shiromani, N. Madden, and V. Shanthi. A finite difference scheme for twodimensional singularly perturbed convectiondiffusion problem with discontinuous source term. arXiv:2401.02331. Jan 2024.
- [3] R. Hill and N. Madden. Layer-adapted meshes for singularly perturbed problems via mesh partial differential equations and a posteriori information. arXiv:2311.01274. Nov 2023.
- [4] L. Loftus, N. Madden, P.A. Scott, A. Cooke, and N. McNicholas. The Gender

Pay Gap and Irish Higher Education: University of Galway, a Case Study. *Adm. Sci.*, 13(11), 239, 2023. DOI: 10.3390/adm-sci13110239

#### **Research** activities

I gave workshop presentations Charles University (Prague) in May 2023, and at the Banff International Research Station (Banff) in August 2023. I gave a conference presentation at the 29th Biennial Numerical Analysis Conference (Glasgow), June 2023.

From September to December 2023 I was a Visiting Scientist at the Department of Mathematics and Statistics, Memorial University of Newfoundland. While there I mainly worked with Scott MacLachlan on some new finite element methods convection-diffusion problems, and their implementation in Firedrake. I also gave an seminar on fitted finite element methods at the departmental colloquium.

#### Maglione, Joshua

#### Current research interests

My research interests are in computational algebra, asymptotic group theory, and algebraic combinatorics. I develop efficient algorithms to aid in various isomorphism problems. The Group Isomorphism Problem is closely related to the Tensor Isomorphism Problem, so I am also interested in tensors, their structure, and their applications to algebra. I also apply combinatorial tools to understand and compute certain *p*-adic integrals coming from zeta functions of groups and rings and Igusa's zeta function. These can be used to better understand enumerative aspects of groups, rings, and algebras such as the number of finite-index subgroups of a group.

#### **Recent** publications

 C. Alfes, J. Maglione, and C. Voll. Ehrhart polynomials, Hecke series, and affine buildings. To appear in *Sémin. Lothar. Comb.*, 2024. arXiv:2402.15412.

- [2] P. A. Brooksbank, J. F. Maglione, E. A. O'Brien, and J. B. Wilson. Isomorphism invariant metrics. Preprint, 2023. arXiv:2304.00465.
- [3] G. Dorpalen-Barry, J. Maglione, C. Stump. The Poincaré-extended ab-index. Preprint, 2023.
   arXiv:2301.05904.
   Extended abstract to appear in Sémin. Lothar.

*Comb.*, 2024.

- [4] L. Kühne, J. Maglione. On the geometry of flag Hilbert–Poincaré series for matroids. Algebr. Comb. 3(6):623–638, 2023.
- [5] J. Maglione, C. Voll. Flag Hilbert–Poincaré series of hyperplane arrangements and Igusa zeta functions. To appear in *Israel J. Math.*, 2024.

#### **Research** activities

- Invited Mini-Course: Colorado State University (May 2024), International Centre for Theoretical Sciences Bangalore (Dec. 2024). Invited talks: University of Warwick (Feb. 2023).
- Conferences organized: Groups in Galway 2024, Symbolic Enumeration in Algebra.
- Research visits: University of Trento (May 2023), Bielefeld University (May 2023; Apr. 2024), Colorado State University (Jun.–Jul. 2023).
- Refereed: Journal of Algebra, Journal of Computational Algebra, International Symposium on Symbolic and Algebraic Computation.

### McCluskey, Aisling

#### Current research interests

My current research interests revolve around generalising the classic notions of betweenness, equidistance and relativeness closeness in Euclidean geometry to the natural context of metric spaces. Such notions can be viewed from an axiomatic perspective and interpreted in a metric space. Of particular interest is when the metric is induced by a vector space norm. Recent work with P. Bankston has provided some interesting characterisations of normed vector space properties purely in terms of of abstract betweenness and relative closeness.

I am also interested in university mathematics education, particularly in the realm of assessment strategy that provokes and promotes deep and engaged learning and also in the context of initial teacher education at post-primary level.

#### **Recent** publications

- D. Anderson, P. Bankston, A. McCluskey. Betweenness-induced convexity in hyperspaces of normed vector spaces, to appear in *Journal* of Convex Analysis, 2024
- [2] A. McCluskey, J. Grant McLoughlin, K. O'Sullivan. The Junior Mathematics Enrichment Programme at Galway, Ireland: book chapter to appear in *International Perspectives* on Mathematics Outreach, 2024. https://www. infoagepub.com/products/International-Perspectives-on-Mathematics-Outreach

### **Research** activities

- Co-host (with Nina Snigireva) of 22nd Galway Topology Colloquium https://maths. nuigalway.ie/galwaytopology/ on June 4-5, 2024
- PhD external examiner at UCC, September 2024

#### Mc Gettrick, Michael.

#### Current research interests

My main research interests are within theoretical quantum computer science. Therein, I predominantly work on quantum walks and quantum games, as basic ingredients in quantum algorithms. Other areas of interest include: (1) Mathematics (graphs, geometry) used in modelling (network) transport systems, (2) and Mathematics and (quantum) algorithms as applied in music (both algorithmic composition and classification of melodies).

### **Recent** publications

 M. Mc Gettrick, P. Mc Gettrick The Kolmogorov complexity of traditional Irish dance music. To appear (2024)

#### **Research** activities

- 1 PhD student graduated in 2024 (Victoria Sánchez Muñoz)
- 1 current PhD student (Ian Craig)
- Member of the Peer Review Panel on "Software Enabled Quantum Computation", Engineering and Physical Sciences Research Council (EPSRC), UK
- Member of the Irish Mathematical Society
- Keynote speaker at the IFAC (International Federation of Automatic Control) 1st. Interational Workshop on Quantum Algorithms, Machine Learning and Control, June 2023, Trinity College Dublin
- Invited lecture "Introduction to Quantum Games" at Winter School on Quantum Computing Technologies, Mehran University (Pakistan), January 2024
- Member of the review panel for GECCO (The Genetic and Evolutionary Computation Conference), Melbourne, July 2024
- Member of the National Advisory Forum for Quantum Technologies (Republic of Ireland)

# Ó Broin, Pilib

### Current research interests

My research interests lie primarily in clinical/translational bioinformatics with a particular focus on the development and application of machine learning methods for genomic data in the cancer, immunology, and neuroscience domains.

#### **Research** outputs

- 'Predictive modelling of brain disorders with magnetic resonance imaging: A systematic review of modelling practices, transparency, and interpretability in the use of convolutional neural networks'. S O'Connell, DM Cannon, P Ó Broin. *Human Brain Mapping* 44 (18), 6561-6574 (2023).
- [2] 'Genes positively regulated by Mef2c in cortical neurons are enriched for common genetic variation associated with IQ and educational attainment'. L Fahey, D Ali, G Donohoe, P Ó Broin, DW Morris. *Human Molecular Genetics* 32 (22), 3194-3203 (2023).
- [3] 'Performance and Advancement of the Kidney Solid Organ Response Test'. Joshua Lee, Mariel Barbachan e Silva, Yi Bao, Ryan Whitmarsh, Sukanta Banerjee, Jeannine O'Connor, Jeffery Holbert, Tiffany K Bratton, Pilib Ó Broin, Enver Akalin. Transplantation 107(10):p 2271-2278, (2023).
- [4] 'CCPlotR: an R package for the visualization of cell-cell interactions'. Sarah Ennis, Pilib Ó Broin, Eva Szegezdi. *Bioinformatics Ad*vances, Volume 3, Issue 1, (2023).
- [5] 'Cell-cell interactome of the hematopoietic niche and its changes in acute myeloid leukemia'. Sarah Ennis, Alessandra Conforte, Eimear O'Reilly, Javid Sabour Takanlu, Tatiana Cichocka, Sukhraj Pal Dhami, Pamela Nicholson, Philippe Krebs, Pilib Ó Broin, Eva Szegezdi. *iScience* 26 (6) (2023).

#### **Research** activities

- My research group this year included: 2 postdoctoral researchers, 10 PhD students, 1 research assistant, and one research intern. 2 PhD students (Sarah Ennis & Shane O'Connell) submitted their theses.
- Research funding: SFI CRT in Genomics Data Science, SFI ADAPT Centre, SFI Frontiers (x2), DBEI (DTIF), HEA (North-South Research Programme).

- External activities: Executive Board Member, Translational Medicine Alliance Ireland (TMAI); Expert Reviewer, Horizon Europe, EURAXESS Internship Program for Refugee and Displaced Researchers; Management committee member, COST action CA22103; International Programme Committee, Bioinformatics 2024
- Memberships: European Association for Cancer Research (EACR); International Society for Computational Biology (ISCB); Irish Society for Human Genetics (ISHG); European Society for Human Genetics (ESHG); Marie Curie Alumni Association (MCAA); ELIXIR Machine Learning Focus Group (MLFG).

### O'Leary, Neil

# Current research interests

A wide range of methodological interests; in particular the design and analysis of clinical trials, multilevel modelling of clustered and longitudinal data, along with other applied research interests in causal inference in observational studies, survey techniques and missing data.

#### **Recent** publications

- H. Hara, N. O'Leary, M. Ono, Y. Onuma, P.W. Serruys. A comparison of risk prediction models for patients with acute coronary syndromes. *EuroIntervention*, 17(16):1362, 2022.
- [2] K. Ninomiya, S. Kageyama, H. Shiomi, N. Kotoku, S. Masuda, P.C. Revaiah, et al. Can machine learning aid the selection of percutaneous vs surgical revascularization? Journal of the American College of Cardiology, 82(22):2113, 2023.
- [3] M. Ono, S. Kageyama, N. O'Leary, M.S. El-Kurdi, J. Reinöhl, E. Solien, *et al.* 1-Year patency of biorestorative polymeric coronary artery bypass grafts in an ovine model. *Basic to Translational Science*, 8(1):19, 2022.

[4] H. Hara, N. O'Leary, M. Ono, Y. Onuma, P.W. Serruys. A comparison of risk prediction models for patients with acute coronary syndromes. *EuroIntervention*, 17(16):1362, 2022.

#### **Research** activities

- Collaboration with the CORRIB Research Center for Advanced Imaging and Core laboratory on a number of applied projects.
- Reviewer for NIHR Journals Library.

#### Pfeiffer, Götz

#### Current research interests

Complex hyperplane arrangements and their symmetry groups, various algebras related to these arrangements and their roles as modules for the group and as cohomology rings, Chow rings of matroids, Hecke algebras of complex reflection groups and their centers.

#### **Recent** publications

- L. Hellebrandt and G. Pfeiffer On the Left Connected Subalgebra of the Descent Algebra of a Coxeter Group of Classical Type. Annals of Combinatorics 27 (2023), 693–706.
- [2] John M. Burns and Götz Pfeiffer. Maximal Order Abelian Subgroups of Coxeter Groups. *Glasgow Math. J.* 65 (2023), Issue 1, 114–120.
- [3] E. Chavli and G.Pfeiffer. Centers of Hecke Algebras of Complex Reflection Groups. *Beiträge* zur Algebra und Geometrie (2023).
- [4] J. Matthew Douglass, Götz Pfeiffer and Gerhard Röhrle. Invariants and semi-invariants in the cohomology of the complement of a reflection arrangement. arXiv:2009.12847.

#### **Research** activities

- Graduate Students: 1
- Papers refereed: 7.

- Invited Talks: Parabolic Normalizers as Subdirect Products (January 2023; "Lie Theory: Frontiers, Algorithms and Applications", Monash Prato Centre, Italy); Computational Aspects of Complex Reflection Groups (4 Lectures, March 2023; "Spring School on Real, Complex, and Symplectic Reflection Groups", Ruhr-Universität Bochum, Germany).
- Conference organized: Groups in Galway 2023, May 18-19, 2023 (with A. Carnevale).
- Editorial Board Member: Journal of Symbolic Computation; Mathematical Proceedings of the Royal Irish Academy.
- Member: Irish Mathematical Society; American Mathematical Society.

### Pfeiffer, Kirsten

### Current research interests

My research interests focus on educational interventions to enhance students' creative reasoning skills and the learning of mathematical argumentation and proof. I'm interested in task design in the teaching of mathematics at university level, in particular in students' practice of evaluation exercises and possible learning effects of these. Together with my PhD student Latifah Mustofa Lestyanto I am currently studying Anna Sfard's theory of *commognition* to consider its applicability and appropriateness as a framework for investigating learning and teaching of mathematical proof.

I'm also interested in the role of mathematics support centres from a sociocultural point of view, in models for tutor training and accrediting systems for this as well as in research about usage and accessibility of online mathematics resources.

#### **Research** activities

 Over the last few years I have investigated the merits of a special type of tasks, namely proof evaluation tasks, for the learning of mathematical proof, together with Rachel Quinlan. In a current project with Latifah Mustofa Lestyanto, we investigate if the commognitive framework is suitable to describe students' learning and performance of mathematical proof, in particular proof by mathematical induction, and to develop suitable tasks and activities to foster learning of proof. This framework may also be suitable to provide further insights from students' proof evaluation performances.

- In collaboration with colleagues from the University of Birmingham, TU Dublin and the University of Maynooth, we have developed an accrediting system of training for postgraduate tutors and lecturers in STEM. Our most recent paper about this has just been accepted by the journal Teaching Mathematics and Its Applications: International Journal of the IMA.
- In October 2023 I gave a presentation about the Resource Website Project of the Irish Maths Learning Support Network (IMLSN) at the Ninth Conference on Research in Mathematics Education in Ireland (MEI 9). Together with Julie Crowley (Munster Technological University) and Mike Welby (University of Galway), we published a paper about this project in the conference proceedings.
- As the chair of the Irish Maths Learning Support Network (IMLSN) I organised the annual IMLSN workshop on Mathematics learning support linking practice to research in the new normal, which took place in June 2022. Together with Ciaran O'Sullivan (TU Dublin) I wrote an article about the outcomes for the MSOR Connections, which has been published in the Autumn of 2023.
- In September 2023 I took part at the annual CETL-MSOR conference in Cardiff, U.K. This conference is aimed at practitioners from the full range of the learning, teaching and support communities within the disciplines of Mathematics, Statistics and Operational Research.

# Quinlan, Rachel.

### Current research interests

I am generally interested in combinatorial and algebraic aspects of matrix theory. Objects of current interest include alternating sign matrices linked to algebraic structures, and matrix spaces with rank behaves in unusual ways. I am also interested in university mathematics education and in mathematics in the visual arts.

### **Research** outputs

- Dana Saleh and Rachel Quinlan, 2-uniform covering groups of elementary abelian 2groups, Communications in Algebra, Vol. 52, no. 2. 630-656, 2024.
- Rachel Quinlan, Interchangeable Origami Wallpaper Patterns, Proceedings of the 2023
   Bridges Conference, bridgesmathart.org, 2023.
- [3] Cian O'Brien and Rachel Quinlan. Alternating sign matrices of finite multiplicative order, Linear Algebra and its Applications, Vol. 631, 332-358, 2022.
- [4] Rachel Quinlan, Moumita Shau and Fernando Szechtman. *Linear diophantine equations in several variables*, Linear Algebra and its Applications, Vol. 630, 67–90, 2022.
- [5] C. O'Brien, K. Jennings and R. Quinlan. Alternating signed bipartite graphs and difference-1 colourings, Linear Algebra and its Applications, Vol. 604, 370–398, 2020.

### **Research** activities

- I am currently supervising (with Cian O'Brien) the PhD research of Badriah Safarji.
- In 2023 I gave a plenary talk at the 25th Conference of the International Linear Algebra Society in Madrid.
- From September to December 2023 I was a visiting scientist at Memorial University of Newfoundland, while on sabbatical leave from the University of Galway.

# Roshan, Davood Current research interests

My primary research interest is in the longitudinal analysis of clinical biomarkers. In particular, I am interested in developing statistical models and algorithms to generate adaptive reference regions from high dimensional streaming data from medical devices. The development of early-warning systems in real-time will be a key enabler for enhanced patient monitoring and care. I also have special interest in Translational Statistics, Data Visualisations and Data Science with a focus on developing predictive tools.

# **Research outputs**

Ivory, John D., Duygu Sezgin, Patricia M. Coutts, Davood Roshan, Chloe M. Hobbs, José Verdú Soriano, James P. O'Gara, David Gallagher, and Georgina Gethin (2023). Signs, symptoms and/or biomarkers reported to indicate biofilm in chronic wounds: An eDelphi consensus protocol. Journal of Wound Management 24, no. 1 (2023): 22-27.

### Research activities

- Grants (pending):
  - HRB Secondary Data Analysis Projects, Riding Towards Safety: Advancing Concussion Identification, Prevention and Care in Irish Horse-Racing (co-PI).
  - 2 Hardiman PhD applications (PI)
  - 1 application in CÚRAM MedDevDoc PhD programme (PI)
- The external examiner for a PhD thesis submitted to the University of Amrita Vishwa Vidyapeetham, India (Doctor of Philosophy under the Faculty of Engineering) (March 2024)
- Invited by the Alzahra Statistical Association (Iran) to run a two-days workshop on "The Grammar of Graphics for Statistical Visualisations in R" (February 2024).

- Local organiser of the **4th Young-ISA annual meeting** at university of Galway (November 2023).
- College of Science and Engineering scholarship (€97,000): to supervise a PhD student in Biostatistics (July 2023).
- Awarded the College of Science and Engineering Millennium Fund (€9,000) to Develop Computational Approaches for the Generation of Adaptive Reference Ranges in Real Time Monitoring in Health Care and Beyond (May 2023).
- Principle Investigator at CÚRAM.
- 2 PhD student, 1 Postdoctoral Researcher.
- Seminar Series Co-organizer in the School of Mathematical & Statistical Sciences, University of Galway.
- Vice-chair of the Young Irish Statistical Association where we organise the Inaugural Young-ISA meetings; twitter poster conferences; and Young-ISA webinar series.
- Memberships: Young-ISA, Irish Statistical Association, International Society for Clinical Biostatistics, International Biometric Society, Statistical Modelling Society.

#### Rossmann, Tobias

#### Current research interests

My research is in algebra and neighbouring fields. I am particularly interested in asymptotic and computational questions. In recent years, my main focus has been on zeta functions arising from algebraic counting problems such as the enumeration of subgroups, representations, linear orbits, or conjugacy classes.

#### **Recent** publications

 T. Rossmann, Enumerating conjugacy classes of graphical groups over finite fields. Bull. Lond. Math. Soc. 54 (2022), no. 5, 1923–1943.

- [2] A. Carnevale and T. Rossmann, Linear relations with disjoint supports and average sizes of kernels. J. Lond. Math. Soc. 106 (2022), no. 3, 1759–1809.
- [3] T. Rossmann and C. Voll, Groups, graphs, and hypergraphs: average sizes of kernels of generic matrices with support constraints. Mem. Amer. Math. Soc. 294 (2024), no. 1465, vi+120 pp.
- [4] A. Carnevale, V. D. Moustakas, and T. Rossmann, From coloured permutations to Hadamard products and zeta functions. To appear in Sém. Lothar. Combin. (2024), 12 pages.
- [5] T. Rossmann, On the enumeration of orbits of unipotent groups over finite fields. Preprint, arXiv:2208.04646, 15 pages.

#### **Research** activities

- I will give an invited research-level course at the Research Programme *Combinatorial Methods in Enumerative Algebra*, ICTS Bangalore, India (December 2024).
- I am an organiser of the upcoming meetings Groups in Galway 2024 (with A. Carnevale and J. Maglione; May 2024) and Symbolic Enumeration in Algebra (with A. Carnevale, P. Lins, J. Maglione, and C. Voll; July 2024).
- I am a member of the Editorial Board of Experimental Mathematics.
- In September 2023, David Cormican commenced his PhD studies under my supervision, funded by a Hardiman Scholarship.

### Ryan, Ray Current research interests

Functional Analysis: polynomial and holomorphic functions on complex Banach spaces and Banach lattices; tensor products of Banach lattices.

### **Recent** publications

 C. Boyd, R. Ryan, N. Snigireva. A Nakano carrier theorem for polynomials. *Proc. Amer. Math. Soc*, 151(4):1621–1635, 2023.

### **Research** activities

- Order Continuity on Banach Lattices, UCD Analysis Seminar, 28 November 2023.
- Order Continuous Polynomials on Banach Lattices, 8th ILJU School of Mathematics, POSTECH 2024, Korea.

#### Scarrott, Carl

### Current research interests

My key three research platforms are in (1) methodological and computational developments for extreme value modelling, with applications in environment, health and finance, (2) biostatistical modelling in health research and (3) applied statistics in environmental science, engineering and exercise science.

#### **Research** outputs

- Pedlar, C.R., Myrissa, K., Barry, M., Khwaja, I.G., Simpkin, A.J., Newell, J., Scarrott, C.J., Whyte, G.P., Kipps, C., and Baggish, A.L. Medical encounters at communitybased physical activity events (parkrun) in the UK. British *Journal of Sports Medicine*, 55, 1420-1426, 2021.
- Scarrott, C.J., Hu, Y. and Akbar, A. Extreme value mixture modelling, threshold estimation and boundary corrected kernel density estimation. CRAN, Version 2.12, 2019, https://cran.r-project.org/ web/packages/evmix/index.html
- Mattle, H., Scarrott, C.J., Claffey, M., Thornton, J., Macho, J., Riedel, C., Soderman, M., Bonafe, A., Piotin, M., Newell, J. and Andersson, T. Analysis of revascularization in ischemic stroke with Embo-Trap (ARISE I study) and metaanalysis of thrombectomy. *Interventional Neuroradiology*, 25(3), 261-270, 2018.

## Seoighe, Cathal Current research interests

Research interests are mainly in genomics (especially cancer genomics) and molecular evolution; in particular, variation in germline and somatic mutation rates and their relationship with cancer risk, development and application of models and computational methods to analyze molecular sequence evolution and gene expression data and the analysis of genomic data in order to generate insights into the links between genomic and phenotypic variation.

#### **Recent** publications

- V. Nembaware, D. Bennett, E. R. Chimusa, T. Chikowore, R. Daodu, V. N. Bitoungui, S. M. Williams, S. Fatumo, S. Healy, C. Seoighe, A. Wonkam, G. é, R. Ndiaye, C. Dandara, L. Mutesa, M. Ramsay, G. El-Kamah, G. Sirugo, J. Makani, K. Sadki, M. Z. Alimohamed, S. Nkya, A. Gaye, R. Ramesar, A. Choudhury, C. Happi, N. S. Munung, N. Kherji, J. Hotchkiss, V. Ras, A. Ghansay, C. Musanabaganwa, K. K. Esoh, S. M. Adadey, and S. C. Coughlan. The African Society of Human Genetics successfully launches global data science workshops. *Trends Genet*, 39(11):803– 807, Nov 2023.
- [2] B. O'Sullivan and C. Seoighe. Comprehensive and realistic simulation of tumour genomic sequencing data. NAR Cancer, 5(3):zcad051, Sep 2023.
- [3] P. M. Staunton, A. J. Peters, and C. Seoighe. Somatic mutations inferred from RNA-seq data highlight the contribution of replication timing to mutation rate variation in a model plant. *Genetics*, 225(2), Oct 2023.

#### **Research** activities

- Scientific Director of the SFI Centre for Research Training in Genomics Data Science
- SFI Principal Investigator award to study variation in germline and somatic mutation rates

- Research group consisting of one postdoctoral researcher, five PhD students (principal supervisor) and two co-supervised PhD students
- Collaborator on Biotope2, a UCD-led SFI Sustainable Development Goals (SDG) Challenge to predict the severity of childhood pneumonia in Malawi.

### Simpkin, Andrew

#### Current research interests

Derivative estimation for multivariate functional data; landmark approaches for joint time-to-event and (multivariate) functional data; application of functional data analysis to DNA methylation data.

#### **Recent** publications

- Armario, X., Carron, J., Simpkin, A.J., et al. Impact of the COVID-19 pandemic on global TAVR activity: the COVID-TAVI study. *Cardiovascular Interventions*, 17(3), pp.374-387, 2024
- [2] Tammes, P., Jones, T., Ben-Shlomo, Y. and Simpkin, A.J. Suicide under the Nazi-regime: a case-control study among Amsterdam Jews. *Archives of suicide research*, 27(4), pp.1231-1244, 2023
- [3] Beatty, R., Mendez, K.L., Schreiber, L.H., Tarpey, R., Whyte, W., Fan, Y., Robinson, S.T., O'Dwyer, J., Simpkin, A.J., Tannian, J. and Dockery, P. Soft robotic mediated autonomous adaptation to fibrotic capsule formation for improved drug delivery. *Science Robotics*, 8(81), 2023

#### **Research** activities

- Current research grants:
  - Simpkin AJ, Hynes N (co-PIs). HealAsyst: A multifactorial wound treatment monitoring system for intelligent healing of chronic wounds. April 2023 to March 2026; €1,214,000;

- Simpkin AJ (PI), Bargary N. Modelling sensor data in recreational runners. Insight Platform Research Budget. February 2022 to January 2026; €112,000;
- Simpkin AJ, Bargary N (co-PIs).
   Functional data Analysis for Sensor Technology. SFI Frontiers for the Future project. December 2020 to November 2024; €467,569;
- Graduate students: Anna Grossbach Epigenetic aging: determinants and consequences; John Andrew Modelling longitudinal functional data; Solomon Beer Lifecourse modelling with time varying covariates
- Postdoctoral researchers: Nastaran Sharifian Modelling multivariate sensor data; Omid Khazaei Modelling the weaning process in intensive care data; Jair Andrade Using sensor BP to assist appointment scheduling for hypertension; Yueyun Zhu Developing methods in multivariate FDA

## Snigireva, Nina Current research interests

Currently I am interested in the existence and properties of attractors and invariant measures for Iterated Function Systems. I am also investigating polynomials and holomorphic functions on Banach Lattices.

#### **Recent** publications

- C. Boyd, R. Ryan, N. Snigireva, A Nakano carrier theorem for polynomials, *Proceedings of the American Mathematical Society*, **151** (2023), no. 4, 1621–1635.
- [2] K. Lesniak, N. Snigireva, F. Strobin, Strongly-fibred iterated function systems and the Barnsley-Vince triangle, *Banach Center Publ.* **125**, Inst. Math., Polish Acad. Sci., Warsaw (2023), pp 81–90.
- [3] C. Boyd, R. Ryan, N. Snigireva, Holomorphic Functions on Complex Banach Lattices submitted, arXiv:2310.03910.

- [4] K. Lesniak, N. Snigireva, F. Strobin, A. Vince, Highly non-contractive iterated function systems on Euclidean space can have an attractor, *submitted*.
- [5] K. Lesniak, N. Snigireva, F. Strobin, Rate of convergence in the deterministic chaos game on doubling spaces, *submitted*.

#### **Research** activities

- Polynomials and holomorphic functions on complex Banach lattices, Invited Talk at the 19th ILJU School of Mathematics on Banach Spaces and Related Topics: Commemorating the 65th Birthday of Professor Yun Sung Choi, 22nd–26th January 2024, IBS POSTECH, Pohang, Republic of Korea.
- Polynomials and holomorphic functions on complex Banach lattices, UCD Analysis Seminar, 28th November 2023.
- Reviewing and refereeing.

#### Tripathi, Bharat B.

#### Current research interests

My current research interest is in modeling and simulation of shear shock waves in brain in context of traumatic brain injury. This involves development of novel nonlinear continuum mechanics models, construction of state-of-the-art numerical algorithms like discontinuous Galerkin method, development of machine learning tools for optimization, prediction, calibration etc. In general, I am motivated to research in the field of computational mechanics to bring together the aspects of physics and mathematical/scientific computing with the theory of statistics. The amalgamat ion of the three for modeling propagation of information/material in biomedical applications, remains the overarching theme of his research.

#### **Recent** publications

 Oisin Morrison, Michel Destrade, Bharat B. Tripathi. An atlas of the heterogeneous viscoelastic brain with local power-law attenuation synthesised using Prony-series. Acta Biomaterialia, 2023.

- [2] Sandhya Chandrasekaran, Francisco Santibanez, Bharat B. Tripathi, Ryan DeRuiter, Ruth Vorder Bruegge, and Gianmarco Pinton. In situ ultrasound imaging of shear shock waves in the porcine brain. *Journal of Biomechanics*, 110913, 2022.
- [3] Bharat B. Tripathi, Sandhya Chandrasekaran, and Gianmarco Pinton. Super-resolved shear shock focusing in the human head. *Brain Multiphysics*, 2, 100033, 2021.
- [4] Sandhya Chandrasekaran, Bharat B. Tripathi, David Espíndola, and Gianmarco Pinton. Modeling ultrasound propagation in the moving brain: applications to shear shock waves and traumatic brain injury. *IEEE Trans. Ultras.*, *Ferr. Freq. Cont.*, 68(1), 201-212, 2021.
- [5] Bharat B. Tripathi, David Espindola, and Gianmarco F. Pinton. Modeling and Simulations of Two Dimensional Propagation of Shear Shock Waves in Relaxing Soft Solids, J. Comput. Phys., 395: 205-222, 2019.
- [6] Bharat B. Tripathi, David Espindola, and Gianmarco F. Pinton. Piecewise parabolic method for propagation of shear shock waves in relaxing soft solids: one dimensional case, *Int. J. Numer. Meth. Biomed. Engg.* **35**(5):e3187, 2019.

#### **Research** activities

- Oral presentation in 6th Oxford International Neuron and Brain Mechanics Workshop (April 19-20, 2021), Oxford, UK.
- Oral presentation in 2020 IEEE International Ultrasonics Symposium (September 7-11, 2020), Las Vegas, USA.
- Oral presentation in 11<sup>th</sup> European Solid Mechanics Conference (ESMC 2022) (July 4-8, 2022), University of Galway, Ireland. (Oral).

### Yang, Haixuan

### Current research interests

My focus is in Bioinformatics & Statistical Modelling, especially of network data such as proteinprotein interactions, co-expression, and functional similarity. A bio-molecular network can be viewed as a collection of nodes, representing the biomolecules, connected by links, representing relations between the bio-molecules. I am working on inferring valuable information from bio-molecular networks.

#### **Recent** publications

- M. Timilsina, V. Nováček, M. d'Aquin, H. Yang. Boundary heat diffusion classifier for a semi-supervised learning in a multilayer network embedding. *Neural Networks*, 156:205-217, 2022.
- [2] M. Torres, H. Yang, A.E. Romero, A. Paccanaro. Protein function prediction for newly sequenced organisms. *Nature Machine Intelli*gence, 3(12):1050-1060, 2021.
- [3] Y. Zhong, C. Seoighe, H. Yang. Non-Negative matrix factorization combined with kernel regression for the prediction of adverse drug reaction profiles. *Bioinformatics Advances*, 4(1):vbae009, 2024.

### Zhang, Quan

#### Current research interests

My current research interest is the theoretical modeling, numerical simulations, and experimental characterization of Magnetoactive Metamaterials for tunable wave manipulations. I am focused on exploiting the unique transformative ability of soft magnetoactive materials integrated into the neat metamaterial design to develop novel tunable and multifunctional soft magnetoactive metamaterials with superior elastic wave properties.

#### **Recent** publications

- Q. Zhang, S. Rudykh. Propagation of solitary waves in origami-inspired metamaterials. J. Mech. Phys. Solids, 187:105626, 2024.
- [2] W. Liu, Q. Zhang, L. Wu, J. Sun, J. Zhou. Design of quasi-zero stiffness metamaterials with high reliability via metallic architected materials. *Thin Wall. Struct.*, 198:111686, 2024.

- [3] Q. Zhang, G. Hu, S. Rudykh. Magnetoactive asymmetric mechanical metamaterial for tunable elastic cloaking. *Int. J. Solids Struct.*, 289:112648, 2024.
- [4] Q. Zhang, A.V. Cherkasov, C. Xie, N. Arora, S. Rudykh. Nonlinear elastic vector solitons in hard-magnetic soft mechanical metamaterials. *Int. J. Solids Struct.*, 280:112396, 2023.
- [5] L. Yang, Q. Zhang, G. Hu, N. Yang. Deformation insensitive thermal conductance of the designed Si metamaterial. *Appl. Phys. Lett.*, 123:062201, 2023.

#### **Research** activities

- *Grants*: My application for the College of Science and Engineering SDG Support Fund was approved.
- Conferences: "Nonlinear Elasticity: Modelling of multi-physics and applications", a Euromech colloquium celebrating the 80th birthday of Prof. Ray Ogden FRS, 25th–28th March 2024, Edinburgh, UK.
- Conferences: Phononics 2023, 12th-16th June 2023, Manchester, UK.

#### Zurlo, Giuseppe.

#### Current research interests

I am interested at how elasticity can be employed to describe the behavior of solids in a broad range of scales, from the sub-cellular level, to the macroscopic level of the material. I have worked on the modelling of damage of rubber, on the nonlinear elastic response of functionally graded materials, on coupled electro- elastic instabilities, on biological growth and additive manufacturing.

I have fruitful collaborations with researchers from my own university (V.Balbi, M.Destrade, E.McIvoy) and from a broad international network: India (A.Khurana, M.Joglekar - IIT Roorkee), France (L.Truskinovsky - ESPCI Paris, A.Elrich - Grenoble, P. Recho - Grenoble, T.Lecuit -Marseille), Israel (R.Segev - U.Negev, M.Moshe - Jerusalem), Italy (G.Tomassetti - RomaTre, R.Paroni - Pisa, M.Ciavarella and S.Campanelli - Bari).

I am currently co-supervising 2 PhD theses (M.Daman in cotutelle with Italy, and T.Hayes in Galway).

## Recent publications

- Renzi D., Marfia S., Tomassetti G., Zurlo G., A discrete model for layered growth, European J. Of Mechanics A-Solids, 105, 105232, 2024.
- [2] Venkata S.P., Balbi V., Destrade M., Zurlo G., Designing necks and wrinkles in inflated auxetic membranes, International Journal Of Mechanical Sciences, 268, 109031, 2024.
- [3] Alibakhshi A., Rahmanian S., Destrade M., Zurlo G., Local and global dynamics of a functionally graded dielectric elastomer plate, International Journal Of Engineering Science, 195, 103987, 2024.
- [4] Venkata S.P., Balbi V., Destrade M., Accoto D., Zurlo G., Programmable wrinkling for functionally-graded auxetic circular membranes, Extreme Mechanics Letters 63, 102045, 2023.
- [5] Harmansa S.; Erlich A.; Eloy C.; Zurlo G.; Lecuit T Growth anisotropy of the extracellular matrix shapes a developing organ, Nature Communications, 14 (1), 1220, 2023

### **Research** activities

• In May 2024, I am taking part to a field trip in Scotland (Thurso) to study peatland instabilities, within an international collaboration of mathematicians, engineers and geologists funded by the INI, Isaac Newton Institute for Mathematical Sciences (UK).

# 7 Visitors

# Hemani, Gibran (Integrative Epidemiology Unit, University of Bristol) Visiting: John Ferguson

Dates of visit: 10 May 2023 – 12 May 2023

#### **Research** activity

Gib had several fruitful discussions with Amanda Forde and John Ferguson, pertaining to Amanda's PhD. Gib also interacted with many other members of the statistics group, and gave a talk at the school seminar, "The future of genetic biobanks" on Thursday 11th.

# Lucci, Giulio. (Politecnico di Torino & Università Sapienza) Visiting: Giuseppe Zurlo

Dates of visit: 13 November 2023 – 17 November 2023

#### **Research** activity

Giuseppe and Giulio met in Torino when the former was in the examining committee of the latter's PhD viva. They decided to collaborate on the mathematical modelling of cancer spread and Giulio exploited an Erasmus+ Grant to visit Giuseppe for one week. Their collaboration is now progressing on topics they have discussed in Galway.

# Marzocchi, Alfredo (Università Cattolica del Sacro Cuore) Visiting: M. Destrade

Dates of visit: 12 November 2023 – 14 November 2023

#### **Research** activity

Collaboration and co-supervision of PhD project.

# Musesti, Alessandro. (Università Cattolica del Sacro Cuore, Milano) Visiting: Giuseppe Zurlo

Dates of visit: 22 May 2023 – 24 May 2023

#### **Research** activity

Alessandro is full professor of mathematical physics and was invited in Galway both to give a talk, and to collaborate with Giuseppe on the modelling of muscle growth and atrophy, a topic where Giuseppe's PhD student Thomas is currently working on.

### Shearer, Tom (University of Manchester) Visiting: M. Destrade

Dates of visit: 20 November 2023 – 24 November 2023

#### **Research** activity

Complete a paper; discussions on grants.

# Soodhalter, Kirk (Trinity College Dublib) Visiting: Niall Madden

Dates of visit: 25 - 27 April 2023

#### **Research** activity

Discussions on enriched finite element methods for singularly perturbed problems.

Voll, Christopher (Bielefeld University) Visiting: Angela Carnevale, Joshua Maglione, Tobias Rossmann

Dates of visit: 12 November 2023 – 26 November 2023

# Research activity

Christopher worked with **Angela** on the organisation of the upcoming research programme "Combinatorial Methods in Enumerative Algebra" which will take place at the ICTS Bangalore at the end of 2024.

**Josh** and Christopher collaborated on a joint research project, which combines the topics of *p*-adic lattice enumeration, the combinatorics of semistandard Young tableaux, and the algebra of the spherical symplectic Hecke algebra. They made significant progress and also wrote an extended abstract for FPSAC 2024, which has now been accepted and will appear later this year.

Christopher and **Tobias** continued their collaboration on conjugacy classes of graphical groups and more generally average sizes of kernels within modules of matrices attached to graphs. In particular, they settled and extended a conjecture on the effects of taking joins of graphs on associated classcounting zeta functions from their joint monograph (Mem. Amer. Math. Soc. 2024).

Our visitor also participated in our "Algebra and Combinatorics" reading group.

# 8 Conferences, meetings, and workshops

## Groups in Galway 2023

**Dates:** 18–19 May 2023

Speakers: Naomi Andrew (University of Oxford), Javier Aramayona (ICMAT), Ilaria Castellano (Bielefeld University), Leo Margolis (Universidad Autónoma de Madrid), Padraig Ó Catháin (Dublin City University), Colva Roney-Dougal (University of St Andrews), Tobias Rossmann (University of Galway), Yuri Santos Rego (Otto-von-Guericke University Magdeburg), Gerald Williams (University of Essex) Organisers: Angela Carnevale, Götz Pfeiffer

 ${\bf Funders:}$  Irish Mathematical Society, University of Galway

Web page: https://angelacarnevale.github.io/gig23/

# 4th Young-ISA event ("Researcher's Toolkit: Publication, Progression, and People") Dates: 17 November 2023

**Speakers:** Kathleen O'Sullivan (University College Cork), Carl Scarrott (University of Galway), Brendan Murphy (University College Dublin), Eleanor Fallon (University of Limerick), Darshana Jayakumari (Maynooth University) Luiza Piancastelli (University College Dublin) Emily Gribbin (Queen's University Belfast), Luke Kelly (University College Cork), Ana Silva Couto (Biomathematics and Statistics Scotland) Lydia King (University of Galway) Estevao Batista Do Prado (Lancaster University) Joshua Tobin (Trinity College Dublin)

**Organisers:** Davood Roshan (University of Galway), Shirin Moghaddam (University of Limerick), Silvia D'Angelo (Trinity College Dublin), Kate Finucane (University College Dublin), Amir Jalali (University of Limerick), James A Sweeney (University of Limerick), Fatima Jaouimaa (Lillys Pharmacy & Health Store), Gabriel Rodrigues Palma (Maynooth University), Autumn.odonnell (University College Cork), Joshua Henderson (Queen University Belfast), Kishor Das (University of Galway), Nastaran Sharifian (University of Galway), Omid Khazaei (University of Galway), Pouyan Nejadi (University of Galway).

**Funders:** Irish Statistical Association; Sonraí Health Data Science Research Cluster; the British and Irish Region (BIR) of the International Biometric Society (IBS)

Web page: https://young-istat.github.io/events/posts/2023-11-17-meeting4/

# 9 School seminar

- Koushik Paul, University of Galway. Novel Construction of Specht Modules for Monomial Groups, 26/03/2024.
- [2] <u>Rachel Quinlan</u>, University of Galway. *Curiosities of Alternating Sign Matrices*, 14/03/2024.
- [3] <u>Katrin Wendland</u>, Trinity College Dublin. Symmetries of Z<sub>3</sub>-orbifold K3s, 07/03/2024.
- [4] <u>Victoria Sánchez Muñoz</u>, University of Galway. Boolean games played in a triangle using bi-partite and tri-partite entanglement, 01/03/2024.
- [5] <u>Damian Markham</u>, Sorbonne University. Secure Networks of Quantum Sensors, 29/02/2024.
- [6] Leo Creedon, ATU Sligo. The ring of derivations of a group algebra, and new partial algebraic structures which are almost semigroups, groups and rings, 22/02/2024.
- [7] <u>Brian O'Sullivan</u>, University of Galway. Computational approaches to identify and explain sources of error in cancer somatic mutation data, 22/02/2024.
- [8] <u>Brendan Masterson</u>, Middlesex University London. Authenticity in Learning, Teaching and Assessment., 15/02/2024.
- [9] Joshua Maglione, University of Galway. Categorifying characteristic subgroups: a characterization, 08/02/2024.
- [10] <u>Robert Osburn</u>, University College Dublin. Strange identities, the Habiro ring and resurgence, 30/01/2024.
- [11] Lydia King, University of Galway. The Role of Genomic Data in Stratifying Patients within Predictive Models for Breast Cancer Survival Outcome, 30/01/2024.
- [12] <u>Victoria Sánchez Muñoz</u>, University of Galway. How Maths Helped Me to Annoy My Insurance Company, 25/01/2024.

- [13] Nina Snigireva, University of Galway. Properties of Polynomials on Banach Lattices, 11/01/2024.
- [14] <u>Noor Kherrah</u>, University of Galway. (PhD Viva) Differences in immunogenicity between cancer mutation signatures shed light on immunoediting, 17/11/2023.
- [15] <u>Ted Hurley</u>, University of Galway. What are your favourite matrices? Why? What are your favourite \*types\* of matrices? How are they made and for what purpose?, 09/11/2023.
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