School of Mathematics, Statistics and Applied Mathematics Research Day
22nd April 2010

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1 Introduction

Welcome to the first of our annual School Research Days. The School, now in its second year of existence, comprises the disciplines of Mathematics, Applied Mathematics, Statistics and Bioinformatics and our research activity ranges across all these areas. We have particular strengths in Computational Algebra, Mathematical Modelling, Statistics, Biostatistics and Bioinformatics. The School has a thriving graduate programme, with almost 30 PhD students, including many from overseas. Among the funded research activities in the School are the De Brún Centre for Computational Algebra and the Galway wing of the BIO-SI initiative, both supported by SFI under the Mathematics Initiative. The School won two posts under the SFI Stokes scheme. Cathal Seoighe was appointed SFI Stokes Professor in Bioinformatics and Milovan Krnjajic is SFI Stokes Lecturer in Statistics.

The De Brún Centre for Computational Algebra

The De Brún Centre for Computational Centre was launched in 2008, funded by SFI for a four year period under the Mathematics Initiative. Algebraic computation is playing an increasingly widespread role in applied mathematics, statistics, engineering and science. Three teams of researchers in the Centre work in inter-related areas of computational algebra, focusing on innovative projects with direct relevance to applied mathematics and engineering.

The de Brún Centre has been hosting a series of two-week workshops on computational aspects of mathematics. The themes are computational group theory, crystallography, quantum computing, computational biology, algebraic and topological statistics. An international conference on algebraic design theory and its applications, incorporating the 2nd International Workshop on Hadamard and Cocyclic Matrices, was held July 1-3, 2009.

Biostatistics and Bioinformatics

The Bio-Statistics and Informatics initiative, BIO-SI, is funded by the SFI Mathematics Initiative. Its objective is to create innovative statistical science in the areas of Biostatistics and Bioinformatics, primarily by forging a partnership collaboration between the University of Limerick and NUI Galway, with the Galway team led by Professor John Hinde. The research work carried out ranges over the five key BIO-SI programme areas, namely: Covariance Modelling, Multivariate Survival Modelling, Statistical Genetics, Mixture Models and Microarray Analysis.

SFI Stokes Professor in Bioinformatics Cathal Seoighe formerly held posts at the University of the Western Cape and the University of Cape Town, both in South Africa. There, he established research groups with a focus on several aspects of genomics and molecular evolution, including the development of models of HIV-1 evolution in the context of immune responses and drug treatment, as part of global collaborations to combat the spread of the HIV pandemic. Recently, Dr Aaron Golden, another Bioinformaticist, has joined the School, creating a critical mass in this area.

Mathematical Modelling

Mathematical Modelling has also been targeted by the School as for strategic growth. There is a small but very active group with interdisciplinary collaborations in Physics, Engineering, Economics and Information Technology, whose members area also participants in MACSI, the Mathematics Applications Consortium for Science and Industry, in the University of Limerick. The appointment of Dr Michel Destrade as Professor of Applied Mathematics, who takes up his post in September 2010, will give new leadership to the modelling group.

Ray Ryan
Head of School

2 Presentations

Explicit Small Classifying Spaces for a Range of Finitely Presented Infinite Groups

Dr. Maura Clancy
NUI Galway.

While a classifying space $B(G)$ exists for any group G, in reality given a group presentation, finding a productive $B(G)$ is by no means trivial. This talk is intended to give a general overview on explicit small classifying spaces for a range of finitely presented infinite groups, and on using these spaces to deduce homological information on the groups. In keeping with the aims of a School Research Day, I also hope to give a brief account of my experiences as a Ph.D. student at NUI Galway.

Groups, Computing and Designs

Dr. Alla Detinko
NUI Galway.

In this talk we present an overview of the activities of the research group 'Groups, Computing and Designs' recently established in the School. Special consideration will be given to our research in computational theory of matrix groups.

Statistical Modelling

Prof. John Hinde
NUI Galway.

Much statistical research within the School comes under the general area of statistical modelling. This encompasses both application and methodological development with a strong computational component. Important research themes revolve around mixture and random effect models. This talk will introduce some of these modelling techniques through the reanalysis of a large educational dataset on teaching style and pupil performance. Specific methods include: a latent class (mixture) model for clustering based on binary indicators of teaching style; variance component models relating the teaching styles, determined by the cluster analysis, to pupil progress; and normal mixture and factor models for pupil personality. There are many common strands to the different models used and in the computational approaches, with heavy reliance on the EM algorithm. We will illustrate some of these and highlight how they link to other ongoing research in the School.

Some Mathematical Models for Drug Delivery

Dr. Martin Meere
NUI Galway.

Much of this talk will consist of a general introduction to the mathematical modelling of drug delivery systems. Optimal drug delivery requires the drug to be delivered to the right place, at the right time, and with the required dosage and release duration. Mathematical modelling has been extensively used to help realise these goals. In this talk, I shall describe some problems for barrier release (reservoir) systems, monolithic systems, stent systems, and systems involving polymer swelling.

Experiences in Industrial Mathematics

Prof. Stephen O' Brien
University of Limerick and MACSI.

Set-Valued Maps and Fixed Point Theory

Prof. Donal O'Regan
NUI Galway.

An Overview of the Research Office, NUI Galway

Dr. Ann Ryan
NUI Galway.

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3 Poster Session

An Application of Survival Trees to the Study of Cardiovascular Disease

Alberto Alvarez Iglesias, John Newell, John Hinde and Liam Glynn.

Recursive partitioning methods are a popular non-parametric alternative to the classical parametric and non-parametric models in regression, classification and survival problems. They have been recognized as a useful modelling tool as they produce a model that is very easy to interpret. In general, the aim of any statistical model is to explain the complicated interstructure between a large number of explanatory variables and the response, in the simplest way possible, and to use the model to predict the outcome of interest when new observations are considered. Single trees are an excellent way to describe the structure of the learning data but their predictive power can be disappointing. In the last decade, many efforts have been made to overcome this problem. These methods are generally known as "ensemble methods" and they use a set of trees, created by bootstrapping the original data, in order to improve predictability. The price to be paid, however, is the absence of a singular tree.

In this work, a data set of 1586 patients with cardiovascular disease will be analyzed. The primary endpoint was a cardiovascular composite endpoint, which included death from a cardiovascular cause or any of the cardiovascular events of myocardial infarction (MI), heart failure, peripheral vascular disease and stroke. Seventeen factors/covariates will be considered for development of a prognostic model and the results of different methods for growing survival trees will be compared.

[1] Breiman, L., Friedman, J.H., Olshen, R.A. and Stone, C.J. (1984), *Classification and Regression Trees*. Wadsworth, Belmont, CA.

[2] Breiman, L. (2003). Manual setting up, using and understanding random forests V4.0.

[3] Breiman, L. (1996). Bagging predictors. *Machine Learning* **24(2)**, 123-140.

[4] Breiman, L. (2001). Random forest. *Machine Learning* **45(1)**, 5-32.

[5] Harrell, F.E., Lee K.L., Mark, D.B. (1996). Tutorial in biostatistics. Multivariable prognostic models: issues in developing models, evaluating assumptions and adequacy, and measuring and reducing errors. *Statistics in Medicine* **15**, 361-387.

[6] Ishwaran, H., Kogalur, U.B., Blackstone, E.H. and Lauer, M.S. (2008). Random survival forest. *The Annals of Applied Statistics* **2**, 841-860.

[7] Leblanc, M. and Crowley, J. (1992). Relative risk trees for censored survival data, *Biometrics*, **48**, 411-425.

Supported by IRCSET grant.

A Quiver Presentation of the Descent Algebra of the Symmetric Group

Marcus Bishop, Götz Pfeiffer

We show how a presentation of the descent algebra of the Symmetric Group can be derived from a map from an algebra of binary trees into the free Lie algebra. We then introduce a quiver whose path algebra injects into the algebra of binary trees. Composing these two maps provides a presentation of the descent algebra in terms of a quiver subject to relations which we calculate explicitly.

[1] Götz Pfeiffer. A quiver presentation of Solomon's descent algebra. *Adv. Math.*, 220:1428–1465, 2009.

[2] Louis Solomon. A Mackey formula in the group ring of a Coxeter group. *J. Algebra*, 41(2):255–264, 1976.

Supported by IRCSET

Lattice of Topologies

Jorge Bruno, Aisling McCluskey

Given a set X, the lattice $LT(X)$ of all topologies on X (under set inclusion) has been studied extensively and is well understood. In this scenario, it is still interesting to investigate topologies on $LT(X)$ for which a particular family of functions is continuous. In particular, topological lattices are those for which $\wedge_x(y) = x \wedge y$ and $\wedge : LT(X) \times LT(X) \to LT(X)$ are continuous.

Another less natural, but just as interesting, order on $LT(X)$ is given by the embeddablity ordering. Where

$A \leq B \iff A \hookrightarrow B$. This order arises naturally within $\mathscr{P}(X)$ to find representations of partial orders within such set. Moreover, many independent results have been encountered within this topic. At this stage, regarding embeddability, the general hypothesis is to investigate the possibility of *evolution of topologies* (for a fixed set X). By this is meant a way to topologise $LT(X)$, so rendering the discussion of continuous maps $f : [0,1] \to LT(X)$ meaningful and useful. One could then track the *evolution* of topologies from $f(0)$ to $f(1)$, say. Achieving such an aim would enable a host of different research questions to be raised, such as whether there is a continuous function from $f(0)$ to $f(1)$, or whether, given topological properties P and Q, we can determine a continuous function f such that $f(0)$ is P while $f(1)$ is Q.

Supported by IRCSET

Some Mathematical Models of Anaerobic Digestion

Kevin Doherty, Martin Meere

Anaerobic digestion is a process in which biodegradable material is broken down into simpler products by microorganisms in the absence of oxygen. The process can take place naturally in areas where oxygen is not readily available as the main electron carrier for chemical reactions, such as in landfills, or underwater. We formulated and analysed some models for the digestion process.

We considered one of the simplest feasible models for anaerobic digestion. This model tracks the evolution of two types of substrate (influent and volatile fatty acids) and two populations of microbial species (acidogens and methanogens). We considered the solution to this model subject to conditions appropriate to continuous operation in a reactor. The analysis consists largely of investigating the stability of the equilibrium points. We also performed an asymptotic analysis of the model subject to conditions appropriate to batch operation.

Finally, we considered a much larger model - the Anaerobic Digestion Model No.1 (ADM1) [1]. This model tracks the evolution of twenty four different substrates and seven different microbial populations, and takes account of biochemical processes, physico-chemical processes and various types of inhibition. The model was successfully implemented in both Maple and Matlab.

[1] D.J. Batstone, J. Keller, I. Angelidaki, S.V. Kalyuzhnyi, S.G. Pavlostathis, A. Rozzi, W.T.M. Sanders, H. Siegrist & V.A. Vavilin. *Anaerobic Digestion Model No.1 (ADM1)*, Scientific and Technical Report No.13. IWA publishing, 2002.

Vertex Operator Algebras

Hoang Dinh Van, Michael Tuite

I am working on Vertex Operator Algebras. Here is a short description of my reading including: Formal Distributions, Locality, Vertex Algebras, and Vertex Operator Algebras.

[1] Goeffrey Mason and Michael Tuite, *Vertex Operators and Modular Forms*, "A Window Into Zeta and Modular Physics", MSRI Publications Volume 57 (2010).

[2] Victor Kac, *Vertex Algebras for Beginners*, University Lecture Series 10, AMS (1998).

Supported by Science Foundation Ireland.

Matching: An Example Analysis of a Colorectal Cancer Observational Study

Cara Dooley, John Hinde, John Newell

The aim of the study was to compare survival of colorectal cancer patients in the whole population against the survival of patients in a sub-population who also had inflammatory bowel disease (IBD). All individuals who suffered from colorectal cancer were drawn from the entire Irish population using data from January 1994 to December 2005 provided by the National Cancer Registry of Ireland (NCRI).

The control group contained many more observations ($n > 20000$) when compared to the IBD group ($n = 170$). Given the number of control patients, there was large diversity in this group. In a conventional designed experiment or trial, patients entering the trial would be taken to be as similar as possible. Usually patients would be similar in age, health etc. As this was an observational study, there was no design prior to collecting the data.

To compensate for this lack of design, each IBD patient is matched to the ”closest” control patient. For each pair of IBD and control patients a distance is calculated and those two patients which have the smallest distance between them (and are so are the most similar) are matched. The distance used in this case is a Malanhobis distance based on ranks. The matching is carried out using the Optmatch Package in R.

Supported by SFI grant 07/MI/012

Tree-Based Classification and a Logistic Regression Model for HER2 Diagnosis Using Gene Expression Data

Orla Doolin, John Newell

HER2-positive is a breast cancer tumour that tests for the human epidermal growth factor receptor 2, a protein that promotes higher aggressiveness and faster growth of cancer cells. HER2 is overexpessed in 25-30% of breast tumors and has been shown to be associated with poor prognosis and increased disease recurrence. Accurate evaluation of HER2 receptor status in invasive tumors is critical in its prognostic role as well as its ability to predict response to antibody treatments for the patient. This study is part of an increasing effort to create an alternative molecular basis for tumour classification, moving away from the classical morphologic systems based on macro and microscopic histology. There now exist microarray technologies that can simultaneously assess the level of expression of thousands of genes and demonstrate the potential power of expression profiling for classifying tumours. For this cancer cohort, with data from the National Breast Cancer Research Institute Galway, the goal is to quantify the dependence of HER2 status positive or negative across a set of gene markers, ER ALPHA, GRB7, Her2, LASP1, RARA, RPL19, STARD3, TUBG1 and TOP2A. Receptor status on estrogen, progesterone and HER2 divide the cohort of 95 women into four intrinsic molecular subtypes, Luminal A and Basal corresponding to HER2-negative and Luminal B and HER2 Overexpressing corresponding to HER2-positive. Described in particular is the use of recursive partitioning techniques and tree-based methodology in HER2 diagnosis based on microarray gene expression data. Improvements in classification accuracy are obtained by use of the recently published R package party which implements Breiman and Cutler’s random forests, using unbiased conditional inference trees from ctree as base learners.

Supervised by Dr.John Newell

Supported by National Breast Cancer Research Institute, Galway.

Heritability and Genome-Wide Association (GWAS) Assay of MicroRNA Regulatory Efficacy

Paul Geeleher, Prof. Cathal Seoige and Dr. Aaron Golden

MicroRNAs are small non-coding RNA molecules that regulate the expression level of genes by binding to messenger RNA targets, which prevents these messenger RNA molecules from being translated into mature proteins. We have performed an analysis to investigate the genetic compont involved in the regulatory effect of microRNAs. The Regulatory Effect (RE) score [1] is used to measure the inhibitory effect of a microRNA in a sample by measuring the expression levels of the microRNA’s messenger RNA targets, independent of the expression level of the actual microRNA; it is calculated from the the average difference in expression level of the targets versus non-targets, where the targets have been determined previously by target-prediction algorithms such as PITA [2]. The Hapmap project is an international collaboration which aims to catalogue the main sources of variation in the human genome with and between distinct geographic populations based on single nucleotide polymorphisms (SNP). The project members have used SNP microarrays to genotype groups of trios of individuals (two parents and one child) from several worldwide geographic regions. Other affiliated groups have used the cell lines produced by the project to perform gene expression studies that measure messenger RNA levels. Using this data and because these cell line samples are related by genetic lineage we have been able to ascertain that there is a heritable component to the regulatory effect of microRNAs. This seems to suggest that the entire miRNA processing machinery operates at a lower level of activity overall in a sub-population defined by specific genotype SNPs. We have performed a genetical genomics assay but have thus far been unable to identify expression quantatitive trait loci (eQTL) that show a statistically significant association with this altered RE-score. We are currently assessing the likely causative effects of such diminished microRNA regulatory efficacy.

[1] Chao Cheng, Xuping Fu, Pedro Alves and Mark Gerstein: *mRNA expression profiles show differential regulatory effects of microRNAs between estrogen receptor-positive and estrogen receptor-negative breast cancer.*, Genome Biology 2009, 10:R90

[2] Michael Kertesz, Nicola Iovino, Ulrich Unnerstall, Ulrike Gaul & Eran Segal *The role of site accessibility in microRNA target recognition.*, Nature Genetics 39, 1278 - 1284 (2007)

Supported by IRCSET

Computational Homology and Permutahedral Complexes

Fintan Hegarty, Graham Ellis

Homology is the study of connectivity and "holes " in spaces. This thesis is aimed at the homological study of subsets of $\mathbb{R}^n$ arising from experimental data. We develop a mathematical machinery for efficiently computing the homology of cellular spaces with a view to applications in image analysis. We discuss and implement in GAP a cubical approach to homology computations, and then introduce and implement a new approach based on permutahedral complexes. We compare the efficiency of these new computations using permutahedral complexes with those using the more traditional cubical and simplicial complexes. Our guiding example is an analysis of computed tomography images used for radiation therapy.

Supported by SFI

Analysis of Grazing Bifurcations within a Discontinuity-geometry Framework

Neil Humphries, Petri Piiroinen

Inherent discontinuities in a *piecewise-smooth* (PWS) dynamical system can cause considerable difficulties in forming a qualitative picture of how the behavior of such a system changes under parameter variation, with an extra range of behaviors not shown by smooth systems, such as period-adding and robust chaos. One type of PWS system is a *periodically-forced impact oscillator* (PFIO), which has two fundamental components; a smooth dynamical system that models the system in free-flight between impacts and a reset rule that models the impact. If the impact surface is sufficiently far from the natural centre of oscillation, then the only orbit of such a system will be a non-impacting one. Eventually, as the impact surface is brought ever closer to the natural centre, this orbit is destroyed at a grazing bifurcation and impacting orbits will appear. However, under parameter variation there is a wide range of different behaviours that could be manifested around this bifurcation.

This study is exploring a geometric methodology — 'Discontinuity-Geometry' — to assist in both analysing and understanding PFIOs. After a brief introduction to this framework, with definitions of the geometric objects used, we will use the discontinuity-geometry framework to both analyse and explain the differences in behaviour manifested by such a system in two damping scenarios.

This project is supported by IRCSET

Classification Problems for Finite Linear Groups

Barry Hurley, Dane Flannery

This thesis is concerned with classification problems for finite linear groups. Our main concern is with groups of prime degree, and groups defined over finite fields; although we obtain results for groups of other degrees and over other fields, some of which are of independent interest.

It is broken down into three parts:

- a solution to the listing problem for the finite insoluble irreducible subgroups of $GL(3,\mathbb{F})$, where $\mathbb{F}$ is a non-modular splitting field for the groups.
- soluble groups in prime degree, and degree the product of two (different) primes.
- Elimination of exceptional characteristics in degrees 2 and 3.

We use the system MAGMA[1] to carry out the implementation of our classifications. The work carried out in [2], [3], and [4] are essential reference points.

[1] W. Bosma, J. Cannon and C. Playoust. *The Magma algebra system. I. The user language,* (J Symbolic Comput. 24 (1997) 235-265).

[2] H.F. Blichfeldt. *Finite collineation groups*, (University of Chicago Press, 1917).

[3] J.D. Dixon. *The structure of Linear Groups*. (Van Nostrand Reinhold, London. 1971).

[4] D.L. Flannery, E.A. O'Brien. *Linear Groups of Small Degree over Finite Fields*. (International Journal of Algebra and Computation, Volume 15, No.3, 2005).

Virasoro Correlation Functions for Vertex Operator Algebras

Donny Hurley, Michael Tuite

We are interested in n-point Correlation functions for these types of Vertex Operator Algebras on Riemann surfaces of genus zero and one. These functions are not manifestly symmetric, however, it can be shown that they are symmetric for $z_1,\dots,z_n$ and described using graphical representations with weights attached to the edges in the graph.

For a function over a sphere (genus zero), the n-point function can be defined as an inner product $\langle \mathbf{1}, Y(\omega,z_1)\dots Y(\omega,z_n)\mathbf{1}\rangle$, a rational function in $z_1,\dots,z_n$. Using a recursive reduction formula the n-point function can be expressed as a sum of all directed graphs with n vertices and each vertex has exactly 2 edges. It is also possible to describe the n-point function using the set of **derangements** of the label set $\Phi = \{1,\dots,n\}$.

For a function over a torus (genus one), the n-point function $G_n(z_1,\dots,z_n)$ can be calculated using Zhu's Reduction Formula. In this case there are terms involving the Eisenstein series E_2, modular functions $P_2(z_i - z_j)$ and q-derivative terms. Again we will express this as the sum of all directed graphs with n vertices and now each vertex has 0, 1 or 2 edges. This can be described as the set of all **permutations** of the label set $\Phi = \{1,\dots,n\}$.

[1] Y. Zhu, *Modular invariance of characters of vertex operator algebras*, J. Amer. Math. Soc. 1996, 9, 237302.

Supported by SFI

Computing in Symmetric Groups

Liam Naughton, Gotz Pfeiffer

This research is concerned with the development of new algorithms for the computation of the table of marks of the symmetric group. The table of marks of a finite group G is a matrix who's rows and columns are labelled by the conjugacy classes of subgroups of G and where for any 2 subgroups H_1 and H_2 of G the (H_1,H_2)-entry in the table of marks is the number of fixed points of H_2 on the right cosets of H_1 in G. The table of marks characterises the set of all permutation representations of G.

[1] Pfeiffer, G *The subgroups of M_{24} or how to compute the table of marks of a finite group.*, Experimental Mathematics **6**, 1997

[2] Labelle, J, Yeh, Y.N. *The relation between Burnside rings and combinatorial species.*, Journal. Combin. Theory. Ser. A 1989

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Design and Function of Transcription Factors in the Chromatin Environment

Nguyen Trung Thong, Andrew Flaus, and Cathal Seoighe

Nucleosomes are the fundamental organising units of eukaryotic genomes. They control the packaging of DNA as chromatin and play key roles in modulating transcription, replication and repair. We hypothesize that binding sites for different transcription factors have distinct positional preferences relative to the nucleosome which can influence their efficiency. Here, we use public ChIP-seq data of nucleosome occupancy and transcription factor binding sites (TFBSs) and develop a robust methodology for predicting functional TFBSs and inferring the relationship between nucleosome occupancy and TFBSs.

A Note on the Numerical Solution of the ICU-Minimal Model (ICU-MM)

Anh Thai Nhan, Niall Madden

This work is part of a larger project concerning the modelling of the reaction of ICU patients to certain drug therapies [1]. Colleagues in Applied Mathematics are working on analysis of existing mathematical models [2], and the design of new one. Researchers in Information Technology are then incorporating these models into a Dynamic Bayesian Network [3]. Our role is to design numerical methods that can be used to solve the equations in the model numerically and can integrated efficiently into the DBN. The models present several challenges. Here we focus on problems caused by discontinuities in the data.

[1] Van Herpe et al, *Nonlinear model predictive control with moving horizon state and disturbance estimation - Application to the normailization of blood glucose in the critically ill*, Proc. 17th IFAC World Congress, Seoul, Korea, July 6-11, 2008.

[2] Liam O'Callaghan and Dr. Petri T. Piiroinen, *Models of Glycemic Regulation*, School of Mathematics, Statistics and Applied Mathematics Poster Session, April 2010.

[3] Catherine G. Enright, et al., *Modelling glycaemia in ICU patients — a dynamic Bayesian network approach*, Proc. BIOSIGNALS 2010, Valentia, Spain.

Supported by SFI RFP/CMS/1254.

Models for Glycemic Regulation

Liam O'Callaghan, Petri Piiroinen

The mechanisms by which blood sugar is regulated (by a complex process involving many hormones, including insulin and glucagon) are quite well understood. The dynamics of the system, however, are not. Essentially, a practitioner administering insulin would have an idea of the chain of events that, following the drug's administration, result in lowering a patient's blood sugar level. However, the magnitude of such an effect can at present not be predicted with a significant level of accuracy.

We present an analysis of a "minimal model" which was recently developed for glycemic control in the critically ill. A minimal model is essentially the smallest possible model that expresses the features that are required. The analysis consists of looking for blood glucose values to which the model will move towards, or move away from, and also the nature of this motion. Whether or not the predictions made by this model are realistic is obviously of critical importance.

The prospects for future advancement and the development of a full-scale description of the glucose regulatory system will also be presented. In particular, the binding process between insulin and its corresponding receptors needs to be effectively modelled, and the subsequent signalling which results in the lowering of blood glucose explained, if the effect of insulin is to be properly quantified.

Hadamard Matrices from Difference Sets

Padraig Ó Catháin, Dane Flannery

In this poster, we show that no Hadamard matrix constructed using the twin prime power method is cocyclic, with the exception of the matrix of order 16. We achieve this by showing that the action of the automorphism group of a cocyclic twin prime power matrix induces a 2-transitive action on the rows of the matrix. We then use Ito's classification of Hadamard matrices with 2-transitive automorphism groups to show that exactly one twin prime power Hadamard matrix is cocyclic. This work answers a research problem posed by K.J. Horadam, and exhibits the first known infinite family of Hadamard matrices which are not cocyclic.

[1] Ó Catháin, P. & Röder, M. *The cocyclic Hadamard matrices of order less than* 40, Designs, Codes & Cryptography, to appear.

[2] Ó Catháin, P. & Stafford, R. *On twin prime power Hadamard matrices* Cryptography and Communications - Discrete Structures, Boolean Functions and Sequences, to appear.

A Method to Analyse Students' Proof Evaluation

Kirsten Pfeiffer, Rachel Quinlan

Interested particularly in the students' transition from school to university I explore first year students' behaviour and knowledge when validating and evaluating mathematical proofs. A significant aim of my developmental study is to develop and test a method to describe and analyse students' proof validation and evaluation skills and habits. I will here outline the ideas which led to a new perspective and terminology of description and analysis of transcripts of recently held interviews.

Convolutional Codes from Group Rings

Jessica O'Shaughnessy, Ted Hurley

An original group ring construction for convolutional codes was proposed in 2009 . This group ring construction uses an isomorphism between group rings and group ring matrices to construct generator and control matrices from units in the group ring. This construction is extended to a new group ring construction. This new construction has several interesting free distance properties. Additionally, it can be used to construct LDPC convolutional codes, systematic convolutional codes, and some other optimal convolutional codes.

[1] T. Hurley. *Convolutional Codes from Units in Matrix and Group Rings*, Inter. J. Pure & Appl. Mathematics, **50**, n.3 (2009), 431–463.

Algorithms for Nilpotent Linear Groups

Tobias Rossmann, Dane Flannery, Alla Detinko

We describe an algorithm for irreducibility testing of finite nilpotent linear groups over various fields of characteristic zero, including number fields and rational function fields over number fields. For a reducible group, our algorithm constructs a proper submodule. An implementation in MAGMA is publicly available. Details on the algorithm and its implementation can be found in [1].

We extended our work on irreducibility testing and also obtained an algorithm for primitivity testing of finite nilpotent linear groups over cyclotomic fields. For an imprimitive group, a system of imprimitivity is constructed.

This work is supported by the Research Frontiers Programme of Science Foundation Ireland.

References

[1] T. Rossmann. *Irreducibility testing of finite nilpotent linear groups.* Accepted by *J. Algebra*, 2010.

An Additive Penalty Approach to Derivative Estimation of Noisy Data

Andrew Simpkin, John Newell

It is often the case that when analysing data the derivative, or rate of change, of the underlying function describing the observed data is of primary interest. A popular tool for derivative estimation is spline smoothing, with a large number of variants being available. We present a method for derivative estimation which extends the *P*-spline fitting procedure to include an extra additive penalty term for increased robustness in smoothing. The method is applied to biomedical data and compared with several alternative techniques. A small simulation study is presented to gain further insight about the relative performance of the extended *P*-spline procedure.

Modelling of Drug Delivery

VO Thi Ngoc Tuoi, Martin Meere

The effect of binding sites to drug diffusion in the artery tissue is considered. A reversible chemical reaction that explains the prolonged presence of drug in the vascular tissue was used to model the presence of the binding site action. In addition, the effect of polymer swelling for the control of drug release is investigated. One of the useful thermoresponsive polymers is Poly(N-isopropylacrylamide) (PNIPAm). This polymer is hydrophilic below the lower critical solution temperature (LCST) 32^0 C, but hydrophobic above 32^0 C, a property that can be exploited to act as an on/off switch to control drug delivery by varying temperature. Initially, there is a good agreement between numerical solutions of the model and experimental datas.

[1] A. Borghi, E. Foa, R. Balossino, F. Migliavacca and G. Dubini, *Modelling drug elution from stents: effects of reversible binding in the vascular wall and degradable polymeric matrix*, Computer Methods in Biomechanics and Biomedical Engineering **11** (2008) 367–377.

[2] J. Siepmann, F. Siepmann, *Mathematical modelling of drug delivery*, International Journal of Pharmaceutics **364** (2008) 328–343.

[3] J. Crank, *Free and Moving Boundary Problems*, Oxford University Press, Oxford, UK (1984).

Supported by MACSI

A Study of Item Selection using Principal Component Analysis and Correspondence Analysis

Nur Fatihah Mat Yusoff, John Hinde

This study investigates dimension-reduction techniques in psychometric testing by using Principal Component Analysis (PCA) and Correspondence Analysis (CA). Psychometric research is one of the fields of social science study that is interested in the theory and techniques of education and psychological measurement. Researchers in this area are frequently concerned with the construction and validation of measurement instruments. Theoretically, PCA is a mathematical algorithm that transforms a number of possibly correlated variables into a smaller number of uncorrelated variables by performing a covariance analysis between variables. The PCA concept is closely related to Factor Analysis (FA) which aims to detect structure in the relationships between variables. It is a common technique that has been used by social science researchers in conducting validity and reliability analysis of their study. The CA can be considered as a factor method for the categorical variables and is often linked with producing a low-dimensional graphical display of variables and units. Simple CA is a technique designed to analyse a two-way table, while Multiple Correspondence Analysis (MCA) is an extension of simple CA in that it is applicable to a large set of variables. The result will provide information which is similar in nature to those produced by principal component analysis, and allows us to explore the structure of the categorical variables included in the table.

This study is concerned with reducing the dimension, or number of variables, in an instrument by using the data from a pilot study on personality traits. The original instrument was developed by Oliver P. John and Sanjay Srivastava from University of California, Berkeley in 1999. The pilot survey was conducted at the University Malaysia Sarawak, Malaysia where 80 students from second year and above were randomly selected as respondents. In the original instrument, there are 44 items to assess five personality traits, or the big five dimensions. We believe that some of the items, or even dimensions are not relevant in the Malaysian context. At the end of this study, our aim is to produce the best instrument that can represent all of the variables that we are interested in for subsequent use in structural equation modelling of student achievement.

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[3] Hair, J. F., Anderson, R. E., Tatham, R. L., and Black, W. C. (1998), *Multivariate data analysis with readings*, 5th ed., Englewood Cliffs, NJ: Prentice Hall.

[4] Lynn, S. H. and McCulloch, C. E. (2000), Using principal component analysis and correspondence analysis for estimation in latent variable models, *Journal of the American Association*. 95(450), 561–572.

[5] Vyas, S. and Kumaranayake, L. (2006), *Constructing socio-economic status indices: how to use principal components analysis*, London:Oxford University Press.

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4 Abstracts of Recent PhD Theses

On Abelian Ideals in a Borel Subalgebra of a Complex Simple Lie Algebra

Patrick Browne
Supervisor: Dr. John Burns

This is an abstract of the PhD thesis *On Abelian Ideals in a Borel Subalgebra of a Complex Simple Lie Algebra* written by Patrick Browne under the supervision of Dr. John Burns at the Department of Mathematics, National University of Ireland, Galway and submitted in December 2008.

Let $\mathfrak{g}$ be a complex simple Lie algebra and $\mathfrak{b}$ a fixed Borel subalgebra of $\mathfrak{g}$. We construct all maximal (with respect to containment) abelian ideals of $\mathfrak{b}$ by a variety of methods each having their own merits. We also derive formulas for their dimensions. Then we give a new proof of Kostant's theorem on the dimension of an abelian ideal. Finally we apply our results to give new examples of Einstein solvmanifolds.

We now give a brief historical account of interest in this area. In 1945 A. Malcev [1] determined the commutative subgroups of maximum dimension in the semisimple complex Lie groups. The maximal dimension of these commutative subgroups coincides with the maximal dimension of a commutative subalgebra of $\mathfrak{g}$. The next development was Kostant's [2] paper published in 1965, where he gave a connection between Malchev's result and the maximal eigenvalue of the Laplacian acting on the exterior powers ($\bigwedge^k \mathfrak{g}$) of the adjoint representation. In 1998 Kostant reported on the results of Peterson that the number of abelian ideals in the fixed Borel subalgebra of $\mathfrak{g}$ is $2^{rank(\mathfrak{g})}$, and this paper was the genesis of much of the recent interest in this area. In [3], Panyushev and Röhrle while studying the relationship between spherical nilpotent orbits and abelian ideals of $\mathfrak{b}$, constructed all maximal abelian ideals, with the aid of a computer program [4], and observed a bijection between them and the set of long simple roots. Our method does not require the use of computer calculations. Suter in [5] found the maximal dimension of a maximal abelian ideal using the affine Weyl group, in terms of certain Lie theoretic invariants and gave a uniform explanation of the one to one correspondence between the long simple roots and the maximal abelian ideals. In [6] Papi and Cellini gave formulas for the dimension of all maximal abelian ideals in $\mathfrak{b}$, similar to that of Suter. The new formulas in this thesis are simpler and different in nature.

The methods used in the thesis rely heavily on the theory of graded Lie algebras. We also give an alternative proof of Kostant's theroem that does not require the representation theory used by Kostant. Finally our results are used to contruct new examples of non compact Einstein solvmanifolds.

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[2] Kostant, B., *Eigenvalues of a Laplacian and commutative Lie subalgebras*, Topology, vol.3, 1965,pp.147-159.

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[5] Suter, R., *Abelian ideals in a Borel subalgebra of a complex simple Lie algebra*, Inventiones Mathematicae, vol.156, 2004,pp.175-221.

[6] Cellini, P. and Papi, P. , *Abelian ideals of Borel subalgebras and affine Weyl groups*, Adv. Math., vol.187, 2004,pp.320-361.

Explicit Small Classifying Spaces for a Range of Finitely Presented Infinite Groups

Maura Clancy
Supervisor: Dr. Graham Ellis

This is an abstract of the PhD thesis *Explicit small classifying spaces for a range of finitely presented infinite groups* written by Maura Clancy under the supervision of Dr Graham Ellis at the School of Mathematics, Statistics and Applied Mathematics, National University of Ireland, Galway and submitted in February 2009.

While a classifying space B_G exists for any group G, in reality given a group presentation, finding a productive B_G is by no means trivial. This thesis unearths explicit small classifying spaces for a range of finitely presented infinite groups and uses these spaces to deduce homological information on the groups.

In Chapter 2 we derive formulae for the second integral homology of any Artin group for which the $K(\pi,1)$-conjecture is known to hold, and for the third integral homology of the braid group A_n and the affine braid group $\tilde{A}_n$. The derivation and proofs are based on the cellular chain complex $C_*(\tilde{X}_D)$, where $\tilde{X}_D$ is the universal cover of a classifying space B_G for the group $G \in \{A_n, \tilde{A}_n\}$. Chapter 3 defines *polytopal* groups, actions and classifying spaces. We prove that a group G is polytopal when G is the semi-direct product of two polytopal groups N and Q. We show that $\tilde{B}_N \times \tilde{B}_Q$ is the universal covering space of a polytopal classifying space $\tilde{B}_G$ for G, where $\tilde{B}_N$ (resp. $\tilde{B}_Q$) is the universal covering space of a polytopal classifying space B_N for N (resp. B_Q for Q). We further show that the cellular chain complex $C_*(\tilde{B}_G)$ can be obtained as the total complex of a double complex with $Dim(B_N)$ rows and $Dim(B_Q)$ columns, a fact alternatively proven by Thomas Brady in his paper "Free resolutions for semi-direct products". Chapter 4 centres on Bieberbach groups; we realise six of the ten 3-dimensional Bieberbach groups as semi-direct products $G = N \rtimes_\alpha Q$, where N is 2-dimensional Bieberbach and $Q = C_\infty$. This technique can be extended to determine, inductively, classifying spaces for higher dimensional Bieberbach groups. Chapter 5 introduces *twisted Artin groups* $\mathfrak{A}_{\vec{D}}$ and shows that in some cases there exists a polytopal classifying space whose t-dimensional cells are indexed by the finite type subsets, of size t, of the generating set S. We show that 3-generator twisted Artin groups of large type admit a two-dimensional classifying space. Using star graph techniques we show that such classifying spaces are non-positively curved for standard Artin groups of large type. In Chapter 6 we conjecture that certain groups are quasi-lattice-ordered and then use a GAP routine to experimentally investigate the word-reversing algorithm.

Combinatorial Polytopes and Group Cohomology

Séamus Kelly
Supervisors: Dr. Graham Ellis and Dr. J. Cruickshank

This thesis investigates the practicality of a method for computing group homology described in the paper "Polytopal resolutions for finite groups" by Ellis, Harris and Sköldberg. Using a mix of theoretical and computational results we show that the method is certainly practical for the low-dimensional homology of Mathieu groups, isometry groups of $\mathbb{R}^3$, and finite reflection groups and their even subgroups. The main new results in the thesis are:

[1] the description of the combinatorial structure of an orbit polytope for the even subgroup of a finite reflection group;

[2] the existence of a simple orbit polytope for some Mathieu groups, and a partial description of its combinatorial structure;

[3] efficient GAP/Polymake code for computing the combinatorial structure of orbit polytopes.

Dihedral Codes

Ian McLoughlin
Supervisor: Prof. Ted Hurley

This is an abstract of the PhD thesis *Dihedral Codes* written by Ian McLoughlin under the supervision of Professor Ted Hurley at the School of Mathematics, Statistics and Applied Mathematics, National University of Ireland, Galway and submitted in June 2009.

In this thesis we give new constructions of a number of extremal type II codes. Algebraic proofs are provided that the constructions do in fact yield the codes. The codes are constructed using group rings of which the underlying groups are dihedral. Type II codes are not cyclic, but the constructions here are similar to the constructions of cyclic codes from polynomials.

The first code we construct is the extended binary Golay code. It is constructed from a zero divisor in the group ring of the finite field with two elements and the dihedral group with twenty-four elements. We create a generator matrix of the code that is in standard form and is a reverse circulant generator matrix. The generator matrix generates the code as quasi cyclic of index two.

Algebraic proofs are given of the code's minimum distance, self-duality and doubly evenness. A list of twenty-three other zero divisors that we have found to generate the code is given. Trivial changes adapt the aforementioned algebraic proofs to any of these zero divisors. We also prove that the twenty-four zero divisors are the only ones of their form that will generate the code.

Next we construct the $(48, 24, 12)$ extremal type II code as a dihedral code. The new construction is similar to that

of the extended Golay code. Again, proofs of the self-duality and doubly evenness are given. An algebraic proof of the minimum distance is achieved through the use of two different group ring matrices.

A number of different codes are then constructed, building on the first two constructions. We list some zero divisors that generate type II codes of lengths seventy-two and ninety-six. According to investigations by computer, these codes have minimum distances of twelve and sixteen respectively. No type II codes of each of these lengths are known that have greater respective minimum distances. Some techniques are detailed that vastly reduce the calculations involved in their analysis.

The constructions of the $(72,36,12)$ and $(96,48,16)$ codes are facilitated by the construction of extremal type II codes of all lengths a multiple of eight up to length forty. Type II codes only exist at lengths that are multiples of eight. Overall we have shown that extremal type II codes can be constructed in dihedral group rings at every length a multiple of eight up to and including length forty-eight, and at some lengths beyond forty-eight. We also successfully investigate the possibility to construct some type I codes in the same way.

The Hochschild Cohomology Ring of a Quadratic Monomial Algebra

David O'Keeffe
Supervisor: Dr. Emil Sköldberg

This is the abstract of the PhD thesis *The Hochschild Cohomology Ring of a Quadratic Monomial Algebra*, written by David O'Keeffe under the supervision of Dr. Emil Sköldberg at the Department of Mathematics, National University of Ireland, Galway and submitted in January 2009.

Until recently, little was known about the multiplicative structure of the Hochschild cohomology ring for most associative algebras. During the last decade or so, more light has been shed on this topic, with several papers published regarding the structure of the Hochschild cohomology ring for various algebras.

In this thesis, we compute the Hochschild cohomology groups for a special class of associative algebras: the so-called class of Quadratic monomial algebras. These results are then used to compute the Hochschild cohomology ring for the above class of algebras. In doing this, we extend results obtained by Claude Cibils, where he computes the cohomology ring for the class of radical square zero algebras. The latter class of algebras form a subclass of the class of quadratic monomial algebras.

Chapter 1 consists of all the necessary background material that is referred to throughout this work. There are also some new proofs of already known results. However most of the original work is contained in chapters 2, 3 and 4.

Chapter 2 describes the Hochschild cohomology groups of a quadratic monomial algebra in terms of the cohomology of a graph. An alternative calculation of these groups was performed by Emil Sköldberg. Also in this chapter we describe the generating elements of the cohomology algebra.

Chapter 3 builds on the calculations of the previous chapter by computing the algebra structure on the cohomology algebra. We describe the product structure on the cohomology algebra as a composition of chain maps on a projective resolution.

Finally using the algebra structure calculated in Chapter 3 and the Hilbert series of a vector space, we show in Chapter 4, the cohomology algebra of a quadratic monomial algebra exhibits all possible behaviours as an algebra: It may be

- finite dimensional over k,
- finitely generated over k,
- infinitely generated over k,

where we write k to denote a field of arbitrary characteristic.

REFERENCES

[1] Claude Cibils, *Hochschild cohomology algebra of radical square zero algebras,* Algebras and modules, II CMS Conf.Proc.,vol.24, Amer.Math.Soc., Providence, RI, 1998,pp.93-101.

[2] Emil Sköldberg, *Some Remarks on the Hochschild cohomology of graded algebras*, (preprint), available from http://www.maths.nuigalway.ie/emil

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Three Problems in Algebraic Combinatorics

David Quinn
Supervisor: Dr. Emil Sköldberg

In this thesis we consider three problems in the broad area of algebraic combinatorics. In the first section we consider the incidence algebras of finite graded posets. We define the incidence algebra of a poset P to be the quotient of the quiver algebra on the Hasse diagram of P with the ideal generated by the differences of paths p_i, p_j such that source(p_i) = source(p_j) and destination(p_i) = destination(p_j). Our main result shows that these algebras have a quadratic Gröbner basis if and only if the poset is pure and lexicographically shellable as defined in [1]. We also generalise our result to pure augmented acyclic categories also defined in [1].

In the second section we consider a symmetric variant of the Orlik-Solomon algebra. The standard Orlik-Solomon algebra [3] can be defined as a quotient of the exterior algebra. It was first introduced as the cohomology algebra of the compliment of a hyperplane arrangement where it was shown to rely only on the dependencies among the hyperplanes. This dependence structure defines a matroid and the Orlik-Solomon algebra has since been studied for arbitrary matroids. Here we introduce a symmetric variant as a quotient of a polynomial ring $S = k[x_1, \ldots, x_n]$ and discuss a number of its ring theoretical properties and homological invariants. In particular, for uniform matroids U of rank 2, we show that the algebra is Gorenstein and calculate its minimal graded Betti numbers. We also describe the reduced Gröbner basis and Hilbert series of the algebra when the matroid U has even rank. In order to achieve some of these results we also calculate the graded Betti numbers of ideals with linear quotients.

Finally, following results of Sköldberg [2], we use algebraic discrete Morse theory to construct an explicit minimal Hochschild resolution of the commutative algebra $A = S/I$, where I is a stable ideal; that is, for any minimal generator mx_j of I with x_j such that $j \geq \max i \mid x_i | m$ then the monomial $mx_i \in I$ for all $i < j$. We start with the normalised Hochschild complex $HC_n := A \otimes A_+^{\otimes^n} \otimes A$, where A_+ is the positively graded part of A. This complex is a resolution, however it is far from minimal in general. Sköldberg describes an acyclic partial matching on the basis of this complex which may be used to define a homotopy to a smaller complex. Using this we construct a homotopy equivalent complex and give an explicit description of the differential. From the differential we see that this is a minimal resolution.

[1] D. Kozlov. *Combinatorial Algebraic Topology*. Springer, 2008.

[2] E. Sköldberg. *Morse theory from an algebraic viewpoint*. Trans. Amer. Math. Soc., 358:115-129, 2006.

[3] S. A. Yuzvinsky. *Orlik-Solomon algebras in algebra and topology.*, Russ. Math. Surv., 56:293-364, 2001.

Numerical Methods for Singularly Perturbed Differential Equations

Meghan Stephens
Supervisor: Dr. Niall Madden

This thesis is concerned with the design and analysis of numerical methods for some classes of singularly perturbed differential equations.

We first consider a parameterised reaction-diffusion problem, based on the Rayleigh and Orr-Sommerfeld models of hydrodynamic stability, where it is necessary to determine a function u and a parameter κ. Since κ depends on the derivative of u at a boundary, it is important to accurately estimate u in that region, and so we must resolve the layer. We develop an iterative technique that uses a finite difference method on a piecewise uniform, Shishkin mesh. An analysis of the method shows that the errors are parameter uniform and are almost second order convergent, which is supported with numerical results.

In the main body of the thesis we investigate the use of iterative overlapping Schwarz methods for coupled systems of reaction diffusion problems. We first consider the case when all the differential equations in the system have identical singular perturbation parameters $\varepsilon_1 = \varepsilon_2 = \cdots = \varepsilon_m = \varepsilon$. By appropriately choosing the overlaps of the subdomains we can ensure parameter uniform results and furthermore, when ε is sufficiently small we only require one iteration.

When the problem is generalised so that each equation may have distinct perturbation parameters the solutions have overlapping layers of different widths. Consequently we require more subdomains and, although the results are parameter uniform, the fast convergence of the iterates is

lost. We overcome this problem by developing a semi-iterative algorithm.

Finally we extend the Schwarz methods to two dimensional systems and demonstrate the benefits of the domain decomposition algorithms, in particular the reduction in computational effort.

5 Research Activity from 1 Jan 2009 to 1 April 2010

Permanent and Contract Staff

Aramayona, Javier

My research interests are situated at the intersection of geometry, topology and group theory. The action of a finitely generated group on a space with some flavour of nonpositive curvature provides a unifying theme for my work. More concretely, I study certain spaces of moduli of surfaces, known as Teichmuller spaces, and their symmetry groups, known as mapping class groups. My research activities from January 2009 until April 2010 include: - (co-)author of two published articles, one preprint and one article in preparation; - (co)organiser of six international conferences, in Dublin, Galway, Warwick and Singapore; - (co)recepient of four grants (Millenium Fund, Ulysses and Registrar Office NUIG); - visits to the Universidad Autonoma de Madrid (July-August 2009) and to the Institute for Mathematical Sciences (Singapore, July-August 2010) - research talks at various institutions of Ireland, United Kingdom, United States, France and Spain.

Browne, Patrick

My doctoral thesis was concerned with Abelian ideals in the Borel subalgebra of a complex simple Lie algebra (for more information see *http://arxiv.org/abs/math/0210463*). Currently I am working on extending the results from my doctoral thesis to the isotropy representation of a symmetric space. I am also investigating constructions of *Einstein solvmanifolds*. A Riemannian manifold is called a *solvmanifold* if it admits a transitive solvable group of isometries, and *Einstein* if the Ricci tensor is proportional to the metric.

Burns, John

Research Areas

- Differential geometry (homogeneous manifolds, Einstein metrics, contant mean curvature surfaces)
- Algebra (Lie Algebras, Coxeter Groups)

Recent Publications

[1] Exponents and highest root coefficients. Comm. Algebra 37 (2009), no. 11, 3815–3819.

[2] Recurrence relations and Dynkin diagrams (with M.J. Clancy D.C.U.) Proc. Roy. Irish Acad. Sect. A (to appear).

Other Research Activity

[1] Graduate Students: Dr. Patrick Browne (graduated Nov.2009)

[2] Conferences: Irish Geometry Conference 2009 Cork

Clancy, Maura

My area of research is Algebraic Topology. The title of my doctoral thesis is *Explicit small classifying spaces for a range of finitely presented infinite groups*, which I submitted in February 2009. My thesis unearths explicit small classifying spaces for a range of finitely presented infinite groups and uses these spaces to deduce homological information on the groups. We also derive formulae for the second integral homology of any Artin group for which the $K(\pi,1)$-conjecture is known to hold, and for the third integral homology of the braid group A_n and the affine braid group $\tilde{A}_n$.
I am also interested in pursuing research into the teaching and learning of Mathematics.

Publications:

M. Clancy and G. Ellis, "Twisted Artin groups". To appear in Journal of J-Theory.

Conferences:
BMC 2009/IMS: 6-9th April 2009, NUI,G
Groups in Galway: 7-9th May 3009, NUI,G
De Brún Workshop on Representations and Commutative Algebra: 21st July - 1st August 2009, NUIG
Effective College Teaching & Cooperative Learning Workshop: 14-15th September 2009, Athlone Institute of Technology (organised by The Learning Innovation Network)

Cruickshank, James

Generally my research interests involve problems that have some geometric and/or some combinatorial elements. I am interested in polytopes (which are generalisations of polyhedra). I have recently been interested in studying geometric realization problems associated to objects like polyhedra and polygons.

Also, I have recently worked (with Ray Ryan) on polynomials on infinite dimensional spaces and on functional characterisation of polynomial mappings. This work also has a combinatorial geometric flavour.

Recent students: Séamus Kelly, PhD (2009), Jonathan McLaughlin PhD (submitted 2010)

Recent papers:

Series Parallel Linkages, J. Cruickshank and Jonathan McLaughlin. available at http://arxiv.org/abs/0911.5293

Recent Talks: April 2010, Stockholm University - colloquium talk, October 2009, San Diego State University - colloquium talk, April 2009 - British Mathematical Colloquium, Analysis splinter group.

Other Activities: I participated in the Tropical Geometry session at MSRI in 2009 and I have visited Stockholm University in April 2010.

Ellis, Graham

Research interests in homological algebra, homotopical algebra, computational group theory and their applications. I am the author of the 'HAP' package for homological algebra programming in GAP. I was co-organizer of the First and Second de Brún Workshops on Computational Algebra. My research team includes three postdoctoral researchers and one PhD student.

Recent publications and preprints

- A. Romero, G. Ellis and J. Rubio, *Interoperating between computer algebra systems: computing homology of groups with Kenzo and GAP*. To appear in ISAAC Proceedings 2009.
- G. Ellis and P. Smith, *Computing group cohomology rings from the Lyndon-Hochschild-Serre spectral sequence*. To appear in J. Symbolic Computation, modulo some improvements.

- M. Dutour and G. Ellis, *Wythoff polytopes and low-dimensional homology of Mathieu groups*. To appear in J. Algebra.
- M. Clancy and G. Ellis, *Twisted Artin groups*. To appear in Journal of J-Theory.
- G. Ellis and R. Mikhailov, *A colimit of classyfying spaces*. To appear in Advances in Mathematics.
- G. Ellis, H. Mohammadzadeh and H. Tavallaee, *Computing covers of Lie algebras*. To appear in AMS Contemporary Mathematics.
- G. Ellis, *Homological Algebra Programming*. Appeared in AMS Contemporary Mathematics.

Flannery, Dane

Carried out a range of activities in the 'Groups, Computing and Designs' group in the de Brún Centre for Computational Algebra. Three journal publications (*Journal of Algebra*, *Journal of Pure and Applied Algebra*, *Journal of Symbolic Computation*), and one to appear (London Mathematical Society Lecture Note Series). One book publication pending ('Algebraic Design Theory', Mathematical Surveys and Monographs, American Mathematical Society). Published software as a Magma package for computing with matrix groups over infinite fields.

"`http://magma.maths.usyd.edu.au/magma/htmlhelp/text704.htm`"

Co-organized the International Conference on Design Theory & Applications, and the 3rd de Brún Workshop (both NUI Galway). Co-editor of the Special Issue on Design Theory of *Cryptography and Communications: Discrete Structures, Boolean Functions and Sequences*. Gave talks at the British Mathematical Colloquium, and the Matrix Group Recognition Informatics Forum, University of Edinburgh. Research visits to the University of Auckland, and RMIT University. Attended conferences in the UK (University of Bath) and USA (Ohio State University). Collaborators and co-authors include Dr A. Detinko (Galway), Prof. B. Eick (Braunschweig), Prof. K. Horadam (Melbourne), Dr W. de Launey (San Diego), Dr A. LeBel (Melbourne), Prof. E. O'Brien (Auckland). Supervisor and co-supervisor of three Ph.D. students.

Golden, Aaron

Research Interests

Computational Biology & Bioinformatics: Automated identification of cis-regulatory elements in genomic sequences; Annotation of metagemome libraries using machine learning techniques; Development of integrative techniques to assimilate multiple genomic and epigenomic datasets; Probabilistic & physical modeling of multiple genome/epigenome states; Data analysis pipeline development and imaging techniques for high-throughput genomic & biomedical imaging systems.

Astrophysics: Magnetic properties of ultra-cool dwarfs in particular elucidating the conditions under which beamed coherent radio emission caused by the electron cyclotron maser instability occurs; Radio emission from super-Jupiters and exo-planets; Pulsar emission physics; Dust/particulate suspension & scattering properties in stellar/planetary atmospheres; Data analysis pipeline development for astronomical data; Novel imaging techniques for interferometric data.

Publications

Kim, M.K.-H., McGarry, T.J., O Broin, P., Flatow, J.M., Golden, A. A.-J., Licht, J.D. *An Integrated Genome Screen Identifies The Wnt Signalling Pathway as a Major Target of WT1*, Proceedings of the National Academy of Sciences,106(27):11154-9, 2009

Geeleher, P., Morris, D., Hinde, J.P., Golden, A., *BioconductorBuntu - a Linux Distribution that Implements a Web-Based DNA Microarray Analysis Server*, Bioinformatics, 25(11):1438-9, 2009

McDonald, J., Golden, A., Jennings, S.G. *OpenDDA: A Novel High-Performance Computational Framework for the Discrete Dipole Approximation*, International Journal of High Performance Computing Applications, 23, 42-61, 2009.

Hallinan, G., Doyle, J.G., Antonova, A., Bourke, S., Jardine, M., Donati, J.-F., Morin, Julien, Golden, A., *COOL STARS, STELLAR SYSTEMS AND THE SUN: Proceedings of the 15th Cambridge Workshop on Cool Stars, Stellar Systems and the Sun*, AIP Conference Proceedings, Vol. 1094, pp 146-151 (2009)

Manuscripts submitted

Mulvee, E., Geeleher, P., Howley, B., Benes, V., Schmidt, S., Blake, J., Miller, N., Kerin, M.J., Fearnhead, H., Golden, A., *miRNA Profiling of HER2 Positive Breast Cancers Correlation between increased has-miR-451 levels and late stage tumour status* (submitted to BMC Research Notes)

Howley, B., Elliman, S.J., Lowery, A.J., Bera, A., O'Connell, E., Kerin, M.J., Golden, A., Miller, N., Fearnhead, H.O., *miR-99a Induces Apoptosis and Targets mTor in breast cancer cell lines* (submitted to Cancer Letters)

Supervision

G. Hallinan (Ph.D. 2009) Radio Transient Emission from Ultracool Dwarfs - graduated 2009.

P. Geeleher *Integrative Genomics to Deconvolve Prostate Cancer Dysregulated Pathways* (Hewlett-Packard Enterprise/IRCSET Scholar)

N. McCoy *Metagenomic Annotation using Self Organising Map Techniques* (IRCSET Scholar)

A. Fergus *Computational Simulation of Boundary Layer Tracer Suspension & Dynamics*

P. O Broin *Automated Cis-regulatory Module Identification*

L. Harding *Weather, Starspots or Aurorae - Understanding the Optical Modulation from Radio Active Brown Dwarfs*

S. Bourke *High Resolution Astronomical Imaging using Radio Interferometry* (submitted)

Postodoctoral Fellows

Dr. Gregg Hallinan (currently Visiting Fellow, UC Berkeley)

Conferences attended

Next Generation Sequencing Congress, London, November 16th-17th 2009

Pathways to Habitable Planets, Barcelona, September 14th-18th 2009

Invited Talks

Departmental Seminar Series, Department of Genetics, Albert Einstein College of Medicine, February 17th 2010

Invited speaker, Next Generation Sequencing Congress, London, November 16th-17th 2009

Research Visits

Center for Epigenomics, Albert Einstein College of Medicine, February 2010.

Grants Awarded

2009 Short Term Travel Fellowship, Science Foundation Ireland (Euro 7898) PI

2009 Teagasc Walsh Ph.D. Fellowship, *Functional Genomics for Agriscience* (Euro 63K) PI

Grants Active

Hewlett-Packard/Irish Research Council for Science, Engineering and Technology (IRCSET) Enterprise Ph.D. Fellowship, *Integrative Genomics applied to High Throughput Prostate Cancer Data* (Euro 63K) PI

SFI Research Frontiers Programme (Astrophysics), *Investigating pulsed coherent radio emission at the substellar boundary and beyond - are brown dwarfs pulsar analogues?* (Euro 193K) PI

SFI Research Frontiers Programme (Computer Science), *De-coding cis-regulatory modules in Human DNA using Artificial Intelligence Techniques* (Euro 160k) PI

Hayes, Michael

Hinde, John

Current Research Interests

Statistical modelling, particularly generalized linear models and random effects models; statistical computing and statistical software; likelihood theory and inference; applications of statistics in biological and social sciences. Experience of statistical consulting to large projects in health policy evaluation, engineering, medicine and numerous smaller studies.

Current Research Grants

SFI Research Frontiers Programme - *Random Effect Mixture Models for Multicategory Data*

SFI Mathematics Initiative - *Bio-statistics and Informatics (BIO-SI)* co-PI and lead of Galway group.

Publications and Activities

Publications: 1 book; 2 journal articles
Submissions: 1 journal article; 2 statistical encyclopedia entries; 2 conference papers
Postdocs: 2
Editorial roles: Associate Editor, *Statistics & Computing*; Advisory Board Member (ex-Editor), *Statistical Modelling*.
Research students: 3
Research visits: US, Brazil and Belgium
Research Visitors: 3
Conferences attended: 5 (Ireland; Belgium; USA; Cyprus; UK)
Workshops attended/organised: 3 (Limerick, Dublin, Galway)
Invited Talks: Federal University of Ceará, Fortaleza, Brazil; Statistical modelling advances for social and health data meeting, Royal Statistical Society, London.
Current Professional Society Activity: Council Member, International Biometric Society (2004—2011); Incoming President of British and Irish Region of Biometric Society (2010—2012).

Holian, Emma

My research explores methods of clustering individuals into homogeneous groups according to the value of their observed responses, in particular in longitudinal applications. The clustering methodology applied is a mixture model of mixed models in which a parametric regression models the distinct profiles, and a random effect and/or correlation structures, are incorporated into the model, where each cluster is allowed a unique structure, the resulting model being referred to as the Regression Cluster Model. Allocation into groups and values of the model parameters are sought by employing the Expectation-Maximisation algorithm while the number of unique groups present in the data and the choice of cluster model structures are determined by minimising certain model fit criteria. Modelling The benefit of such a clustering approach is that not only do you result in groups of similar individuals but also a parametric model is fitted to model the attributes shown by that group. Also, including a random effect or correlation structure, can relax the extent to which the overall average trend dictates the optimal choice of groups and allows the longitudinal trend exhibited in that profile to have more of a say. Therefore individuals displaying the same pattern over time, even though they may differ in magnitude of response, may be deemed similar in nature as a result.

Previous work, with collaboration with the NCBES and the National Diagnostics Centre, NUI Galway, applied the modelling approach to clustering longitudinal differential genetic expression profiles produced by microarray experiments. The application to microarray experiments proved extremely useful, the group configuration of genes that resulted from this application revealed interesting response patterns to stress stimuli in farmed fish, and also gave some indication to how genes may be actively co-expressed, that is, groups of genes that each have their role to play in the response required to that stimulus.

Recent activities work towards enhancing the regression cluster model to include speeding up the convergence procedure , devising appropriate model fit criteria, modelling with missing responses, spline function regression - work with Dr Norma Coffey, NUI Galway - and modelling discrete longitudinal responses rather than continuous. The latter requires a refinement in the underlying distribution properties of the model. Funding received from Millennium Fund allows collaboration on this topic with Dr Marie-Jos Martinez, University of Grenoble II, France, and Dr Cathal Walsh of Trinity College. Marie, while at NUI Galway previously, worked in modelling discrete responses and Cathal has been working on a research project that aimed to identify distinct Multiple Sclerosis patient profiles by way of their score response to pain medication measured over time of treatment.

Hurley, Ted

Research Areas

Generally: *Algebra*. In particular: *Combinatorial Group Theory, Computer Algebra, Group Rings* and applications thereof in *the Communications/Information* areas.

Research papers

Three papers in (refereed) Journals and two submitted; one (joint) paper in (refereed) Conference Proceedings; two papers submitted and appeared in *arXiv*. For example:

- (with Paul Hurley) 'Codes from zero-divisors and units in group rings', *Int. J. of Information and Coding Theory,* Vol. 1, no. 1, pp 57-87, 2009.
- 'Convolutional Codes from Units in Matrix and Group Rings', J. Pure & Appl. Math., Vol. 50, no. 3, pp 431-463, 2009.

Chapters in book

Two Chapters in book, *Selected topics in Information and Coding Theory*, Inderscience, March 2010.

PhD Students

Ian McLoughlin (awarded Sept 2009), Jessica O'Shaughnessy (to submit May 2010).

Conferences

Attended six conferences and gave four research talks.

Reviews, referee

Refereed or reviewed five research papers.

Patents

- *Generation of parity-check matrices*, with Jakub Wenus and Paul McEvoy (Technology from Ideas), International filing August 2009, no. 20090019333.
- *Method and apparatus for generating error-correcting and error-detecting codes using zero-divisors and units in group rings*, (NUIG), International filing January 2009, no. 20090089744.

Jennings, Kevin

My research interests are in difference sets with classical parameters. These are finite sets D with k elements taken from a finite group G with v elements. Each nonidentity element of the group can be expressed the same number of times as a difference $a-b$ where $a,b \in D$. These objects are often realised as the image of a hyperplane in a finite field under an identification of scalars. The central problems include finding new constructions, showing that new instances are inequivalent to known constructions and ruling out various parameter families. Basic working techniques are linear algebra over finite fields and some combinatoric arguments.

Conferences attended: Design Theory workshop here in the De Brún Centre, NUI Galway and the international Finite Fields conference $\mathbb{F}_q 9$ in the Claude Shannon Institute, UCD.

This year, while guiding Anthony Winterlich in his Master's thesis, I have developed an interest in the foundations of mathematics. This area is new to me. Obvious interplay here might help to formalise generalisations of difference sets from finite groups to infinite groups in interesting ways, or to extend the concept of difference sets to quasigroups and other weaker algebraic structures.

Krnjajic, Milovan

I am interested in developing flexible statistical models in variety of application areas, in particular, models and methods based on Bayesian non-parametrics, inverse models, and various machine learning approaches to classification and prediction.

Madden, Niall

My primary interest is the mathematical analysis of finite difference and finite element methods for *singularly perturbed* differential equations—problems for which classical methods typically behave poorly. Recently, I've been concerned with methods that are highly computationally efficient. This includes domain decomposition techniques, which are suitable for implementation on parallel computers or distributed environments [1]; sparse grid finite element methods [2], which reduce the number of degrees of freedom needed to solve certain PDEs from $\mathcal{O}(N^2)$ to $\mathcal{O}(N^{3/2})$, but without loss of accuracy; and alternating direction methods which reduce time-dependent PDEs to systems of ODEs [3].

As well as investigating the mathematical properties of numerical methods, I am interested in their use in the

study of applied problems. This includes a project on the transport and diffusion of pollutants in tidal regions (SFI Grant RFP/CMS/1205), and on computing solutions to models for ICU patient responses to certain drug therapies (RFP/CMS/1254).

[1] M. Stephens and N. Madden, *A parameter-uniform Schwarz method for a coupled system of reaction diffusion equations*, J. Comput. Appl. Math., 230(2):360–370, 2009.

[2] F. Liu, N. Madden, Stynes M., and A. Zhou. A two-scale sparse grid method for a singularly perturbed reaction-diffusion problem in two dimensions. *IMA J. Numer. Anal.*, 29(4):986–1007, 2009.

[3] T. Linß and N. Madden, *Analysis of an alternating direction method applied to singularly perturbed reaction-diffusion problems*, IJNAM, to appear, 2010.

McCluskey, Aisling

Set-theoretic/general topology and order/lattice theory.

Mc Gettrick, Michael

Research Areas

I have been working recently (2009/2010) mainly in quantum computation (also called quantum information theory). In particular my interests here are in Quantum Algorithms, and the construction and analysis of quantum random walks and quantum games.

Other smaller current interests are in discrete event dynamical systems, tropical mathematics and computer algebra in general.

In 2009, I worked for 4 months at the University of Linz (Austria) on computer algebra (tropical mathematics calculations) and for 4 months at the University of Paris on quantum computation.

Publications

- *One Dimensional Quantum Walks with Memory* Quantum Information and Computation, Vol. 10, No. 5&6 (2010) 0509-0524.
- *Lazy Quantum Random Walks using Qutrits*, submitted to the International Journal of Quantum Information (2010).

Presentations

- *Quantum Random Walks with Memory*. January 2010, talk at North-South Quantum Information Winter School, Maynooth (Ireland)
- *The Quantum Prisoners Multilemma, and other Quantum Games*. June 2009, Seminar at Groupe Calcul Quantique, Laboratoire de Recherche en Informatique, Universite Paris Sud (France)
- *Tropical Triangles*. March 2009, Seminar at Research Institute for Symbolic Computation, University of Linz (Austria).
- *Geometry, Musical Rhythm and a problem of Erdos*. January 2009, Colloquium at Research Institute for Symbolic Computation, University of Linz (Austria)

Meere, Martin

Activities

- Investigation of drug diffusion from thermo-responsive swellable polymers, in collaboration with Dr. Yury Rochev at NCBES, NUI, Galway. This project involves the training of two PhD students.
- Work has begun on a project with Dr. Petri Pirroinen on modelling aspects of the cell cycle. This project involves the training of one PhD student.
- Analysis of impurity diffusion in stressed crystal lattices, in collaboration with Prof. John King at the University of Nottingham.

Publications, Supervision, Visits and Refereeing

- Two joint papers published in refereed journals (one an electronic journal). Involved with the superivision of two PhD students as a supervisor, and another one indirectly.

- Attended the BAMC in Nottingham, April 2009, and the European Study Group with Industry, UL, June-July 2009.
- One week visit to University of Nottingham, April 2009. Gave an invited talk to MACSI in UL in November 2009.
- Acted as a referee for a few journals.

Newell, John

Research interests include biostatistics, statistical modelling, statistical computing, survival analysis and the application of statistics in Sports Science. I hold an adjunct post as Senior Research Fellow in the Department of Mathematics and Statistics, University of Canterbury, Christchurch, New Zealand. I have two PhD students in Statistics (one jointly supervised with Professor John Hinde) and one MSc student in Biostatistics.

Member of the Executive Committee of the Statistical Modelling Society and the Irish Statistical Association.

Recent Publications

Journal Papers:

Sean F Dinneen, Mary Clare O' Hara, Molly Byrne, John Newell, Lisa Daly, Donal O' Shea, Diarmuid Smith and Irish DAFNE Study Group. The Irish DAFNE Study Protocol: A cluster randomised trial of group versus individual follow-up after structured education for Type 1 diabetes. Trials 2009, 10:88

O' Riordan C, Glynn LG, MacFarlane A, Newell J, Iglesias AA, Whitford D, Cantillon P, Murphy AW. Research activity and capacity in primary care. Forum 2009;26 (9):27-30.

Glynn, L G, O'Riordan, C, MacFarlane, A, Newell, J, A Iglesias, A, Whitford, D, Cantillon, P, Murphy, A W. (2009) Research activity and capacity in primary healthcare: The REACH study: A survey. BMC Family Practice 2009, 10:33

A W Murphy, M E Cupples, S M Smith, M Byrne, M C Byrne, J Newell. Effect of tailored practice and patient care plans on secondary prevention of heart disease in general practice: cluster randomised controlled trial. BMJ 2009;339 b4220.

In press:

Heneghan, H., Newell, J. et al. Systemic Mirna 195 Differentiates Breast Cancer From Other Malignancies and is a Potential Biomarker for Detecting Non Invasive and Early Stage Disease . To appear in The Oncologist.

Eilis Foran, Megan M. Garrity-Park, Coralie Mureau, John Newell, Thomas C. Smyrk, Paul J. Limburg, and Laurence J. Egan. Upregulation of DNA Methyltransferase-Mediated Gene Silencing, Anchorage-Independent Growth, and Migration of Colon Cancer Cells by Interleukin-6. To appear in Molecular Cancer Research.

Jocelyn Anderson, Liam G Glynn, John Newell, Alberto A Iglesias, Donal Reddan and Andrew W Murphy. The impact of renal insufficiency and anaemia on survival in patients with cardiovascular disease: a cohort study. To appear in BMC Cardiovascular Disorders.

Books:

Statistics for Sports and Exercise Science: A Practical Approach John Newell, Tom Aitchison, Stanley Grant. Pearson Publishers, Oct 2009, ISBN13: 9780132042543.

O'Keeffe, David

My area of interest is in cohomology theory and recently I have been working on problems concerning the calculation of Hochschild cohomology rings for certain classes of associative algebras. For my doctoral thesis I calculated the cohomology ring for the so called class of quadratic monomial algebras. A quadratic monomial algebra is a quotient of a path algebra. I also showed that the cohomology algebra of a quadratic monomial algebra exhibits all possible behaviours as an algebra, that is, it may be finite dimensional over k, finitely generated over k, or infinitely generated over k, where k is written to denote a field of arbitrary characteristic.

I am also interested in researching and understanding the different approaches used in the teaching of mathematics to undergraduate students. Presently I am involved (with Dr. Ray Ryan) in delivering a blended online learning course to part-time commerce students.

O'Regan, Donal

Differential Equations, Nonlinear Analysis and Fixed Point Theory.

Pfeiffer, Götz

I am working on problems in Computational Algebra. In particular, I am interested in finite groups, representation theory, computational group theory, algebraic combinatorics and the theory of formal languages and semigroups. I have participated in the development of the GAP system for computational group theory, and has contributed to several software packages for GAP. I am a member of the GAP council. I am a co-author of a book on "Characters of Finite Coxeter Groups and Iwahori–Hecke Algebras".

Currently, I am working on algorithms for the structural analysis of finite Coxeter groups and related algebraic objects. I am supervising two Phd students. I am a director of the De Brun Centre for Computational Algebra and have helped organizing several conferences and workshops (BMC 2009; 1st and 3rd de Brun Workshop; Groups in Galway 2010). I am frequently invited to speak at conferences, or to give seminar talks.

Recent Publication. *A Quiver Presentation for Solomon's Descent Algebra.* Adv. Math. **220** (2009), no. 5, 1428–1465.

Piiroinen, Petri

My main research interests are in numerical and analytical analysis methods for recurrent nonlinear dynamical system with discontinuities. These kinds of systems can be found in, for instance, mechanics, biology and economics, and even though they initially seem relatively easy to analyse they often give rise to a remarkably varied display of dynamical behaviours. Recently I have gained an interest in how to model and analyse various aspects of the cell cycle, the glucose-insulin system in humans and other biological models. I am currently supervisor for one SFI-funded MSc and an IRCSET-funded PhD student, and a co-supervisor, with Dr Martin Meere, for one College-of-Science-funded PhD student. From December 2010 my research team will be extend with an IRCSET-funded Postdoc. Since January 2009 I have published three peer-review journal papers, attended two conferences and given a number of talks.

Quinlan, Rachel

My research activities are concentrated in two distinct areas : algebra and mathematics education. In recent years my work in algebra has focussed on interactions between linear algebra, Galois theory and the theory of finite groups.

I am also interested in the character theory and representation theory of finite groups. I am currently supervising the research of James Lovett, who is a M.Litt. student working on the history of representation theory.

I also have some research activity in the area of mathematics education at university level. I am currently supervising the PhD research of Kirsten Pfeiffer, whose investigations involve a theoretical and practical analysis of first year students' efforts to comprehend, validate and evaluate mathematical proofs.

Publications

[1] R. Gow and R. Quinlan, Galois theory and linear algebra, Linear Algebra and its Applications, Vol. 430, Issue 7, 2009.

[2] R. Gow and R. Quinlan, Galois extensions and subspaces of alternating bilinear forms with special rank properties, Linear Algebra and its Applications, Vol. 430, Issues 8-9, 2009.

[3] R. Quinlan, What makes mathematics attractive at university?, Proceedings of the 3rd National Conference on Research in Mathematics Education, St. Patrick's College Drumcondra.

Conference Presentations and Seminars

[1] *The early days of character theory*, Groups in Galway Conference, NUI Galway, May 2009.

[2] *What makes mathematics attractive at university?*, 3rd National Conference on Research in Mathematics Education, St. Patrick's College Drumcondra, September 2009.

[3] *Minimum polynomials and the trace form for cyclic extensions*, 9th International Conference on Finite Fields and their Applications, University College Dublin, July 2009.

[4] *A problem in linear algebra*, UCD Algebra Seminar, February 2010.

[5] with K. Pfeiffer, *Workshop on analysing students' proof evaluation*, British Congress of Mathematics Education (BCME7), Manchester, April 2010.

Rover, Claas

Group Theory, Computational Group Theory and Formal Languages and Automata.

Ryan, Ray

Functional Analysis; Tensor Products of Banach Spaces; Polynomials and Holomorphic Mappings on Banach Spaces and Riesz Spaces.

Conference Talks:

Polynomials on Vector Spaces, Complex Analysis on Infinite Dimensional Spaces, UCD, June 2009.
The Mazur-Orlicz Theorem for Polynomials, Function Theory on Infinite Dimensional Spaces XI, Madrid, December 2009.

Seoighe, Cathal

The focus of my research is on modeling molecular biological data, including gene expression, alternative mRNA splicing and molecular evolution, in particular the evolution of HIV-1. Bioinformatics is interdisciplinary in nature and I collaborate or am in the process of establishing collaborations with several life sciences research groups on campus. For example, I am currently working with the Dr. Andrew Flaus in the Chromosome Biology Group on the relationship between chromatin structure and the control of gene expression, using newly generated and existing next-generation sequence data. Nine journal articles on which I am a co-author have been published between January 2009 and April 2010. An example of some recently published work is the development of a phylogenetic Hidden Markov Model to predict immune epitopes and its application to southern African data from HIV-1 (*Molecular Biology and Evolution*, April 2010; together with Miguel Lacerda).

Research support

My research is currently supported by Science Foundation Ireland through the Stokes Professorship Programme. Postgraduate students are funded through IRCSET and strategic startup funding provided by NUIG.

Current PhD students

- Miguel Lacerda (Phylogenetic Hidden Markov and other models of HIV-1 immune escape)
- Thong Nguyen (Relationship between chromatin structure and gene regulation in human)
- Renaud Gaujoux (University of Cape Town; Microarray analysis of heterogeneous tissues)

Sheahan, Jerome

Recent recent centres on combinatorial techniques to unify apparently different enumeration problems in various areas of scientific endeavour. The mathematics employed involves generating functions and Markov Chain techniques for the derivation of (mainly) exact distributions associated with random variables whose values arise as functions of patterns in sequences (currently only binary). Applications of the work arise in many areas including decision making, optimal control in e.g. industrial processes, tests for randomness, the study of pseudo-randomness relating to e.g. digital systems, and improved results relating to minimum distance and covering radius in codes.

Other activities include regular statistical consulting service to researchers in every College on Campus. Problems solved run the gamut of statistical methods, including Generalised Linear Modelling for the analysis of experimental data, time series, multivariate analysis, and the design and analysis of social surveys.

Sköldberg, Emil

Group Theory, Computational Group Theory and Formal Languages and Automata.

Tuite, Michael

My area of research is in vertex operator algebras which lies on the interface of theoretical physics and pure mathematics. My recent work has mainly concentrated on

understanding partition and n-point functions on higher genus Riemann surfaces formed by sewing together lower genus surfaces. This is an on-going project over many years in collaboration with Geoffrey Mason of UC Santa Cruz, a postdoctoral researcher Sasha Zuevsky and PhD student Donny Hurley in NUI Galway. In the past year we computed all genus two n-point functions for the fermionic vertex operator superalgebra in terms of the Szegö kernel data. We have also computed the bosonic string partition function for certain general genus Riemann surfaces. Donny has been working on Virasoro n-point functions at genus zero and one with applications to genus two theory. I also have a new PhD student Hoang Dinh Van who will be working on a new approach I have been developing to vertex operator algebras with exceptional Lie or finite group symmetries.

Funded Research Projects

- SFI Research Frontiers Programme, *Vertex Operator Algebras on Genus Two Riemann surfaces*, 2005-2009. Supporting Ph.D. student Donny Hurley.
- SFI Research Frontiers Programme *Higher Genus Vertex Operator Algebras*, 2008-2011. Supporting postdoctoral researcher Sasha Zuevsky working on vertex operator algebras on arbitrary genus Riemann surfaces.
- SFI Research Frontiers Programme *Vertex Operator Algebras and Deligne's Exceptional Lie Groups*, 2009-2013. Supporting Ph.D. student Hoang Dinh Van.

Publications and Presentations

- 1 paper published, 3 papers and 1 book (as editor of conference proceeding) in press, 2 papers under review.
- 4 conference presentations and seminars (Tokyo, Dublin, Edinburgh and Zurich).

Ward, James

Research interests in Subnormal Subgroups, Noncommutative Rings and the History of Mathematics. One of the main organizers of the joint meeting of the 61st British Mathematical Colloquium and the Irish Mathematical Society was hosted by NUI Galway in April 2009.

Waters, Thomas

My research interests fall into three overlapping areas:

- **Integrability of Geodesic Flow** The equations defining geodesic curves admit a Hamiltonian formulation; as such a natural question is that of integrability. I have addressed this issue on surfaces defined in terms of the spherical harmonics by using numerical (Poincaré section) and analytical (variational equations) techniques. I use methods from dynamical systems, differential geometry and differential Galois theory.
- **Solar sails in the Earth-Sun system** Taking the third body in the circular restricted three body problem to be a solar sail represents a three-parameter extension to this classical dynamical problem. Of particular interest is the existence and stability of equilibrium points and periodic orbits. Recently I have made use of the specialised software AUTO to find connections between different families of periodic orbits to develop a global understanding of the dynamics.
- **Systems with quasiperiodic coefficients** I have extended the well-known Mathieu equation to systems of ODE's whose coefficients contain periodic terms in a number of frequencies. As these frequencies vary continuously the system passes through resonance and the stability of the system depends very strongly on this resonant behaviour. Parameter space is divided into zones of stability and instability whose boundary is exceedingly complex.

Recent Projects:

- I led a research project titled 'Earth observation using solar sails', funded by the NUI Galway Millennium fund. This involved hiring a maths graduate for the summer to examine the orbits available to a solar sail in the Earth-Sun system.

Postdoctoral Researchers

Chadha, Naresh

Research Interests

Designing and analyzing numerical methods for Singularly perturbed differential equations; adaptive mesh construction; mesh-free methods based on radial basis functions.

Currently working on designing novel numerical methods to introduce an adaptive time-stepping for a solute transport problem in *DIVAST* (Depth Integrated Velocities and Solute Transport). This is a code written in Fortran, and it has been widely used to simulate two-dimensional distributions of currents, water surface elevations and various water quality parameters within the modelling domain as functions of time, taking into account the hydraulic characteristics governed by the bed topography and boundary conditions. To be specific, DIVAST has two modules, one deals with hydrodynamics of a water body; and second is mainly concerned with a solute-transport problem. The coefficients for the solute-transport problem are provided by the computed solution of hydrodynamics-module.

The governing equations used for hydrodynamics are depth-integrated Navier-Stokes equations. These equations are to be solved in conjunction with a realistic treatment of certain complex-boundaries of a water-body. Moreover, these boundaries may even change over a tidal-period.

In principle, the governing equation for the solute-transport problem is a time dependent advection-diffusion problem. However, the formulation may vary in order to incorporate certain physical entities into modeling, e.g., for modeling certain aspects related to certain toxic elements, one would be dealing with advection-diffusion-reaction problem.

As a part of a larger problem (outlined above), we are working on introducing adaptive time-stepping for a solute-transport problem in DIVAST.

Coffey, Norma

Current research interests include

- Functional data analysis:- with applications in biomechanics, human kinematics and time-course microarray gene expression data. Applications in biomechanics and human kinematics are part of ongoing work with Dr. Drew Harrison, Biomechanics Research Unit, University of Limerick. Presently employed as a postdoctoral researcher applying functional data analysis methodology to time-course microarray gene expression data.
- Mixed effects modelling:- particularly using the linear mixed effects model to perform functional data analysis.

Recent Talks:

- International Symposium on Biomechanics in Sport, University of Limerick, 21st August 2009 - introducing functional data analysis techniques and their merits in analysing biomechanical data to sports scientists.
- International Conference on Stochastic Modeling Techniques and Data Analysis in Chania, Crete, June 2010 - presenting a review of the use of functional data analysis to analyse time-course microarray gene expression data.

Recent Publications:

- Donoghue, O., Harrison, A.J., Coffey, N., and Hayes, K. (2008) Functional data analysis of running kinematics in chronic Achilles tendon injury. *Medicine and Science in Sports and Exercise*, Vol. 40, Issue 7, pp.1323–1335.
- Coffey, N. (2009) Functional principal components analysis via the linear mixed effects model. PhD Thesis.
- Coffey, N., Donoghue, O., Harrison, A.J. and Hayes, K. (2010) Common functional principal components analysis - a new approach to analysing human movement data. Submitted to *Human Movement Science*.

Detinko, Alla

Area of research: computational group theory. Current project: development of computational theory of linear groups over infinite domains.

2 papers published, 1 accepted, 1 published software (Magma package), 2 papers due for submission.

3 conference presentations:(1)Groups St Andrews (University of Bath, UK, August 2009); (2) 3rd de Brun Workshop (NUIG, December 2009); (3) Combinatorics, Groups, Algorithms, and Complexity (University of Ohio, USA, March 2010).

Co-organizer of two conferences: International Conference on Design Theory and Applications (NUI Galway, July 2009); 3rd de Brun Workshop (December 2009). Co-organizer of the public lecture by Prof. E. Zelmanov.

PhD student: Tobias Rossmann (co-supervision).

Dickinson, Mark

My interests lie in the field of algebraic number theory, particularly those parts of it dealing with modular forms, Galois representations and L-functions. He is also interested in computational algebra and formal proof verification. He's currently working on a GAP package designed for performing computations in Galois cohomology, with an interface to the GP/Pari computational algebra system.

Recent publication (lying somewhat outside main research interests): "A congruence problem for polyhedra", with Alexander Borisov and Stuart Hastings. (American Mathematical Monthly, March 2010.)

King, Simon

I am postdoctoral fellow under a Marie Curie project currently working on computational group cohomology, improving old and developing new algorithmic methods to compute modular cohomology rings of finite groups. I succeeded with the first cohomology computation for all groups of order 128 and of various classical groups, most notably the mod-2 cohomology of the Higman–Sims group and the third Conway group. I also work in commutative algebra and low dimensional topology.

I gave conference presentations on cohomology in Barcelona (June 12-13, 2009) and Galway (30 June - 9 July, 2009) and on commutative algebra and topology in Joseph, Oregon (12-21 July 2009), and several talks in seminars.

My computational results are presented on my web pages. There are two recent preprints (one is joint with David Green), and two are in preparation. I am one of the editors of the proceedings of a workshop on low-dimensional topology in Oberwolfach, that I co-organised in 2008.

Mondal, Kajal Kumar

My area of research is fluid dynamics. I am interested to analyze the solute-transport problems using finite difference/finite element method, because these problems have a wide range of applications in the fields of environmental fluid dynamics and physiological fluid dynamics. Recently, I am working in an interdisciplinary group at National University of Ireland, Galway, Ireland, led by Dr. Niall Madden (Mathematics) and Dr. Michael Hartnett (Civil Engineering). Our main objective is to investigate a numerical framework for the interpretation of contaminant spreading in tidal flows and to combine recent mathematical advances in the numerical solution of the PDE, with working engineering codes.

O' Shea, Edwin

My research interests are in applicable and computational algebra and combinatorics. These include how toric Groebner bases and Rees algebras of monomial ideals can be utilised in discrete optimisation, and vice versa. I have used this bridge, along with collaborators, to understand computational aspects of toric varieties, structure in integer programming, perfection in graphs and statistical disclosure limitation. I enjoy experimenting with computational algebra packages like Macaulay 2 to gain insight on these problems.

Since arriving in Galway in June 2009, under the auspices of the De Brun Centre for Computational Algebra, I have spent roughly half of my time working on algebraic methods in statistical disclosure limitation. This area uses algebraic and combinatorial methods to gauge the security of an individual's private census data when margins are released to the general public. My work on this topic was submitted to The SIAM Journal of Discrete Mathematics in December 2009 and a revised version is currently in progress.

A second strand of my research this year concerned a classical problem that arose while we were teaching the enrichment program for local secondary school students. Bachet's problem asks: "What is the least number of pound weights that can be used on a scale pan to weigh any integral number of pounds from 1 to 40 inclusive, if the weights can be placed in either of the scale pans?"

This problem is popularly known as Bachet's problem and stretches all the way back to Fibonacci in 1202! While it can be justifiably considered the first problem of the thoroughly modern and active area of integer partitions, its generalisation when we replace 40 by any integer has only emerged in the last 15 years and was little known at that. I thought that this sad state of affairs ought to be rectified and could be done so in a manner accessible to undergraduates so I set about writing an expository article which was submitted in April 2010 to the MAA's Mathematics Magazine. A pleasant corollary of this expository work is current and new work with Jorge Bruno that extends again, in an "error correcting manner", the recent generalisation of Bachet's problem.

Papageorgiou, Georgios

My current research reflects an interest on methods for the analysis of correlated observations. Generalized linear mixed models are widely used for the analysis of such observations. My research has focused on extending the family of multivariate generalized linear mixed models to include random effects that are generated by smooth densities. Two such families of densities have been considered and an automated Monte Carlo EM algorithm that can be used with both densities has been implemented. The properties of these flexible models have been investigated and a comparison to the traditional parametric models has been carried out using simulation studies and an application to a real data set.

Another class of models that is frequently used for the analysis of correlated, time ordered observation is the class of joint mean-covariance models. These models use the modified Cholesky decomposition of the within subject covariance matrix in order to arrive to an unconstrained, statistically meaningful reparameterisation. However, just as in all classes of models, maximum likelihood estimation provides overoptimistic variance components estimates as it does not take into account the loss of degrees of freedom that results from estimating the mean structure. We have propose adjustments to the estimating equations in order to alleviate the problem of inefficient estimation and downward bias in the class of joint mean-covariance models. The performance of these adjustments have been investigated though simulation studies.

[1] Number of papers published: 2

[2] Papers under review: 1

[3] Proceedings papers: 1

[4] Conference talks: 1

Zuevsky, Alexander

- Representation theory: Vertex algebras, applications in number theory, modular forms, Riemann surfaces; q-deformed algebraic structures
- Mathematical Physics: Conformal field theory; Dynamical Systems: algebraic methods in integrable models; applications in non-commutative geometry

Project: Vertex operator algebras on higher genus Riemann surfaces

In joint research with M. P. Tuite and Prof. G. Mason (Department of Mathematics, University of California Santa Cruz), we develop a procedure for the construction of all n-point correlation functions for super vertex operator algebras (VOSA)/conformal field theories on higher genus Riemann surfaces.

Publications and preprints in 2009-2010: Publications: 4; Journal submissions: 4; Talks given: 5; Conferences attended: 2.
