IMS September Meeting

September 1–2, 2022, TU Dublin

1 PROGRAMME

Thursday, 1st September 2022

10:30 am – 11:00 am: Registration/Coffee

11:00 am – 11:20 am: Welcome address (Prof Pramod Pathak, Dean, Faculty of Computing, Digital and Data, TU Dublin)

11:20 am – 12:00 pm: Nicole Beisiegel (TU Dublin) – Numerical Testcases to Study Proudman Resonance Using Shallow Water Models

12:00pm – 12.40 am: Leo Creedon (ATU Sligo) – New algebraic structures which are almost semigroups and rings

12:40 pm – 2:00 pm: Lunch

2:00 pm – 2:40 pm: Ray Ryan (*NUI Galway*) – Analysis on vector lattices

2:40 pm – 3.20 pm: Norma Bargary (*UL*) – Functional data analysis with applications in sports

3:20 pm – 3.50 pm: Coffee

3:50 pm – 4.30 pm: Rachel Quinlan (*NUI Galway*) – How to make up questions about matrices

4:30 pm – 5.10 pm: Catalina García (*Granada University*) – An overview of multicollinearity: contributions and alternatives to ridge regression

5:30 pm – 6:30 pm: Coffee/Posters/IMS Committee Meeting

7:30 pm: Conference Dinner

Friday, 2nd September 2022

09:30 am – 10:10 am: Roisin Hill (*UL*) – Generating layer-adapted meshes using MPDEs

10:10 am – 10:50 am: Peter Lynch (*University College Dublin*) – Parity and Partition of the Rational Numbers

10:50 am – 11:20 am: Coffee

11:20 am – 12:00 pm: David Malone (*Maynooth University*) – Ranking and Rankability

12:00 am – 12:40 pm: Sarah Fink (*Athena Swan Ireland*) and **Niall Madden** (*NUI Galway*) – Introducing Athena SWAN, and the Mathematical Sciences Athena SWAN Network

12:40 pm – 2:00 pm: Lunch/AGM

2:00 pm – 2:40 pm: Eabhnat Ní Fhloinn (*Dublin City University*)– Is Maths Different? Experiences and opinions of mathematics lecturers teaching online during the COVID-19 pandemic.

2:40 pm – 3:20 pm: Lennon Ó Náraigh (*University College Dublin*) – Mathematical and physical modelling of industrial drying

3:20 pm – 3:30 pm: Concluding remarks/Poster Prize

2 TALK ABSTRACTS

Numerical Testcases to Study Proudman Resonance Using Shallow Water Models

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Meteotsunamis are atmospherically induced, potentially destructive and extreme waves in the tsunami frequency band. While the main underlying physical mechanisms have been widely known for a long time (see for example [1]), computational modelling capabilities are still not widely available or scarce. In this talk, we consider an adaptive discontinuous Galerkin (DG) model with advanced filtering, or slope limiting, capabilities as in [2, 3] to simulate idealised meteotsunamis caused by Proudman resonance. A number of idealised testcases demonstrate the model's performance and the general effects of resonant wave events. The model uses an adaptive, triangular mesh that is driven by heuristic, or application-based refinement indicators. The discussion of the model's computational efficiency will be guided by efficiency metrics as in [4] that we define and apply to model results.

REFERENCES

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[3] N. Beisiegel, S. Vater, J. Behrens and F. Dias, An Adaptive Discontinuous Galerkin Method for the Simulation of Hurricane Storm Surge, Ocean Dynamics, 70, Issue 5, 641–666 (2020)
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New algebraic structures which are almost semigroups and rings

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New algebraic structures (called semigrouplets, grouplets, ringlets and pringlets) are defined. They are generalisations of semigroups, groups and rings. The multiplicative structure of these objects is motivated by exponentiation (multiplying an element by itself repeatedly). Elementary properties of these structures are developed and some examples are given. These structures are related to locally cyclic groups and may have applications in finite dynamical systems, derivations and restricted Lie algebras. They are examples of partial algebraic systems. Other examples include effect algebras and Brandt groupoids.
This is joint work with Kieran Hughes.

Analysis on vector lattices

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For a sequence of real numbers, we have two ways to define convergence: one is the "epsilon definition"; the other is the "lim inf = lim sup" condition. The first comes from the metric structure, the second from the order structure. Happily for first year Analysis students, the two notions agree (and so one can be immediately forgotten). When we move to bigger vector spaces with metric and order structures, the situation is more complicated and the two modes of convergence might not agree. We will look at examples of this phenomenon and will explore some of the ramifications when we work with continuous functions.

Functional data analysis with applications in sports

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Functional data analysis (FDA) is a statistical methodology that is suitable for modelling high-dimensional data collected over some continuum (typically time). FDA is particularly suitable for the modelling and analysis of data that are measured continuously, more recently via state-of-the-art sensor technologies. This talk will give an overview of FDA with applications to data collected in a variety of sports settings, and discuss the methodological challenges associated with the statistical modelling of these modern human movement datasets.

How to make up questions about matrices

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This talk will discuss some extremal problems in linear algebra, such as identifying or characterizing maximal (with respect to inclusion or dimension) subspaces of matrices in which every element has some specified property. The talk is intended for a general mathematical audience and the hope is to convey a sense of the accessibility and broad appeal of this area of research.

An overview of multicollinearity: contributions and alternatives to ridge regression

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Multicollinearity exists in a linear regression model when there is a strong relationship between at least two exogenous variables. In this case, the ordinary least squares estimation can present instability, leading to erroneous conclusions that could even call into question the validity of the analysis. For this reason, alternative estimation methodologies are traditionally applied, such as ridge regression which is systematically applied in many different fields where multicollinearity appears. Despite its consequences, multicollinearity is not always adequately treated in some studies and it is even completely ignored in others. In this same way, the ridge regression is not always adequately applied.
This presentation aims to clarify some aspects of the diagnosis and treatment of multicollinearity. First, we share some contributions in relation to the measures traditionally apply to diagnose multicollinearity. Second, we provide an alternative measure to diagnose multicollinearity after the application of the ridge regression and propose the mitigation of multicollinearity as criteria to select the ridge factor. We also review some limitations of ridge regression and propose the application of the raise regression that allows the mitigation of the multicollinearity maintaining the global characteristics of the original model and modifying the information matrix $(X'X)$ from a geometrical point of view of multicollinearity. Finally, some future research lines are presented with the goal of generating potential synergies with the audience.

Generating layer-adapted meshes using MPDEs

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This work was undertaken as part of my PhD under the supervision of Niall Madden in the National University of Ireland Galway

We consider the numerical solution, by finite elements methods, of singularly-perturbed differential equations (SPDEs) whose solutions exhibit boundary layers. Our interest lies in developing parameter-robust methods, where the quality of the solution is independent of the value of the perturbation parameter,

One way of achieving this is to use layer resolving methods based on meshes that concentrate their mesh points in regions of large variations in the solution.

We investigate the use of Mesh PDEs (MPDEs), based on Moving Mesh PDEs first presented in [2], to generate layer resolving meshes that yield parameter robust solutions to SPDEs. Specifically, we present MPDEs based on the derivative to the numerical solution to the related SPDE. Their solutions yields meshes that are similar to Bakhvalov meshes [1]. The algorithms and code build on those presented in [4].

Since the MPDEs are non-linear problems, we use a fixed-point iterative method to solve them numerically. We present an approach involving alternating between h- and r-refinement which is highly efficient, especially for larger meshes.

We demonstrate the flexibility of the approach with numerical examples implemented in FEniCS [3].

Acknowledgements: My research is supported by the Irish Research Council, GOIPG/2017/463 and GOIPD/2022/284.

References

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Parity and Partition of the Rational Numbers

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We define an extension of parity from the integers to the rational numbers. Three parity classes are found — even, odd and 'none'. Using the 2-adic valuation, we partition the rationals into subgroups with a rich algebraic structure. The natural density provides a means of distinguishing the sizes of countably infinite sets. The Calkin-Wilf tree has a remarkably simple parity pattern, with the sequence 'odd/none/even' repeating indefinitely. This pattern means that the three parity classes have equal natural density in the rationals. A similar result holds for the Stern-Brocot tree.

Ranking and Rankability

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There are many proposed schemes for ranking items given a dataset containing some incomplete information about their ordering. Recently, people have started to look at the rankability of such datasets, which aims to measure how amenable the data is to ranking. I will summarise some of the proposed measures of rankability and show some results from a recent preprint with Nathan McJames and Ollie Mason.

Introducing Athena Swan and the Mathematical Sciences Athena SWAN Network.

Sarah Fink[1] and **Niall Madden**
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Is Maths Different? Experiences and opinions of mathematics lecturers teaching online during the COVID-19 pandemic.

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The COVID-19 pandemic necessitated a move to emergency remote teaching of mathematics in March 2020, followed by a full academic year of online teaching for many universities. The teaching and learning of mathematics online presents some unique challenges, due in part to the symbolic notation and representations used within the discipline. In June 2020, and again in June 2021, we undertook an online survey with mathematics lecturers to ascertain their experiences and opinions of teaching mathematics online, receiving 257 and 190 responses respectively, from over 30 countries. In this talk, I will present a selection of their responses, with a particular focus on the impact of the nature of mathematics upon the challenges experienced in online teaching.

Mathematical and Physical Modelling of Industrial Drying

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Industrial drying - a seemingly dry subject if ever there was one - is an area of research where there is still much to learn. There is also much to be gained, as understanding various drying processes in the food industry can help to optimize them, and hence, cut energy usage while maintaining product quality. Describing drying in a quantitative way requires the use of a surprisingly wide range of mathematical and physical concepts. In this talk I will outline those concepts, and present some findings I have made in my own foray into industrial drying. In particular, I will talk about mathematical modelling, optimization, and simulation. The modelling is based on Partial Differential Equations (PDEs) - there is no escaping the fact that a lot of dryers are basically a hyperbolic system, which convects moist product at the inlet to (hopefully) dry product at the outlet. Maintaining the outlet variables in a target state requires optimal control theory, which for PDEs is formulated as a kind of constrained optimization in Banach spaces. There are some standard results that guarantee the existence of an optimal control, and I will describe these. There is also a lot of Physics involved in the problem, including the modelling of the evaporation rate and the drying rate, there are standard models of such things but they require a lot of figuring out. Finally, there is the matter of putting all of these ideas together in a code package, which can be used for simulations and (hopefully) some insights into developing practical control protocols. I will present one of these practical protocols and outline some ideas for future work.

3 POSTER ABSTRACTS

Powers of Karpelevič Arcs and their Sparsest Realising Matrices

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A celebrated result of Karpelevič describes Θ_n the collection of all eigenvalues arising from the stochastic matrices of order n. The boundary of Θ_n is a disjoint union of arcs, known as the Karpelevič arcs.
Johnson and Paparella considered relationships between different arcs, and posed a conjecture on their powers. This conjecture was later proved by Kim and Kim. We continue their work and give a complete characterization of the Karpelevič arcs that are powers of some other Karpelevič arc. Furthermore, we study the powers of the corresponding realising matrices. In particular, we show that in the case when a Karpelevič arc is a power of another Karpelevič arc, only selected corresponding realising matrices can be written as a power of another stochastic matrix.
This is joint work with Stephen Kirkland (University of Manitoba) and Helena Šmigoc (University College Dublin). Supported by Science Foundation Ireland (SFI) under Grant Number SFI 18/CRT/6049.

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Analysing the Effects of Aerosol Particle Deposition on the Pulmonary Tree using Computational Fluid Dynamics (CFD)

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The treatment of respiratory diseases is currently receiving considerable attention from researchers around the world. Pharmaceutical aerosols play a critical role in the effective treatment of pulmonary diseases. The size and pattern of the human's inhalation pattern determine the amount and location of particle deposition in the respiratory tract during the treatment period. Because of the complexity of the process involved, there is not much experimental evidence available. The application of computational fluid dynamics (CFD) provides an alternative method for predicting the fluid flow characteristics and tracing the particle trajectory as well as its deposition over the tissues at different inhalation patterns. To represent part of the bronchial region in this study, a three-dimensional model was created using a triple bifurcation with four generations as proposed by Weibel (1963). In this present study, the dense discrete phase model (DDPM) is combined with the discrete element method (DEM) to simulate the dynamics of micron–sized particle transport, interactions and deposition efficiencyusing ANSYS Fluent 2020 software enhanced with user-defined functionsin a four-generation model. The purpose of this study is to examine the effect of aerosol particle deposition on the pulmonary tree at an inhalation flow rate of 15 lpm and aerosol particle size of 10μm. The inlet is injected with a total of 10000 particles. A comparison is made between the results of aerosol particle deposition efficiency with one-way and four-way couplings (DDPM and DEM). The couplings include fluid-particle, particle-particle, and particle-wall interactions. In each generation, airflow velocity patterns in the pulmonary airways are analysed.Utilizing the results of this study, involving accurate and cost-effective lung-aerosol dynamic simulations, will assist in providing improved respiratory dose estimation for treating pulmonary disorders.

Investigating the Effects of Delayed Feedback on the Shutdown of the Atlantic Meridional Overturning Circulation

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The Atlantic Meridional Overturning Circulation (AMOC) is a large system of density driven ocean currents in the Atlantic which powers the Gulf Stream. The Gulf Stream plays an important regulatory role in our climate here in Western and Northern Europe. Evidence suggests that the AMOC is approaching a tipping point, at which it will shut down and no longer provide Western and Northern Europe with its relatively warm climate. Furthermore, a recent study found evidence for a gradual but consistent strengthening of the Antarctic Circumpolar Current (ACC). It is currently unclear how this change in ACC strength might affect the AMOC. Through this research we investigate this effect, via the inclusion of a delayed feedback term in two simple ocean box models. The delayed feedback serves to model the ACC. We analyse these adapted models using bifurcation theory and numerical continuation using the software DDE-Biftool.

Overview of Minimal Surfaces

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Minimal Surfaces are the surfaces which come from critical points of an area functional. They appear throughout science and nature, having applications within a wide range of areas including material sciences and astrophysics. This project gives an overview of the main methods and results of minimal surfaces including periodic minimal surfaces, Weierstrass-Enneper representation, adjoint surfaces, associated families and applications of minimal surfaces.

Bump-and-Revalue: Estimating the Greeks

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Financial derivatives are contracts whose value is derived from the performance of an underlying asset. Valuing these derivatives as well as finding how their value changes given shifts in certain parameters is of the utmost importance in quantitative finance. As many of these values do not have closed-form expressions, we must go about valuing them using methods of simulation, in this case Monte-Carlo Simulation. As financial models are mainly represented via Stochastic Differential Equations (SDEs), there is a heavy foundation in stochastic modelling. Where necessary, Numerical approximation methods based upon the SDEs of our financial derivatives were found and we were able to work from those but, where possible, we tried to keep this type of approximation to a minimum. Option price sensitivities (Greeks) were simulated by the bump-and-revalue method using Monte-Carlo simulation. In order to bring the accuracy to as high a degree as possible, we further employed variance reduction techniques (namely importance sampling) as well as several methods for reducing any approximation error. Through this we found numerous factors which heavily influenced the effectiveness of our simulations.

A Mathematical Model for Holographic Recording in Photopolymer Media with Zeolite Nanoparticles

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Researchers from the Industrial and Engineering Optics group and the School of Mathematical Sciences at TU Dublin have done extensive work on a mathematical model to describe holographic recording in a photopolymer materials, more recent studies have shown that the addition of zeolite nanodopants can improve the dynamic range and reduce photopolymerization-induced volume shrinkage. In this research project, a new mathematical model is presented capable of explaining these observations. A coupled system of reaction-diffusion equations will be presented that can describe the mass spatial-temporal profile of monomer, short polymer chains (oligomer), long polymer chains and inert nanoparticles over the duration of holographic recording. These new equation will take into account how both the mass transport properties of the mobile monomer and oligomer and rate of photo-chemical reactions are impacted by the presence of zeolite nanodopants. The new model is validated via a comparison of its predictions against experimental observations.

Stable Reconstruction of Anisotropic Conductivity

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We study the issues of stability and reconstruction of the anisotropic conductivity σ of a biological medium $\Omega \subset \mathbb{R}^3$ by the hybrid inverse problem of Magneto-Acoustic Tomography with Magnetic Induction (MAT-MI). More specifically, we consider a class of anisotropic conductivities given by the symmetric and uniformly positive definite matrix-valued functions $A(x, \gamma(x))$, $x \in \Omega$, where the one-parameter family $t \mapsto A(x, t)$, $t \in [\lambda^{-1}, \lambda]$, is assumed to be *a priori* known. Under suitable conditions that include $A(\cdot, \gamma(\cdot)) \in C^{1,\beta}(\Omega)$, with $0 < \beta \leq 1$, we obtain a Lipschitz type stability estimate of the scalar function γ in the $L^2(\Omega)$ norm in terms of an internal functional that can be physically measured in the MAT-MI experiment. We demonstrate the effectiveness of our theoretical framework in several numerical experiments, where γ is reconstructed in terms of the internal functional. Our result extends previous results in MAT-MI where the conductivity σ was either isotropic or of the simpler anisotropic form γD, with D an *a-priori* known matrix-valued function in Ω. In particular, the more general type of anisotropic conductivity considered here allows for the anisotropic structure to depend non-linearly on the unknown scalar parameter γ to be reconstructed.

Dynamics of Generalized Random Sequential Adsorption

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The biophysical surface phenomenon of Random Sequential Adsorption (RSA) is investigated, during which the irreversible accumulation of surface-active macromolecules at interfaces occurs. This process underpins the development of many immunoassay technologies, which rely on the physical adsorption of detection antibodies (the adsorbate) on solid substrates (the adsorbent) for binding analytical targets such as pathogenic organisms or biomarkers for cancer diagnostics. Of particular interest for us is the modelling of a generalization of standard RSA where specific chemical reactions between the deposited adsorbates and the adsorbent results in non-uniformly distributed adsorption locations. In one dimension (where this phenomenon is known as Rényi's parking problem), we adapt an existing integro-differential equation that measures the rate of creation and destruction of available deposition positions to account for non-uniform adsorption and clustering behaviour.

Stability estimates in the inverse problem of diffuse optical tomography via singular solutions

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Inverse Problems are a field of mathematics that form a basis for imaging and materials' characterisation. Diffuse Optical Tomography (DOT) is a promising medical imaging technique that shows potential to be a cheap, versatile alternative to other forms of medical imaging techniques or a good partner to already established medical imaging modalities. In DOT, infrared light is delivered to the surface of the head (or another body part) and detectors, also on the head's surface, measure the re-emitting light. The optical properties (μ_a-absorption coefficient and μ_s-scattering coefficient) of the head are then recovered using reconstruction algorithms and an image of the head's interior can be created from these optical properties. In this poster we address the inverse problem in the time-harmonic case of DOT of stably recovering the optical properties of an anisotropic medium, under the so-called diffusion approximation. Assuming that the scattering coefficient is a-priori known, we stably determine the absorption coefficient, together with its derivatives (of any order) at the boundary in terms of the so-called Dirichlet-to-Neumann (DN) map (the measurements). Our argument is based on the construction of singular solutions of a second order elliptic system (governing the light propagation), having an isolated singularity of arbitrarily high order. In particular we establish Hölder type stability estimates of any derivatives of the absorption coefficient at the boundary (in the $L^\infty(\partial\Omega)$-norm) with respect to the DN map

Affine Volterra Processes with jumps

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Applications in Biology, Finance, or Physics often require to model uncertain eventssuch as the birth-and-death of a particle; infection and recovery from a disease of an individual from a population; uncertainty of events in large particle systems in Statistical Physics; the future value of an asset in Financial Modelling. All these *uncertain events* are associated with randomness and hence described by *probabilistic models*. At this point it is often assumed that new random events appear independently of each other, and hence future events are independentof the past. Such a behavior is adequately captured by the terminology of Markov processes for which a powerful mathematical framework is available. Unfortunately, many modern applications do not fall into the class of Markov processes as they explicitly require stochastic models with memory effects. Such a behavior was observed,e.g., in the fractional SIR model in Epidemiology, fractional Langevin equations and anomalous diffusions in Physics, rough volatility models in Finance, spot price dynamics in electricity markets, and multi-scale climate change models. Consequently, there is currently a strong demand driven by applications to develop a theory of stochastic models with memory effects and subsequently study their implications with respect to the aforementioned applications. In this project we aim to significantly advance this recent research direction in Stochastics by investigating on the one-hand side a general mathematical theory of stochastic processes with memory and on the other-hand side to validate our research findings against particular models from *recent applications*. Among all of these applications, we focus on stochastic models with memory appearing in the modeling of Financial markets with particular emphasis on stochastic *volatility processes* and *renewable electricity markets* both being fundamental for our society.

Pricing multi-asset options using the MONTE CARLO-TREE (MC-TREE) method

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This presentation introduces the Monte Carlo-Tree (MC-Tree) method to price the multi-asset options. For pricing single asset options, MC-Tree combines the MC method with the recombining binomial tree based on Pascal's triangle (Trinh, 2022). Similarly, MC-Tree combinesthe MC method with the recombining multinomial trees based on Pascal's simplex for pricing multi-asset options (Sierag, 2018). In the higher dimensional case, we develop and apply an optimization algorithm for the convex combination of a collection of (mixing) densities to find the maximized entropy of compound densities. As well-known from the literature, the standard bivariate normal density has the maximal entropy at $\log(2\pi) + 1 \approx 2.837877$. We find the entropy at 2.829718 after applying our optimization algorithm at the tree depth $N = 10$. We also work with a much simpler mixing density for which the entropy is 2.829633. The difference between those two values is possibly insignificant of 10^{-3}. The core of the MC-Tree method is to very accurately approximate standard Gaussian expectations. In one asset case, we use that mixing zero mean distributions gives a zero-mean distribution, and mixing distributions with the second moment at one produces a distribution with second moment at one. In the d assets case, we can conclude that maximizing the entropy over the rotation-and reflection-invariant densities, conditional on the mean at $(0, 0, ..., 0)^T$ and the covariance matrix at I_d is equivalent to maximizing the so-called RI entropy over all densities for a radius of vector-nodes after N steps in the tree, R, on $[0, \infty)$, where $R = \|X\|_2$, conditional on $E[R^2] = d$. In two-assets case, we apply an alternative approach and conclude that maximizing the entropy over the rotation-and reflection-invariant densities, conditional on the covariance matrix $= I_2$ is equivalent to maximizing the entropy over all densities for P on $[0, \infty)$, where $P = \frac{R^2}{2N}$, conditional on mean at one. As well-known from the literature, the exponential distribution with mean and variance at one is the distribution with the maximal entropy at one among all distributions on $(0, \infty)$. Based on numerical results from pricing multi-asset options, the MC-Tree method is more accurate than the recombining multinomial tree and the plain MC Method, using the same tree depth or numbers of simulations.

References

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Mathematical model of bovine hormonal dynamics

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There have been many previous attempts to model the bovine estrus cycle. Some scientists such as Boer and Stötzel have created "hormonal dynamic" models which consist of an ODE for each hormone being modelled and Hill functions to describe the inhibitory or stimulatory effects they have on one another. While other modellers such as Soboleva and Lange have focused on just the follicular phase of the cycle and modelled the individual E2 (Estradiol) production of each follicle. By doing this, they could model the way follicles compete to become dominant. While Soboleva has modelled the follicular competition of the follicles, they have neglected the other interactions taking place which directly effect E2 production and instead have chosen to describe these interactions using 2 constants. In our model we propose a combination of these 2 approaches. Here, we model hormones as ODEs and the growth of each individual follicle and their E2 production separately. We have done this by creating the compartmental model in Figure 2. If for example Follicle 1 is deemed to have ovulated, it becomes a CL (Corpus Luteum) and the compartment switches from E2 to P4 (progesterone) production. The model was parameterised using in-vivo data from our Polish partners at the Institute of Animal Reproduction and Food Research, Polish Academy of Sciences, Olsztyn, Poland. They supplied us with of E2 and P4 blood concentrations data from bovine blood samples, following the injection of varying doses of IGF-1 (Insulin like growth factor) into ($N = 12$), ($N = 33$) cows. This novel approach we have taken is particularly useful for bovine reproductive modelling as by modelling the follicles individually, we can directly model multiple ovulations which can indicate twinning in fertilised cows. In beef farming twins are desirable while in dairy farming they are not as it results in wasted resources and can cause serious health complications for pregnant cows. This research is particularly relevant considering the heightened focus on the high methane emissions by cattle and the 2030 EU target of a 30% reduction in methane emissions