UK Graduate Modelling Camp 2022
Mentor Abstracts

Modelling Business Space Occupancy
Sam Kamperis, Oxford Brookes University

Businesses that occupy physical premises are key to local employment. With data listing the current and empty business properties in the city of Luton, can you model the impact of different interventions? What strategies could lead to an increase in local employment? Interventions could be support for new/existing businesses or change of use (business type) at a premises. The data includes location, property value, business type and the date each vacant site was last occupied. How businesses coexist varies with different types and size. There have also been dramatic changes to how space is used, for example a rise in home delivery has encouraged growth in warehousing occupancy. However, in recent years demand for office space has declined sharply due to more people working home.

Modelling the Airborne Transmission of Viruses
Katerina Kaouri, Cardiff University

Inspired by collaborative research undertaken during the COVID-19 pandemic to inform policy-making, in this challenge we are going to study the airborne transmission of viruses. We are going to develop models of airborne transmission and solve them using numerical and, where appropriate, analytical methods. If time allows, we are going to also look into air purifiers and how they can enhance ventilation in indoor spaces.
Background reading: https://pubmed.ncbi.nlm.nih.gov/35310953/

Mathematical Modelling for Preventing Homelessness
William Lee, University of Huddersfield

The group is asked to use mathematical modelling to understand the problem of homelessness and potentially suggest some interventions that may have a positive impact. This builds on work carried out at the Communities of the Future virtual study group [1]. Possible approaches the group might like to investigate would include using data to parameterise a dynamical systems models of homelessness such as the one formulated in ref [2] or modelling the process by which a household becomes homeless using a discrete event simulation model. It would also be interesting to use available data to better understand the characteristics of homeless households or households at risk of becoming homeless. Examples of interventions that could be investigated include local authorities offering support to households at risk of becoming homeless within three months rather than one month.

References:
[1] V-KEMS Report Communities of the Future.
[2] A. Lacey, J. Byatt-Smith, M. Grinfeld, S. Llewellyn Smith, T. Lowe, D. Parker, K. Parrott, C. Please, W. Smith, and J. Wattis, Mathematics in Industry Reports (2021).

Neutralising Toxic Chemicals in Porous Media
Ellen Luckins, University of Oxford

After a spill or leak of a toxic chemical, it is crucial for both public health and the environment that the chemical is properly cleaned up. Decontamination is typically achieved by reacting the toxic chemical with a cleanser, which neutralises it in a chemical reaction, producing harmless product chemicals. While the rates of these neutralisation reactions can be ascertained by laboratory experiments, it is not clear how environmental factors may impact the decontamination process in the field. There is particular interest in situations where the toxic chemical has seeped into porous building materials such as rock, concrete, or brick, since it is difficult to measure or observe from the surface if any of the toxic chemical remains inside the pores.

The challenge is to develop better understanding of the process of decontaminating porous materials. Questions the mathematical modellers may tackle include: How long does it take to decontaminate a porous material? What are the limiting processes? What environmental factors affect decontamination time? How much cleanser should be applied to the porous material? How can the cleaning process be improved or optimised?

Predicting Chemical Properties of Compounds from their Molecular Structure with Machine Learning
Ambrose Yim, University of Oxford

In chemistry, the molecular structure of a compound plays an important role in determining its chemical properties. Developing algorithms that learn to predict chemical properties from molecular structures is a problem at the forefront of data science. Since molecular structures are naturally encoded as graphs, standard machine learning algorithms that work on data encoded as vectors cannot be applied directly to this task.

Thus, the challenge here is to develop a translator between graphs and vectors: a method that learns and extracts pertinent features of molecular structures as predictive vector features. Having this translator, we can apply standard machine learning methods to molecular structures and use them to make predictions.

In this challenge, students will have the opportunity to apply the method they have developed on a real dataset, to validate and understand their methodology in the context of a real world scientific problem.