Computational Models for Complex Systems

Topic suggestions for student presentations/projects

A.Y. 2019-2020

Preliminary notes

- This document contains a number of suggestions of topics for student presentations or modeling/development projects
- Each suggestion may include a reference to a scientific paper. That paper could be the starting point of an individual search. The presentation could be based on a different (but related) paper on the same topic.
- Some topics can be taken by more than one student (by coordinating presentations)!
- Scientific papers are available in a shared folder that will be made available by the teacher on request
- Sometimes scientific papers are full of technical/mathematical details. The student presentation doesn't need to enter in all the details. Better to focus on main concepts and examples!
- Modeling/development projects do not require to make a public presentation at the end. The project can be discussed with the teacher privately.
- Ideas from students are welcome!

Mathematical models

Seminar: SIR models applied to COVID-19

Available here:

https://arxiv.org/abs/2003.14391

See also for other models:

https://scholar.google.it/scholar?q=sir+covid

A Modified SIR Model for the COVID-19 Contagion in Italy

Giuseppe C. Calafiore, Carlo Novara and Corrado Possieri

***Abstract*— The purpose of this work is to give a contribution to the understanding of the COVID-19 contagion in Italy. To this end, we developed a modified Susceptible-Infected-Recovered (SIR) model for the contagion, and we used official data of the pandemic up to March 30th, 2020 for identifying the parameters of this model. The non standard part of our approach resides in the fact that we considered as model parameters also the initial number of susceptible individuals, as well as the proportionality factor relating the detected number of positives with the actual (and unknown) number of infected individuals. Identifying the contagion, recovery and death rates as well as the mentioned parameters amounts to a non-convex identification problem that we solved by means of a two-dimensional grid search in the outer loop, with a standard weighted least-squares optimization problem as the inner step.**

Seminar/Project: Rock-Scissor-Paper evolution model

Rock–scissors–paper and the survival of the weakest

Marcus Frean[1*] **and Edward R. Abraham**[2]

[1]*School of Mathematical and Computing Sciences, Victoria University, PO Box 600, Wellington, New Zealand*
[2]*National Institute for Water and Atmospheric Research (NIWA), PO Box 14-901, Kilbirnie, Wellington, New Zealand*

In the children's game of rock–scissors–paper, players each choose one of three strategies. A rock beats a pair of scissors, scissors beat a sheet of paper and paper beats a rock, so the strategies form a competitive cycle. Although cycles in competitive ability appear to be reasonably rare among terrestrial plants, they are common among marine sessile organisms and have been reported in other contexts. Here we consider a system with three species in a competitive loop and show that this simple ecology exhibits two counter-intuitive phenomena. First, the species that is least competitive is expected to have the largest population and, where there are oscillations in a finite population, to be the least likely to die out. As a consequence an apparent weakening of a species leads to an increase in its population. Second, evolution favours the most competitive individuals within a species, which leads to a decline in its population. This is analogous to the tragedy of the commons, but here, rather than leading to a collapse, the 'tragedy' acts to maintain diversity.

Keywords: rock–scissors–paper; intransitive competition; Prisoner's Dilemma; voter model

In the seminar, you can present the paper and also show some simulations you performed using ODEs and/or NetLogo

Available here: https://doi.org/10.1098/rspb.2001.1670

Seminar/Project: time series forecasting

- Several methods exist to forecast the future trend of a time series of measured values based by inferring a model (e.g. recurrence equations or ODEs) from available observations
  - Weather forecasts (time series of temperatures/humidity)
  - Economic and market trends
  - Growth of plants in agriculture
  - ….
- See, e.g.: https://machinelearningmastery.com/time-series-forecasting-methods-in-python-cheat-sheet/
- This can be the subject of a seminar or experimental project

Stochastic simulation

Seminar: Improvements to Gillespie's Stochastic Simulation Algorithm

Stochastic Simulation of Chemical Kinetics

Daniel T. Gillespie

Available here:

https://doi.org/10.1146/annurev.physchem.58.032806.104637

Abstract

Stochastic chemical kinetics describes the time evolution of a well-stirred chemically reacting system in a way that takes into account the fact that molecules come in whole numbers and exhibit some degree of randomness in their dynamical behavior. Researchers are increasingly using this approach to chemical kinetics in the analysis of cellular systems in biology, where the small molecular populations of only a few reactant species can lead to deviations from the predictions of the deterministic differential equations of classical chemical kinetics. After reviewing the supporting theory of stochastic chemical kinetics, I discuss some recent advances in methods for using that theory to make numerical simulations. These include improvements to the exact stochastic simulation algorithm (SSA) and the approximate explicit tau-leaping procedure, as well as the development of two approximate strategies for simulating systems that are dynamically stiff: implicit tau-leaping and the slow-scale SSA.

Project: A (modular) simulator of chemical reactions with external events

- Idea: develop (in any programming language) a stochastic simulator of chemical reactions that takes as input
  - A set of chemical reactions
  - An initial configuration (concentrations of molecules)
  - A list of events (changes in concentrations), each scheduled at a precise time
- Simulation of the chemical reaction should be interrupted every time a scheduled event has to be executed. The state has to be updated in accordance with the event content. Then simulation can continue
- The source code should be modular: it should be easy to add a new simulation algorithm
- More details to be discussed…

Stochastic/probabilistic model checking

Seminar: Prism Games

PRISM-games: Verification and Strategy Synthesis for Stochastic Multi-player Games with Multiple Objectives

Marta Kwiatkowska[1], **David Parker**[2], **Clemens Wiltsche**[1]

[1] Department of Computer Science, University of Oxford, UK
[2] School of Computer Science, University of Birmingham, UK

Abstract. PRISM-games is a tool for modelling, verification and strategy synthesis for stochastic multi-player games. These allow models to incorporate both probability, to represent uncertainty, unreliability or randomisation, and game-theoretic aspects, for systems where different entities have opposing objectives. Applications include autonomous transport, security protocols, energy management systems and many more. We provide a detailed overview of the PRISM-games tool, including its modelling and property specification formalisms, and its underlying architecture and implementation. In particular, we discuss some of its key features, which include multi-objective and compositional approaches to verification and strategy synthesis. We also discuss the scalability and efficiency of the tool and give an overview of some of the case studies to which it has been applied.

See also:
http://www.prismmodelchecker.org/games/

Petri nets

Seminar: Petri Nets modeling of Hospitals

A Three-Level Strategy for the Design and Performance Evaluation of Hospital Departments

Maria Pia Fanti, *Senior Member, IEEE*, Agostino Marcello Mangini, Mariagrazia Dotoli, *Senior Member, IEEE*, and Walter Ukovich, *Member, IEEE*

***Abstract*—The efficient management of hospital departments (HDs) has recently become an important issue. Indeed, the increased demand and design for hospital services have saturated the capacity of HD that requires suitable tools for the efficient use of resources and flow of patients, staff, and drugs. This paper proposes a model based on a three-level strategy to design at the tactical level in a concise and effective way the structure, the resources, and the dynamics of a critically congested HD. The design strategy is composed of three basic elements: the modeling module, the optimization module, and the simulation and decision module. The first module employs a Unified Modeling Language tool and a timed Petri net (PN) model to effectively capture the detailed flow and dynamics of patients, starting from their arrival to the HD until their discharge. The optimization module employs the fluid relaxation to concisely approximate in a continuous PN framework the HD model and optimize suitable performance indices. The simulation module verifies that the optimized parameters allow an effective workflow organization while maximizing the patient flow. In case of inconsistencies due to the fluid approximation between the continuous model used in the design phase by the optimization module and the discrete one used in the subsequent verification phase by the simulation module, the latter module revises the values of some HD model parameters. A real case study on the Emergency Cardiology Department of the General Hospital of Bari (Italy) shows the efficiency and accuracy of the proposed method.**

Available here:

https://doi.org/10.1109/TSMCA.2012.2217319

Seminar: Process Mining

Business process mining: An industrial application

W.M.P. van der Aalst[a,*], H.A. Reijers[a], A.J.M.M. Weijters[a], B.F. van Dongen[a], A.K. Alves de Medeiros[a], M. Song[a,b], H.M.W. Verbeek[a]

Abstract

Contemporary information systems (e.g., WfM, ERP, CRM, SCM, and B2B systems) record business events in so-called *event logs*. *Business process mining* takes these logs to discover process, control, data, organizational, and social structures. Although many researchers are developing new and more powerful process mining techniques and software vendors are incorporating these in their software, few of the more advanced process mining techniques have been tested on real-life processes. This paper describes the application of process mining in one of the provincial offices of the Dutch National Public Works Department, responsible for the construction and maintenance of the road and water infrastructure. Using a variety of process mining techniques, we analyzed the processing of invoices sent by the various subcontractors and suppliers from three different perspectives: (1) the process perspective, (2) the organizational perspective, and (3) the case perspective. For this purpose, we used some of the tools developed in the context of the ProM framework. The goal of this paper is to demonstrate the applicability of process mining in general and our algorithms and tools in particular.

See also: http://www.processmining.org

Discrete event simulation and Agent-based modeling

Seminar/Project: Experience with a Discrete Event Simulation tool

- The presentation may consist in a tutorial/demo/case study with one of the following tools for Discrete-Event Simulation
  - SimPy (https://simpy.readthedocs.io)
  - Arena (https://www.arenasimulation.com)
  - FlexSim (https://www.flexsim.com)

Project: Java DES engine prototype

- As a development project, take the DES engine prototype I have described in this course and refine/extend it

Seminar/Project: Experience with NetLogo

- A seminar may consist in a tutorial/demo of one (or more) NetLogo (https://ccl.northwestern.edu/netlogo/) models to be agreed with the teacher

- A project may consist in developing a NetLogo model of a complex system to be agreed with the teacher