Wallenberg AI, Autonomous Systems and Software Program (WASP) PhD Student Day

11 October 2022

Cripps Court Auditorium, Magdalene College, Cambridge

Agenda

8:30 – 9:00	Delegates arrive - Refreshments	
9:00 – 9:05	Welcome	Jim Weatherall, AZ
9:05 – 9:10	Introduction to WASP	Christian Berger, WASP
9:10 – 9:25	AZ's approach to Data Science and AI	Jim Weatherall, AZ
9:25 – 9:45	AI for Drug Combination Predictions	Marta Milo, AZ
9:45 – 10:05	Knowledge Graphs for Precision Oncology	Krishna Bulusu, AZ
10:05 – 10:15	Introduction to workshop	
10:15 – 10:30	Break	
10:30 – 10:50	Challenges and Advances of Deep Learning in Digital Pathology	Nikolay Burlutskiy, AZ
10:50 – 11:10	AI for prediction of pharmacokinetics	Olga Obrezanova, AZ
11:10 – 11:30	Using a fully automated ML approach to ensure clinical trial success	Kleio Kipourou, AZ
11:30 – 12:00	Machine learning and AI for medicine	Mihaela Van Der Schaar, University of Cambridge
12:00 – 12:25	LUNCH	
12:25 – 13:05	Break out workshop - Lunch	
13:05 – 13:50	Report back pitches	
13:50 – 14:00	Summary and close	Jim Weatherall, AZ

Aim: For PhD students to learn more about how data science/AI are used at AZ. For AZ, it is also an opportunity to network with potential future talent.

Attendees

58 PhD students from WASP
Prof. Christian Berger (WASP)
Jim Weatherhall
Jacqui Hall
Michael Tonge
Anne Thuery
Nikolay Burlutskiy
Krishna Bulusu
Richard Dearden
Olga Obrezanova
Marta Milo
Vera Hazlewood
Kleio Kipourou
James Savery
Nina Mian
Paul Metcalfe
Ben Sidders
Iker Huerga
Joachim Reischl
Mihaela Van Der Schaar

Accessing Cripps Court, Magdalene College
Please see attached maps at the end of the document.

Presentation abstracts

Nikolay Burlutskiy: In recent years, Artificial intelligence (AI) has attracted many researchers to improve healthcare. In this talk, we will discuss the role of AI in digital pathology and drug discovery with a few relevant use cases. We will look at current challenges and concerns around AI such as generalisability, interpretability, potential bias, and ethical considerations.

Kleio Kipourou: Multicentre phase II/III clinical trials are large scale operations that often include hundreds of recruiting centres in several countries. Conducting trials of that scale requires thorough planning and efficient execution to ensure patient safety and trial success. Monitoring the progress of a trial is essential to maximise the probability of success. Therefore, we developed a fully automated Machine Learning algorithm that predicts trial activities (e.g. patient recruitment/randomisation) and detects early deviations from the plan. In this talk, we will discuss about the challenges of creating such a tool, which is updated daily and can be applied to any trial, and show how study teams use it to ensure trial success.

Olga Obrezanova: AI-driven approaches to predict *in vivo* animal and human pharmacokinetic (PK) parameters from chemical structure can guide the design of molecules with optimal PK profiles, enable the prediction of virtual compounds, and help to prioritise compounds for *in vivo* assays. We will present the framework for modelling of *in vivo* PK data utilised in AstraZeneca and focus on machine learning models for rat and human PK.

Workshop activity

In groups of 5 to 6 please consider the following questions:

1. What questions would you ask the presenters and what do you want to know more about?

2. What are the next breakthroughs in the area of data science and medicine?
    If you were CEO of AstraZeneca, what would you invest in?

3. How do you think your current expertise can be applied to these challenges?

Groups have 40 minutes to consider these questions and discuss amongst themselves with the help of facilitators.

One group will lead on feeding back for each question with other groups adding additional information.

Background on WASP

Wallenberg AI, Autonomous Systems and Software Program is Sweden's largest individual research program ever, and provides unique opportunities for achieving international research excellence with industrial relevance. WASP is funded by the Knut and Alice Wallenberg Foundation.

The WASP graduate school actively supports forming a strong multi-disciplinary and international professional network between PhD students, researchers and industry. This is done through an ambitious program with specifically designed courses, international research visits, study visits at Swedish industry partners, cooperation with several partner universities in and outside Sweden, and visiting lecturers. There are also recurrent chances for our PhD students to network with industrial and academic representatives in the many events arranged by WASP.

PhD summaries

1	P4 is a Domain Specific Language used to program data planes in programmable switches. We are trying to verify P4 software is correct and adheres to the specifications using formal methods.
2	Software engineering for robotics. Lately, I have investigated how researchers and practitioners use runtime monitoring and field-based testing for gaining confidence in ROS-based software.
3	Discovery of patterns and anomalies in graph structured data. Current focus is on how node embeddings can be extracted from graphs without requiring labels.
4	My research focus is on the control and coordination of connected and automated vehicles in challenging traffic scenarios such as intersections with intensive multi-vehicle interactions.
5	- Visual Inertial Lidar State Estimation (SLAM) - Intention Prediction of Traffic Agents - Automatic Sensor Calibration
6	Different AI methods and their application in the field of robotic assembly. Learning from demonstration. Knowledge-based approaches. Learning and using abstractions/representations of skills/objects.
7	I use dynamic and static software analysis and AI, ML, and DL methods to automatically generated descriptions about what is changed in a program.
8	Applied machine learning in AI. Image and language comprehension using NNs. Do reasoning on the extracted information from these modalities. My research is grounding language in a situated dialog.
9	The topic of my PhD research project is "anomaly detection and countermeasures for edge clouds".
10	Fully Autonomous AI-driven Continuous Integration (CI). Focus on data mining in industrial CI, fault localization, and automatic program repair.
11	It is about 5G and Beyond 5G simultaneous localization and mapping (SLAM), which is to utilize 5G or 6G signals to localize the user and map the unknown environment by using Bayesian or DL approaches.
12	The goal of my research is to facilitate the migration to model-based design and systems to enable reusable and maintainable robotic missions.
13	My main area of research is type-directed program synthesis and program repair, as well as fault-localization and other tools for program correctness.
14	I am interested in networked control systems, i.e. problems within control theory where there is an underlying topology that restricts the behavior.
15	In my research, I explore the usage of ML techniques for improving software reliability in DevOps by timely detecting anomalies in run-time monitoring data representing the health of a software system
16	creating methods to automatically synthesise task switching policy representations to control mobile manipulators operating in unpredictable environment, to reduce the time spent to program a robot.
17	Deep learning for computer vision, e.g. image classification and segmentation. My research also involves vision-based reinforcement learning for robot navigation.
18	State and parameter inference in partially known probabilistic state-space models. I.e., combining prior domain knowledge with machine learning techniques for state-space model inference.
19	Set-based estimation in shared situational awareness for connected and automated vehicles in complex urban scenarios using vehicle-to-everything communication.
20	I am a PhD student under supervision of Prof. Håkan Hjalmarsson. My PhD topic is about the sparse system identification in which we estimate the parameters of system such that most of them are zero.
21	Techniques for large-scale semi-definite programming, copositive programming and low-rank matrix optimization with applications to ML. Also federated learning and quantum computing for optimization.
22	My research project is mostly related with representation learning techniques that deal with lack of available sufficient supervision. We have tackled this problem using KT, active learning, etc.
23	Dynamic On-chip Memory Management exploiting reuse distance and dynamic compute order for DNN accelerators
24	My field of research is scientific visualization where the focus is to utilize topology-based methods in order to extract high-level features and then use them in learning-based models.
25	My research spans Control of Multi-Agent Systems, Robust Control, and Computer Vision, all with respect to safety-critical Robotics.
26	Robotics and Automation. In particular, human-robot interaction and kinesthetic teaching.

27	My focus is on complexity certification of mixed-integer quadratic/linear programming. An important application is on hybrid model predictive control (MPC) to determine required computation, offline.
28	My research area is software testing of autonomous driving systems. We are currently working on a critical scenario identification approach that uses search algorithms to find critical test scenarios.
29	Learning and task planning for industrial robots. Mainly focused on behavior trees as the policy representation.
30	My research lies within the field of control. More specifically, I am interested in sparse controllers suitable for large-scale systems which reject disturbances optimally.
31	My area of research lies on the intersection between control theory and ML. Topics include learning for sysid, causality, diffusion models, experimental design. (interested in medical applications)
32	My research interests include perception for underwater robots, bathymetric mapping and localization with sidescan sonar. Recently I am working on SLAM using differentiable rendering with sidescan.
33	My research interest lies on the intersection of reinforcement learning and robotics. I have been trying to utilize prior knowledge to guide learning robotic skills.
34	I focus on Automatic Manufacturing Quality Inspection based on Deep Learning and Computer Vision. Currently, I am doing research on Sim to Real: Automatic Quality Inspection by training with CAD data.

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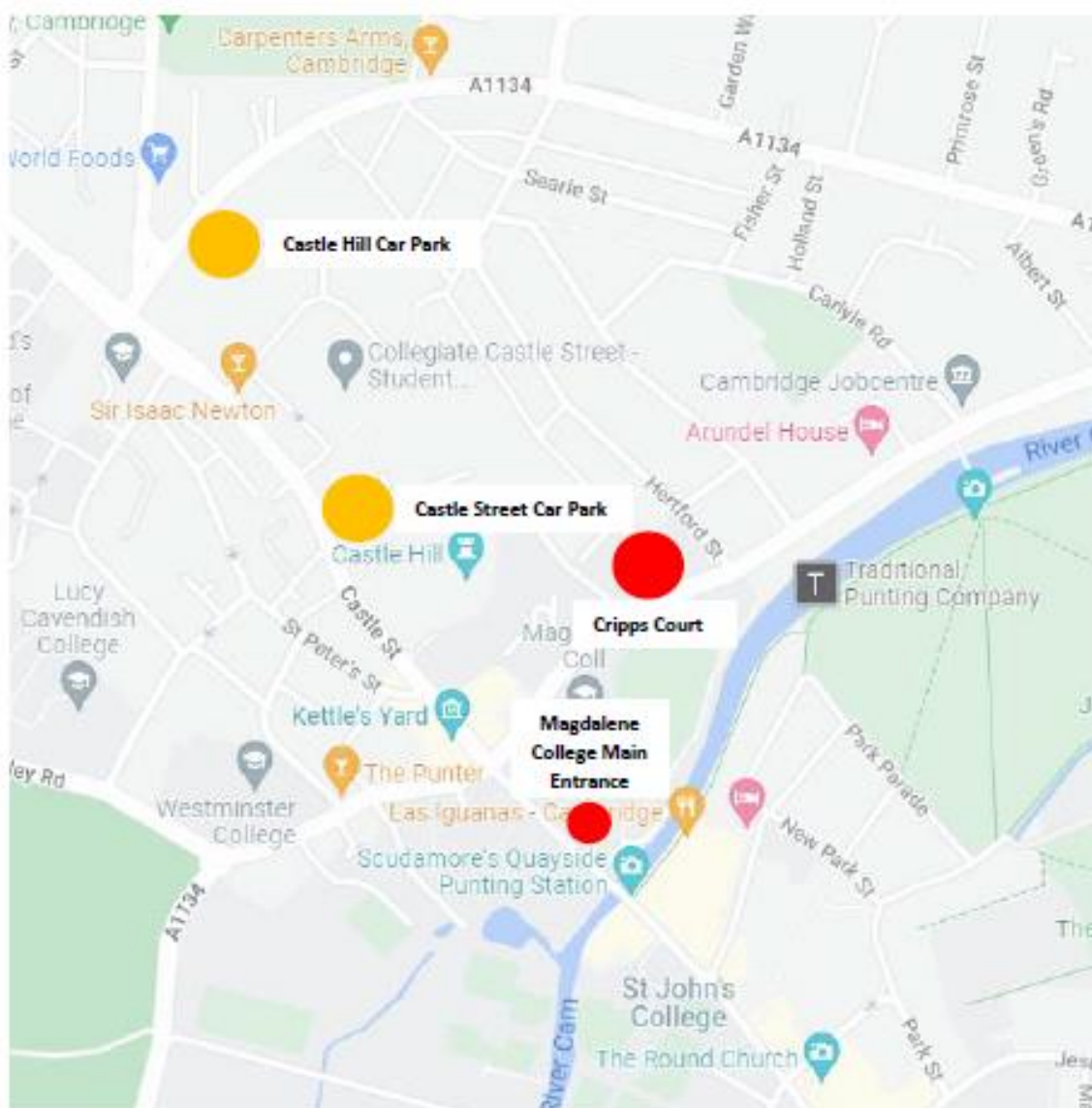
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