
Turing-Roche Partnership Predictive Modelling Workshop Report 2022

Context

The Turing-Roche Strategic Partnership launched in June 2021 with the 'North Star' aim of generating insights to better understand patient and disease heterogeneity and its relevance to clinical outcomes at an unprecedented level of precision in order to improve clinical care.

The partnership is pursuing multiple research themes over our 5 year collaboration. Last year we explored the theme of 'Structured Missingness'- roughly defined as missing data that is structured in some way, which is a common problem emerging in many fields. At the end of 2021 we ran [three collaborative workshops](#) to convene a diverse group of researchers to discuss this problem and scope out approaches to structural missing data, whilst formulating substantive and collaborative research questions that merited further exploration. We then launched an associated funding call and seconded [two project teams into the Turing Institute for 18 months](#).

This year we have chosen the theme of 'Predictive Modelling', looking at this within the lens of uncertainty and heterogeneity in biomedical data. Machine-Learning based predictive models have achieved success in a wide range of real life applications, but often the power and potential of the models comes down to their robustness in the face of data uncertainty i.e noisy data, biased data, missing data etc. This theme was scoped by our Senior Postdoctoral Research Associate Tapabrata (Rohan) Chakraborty and we decided to break the theme down into three sub-themes for further exploration:

- Generalisation despite heterogeneity: developing models that perform robustly in the face of data heterogeneity and generalise across patient heterogeneity
- Prediction uncertainty in personalised healthcare: quantifying the uncertainty of personalised (as opposed to generalised) predictions at the individual patient level made from models trained at the population level
- Algorithmic explainability and fairness for responsible AI: developing models that perform fairly across different patient subgroups and the decision process is interpretable and transparent

Following last year's successful model, we decided to host another collaborative workshop (this time in-person) and launched an [associated funding call](#).

Structure and Workshop Discussions

The workshop took place on the 11th October at the Turing Institute in London. We had a short application process to apply to attend the workshops, ensuring we brought together a diverse community of researchers interested in different sub-themes, including established and early career researchers.

We had 35 researchers attend the workshop, alongside members of the partnership team (Ben MacArthur, Chris Harbron, Rohan Chakraborty, Vicky Hellon and Alvaro Sahun), some of our Expert Panel Members (Mike Barnes and Alejandro Frangi) and colleagues from Roche

(Alex Skates, Eleanor Brooks and Pau Herrero).

The workshop began with a quick introduction and a [virtual talk](#) from our Expert Panel Member Florian Markowetz who challenged the attendees to think about what is actually needed to make a clinical prediction model successful- showing examples of the many models not in use and giving his take on what will help with adoption of a model.

We then separated into three breakout groups to discuss the predictive modelling sub-themes.

- The 'generalisation despite data heterogeneity' group was facilitated by Ben MacArthur, Deputy Programme Director for Health and Medical Sciences Programme at the Turing Institute and co-lead for the partnership. In this group discussions centred on a number of interrelated topics including: how best to define "heterogeneity" as a multiscale phenomenon; the challenges associated with making reliable out of distribution predictions; issues surrounding model updating using real-time heterogeneous data streams, and the clinical and regulatory challenges posed; and model deployment in clinical settings in which patient populations may be highly heterogeneous and differ significantly from training data cohorts.
- The 'prediction uncertainty in personalised healthcare' group was facilitated by Chris Harbron, Expert Statistical Scientist & Advanced Analytics Lead at Roche and co-lead for the partnership. In this group discussions started with a debrief of Florian's talk and sharing of the group's experiences in building prediction models and evaluating the uncertainty in predictions generated by these models. The group identified a wide range of existing approaches and discussed the identification and characterisation of uncertainty, different methods and strategies for evaluating uncertainty and the challenges of communicating uncertainty to different stakeholders.
- The 'algorithmic explainability and fairness for AI in healthcare' group was facilitated by Rohan Chakraborty, Senior Research Associate for the partnership. In this group discussions centred on explainability and fairness of predictive models in healthcare. Within explainability, the two main topics were 1) explainability of algorithms by design vs interpretability of decisions and results (with or without causal analysis), 2) usable explainability: whether it is more important to have simple effective models with clear interpretations rather than complex models with complex explanations (also includes tiered explanations from complex to simple). Within the fairness aspect, the two main topics were 1) data bias: pre-analysis of bias present in data and taking steps to mitigate the same, and for existing methods already trained on past data, use counterfactuals to test fairness, 2) patient-centred fairness: should patients be consulted in the process to get better insight into ethnic and gender considerations? This is a new area and overlaps with social science and ethics of AI. All of the above discussions hold true for learning and non-learning based models.

After lunch the breakout groups split into smaller groups to explore ideas in more detail. We then reconvened as a complete group and each smaller group presented a quick overview of their discussions. The smaller groups were as following:

- Within the sub-theme of generalisation despite data heterogeneity:
 - Out of distribution prediction and model updating
 - Learning model parameterisation
 - Design of experiments for predictive modelling in health
 - Heterogeneity as a multiscale phenomenon
- Within the sub-theme of prediction uncertainty in personalised healthcare:
 - Decision theory (how to make decisions under uncertainty)

- Evaluating uncertainty (what validation sets to use x how, monitoring over time, representativeness)
- Within the sub-theme of algorithmic explainability and fairness for AI in healthcare:
 - Usable explainability (right level at right stage for right user)
 - Multi-modal explanations (heterogeneous data, missing data and distillation/optimisation of explanations)
 - Fairness of models and data (what is fairness-metrics and data bias, fair models, fair parameters)

We ended the day exploring synergies between the groups and a quick round-up from the partnership team.

Next Steps

The partnership team were keen for the collaborations and connections made at the workshop to continue so we organised two virtual co-working sessions in the weeks afterwards for workshop attendees and any other interested researchers to have a space to touch base, work on proposals or have some quiet working time.

The associated predictive modelling funding call is open to the 14th November 2022. We hope to receive applications that were formed at the workshop as well as any applications from researchers who were not able to attend.

For more opportunities to engage and connect with the partnership, for example through our monthly newsletter, Slack workspace and Knowledge Share events- please see our [webpage](#).