

Representing, calibrating & leveraging prediction uncertainty from statistics to machine learning (RCL) programme report

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The RCL programme (6 May - August 29, 2025) focused on methods for representing, calibrating and leveraging prediction uncertainty, bringing more than 100 researchers together from across statistics, machine learning, and applied mathematics. It provided an environment where researchers from various disciplines could interact and collaborate on challenges pertaining to the way uncertainties are defined, calculated, conveyed, used, and (hopefully!) reduced. Application areas included geosciences, computer vision, health, chemistry and more. We fostered novel connections between probabilistic forecast evaluation (well-established in meteorology and econometrics) with problems arising from generative modelling in machine learning, where sound evaluation of predictive uncertainty calls for further exploring the field of multivariate calibration and scoring. The programme included 3 week-long workshops, a one-day Open for Business event, and finished with a 2-day workshop highlighting the research of early career academics.

The first workshop (6-9 May) focused on challenges of uncertainty quantification in non-Euclidean spaces and had talks about various mathematical tools from geometry and topology, in addition to statistical methods. The second workshop (2-6 May) provided an overview of methodologies and frameworks for calibrating probabilistic predictions, bringing together statistical and machine learning communities. The third workshop (23-27 June) presented different approaches to accelerate statistical inference and experimental design. An emerging theme was the use of diffusion models to amortize various statistical tasks such as calibration and design.

A well-attended Newton Gateway Open for Business event on "Uncertainty in Machine Learning: Challenges and Opportunities" was held on 13 August. We had speakers from a range of companies and organisations, talking about uncertainty quantification challenges in electric vehicles, climate/weather predictions, and the renewable energy sector amongst other areas, and finished with a lively panel discussion on cross-sector uncertainty quantification challenges. The programme closed with a 2-day workshop showcasing early career researchers (27-28 August). Talks spanned the full range of topics from the programme, including estimating uncertainty in large language model outputs, targeted experimental design, and physics informed mechanistic modelling. Two EDI events were held during the third and fourth workshops, with a focus on the diversity of career trajectories in statistics and machine learning.

In between workshops, regular activities were sustained, including seminars by participants (including several Ramanujan and Simon fellows), the Kirk and Rothschild distinguished lectures, and flash-talks by PhD students. Coffee breaks and various social activities (including trips to the Orchard, the beer festival, and the open-air Shakespeare performances) around the programme encouraged scientific exchanges between participants. While most had a statistics or machine learning background, we had several participants from other domains, such as physics and the geosciences. Overall, RCL constituted a multidisciplinary platform rooted in mathematical sciences with a methodological core in (mathematical and applied) statistics as well as in machine learning.