Deep Learning in Chemistry: Evolution or Revolution?

Robert Glen

University of Cambridge, Department of Chemistry,
Lensfield Road, Cambridge CB2 1EW, UK
rcg28@cam.ac.uk

Recent advances in deep artificial neural networks coupled to significant improvements in computational power linked to big data resources have generated enormous interest across all areas of science and technology. In chemistry, a community that already has significant expertise in statistical and machine learning approaches, we have rapidly embraced these developments to, in many cases, significantly improve upon previous analyses and in some cases devise novel approaches yielding new insights from our data. Will 'artificial intelligence', which is to some extent a catch-all term covering a plethora of new algorithms and combinations of statistics/machine learning/deep learning be an incremental or revolutionary improvement? We are I believe at an early stage in what promises to be a game-changer in prediction and design in chemistry, if the promise lives up to the hype!