IN CONVERSATION WITH
JIM WEATHERALL

Vice President of Advanced Analytics and Head of the Advanced Analytics Centre, AstraZeneca

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Jim is Vice President of Advanced Analytics and Head of the Advanced Analytics Centre in Global Medicines Development at AstraZeneca, a diverse and global group focussed on their mission of "transforming the development of medicines through applied data science". He is committed to driving the application of advanced analytics as a way of unlocking the full potential of data – through data & text mining, machine learning & artificial intelligence, visual analytics, modelling & simulation, advanced statistical methods, and exploration of new technologies. Jim is an Honorary Reader in Computer Science at the University of Manchester, and Vice-Chair of the Data Science Section at the Royal Statistical Society.

What are your views on the role that machine learning will play in the future of drug discovery?

Machine learning has the potential to play a significant role in the future of drug discovery. This is because drug discovery is a data-intensive endeavour, and the volumes and types of data are now reaching levels of size and complexity where only computers and algorithms are going to be able to identify novel patterns and hypotheses. The idea of using generative-adversarial neural networks for molecular design is exciting, and a number of organisations are currently exploring this approach – essentially taking a positive step towards machine-driven design rather than brute force approaches requiring a physical laboratory, such as high-throughput screening. Furthermore, machine learning is well positioned to infer predictive models from large and diverse data sets – enabling more robust decision making about which molecules to take forward. Imagine if you were able – with a certain degree of accuracy and uncertainty – to confidently predict the clinical efficacy and safety of your medicine, before it ever makes it in to clinical trials. This is an area of huge potential, albeit with some hard work ahead to get the data in shape, and to understand what these complex pattern recognition techniques are really telling us.

In your opinion, what have been the most important developments in AI over the last 12 months?

Firstly, we've seen more organisations embrace the AI branding and create job roles and departments that reflect this, moving past the hype and replacing scepticism with action. Secondly there have been a proliferation of exemplar cases of how these techniques could transform research and development – the aforementioned molecular design using neural networks, being one of these. Thirdly, there have been a number of reports from significant organisations – for example the UK House of Lords released its report "AI in the UK: ready, willing and able?", and Parliament now even has a select committee on AI. And finally, these reports and other sources have significantly advanced the conversation regarding data ethics and algorithmic responsibility.

What are the biggest challenges in integrating AI approaches into a drug development pipeline?

Data and behaviours. These are the two critical success factors for AI to really make a difference. Firstly, data has to be of adequately high volume and quality, otherwise even the most sophisticated AI algorithm will not be able to extract value from it. For behaviours, we are ultimately relying on human beings to make the final call, based on the outputs of AI and machine learning. In order for this to occur, we have to treat AI as much as a 'human problem' as a 'machine problem'. That is, we are trying to understand how best people can interact with AI, what will lead them to trust the outputs, and how to effectively blend their own soft subjective judgement with the outputs of a hard mathematical engine.

Outside of drug discovery, how could AI have an impact on the wider healthcare industry?

There are numerous ways in which AI could have an impact on the wider healthcare industry. We have already seen chat bots and virtual assistants, with whom you can have a 'conversation', in order to discuss your health or medical issues. Then when you enter a clinic or hospital, you could be greeted by a robot who helps to direct you. When you see your doctor, they should be increasingly using the output of AI algorithms to discuss the risk and benefit of various treatments and other interventions with you. And smart devices, sensors, and wearables will be providing a 'closed feedback loop' to keep you continuously abreast of your health status, so that you can take immediate action if required.