Understanding and Mitigating Bias in Autonomous Materials Characterization and Discovery

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Since the publication of the Mission Innovation Materials Acceleration Platform, AI is increasingly responsible for driving automated experimental and computational campaigns. There have been multiple case studies for which autonomy was demonstrated to successfully drive materials optimization or discovery and the world of scientific robots has moved from science fiction to reality. However, within the AI community it is recognized that AI's carry with them their creators' biases which has serious implications for model deployment. Using specific case studies, I will illustrate how these biases arise in materials science and specific steps that can be taken to remove them. Specifically, I will discuss some of our recent work in (1) reducing human bias in label generation by applying robust statistics to spectroscopic data analysis, (2) identifying and mitigating search space bias through model disagreement, and (3) demonstrating how to use active learning to create optimally informative datasets for model training. Finally, I will briefly discuss the broader activities around self-driving lab development within the University of Toronto's Acceleration Consortium.