The Promise of Artificial Intelligence in Chemical Engineering: Is it here, finally?

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Abstract

Artificial intelligence (AI) started off with great promise in the early 1980s, spurred by the success of the expert system paradigm in certain applications. This prompted a flurry of research activities in chemical engineering in the mid-1980s. However, as the ensuing three decades showed, AI didn't quite live up to its promise in chemical engineering.

So, what went wrong with AI?

In this talk, I will review the different phases of AI in chemical engineering in the last 30 years, providing some background and explanation to this question. I will also argue that this time it is different – I believe the time for AI in chemical engineering, and in other domains, has arrived, finally. There are many applications that are ready to yield quick successes in this new data science phase of AI. I will highlight recent work in materials design and in process operations as examples of exciting progress. However, the really interesting and intellectually challenging problems lie in developing such conceptual frameworks as hybrid models, mechanism-based causal explanations, domain-specific knowledge discovery engines, and analytical theories of emergence. These breakthroughs would require going beyond purely data-centric machine learning, despite all the current excitement, and leveraging other knowledge representation and reasoning methods from the earlier phases of AI. They would require a proper integration of symbolic reasoning with data-driven processing. I will discuss these challenges and opportunities going forward.

Professor Venkat Venkatasubramanian is Samuel Ruben-Peter G. Viele Professor of Engineering in the Department of Chemical Engineering, Professor of Computer Science (Affiliate), and Professor of Industrial Engineering and Operations Research (Affiliate) at Columbia University in the City of New York. He earned his Ph. D. in Chemical Engineering at Cornell, M.S. in Physics at Vanderbilt, and B. Tech. in Chemical Engineering at the University of Madras, India. Venkat worked as a Research Associate in Artificial Intelligence in the School of Computer Science at Carnegie-Mellon University. He taught at Purdue University for many years, before returning to Columbia in 2011. At Columbia, Venkat directs the research efforts in the *Complex Resilient Intelligent Systems Laboratory*.

He is also the founding Co-Director of the *Center for the Management of Systemic Risk*, a transdisciplinary center focused on understanding how complex systems fail in order to prevent or mitigate such failures in the future, with faculty from a number of departments at Columbia University.

By inclination and education, Venkat is attracted to fundamental questions that are at the intersection of different disciplines. A leitmotif in his work is understanding emergent phenomena in self-organized complex systems, particularly using artificial intelligence, statistical mechanics, game theory, and systems engineering concepts and techniques. Venkat's research contributions have been in the areas of process fault diagnosis and risk management, materials discovery analytics, pharmaceutical engineering, and income inequality.

Prof. Venkatasubramanian received the *Norris Shreve Award* for Outstanding Teaching in Chemical Engineering three times at Purdue University. He won the *Computing in Chemical Engineering Award* from AIChE and is a *Fellow of AIChE*. In 2011, the College of Engineering at Purdue University recognized his contributions with the *Research Excellence Award*. He is a past-President of the Computer Aids for Chemical Engineering (CACHE) Corporation. He currently serves as an Editor for *Computers and Chemical Engineering*. His new book, *How Much Inequality is Fair? Mathematical Principles of a Moral, Optimal, and Stable Capitalist Society,* was published in 2017. Venkat's other interests include comparative theology, classical music, and cricket.