From Craft to Commodity:
The Evolution of AI in Pharma and Beyond

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"Artificial Intelligence (AI) is not a novel thing," says Reza Olfati-Saber. Coming from an extensive academic background at MIT, Caltech and Dartmouth College, Olfati-Saber now manages R&D teams of data scientists and life scientists as the Global Head of AI and Deep Analytics at pharma giant Sanofi. "It was in the early 1950s that Marvin Minsky introduced the first neural network at Princeton," he explains. HBS Professor Karim Lakhani, who interviewed Olfati-Saber as part of the *AI in Enterprise* series hosted by the Laboratory for Innovation Science at Harvard and who has studied innovation in drug discovery himself, chimes in, "Linear regression was conceptualized by Galton even as early as in the 1800s." Though originally used to predict a relationship between two variables, it is now a popular machine learning (ML) algorithm based on supervised learning.

While neither ML nor AI are new, for a long time they were confined to being abstract ideas rather than an actionable value-add for businesses, the two speakers agree. "AI has evolved from being a craft, pursued by PhDs in labs and at universities behind closed doors, to an off-the-shelf, industrialized solution that's widely available," Lakhani argues. "You have to hand it to the tech giants that believed open source software had merit and could be beneficial to them from a business perspective. It was the advent of open source software that enabled the democratization of AI," Olfati-Saber continues. The dispersion of popular programming language Python, the development of Google's open source software library TensorFlow and the introduction of the open source neural network library Keras (written in Python and capable of running on TensorFlow) led to the eager adoption of deep learning beyond back room university labs. AlphaGo's recent 2016 victory over the world's top-ranked Go player, Lee Sedol, has made deep learning in vogue.

Though Olfati-Saber estimates that 90% of AI needed by companies today are of the less advanced type, this rule does not apply to pharma, where the degree of complexity is arguably higher than in other industries. The potential for AI use is therefore all the more pronounced. "The value chain in drug development spans three stages: discovery, early development and late development. There is potential for AI applications across all stages of this value chain," Olfati-Saber illustrates. And the incentives that loom are enormous. In order to develop a drug, pharma companies invest an average of $1 billion, hoping for multi-billion dollar sales. However, there's only a 15% chance that a drug candidate will make it through all stages, including regulatory approval. "The key question you naturally need to ask is, how can I increase our slim chance for success? That's where AI comes into play. AI can help boost success rates up to 50%. It can also reduce time-to-market through faster and more agile operations," Olfati-Saber explains. Particularly in the context of COVID-19, financial calculations have taken a back seat and time-to-market is the new *non plus ultra*.

"Young pharma companies or biotech starts-ups have the advantage that they can create new processes that are digital or AI-infused from scratch. Big pharma companies need to go through the transformation of turning processes digital after the fact," Olfati-Saber argues. While doing it right from the beginning may be easier, the big pharma players are catching up, though some were reluctant at first. Initially unwilling to invest in AI to the degree necessary for fear it would be nothing but a drain on the bottom line and out of the conviction that "things were going just fine". Most pharma executives have now come around to the fact that AI could be an non-negotiable technology – something that they must embrace in order to remain competitive, much like the more toward digitization over the previous decades.

One area of application for AI in pharma is in drug design. The goal of drug design is the concurrent optimization of multiple physiochemical properties of proteins that impact the development and function of antibodies in an effort to arrive at the optimal formula for a drug. Finding the ideal structure for a drug that optimizes all the desired properties, however, is a lengthy and costly process that involves countless trials. It used to be based on *in vivo* discovery – experimentation using a whole, living organism such as animal studies in traditional clinical trials. Though unable to replicate the precise cellular conditions of an organism, *in vitro* studies – which refer to experiments performed in a controlled environment outside of a living organism – proved more efficient than their *in vivo* counterparts. The newest frontier is now *in silico* studies, experiments entirely performed via computer simulation. Having gained popularity over the last ten years, the deep learning algorithms used for *in silico* studies help significantly increase speed and performance throughout the drug design process. Running thousands of simulations in parallel is no longer a distant dream, but can become standard practice. The only boundary is computational power.

As the computational side advances, it is important we don't forget the people behind the screens. While there are those with statistics, math, physics and engineering backgrounds that revel in the progression of AI, there is another, equally important group of professionals with life sciences and industry expertise. "In order to take full advantage of the potential that AI seeks to unlock, both these groups must work hand in hand," Olfati-Saber is convinced. This requires a new form of bilingualism, spanning the STEM-pharmaceutical divide and enabling both groups to speak each other's language. Though this may not have fully arrived at all pharma companies yet, it will be key to fully tap into the value pools that AI represents for pharma, and this may serve as a means of determining the differences in performance between players in the pharma industry.

Link to Event Podcast & Video:
https://innovationscienceguide.org/resources/ai-in-enterprise-podcast-episode-3-reza-olfati-saber-sanofi