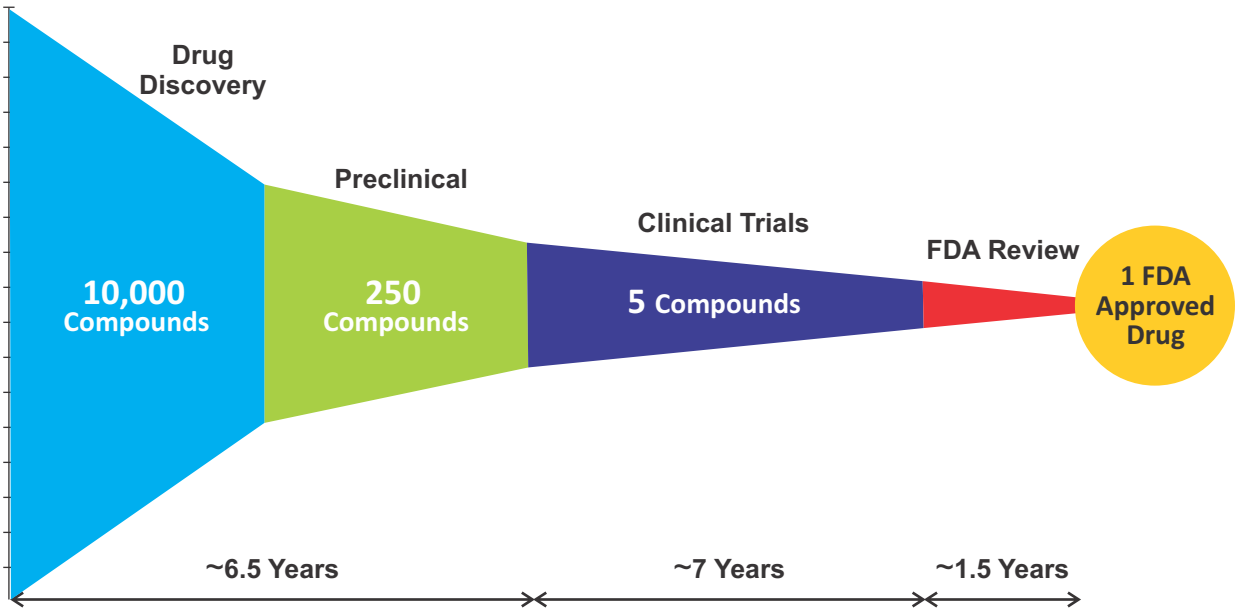
Artificial Intelligence: Transforming the Future of Pharmaceutical Industry

Srinivasan Parthiban is an experienced data scientist, earned his PhD from Indian Institute of Science, specializing in Computational Chemistry. He holds dual Masters Degree- one in Science and the other in Engineering. After his PhD, he continued the research at NASA Ames Research Center (USA) and Weizmann Institute of Science (Israel). He then worked at AstraZeneca in the area of Computer Aided Drug Design for Tuberculosis. Later, he headed informatics business units in Jubilant Biosys and then in GvkBio before he floated the company, Parthys Reverse Informatics. Now his recent venture is VINGYANI, a data science company which deals with Informatics 2.0, that is, Artificial Intelligence for Drug Discovery and Health.

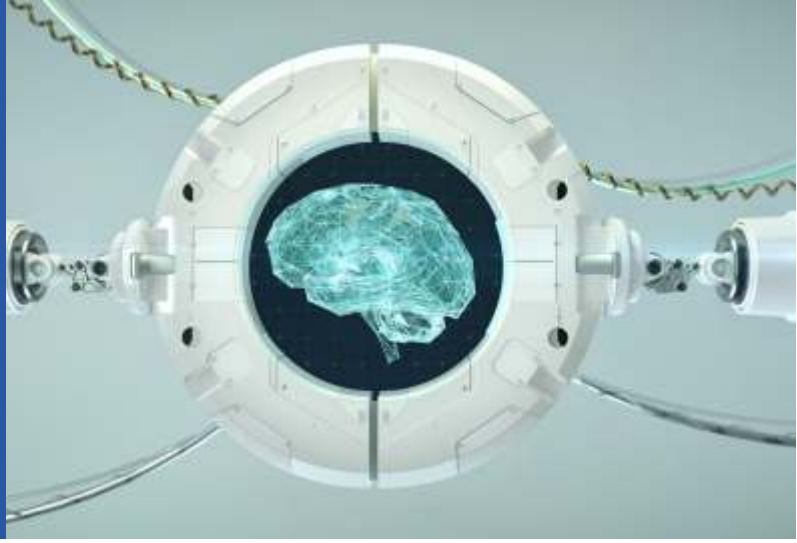
Current drug discovery is long, costly and high failure

Is there a better way to get medicines to patients?



Artificial Intelligence (AI), deep learning in particular as a subcategory of AI, provides opportunities for the discovery and development of innovative drugs,

New medicines are a cornerstone to continuously improve healthcare, to treat diseases better and to increase our health- and lifespan. Finding the right new molecules that eventually become new medicines, however, is a very complex, expensive, and long process. It typically costs 2.6 billion USD and takes 12 to 15 years. How to decrease the costs and speed up new drug discovery has become a challenging and urgent question in industry. Big breakthroughs happen when what is suddenly possible meets what is desperately needed. What is suddenly possible now is AI. When new technologies become easier to use, they transform industries.



Discovering a new drug goes as follows:

Given a medical need, identify the underlying biological mechanism, and design a molecule acting via this mechanism to produce the desired effects. This sounds simple, but in truth it's not easy at all. Leaving aside biology, an important part of the problem is the chemistry: there are just too many molecules to choose from, perhaps as many as 10 to the power of 60 for all drug-like small molecules. Any failure is an enormous financial damage, and in fact, failures in drug discovery research are not rare.

Here comes a disruptive idea: can we automate the process and take the chemist out of the equation? Recent research suggest that this might become possible using artificial neural networks, by which a software first learns from training data, and then is able to perform complex tasks or predictions.

AI is a new digital frontier that will have a profound impact on the world, transforming the way we live and work over the next 10 years. AI has been described as the 'fourth industrial revolution'. It will lead us to self-driving cars, computers understanding human language, and automated drug discovery. The 3Ds powering AI in drug discovery are domain expertise, deep learning and data.

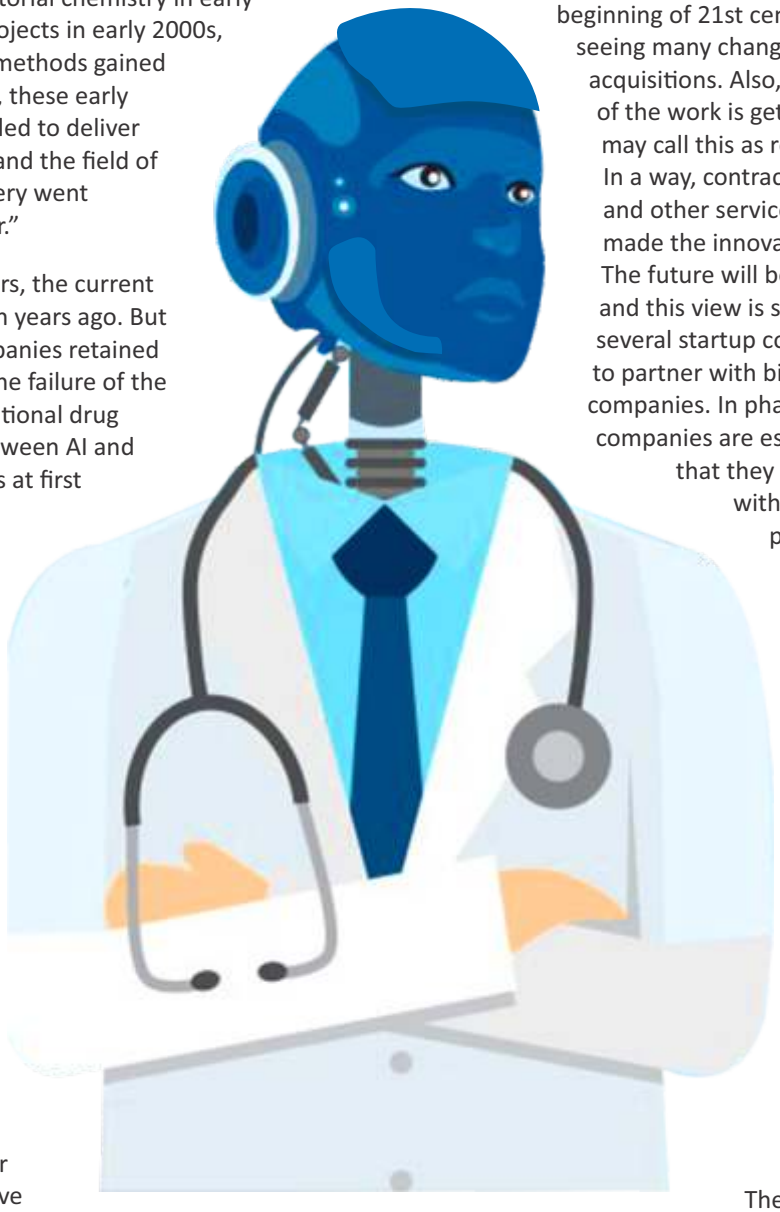
Investments in AI for drug discovery are surging. Big Pharmas are throwing big bucks. They have started to explore what the algorithm behind voice and face recognition can do for drug discovery. Sanofi signed a 300 Million dollars deal with the startup Exscientia, and GSK the same for 42 Million dollars. The Silicon Valley VC firm Andressen Horowitz launched a new 450 Million dollars bio investment fund, with one focus area in applications of AI to drug discovery. Roche acquired Flatiron Health for $2.1 billion, with focus on real world data. In this craze, lots of pharma/biotech investors wonder whether they should jump on the bandwagon or wait and see. In an innovative environment like drug discovery, staying behind is not an option. First-movers enjoy a huge competitive advantage. Indeed, AI in drug design is experiencing a wave of excitement not seen since the emergence of computational chemistry in the late 1980s and early 1990s.

Now, there are two schools of thought on AI. One is that AI has come of age, offering drug developers a chance to harness AI technology to guide research work, offering a much greater chance of success through Phase III. The other side says this is just the latest over-hyped fad that will inevitably fade into the background as large and small companies continue to rely on traditional methods for finding and advancing the next-generation of drugs. We need to evaluate both sides of that argument, debate over the future of AI in R&D and where we are headed over the next 5 years.

Indeed, AI methods bring promises to the pharma industry, but also bring many questions. Can AI help us screen and select the right compounds and assist with identifying successful targets? How can AI help avoid the failures in phase 2 and phase 3 clinical trials? Is AI always going to be limited by data and is collaboration the key to tackle this Issue? How to ensure we are using AI the “right” way? When and where is the right time to use AI? Will we be able to lower drug discovery costs, reduce time to market and develop pharmaceuticals in a way that has never been done before – is AI the answer and is this the future? With AI at the peak of its hype curve, can machine learning live up to expectations?

Many researchers at Biosciences conferences discussed in the last couple of years about the great potential of AI, but equally so about the pain of “wrangling” the meagre data available. AI needs data, and this is the weak point when trying to apply 'AI' to the drug discovery field. This is not object or speech recognition, where we have a huge amount of both labelled and unlabelled data. The problem is that drug discovery is a very different beast.

It is not the first-time drug makers have turned to high-tech solutions to boost R&D productivity. First it was in the late 1970s and early 1980s when the computational methods raised much enthusiasm and gained broad adoption. Then with the arrival of combinatorial chemistry in early 90s and human genome projects in early 2000s, once again computational methods gained momentum. Unfortunately, these early computational methods failed to deliver what they have promised, and the field of computational drug discovery went through a sort of “AI Winter.”



According to many observers, the current AI boom began about seven years ago. But many pharmaceutical companies retained institutional memories of the failure of the previous waves of computational drug discovery. Also, the link between AI and drug discovery isn't obvious at first glance. Early presentations to the pharmaceutical industry on the advances in deep learning in 2014 and 2015 resulted in skepticism and were discarded. In 2016, Google' Alpha Go based on AI beat world champion Lee Sedol in Go game. Things started to change. Since 2017, many pharmaceutical companies started partnering with AI startups and academics or started internal AI programs for R&D. Funding and enthusiasm for computational methods have once again returned. To simply put if AI can play Go or drive cars, it must be able to help solve problems in areas like medicine. With this optimism, the pharmaceutical companies are focusing on AI to drastically reduce costs by billions and reduce time to market by years.

A technology that has arrived, then what is the issue? Why the biopharmaceutical industry is still lagging behind other industries in adopting AI. The answer is shortage of data and analytics talent. Lack of properly skilled teams within the pharmaceutical companies is an existing or emerging barrier to achieving expected results from digital technology initiatives. Although the data and analytics talent pool are expanding, organizations are struggling to find candidates with the right balance of technical skills, biopharmaceutical domain knowledge, and business strategy. As a result, the entire innovation landscape is changing, both in terms of Mergers and acquisition as well as partnering with startup companies.

Pharmaceutical industry is evolving. Until the end of last century, most of the work was done internally, very few partners worked from outside. Since the beginning of 21st century, we have been seeing many changes such as mergers and acquisitions. Also, we have seen that much of the work is getting done externally, we may call this as research externalization. In a way, contract research organizations and other service providers/partners have made the innovation landscape complex. The future will be much more complex and this view is supported by the fact that several startup companies are beginning to partner with big pharmaceutical companies. In pharma's eyes these companies are essentially digital biotechs that they can strike partnerships with and which help feed the pipeline. If the AI technology really proves itself, we may start to see a closer integration of these AI engines into pharma R&D.

In every technological shift, some industries respond more quickly and aggressively than others. The AI revolution is following the same pattern, some industries are leading, whereas others are lagging. The good news is that biopharmaceutical investors see the value in applying AI, machine learning, and deep learning techniques to solving the drug discovery challenges. For the moment, almost every AI-based solution requires “humans in the loop.” The rising popularity of AI-based solutions is creating an insatiable need for people with data science skills, business knowledge, and domain expertise. We are truly at the opening stages of a rare paradigm shift!