Artificial Intelligence Empowers Drug Discovery: New AI-startups Focus On Biotech

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In 1997 a remarkable event caught everybody's attention - the then champion of the world Garry Kasparov lost a tournament to a supercomputer Deep Blue. It was called "a beginning of a new era of computers" by many and now it seems that time keeps justifying those loud statements...

Not just a powerful computer but a human's brain simulation

Being a sub-set of artificial intelligence, machine learning involves algorithms allowing computers to autonomously learn from input data. A fundamental distinction from "usual" software programs, such as Photoshop or, say, Excel, is that in machine learning computers don't have to be explicitly programmed but can change and improve their algorithms by themselves.

The history of machine learning goes back to the 1950th. The first learning program was created by Arthur Samuel in 1952 and it was the game of checkers. Implemented in IBM computer, the program was able to improve itself the more it played studying winning moves and incorporating them into the next rounds.

Five years later Frank Rosenblatt designed the first neural network for computers - the **perceptron**, which simulated the thought processes of the human brain. And just a decade later the "nearest neighbor" algorithm was written, which was a conceptual step towards pattern recognition technology...

Today, machine learning algorithms enable computers to "see" and distinguish objects and text in images and videos, discover and categorize real-world things, communicate with humans, drive cars on auto-pilot, write and publish sport match reports, and ... help discover new drugs.

The stumbling stone of modern drug development

Drug development is a challenge and eventual success is largely determined by the early drug discovery efforts.

A widely used target-based approach to drug discovery starts with biologists identifying possible mechanism of a disease and suggesting a biological "target" - usually a protein involved in a cascade of processes behind a disease. Inhibiting or otherwise impacting such a protein can usually have a substantial effect on the pathogenesis and therefore, the disease might be suppressed and cured.

Once the target is proposed, the next big move is to screen hundreds of thousands or even millions of small molecules against the target to identify so-called "hits", i.e. molecules with substantial affinity to the target protein. Further, the hits undergo numerous additional tests and chemical modifications and some fraction of small molecules eventually make its way to clinical trials.

With this approach, however, it takes on average 12 years and about $2.9 billion to bring a new efficient drug on the market. The drug discovery is largely a “trial and error” process, even today, and “error” here is huge as only a very few experimental drugs ever see the medicine cabinet.

How do computers help find new drugs?

In a pursuit of decreasing the cost and time of drug discovery and more accurately predicting the structure-activity relationship of early drug candidates, scientists developed computer models and programs able to conduct “in-silico” drug discovery. In this approach available structural information about target proteins is used to conduct virtual screening of numerous chemical structures and identify hits which better fit the target in terms of energy of interaction and other calculated functions.

Although promising, standard in-silico methods are still limited and not accurate enough to substitute the real-world experimental screens and trials because of their explicitly pre-programmed nature and pre-determined models, used for calculations. This is where machine learning algorithms and new drug discovery startups come into play.

New drug discovery era is knocking on the door...

Recently, a group of scientists at the University of Toronto created a machine learning algorithm that they hope will revolutionize the way pharmaceutical drugs are discovered. They founded a health tech startup Atomwise offering a solution which can help researchers develop the next generation of drugs and do it

faster and cheaper than ever before. The algorithm Atomwise developed is similar to the Deep Learning Neural Networks used by artificial intelligence startup DeepMind, acquired by Google recently for $628 million. The algorithm teaches itself complex biochemical principles and the factors that are ultimately the most predictive when it comes to the effectiveness of a drug.

“Our system takes into account not a dozen or two dozen, but thousands of factors at the same time and combines them in complicated and nonlinear ways. It’s like having a virtual super-intelligent brain that can analyze millions of small molecules and potential interactions in days instead of years,” said Alexander Levy, chief operating officer at Atomwise. The company’s machine learning algorithm is acting similarly to how computers go about image recognition, which is a unique feature of this approach. Levy says their system has devised some unintuitive methods for understanding what small molecules will properly latch onto a biological target.

To date, Atomwise has raised $6 million to advance artificial intelligence for drug discovery and launched more than a dozen projects to find cures for both common and orphan diseases. The company is collaborating with IBM to find a cure to Ebola and with Dalhousie University in Canada to search for a measles treatment. The startup studied 8.2 million small molecules to find potential cures for multiple sclerosis in a matter of days. Besides, Atomwise is already partnering with a pharmaceutical giant Merck to explore the frontiers of using artificial intelligence for drug discovery.

Not the only one

Besides Atomwise, a number of promising startups focusing on the application of machine learning and AI for drug discovery have emerged within the last several years.

Palo Alto based TwoXAR, founded in 2014, has recently raised $3.4 million in a seed round led by tech investor Andreessen Horowitz. TwoXAR’s solution is DUMATM Drug Discovery platform able to evaluate large public and proprietary datasets to identify and rank high probability drug-disease matches in minutes rather than years. The approach includes four distinct stages:

The company has already tested their technology on more than twenty diseases and is now actively collaborating with academic researchers at the University of Chicago and Michigan State University to further develop the platform. Being a part of the elite Stanford-backed “StartX Med Program”, TwoXAR is collaborating with some unnamed biopharmaceutical organizations.

What’s next?

An important challenge for the AI startups is to convince the big pharma that artificial intelligence is the panacea to its financial and R&D woes. A real rush for AI-based technologies by the big pharma will begin with the first example of an FDA-approved “computer-derived” drug... and we may see this happen in the nearest time.

Possible option for the AI startups to accelerate their integration into drug discovery industry would be to partner with specialized chemical suppliers of large screening databases. It is an opportunity for them to test algorithms with commercially available or easy-to-synthesize compound libraries with intrinsic drug-like properties.