Numerate's ranking technology for pharmaceutical R&D gains U.S. patent

May 27, 2010

We're excited to have been awarded this significant patent. Modern machine learning methods are starting to produce remarkable results in a number of fields. Typically this requires a combination of deep domain expertise and the machine learning expertise to adapt and develop techniques to fit the idiosyncratic challenges of the particular domain. It's exciting to lead such an effort in drug design, and demonstrate that truly modern machine learning techniques can have a significant impact on the quality and cost of healthcare.

Numerate's ranking technology for pharmaceutical R&D gains U.S. patent; Pioneering Use of Machine-Learning Technique to Speed Drug Discovery

San Bruno, CA, May 27, 2010 — Numerate, Inc. announced today the grant of U.S. Patent No. 7,702,467 B2, which provides patent protection for methods of using biological assay data to develop predictive models. These models have accuracies comparable to laboratory testing.

The patent, titled "Molecular Property Modeling Using Ranking," describes methods for using advanced machine-learning technology to design novel small molecule compounds in silico that meet specific candidate drug profiles. This "ranking technology" enables the use of new kinds of experimental data beyond those accessible by any other statistical techniques.

Numerate's ranking algorithms represent the first successful effort to apply these modern machine-learning techniques to problems in drug design. In recent years, related advanced machine-learning algorithms have emerged from academia and been adopted in a number of fields, most notably in finance, web-search, ad placement (at Google), and product recommendations (at Amazon and Netflix).

"The machine learning challenges in drug design are substantially different from those in other fields, such as product recommendation," said Nigel Duffy, Ph.D., Numerate's Chief Technology Officer. "To make accurate predictions, we have developed ways to address key issues, including the bias inherent in biological data, and the experimental noise typical in assay results. As a result, we are able to deliver novel compounds that meet pre-specified objectives and perform in the laboratory as we predict they will."

"The traditional approach to drug design is a process of discovery, and is driven by intuition and, often, serendipity," stated Guido Lanza, Numerate's Chief Executive Officer. "By definition, it is limited by human's ability to make complex design decisions against competing objectives in enormous spaces of chemistry. The only way to improve the efficiency of drug discovery significantly is with a new approach that lets the data drive the design and addresses these multiple objectives simultaneously. Numerate's platform provides the basis for just such a paradigm shift. We are using it today to substantially reduce the time and cost of designing and delivering lead-stage, small molecule drug candidates to our partners.

"This patent significantly extends our leadership position in technology for predicting the properties of small molecule drug candidates," added Mr. Lanza.

Numerate's drug design platform represents an investment of $30 million and ten years of work. The foundation of this platform is a set of proprietary algorithms – including those using modern ranking methods – that provide accurate predictive models for molecular properties, long a holy grail of drug design.

To make their discoveries, Numerate scientists run their platform on Amazon's Elastic Compute Cloud (EC2), allowing them to search through spaces of hundreds of millions of compounds to identify those with the highest probability of activity against a specific target. The compounds are then synthesized and their properties verified in the laboratory.

Numerate's achievements in HIV illustrate the strength of the company's platform. In six months, with only 21 compounds made, Numerate designed, synthesized, and tested novel compounds that demonstrated greater potency and spectrum than the market-leading drug in the class. In addition, these compounds had significantly improved pharmaceutical properties.

"These results are remarkable, given that a typical program could require 10 years and $20 million to achieve similar results. In contrast, our accomplishment took one-tenth of the time and one-hundredth of the cost," said John Griffin, Ph.D., Numerate's Chief Scientific Officer.

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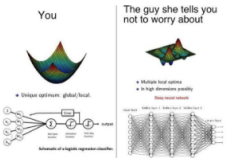

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