

The Promise and Fallacy of AI/ML for Pharma R&D

Introduction/イントロダクション

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Today's Seminar: Program

Opening Remarks, Introduction/開会・イントロダクション

Jun Kurihara (Research Director, CIGS)/栗原 潤 (キヤノングローバル戦略研究所 研究主幹)

I: Presentation/講演

“The Promise and Fallacy of AI/ML for Pharma R&D”

Dr. Ray Liu (Senior Director, Advanced Analytics, Takada Pharmaceutical Inc., Cambridge, MA)/

レイ・リユー(劉睿哲)氏 (武田薬品)

II: Discussion /討論

Moderator: Jun Kurihara (Research Director, CIGS)/栗原 潤 (キヤノングローバル戦略研究所 研究主幹)

Closing Remarks/閉会

Jun Kurihara (Research Director, CIGS)/栗原 潤 (キヤノングローバル戦略研究所 研究主幹)

“An AI System Identified a Potential New Drug in Just 46 Days”

—MIT Technology Review, September 3, 2019

A team from AI pharma startup **Insilico Medicine**, working with researchers at the **University of Toronto**, took 21 days to create 30,000 designs for molecules that target a protein linked with fibrosis (tissue scarring). **They synthesized six of these molecules** in the lab and then tested two in cells; the most promising one was tested in mice. The researchers concluded it was potent against the protein and showed “drug-like” qualities. All in all, **the process took just 46 days**. The research was published in *Nature Biotechnology* this week.

See also,

“A Breakthrough in Imaginative AI with Experimental Validation to Accelerate Drug Discovery”

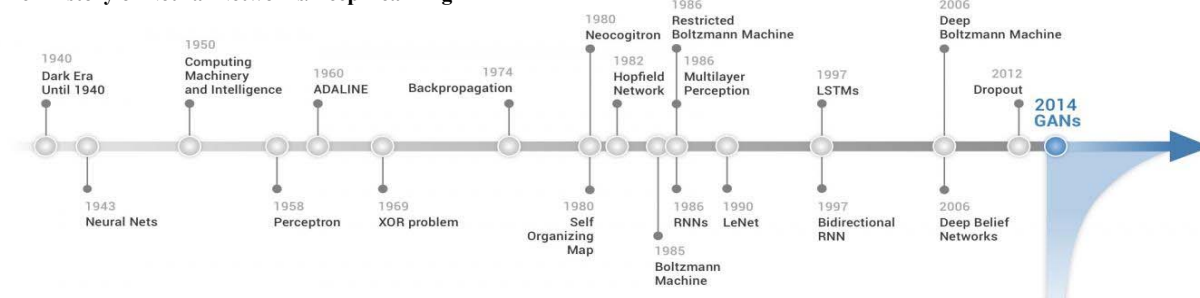
—EurekAlert! September 3, 2019

“Using Advanced GANs in the discovery of drugs is a great example of cutting edge application of AI in the pharmaceutical industry - it speeds up a critical process from years to just weeks.” said Christian Guttman, Executive Director Nordic AI Institute, Professor AI at the University of New South Wales, and Senior AI Research Fellow AI at Karolinska Institute.

Jun KURIHARA, Canon Institute for Global Studies (CIGS)

A Timeline of the Development of Generative Adversarial Networks and A Timeline of the Use of Generative Adversarial Networks in Pharmaceutical Science and Drug Discovery

A Brief History of Neural Networks/Deep Learning



GAN TIMELINE

Jun 2014 Original GAN

GAN FOR DRUG DISCOVERY



Source: Insilico Medicine

“AI-powered Drug Discovery and Manufacturing Conference,” MIT, February 27-28, 2020

Jun KURIHARA, Canon Institute for Global Studies (CIGS)

Prior to the Opening of the Floor for Discussion: the Moderator's Comments (1)

I: Use of AI in the Health Field: Blue-Sky Thinking?

AI systems help **diagnose and prevent** disease and outbreaks early on, **discover** treatments and drugs, **propose** tailored interventions and **power** self-monitoring tools.

(OECD, *Artificial Intelligence in Society*, Paris: OECD, June 2019, p. 16.)

The use of AI in this field extends **beyond facilitating drug discovery** to predicting the right dose for experimental drugs. Since **the optimal drug dose** may depend of so many variables for each individual, such as age, gender, weight, generics, proteomics, the gut microbiome, and more, it's **an ideal subject for modeling and deep learning algorithms**.

(Topol, Eric, *Deep Medicine: How Artificial Intelligence Can Make Healthcare Human Again*, New York: Basic Books, March 2019, p. 220.)

II: Use of AI in the Health Field: An American Experience

Advantages and Limitations of AI Methods in Health and Health Care Applications
(Today's Talk)

Prior to the Opening of the Floor for Discussion: the Moderator's Comments (2)

III: Use of AI in the Health Field: A Global Solution amidst a Dire Shortage of AI-powered Human Resources

A Baltimore-based company, **Insilico Medicine, Inc.**, applies the latest advances in artificial intelligence to drug discovery, biomarker development, and aging research.

The company's CEO, **Alexander Zhavoronkov** (Александр Александрович Жаворонков), is Chief Scientific Officer of the Biogerontology Research Foundation, a UK-based registered charity supporting aging research worldwide. He is also Director of the International Aging Research Portfolio (IARP) knowledge management project, Chief Scientist of Youth Laboratories and an adjunct professor at the Moscow Institute of Physics and Technology.

He holds two Bachelor Degrees from Queen's University, a Master's in Biotechnology from Johns Hopkins University, and a Ph.D. in Biophysics from the Moscow State University.

IV: Use of AI in the Health Field: Issues on the Horizon

- (1) **Intensified global competition** will be fueled by nations and companies in the fields of AI development and the pharmaceutical industry.
- (2) FDA has been paying close attention to the international development of both software in medical devices (SiMD) and software as a medical device (SaMD). **FDA** has been participating (actually chairing) **an international regulators forum** on SiMD and SaMD.
- (3) **International cooperation at a pre-competitive stage (esp. with Japan)**; Kyoto University-led projects (Life Intelligence Consortium (LINC), under the leadership of Prof. Yasushi Okuno, established in November 2016).