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How Beneficial or Threatening is Artificial Intelligence?

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Computer scientists have studied artificial intelligence and machine learning since computers were invented. There have been three waves of developments in this field. First development, in the 1950s, computer chess and reversi™, were realized. In the second development, "expert systems" attracted attention and started the "5th Generation Computer Project." in 1980s. However, the results of both the developments were insufficient (for example, 5th Generation Computer was not created), and the enthusiasm for expecting new type of computers such as artificial intelligence quickly diminished. We are now in the third wave of the AI developments. Will it produce satisfactory results? Will it revolutionize life sciences? In this article, I have tried to answer these questions.

Key Words: AI, Machine Learning, Deep Learning, reinforcement learning

Area of Interest: *In Silico* Chemistry, *In Silico* Biology, History of Science

1. Introduction

In March 2016, computer Go player, AlphaGo, won against Lee Sedol, who had been a world champion several times. In 2020, AlphaFold2, which enables protein 3D structure estimation from amino acid sequences, showed astonishing results in estimation accuracy. These results derived from AI and machine learning (ML) impressed researchers. Subsequently, AI has become an unignorable aspect in almost all fields.

In the 1840s, Charles Babbage devised a programmable calculator for games between humans and machines. Although this device was too simple to perform chess games, considering that he lived in the 19th century, he should be called the first computer game devisor (He is already called the Father of Computers).

In 1912, Leonardo Torres Quevedo produced 'El Ajedrecista' [1], which means chess player. In 1956 (when I was born), Los Alamos National Laboratory created a chess program for a 6 × 6 mini-chess board, the first automatic chess player against a human player. The first match between a computer chess player and a human player was between John McCarthy and ITEP (Institute for Theoretical and Experimental Physics) of the former Soviet Union. Consequently, ITEP won two times and two draws. In 1978, Ostrich, which Monroe Newborn co-programmed, joined in the Tokyo Open but lost 0-3.

In 1988, Deep Thought, developed by Carnegie Mellon University and IBM, won against Bent Larsen, a chess grandmaster. This was the first match wherein a computer won against a professional human chess player with the highest Elo rating. In 1997, Deep Blue, an upgraded version of Deep Thought, had two wins, one loss and three draws, against Garry Kasparov, a world champion. Supercomputers (at that time) were used in these cases. In 2005, computer chess programs won against several world champions (eight wins and four losses). Consequently, standard personal computers were used. Subsequently, it has become challenging for human chess players to win against computer chess players.

Similar situations were realized in the case of Shogi and Go. Go was considered more challenging to program strong computer players. However, AlphaGo, produced by Google Deep Mind, won against Lee Sedol (four wins and one loss), who has won several championships. Soon, winning against a computer in Chess, Shogi, or Go will be well near impossible.

The comprehensive impact made by AI in the last decade is in chemistry and biology. In 2012, the Toronto University group [2] showed tremendous accuracy in image recognition. As aforementioned, Alphafold2 [3] showed surprising results on protein 3D structure estimations (Table 1).

I believe the future of AI has to be discussed, particularly in chemistry, pharmacy, molecular biology, and their surrounding fields. I will try to answer the questions, "What can AI do?", "How should we utilize AI?" In addition, I answer the question, "What should researchers study in the age of AI?".

Table 1. Time series on recent AI development in the Life Science field

year	
2006	Hinton et al. developed Stacked Auto-Encoder (Deep Learning)
2012	**Toronto Shock** Toronto University group (Hinton et al.) showed a 17% error ratio for ILSVRC (about 10% more precise than before).
	Google Shock Google performed unsupervised DL using cat pictures from YouTube and found that one neuron layer in the network showed a portrait like a cat face.
2016	**AlphaGo** (Google DeepMind; DL + Reinforcement Learning) AlphaGo won against Lee Sedol, who was a Go world champion. (4-1).
2020	**AlphaFold2** (Google DeepMind) AlphaFold2 realized precise prediction of protein 3D structures.
	Matlantis™ Matlantis realized Density Functional Theory (DFT) computations by AI.[4]
2021	AlphaFold Protein Structure Database Protein 3D structure database. The structures were estimated by AlphaFold2. {Deep Mind + European Molecular Biology Laboratory (EMBL)}

2. What can AI achieve?

As aforementioned, AI showed incredible results for protein 3D structure estimations. Additionally, 200 million protein 3D structures were predicted and published by Deep Mind and EMBL [5]. In addition, quantum chemical calculations based on the density functional theory (DFT) can be realized using AI [4], and a chemical reaction coordinate of alanine dipeptide isomerization was interpreted using explainable AI (XAI) [6]. There are many other examples like these.

Early this century, although AI was considered a tool for humans, many researchers in the chemistry and biology fields thought AI would be inadequate compared to experimental or theoretical approaches. Only a few scientists thought, “protein 3D structures can be estimated sufficiently accurately" and "Quantum chemical calculations can be executed, not through theoretical algorithm but by AI." However, both of these tasks have been realized.

Recently, our group showed that by using chemical structure descriptors, we could predict drug side effects [7]. These results indicate that with sufficient data, AI could estimate almost all chemical values, such as reactivity's, solubility, etc. If I answer the title question, "What can AI achieve in the chemistry and biology fields?" I will answer: "Any data can be estimated sufficiently accurately with adequate available learning data."

2.1 What can AI achieve in the Organic Chemistry field?

AI has realized the explanation for the chemical reaction coordinate of alanine dipeptide isomerization [6]. Meuwly reviewed the ML method application [8]. Among the several ML applications to organic reactions, the methane combustion network at its initial stage [9] is noteworthy. They provided the methane combustion networks using DFT, smooth overlap of atomic positions (SOAP), and kernel ridge regression. These reports indicate that chemical reactions, including their kinetics, can be predicted using ML soon.

2.2 What can AI achieve in the Drug Discovery field?

Recently, reviews concerning AI, ML, and drug discovery are available. [10-12] Gupta et al. [10] stated that deep learning (DL) has modernized the drug discovery field. Patel et al. [12] claimed that ML is consistently applied in drug target designation and novel drug discovery. Particularly, the recent COVID-19 pandemic has forced rapid drug development of anti-viral drugs against SARS-Cov-2. According to Lv et al., [13] at least 16 anti-SARS-Cov-2 drug candidates were developed (mainly by drug repositioning) using AI and ML as tools.

Typically, I do not suggest that synthesized novel drugs found on the market were through using only computer-based studies. Drug developers have to perform synthesis, pre-clinical and clinical trials. Additionally, post-marketing surveillance has to be realized. However, using AI and ML can decrease drug discovery costs and time. Soon, we would achieve essential drug discovery parts using '*in Silico*' methods such as pre-clinical studies' simulators and semi-auto synthesizers of low, middle, and high molecular drugs.

2.3 What can AI achieve in the other Life Science fields?

In Japan, Life Intelligence Consortium (LInC) [14] started widespread applications to life sciences. For example, they are trying to develop an AI-force field for molecular dynamics, and successful results have been reported, particularly regarding atomic charges. [15] Ordinal force fields are often insufficient for describing hydrogen bonding. AI-force fields are expected to be much more precise. Bayesian network and B-spline (Basis spline) nonparametric regression has enabled cancer subtyping based on a patient-specific gene regulatory network. [16]

The development of IBM WATSON^{TM} in the medical field was an automatic diagnostic system to be applied to various industrial sectors. Although such automated diagnostic systems are still under development, they will be of practical use soon.

The application of AI has occurred in approximately all scientific fields. Some of them are under development and others are in practical application. However, practically all the present success stories are based on Big Data. Considering the complexity of the AI system, considerable data is necessary to make an appropriate model of AI.

3. How should we utilize AI?

According to the above-obtained results, AI can supposedly solve all problems. This assumption may be accurate. I estimate that solvable problems can be solved using AI. For example, Even now, quantum chemistry can solve chemical reaction mechanisms when researchers use huge computer resources. AI and ML can solve such problems. AlphaReaction2 (this name is a mimic of AlphaFold2) will realize the estimation of chemical reaction mechanisms within the first half of this century.

Do researchers have to be apprehensive of AI? I do not think so. This development implies that the number of tools researchers can utilize is increasing. Researchers will be unbothered by calculations or, occasionally, experiments that do not include novel ideas but ordinal procedures. AI can perform such computations and experiments. Researchers will concentrate on finding/producing novel ideas, materials, etc. Scientific databases (such as PubMed, PubChem, and PDB) have become essential during these 30 years, and AI will become necessary tools within the next 20 years. Primarily, researchers should use but not be reliant on AI. These are just the tools that help researchers.

4. What should researchers study in the age of AI?

Do researchers have to learn how to utilize AI? If you have to learn about the algorithms, theories, and methods of AI when attempting to use an AI, it implies that the AI is still immature. Sufficiently developed technologies, including AI, can be conveniently utilized. Researchers do not have to adopt such undeveloped AI but should start to apply ‘sufficiently developed’ AI.

Subsequently, in this century, researchers will have to change their concept about ‘What should we study?’ Conventionally, researchers occasionally focused on studying what even the developed AI would be able to conduct. Consequently, they can concentrate on finding novel concepts. For example, an AI can solve the Riemann hypothesis; however, AI cannot propose the Riemann theory in this century, probably forever. Future researchers should not adopt the theme, such as solving the Riemann hypothesis but a concept as proposing the Riemann theory.

I assume at least three significant themes remain in the life science field. Although I anticipate AI alone cannot solve these themes, they will become integral tools.

(i) Can we design novel drug molecules whose receptors are unknown? In addition, can we invent novel drugs for the diseases for which mechanisms are unknown?

(ii) Details of immune modulations. For example, patients who receive an organ transplant take immune-suppressing drugs that suppress all sorts of immunity (including vs. viruses). Considering such medication should not suppress almost all immunity (such as against viruses) but the one against the transplanted organ. Can AI discover the essential drugs or medical methods, which suppress the immunity a patient must contain?

(iii) The COVID-19 pandemic evidenced that microorganisms, including viruses, easily steal our daily lives. In addition, our resistance was temporarily futile. The problem is that the viruses repeat mutations and we are unable to predict the mutated amino acid sequences. If we know the future microorganisms’ mutations, it will facilitate the end of the pandemic. Can AI predict future variations?

5. My prediction

Table 2. Themes that will be accomplished by AI soon

Year	Accomplished themes by AI
until 2045	Automatic precise simultaneous translation between more than 50 languages.
	Automatic illustration for presentations
	De novo drug design (precise simulations of the intermolecular interactions between drugs and receptors)
	Singularity? (AI transcends human intelligence level)
until 2065	Precise simulations of chemical reactions.
	Simulator of animal experiments with novel drugs
	De novo drug design that includes chemical modifications (AI discovers novel drug chemical structures human medical chemists never considered).
	Quantum computers are in practical use.
	Accurate solutions to the Schrodinger wave molecule equation

Although it is challenging to predict what AI can accomplish soon, I dare to predict what AI will achieve by 2045/2065 (Table 2). This table may underestimate AI development speed. I anticipate these themes' accomplishments to be earlier than my predictions.

We might have realized the area where we should not, must not venture: immortality, genetically edited babies, cloning humans, disease eradication, controlling every chemical reaction, etc. In the movie, Space Odyssey 2001, supercomputer HAL9000 rebelled against astronauts. We may encounter AI rebellion. Accordingly, we have to discuss the legal mechanism for AI. However, we should not avoid scientific developments such as AI. In addition, we still do not know how beneficial or terrifying AI is. We have to prepare for this innovation in the coming years.

6. Conclusion

In this century, AI made a revolution in the life sciences field. Can AI realize all we want? I do not believe that. AI need considerable data for learning. It is occasionally assumed that AI cannot perform what they have not learned. However, 'AI shogi,' for example, by reinforcement learning, found novel moves that even professionals had never considered. Thus, AI can perform what they have not learned.

Nevertheless, AI need considerable data to show their ability. Conversely, if there is sufficient data, AI can do everything we want. Henceforth, researchers cannot ignore the development of AI.

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