Why and how should we use Artificial Intelligence, Machine Learning, and Deep Learning Approaches Differently on COVID-19 Coronavirus and Other Pathogens Research?

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Abbreviations: AI: Artificial Intelligence; ML: Machine Learning; DL: Deep Learning; MD: Molecular Dynamics; CIHR: Canadian Institute of Health Research.

Editorial

Artificial intelligence (AI), machine learning (ML), and deep learning (DL) have become increasingly popular tools and research methodology in many scientific research fields. Examples include improving prediction models by integrating mechanistic immunological information into machine learning [1], using multiomics and spatial integration approaches in conjunction with AI and ML methods to guide future informed cell engineering and precision medicine based on immunological studies data [2], and various other studies summarized by Jabbari P, et al. [3]. Using AI, ML, and DL as novel methods to gain new insights to generate novel vaccine and/or drug designs and discovery has been a revolutionary approach over the past decades [4]. Traditionally, researchers resolve to other computational methods (e.g., molecular dynamics (MD) simulation) to help solve problems of and arise from inadequate and/ unsatisfactory drug binding and affinity to target site(s).

In today's mid-Covid-19 pandemic world, our research communities do not lack researchers from all parts of the world attempting to use AI, ML, and DL to discover and/or invent new vaccine and/or drug designs to fight against this notorious virus. In my opinion, the question does not lie on whether we have people (We have numerous experts in AI, ML, and DL fields), whether we have tools (We have been studying AI, ML, and DL for many years, resulting in numerous tools (e.g., hundreds, if not thousands, of program codes or coding packages, and vast amount of data for training various computational machineries)), or whether we have funding (We have federal and private funding specifically dedicated to these studies e.g., the most recent, 2020, 2.1 million dollar Canadian Institute of Health Research (CIHR) funding was awarded to Dr. Artem Cherkasov and Dr. François Jean and their teams to design new drug cocktails against Covid-19 using computational approaches, probably to date the largest single-handed funding for molecular design studies using a single approach).

The question lies on that we are still currently following the reserved route-
• Learn physical and chemical properties of therapeutic target (s) and (prospective) vaccine (s)/drug (s),
• Generate algorithm(s) to explain these properties based on experimental data from 1. and create working model(s) from these data,
• Use these algorithms to create predictive model (s) based on previous working model(s) to predict modification (s) needed to generate vaccine/drug (candidate(s)) demonstrating improved binding, affinity, and activity. The iteration continues until the best possible candidate (s) is discovered and/or the maximum possible improvement is achieved. This cycle would be repeated when researchers discover new information (or simply just data) on these properties and/or discover (and

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possibly validate) new therapeutic target (s). While the robustness of this classic, more reserved route has been proven over years of hardened and seasoned research, we cannot deny the fact that we will not be able to break through this repetition cycle, unless we attempt to approach from a different perspective, albeit riskier and involves more daring (potentially less acceptable to the public consensus in current research communities) concept (s).

I want to challenge the readers to re-think and re-evaluate our understanding, approach, and position on vaccine/drug-pathogen relationship. Is not discovering vaccine and/or drug candidate(s), characterizing physical and chemical properties of both (bio)molecules, finding therapeutic target(s), understanding the mechanism of action, and improving the vaccine/drug design a passive way to battle Covid-19 (and other pathogens alike)?. Despite the fact that many other research also attempt to explain Covid-19 and other pathogens using different approaches other than AI, ML, and DL, such as X-ray crystallography approach to help understand the mechanism of action [5], as well as immunogenomics and systems biology approaches to understand host-pathogen relationship [6,7], none of these approaches, let us be honest, have the capability to predict the next Covid-19 variant(s), its biological properties, and its next target(s). We are fighting a war where opponents know the direction both parties advance to, but we do not have the knowledge on the next direction our opponents are heading. Instead of blindly following where the pathogen is heading, we should use AI, ML, and DL to predict the next (several) directions the pathogen is heading or attempting to head into. What if we could predict the next Covid-19 variant(s), when, where, and how it will (re-)emerge, its target population (pandemic or not), its effect range and extent (infectivity, virulence, morbidity, and mortality, etc.), its susceptibility (to (bio) molecule(s) and/or other biological and other factors e.g., health policies and orders), and others? This prediction capability is much like what the movie "Minority Report" by Tom Cruise demonstrated. In the movie, the fictional future police could stop the crime before it happens or stop the crime immediately just as it initiates. We should use AI, ML, and DL at their full potential and capacity to fully capitalize primary preventive measures while keeping generating new vaccine(s) and drug(s) for secondary prevention and treatment measures. Although one may argue that chain reactions and events in "Minority Report" are ethically questionable and possibly incorrect in many people's eyes, we still cannot deny that the well-advanced technology and its concepts could give us new ways to actively fight Covid-19 and other pathogens from a very different perspective while still using the same AI, ML, and DL approach.

As you read along, you may probably start seeing that AI, ML, and DL should not be limited to only 1 or 2 research routes. This is how I foresee and envision our scientific research using AI, ML, and DL approaches, not necessarily limited to vaccine/drug-pathogen relationship, in the future. I want this editorial to be a mind perturbing ground for the readers to re-think and challenge our views to re-evaluate the importance of using different AI, ML, and DL approaches in all research fields. We need to truly think outside the box again to dare ourselves to adopt very different research perspectives and realms, which can be tagged along by many risky and daring concepts that may or may not be welcomed by others to be discovered in the future by different scientific researchers and communities.

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