

Bioinformatics and Artificial Intelligence to Combat Covid-19 and Beyond

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Editorial

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Editorial

COVID-19 perhaps is the greatest and tremendously significant crisis against Homo sapiens sapiens in the contemporary history of the globe. The group of coronaviridae includes viruses with very long RNA genomes up to 33000 nucleotides. SARS-CoV-2 belongs to the Sarbecovirus provided with approximate genome size of 30000 nucleotides [1]. SARS-CoV-2 has four main structural proteins: spike (S), envelope (E), membrane (M) and nucleocapsid (N). Additionally some other non-structural proteins are encoded in the pp1a and pp1ab polyproteins, essential for viral replication [1]. SARS-CoV-2 seems to use the human receptor ACE2 as its main entry point [2]. The binding domains for ACE2 are located on the spike proteins, which further contain a novel furin cleavage site, associated with increased pathogenicity and transmission potential [3]. Because of the rapid rate of mutations on the rate of infectivity has also increased leading to so many variants caused first, second and third wave of infection throughout the world. On the other hand the vaccine formulation and creation of vaccine has rather been appeared as difficult and the impending Coronavirus Disease 2019 (COVID-19) pandemic has posed a major threat to public health around the world [4], necessitating the provision of an urgent vaccination. Governments, healthcare institutions, and the public all across the world are concerned about the COVID-19 pandemic. The globe has not witnessed an outbreak of this magnitude since the Spanish Flu decimated the planet in the early half of the twentieth century. With the emergence of COVID-19 in the United States, India, Italy, and other nations around the world, scientists have now focused on containing the pandemic [5,6].

The biology of Coronaviruses has been studied for many years and the bioinformatics tools are designed explicitly

for SARS-CoV-2 which is in use to develop rapid reaction to the need for fast detection, understanding and treatment of COVID-19. To control the on-going COVID-19 pandemic, it is of utmost importance to get an insight into the evolution and pathogenesis of the virus. Hufsky F, et al. [7] has been attempting to project and cover bioinformatics workflows and tools for the routine detection of SARS-CoV-2 infection, analysis of sequencing data, the tracking of the COVID-19 pandemic and evaluation of containment measures, evolutionary study of Coronavirus evolution, the discovery of potential drug targets and development of therapeutic strategies. They have very carefully been suggestive for active response to the pandemic which in fact requires high-quality SARS-CoV-2 data and meta-data. Schriml LM, et al. [8] and newly released software to be available freely and as open source repository like GitHub, allowing for transparency and managing versioning process and development. In particular, when software and resources are evolving as fast as the virus, versioning and reproducibility of all steps are also in increasing importance. Hufsky F, et al. [7] in their lucid elaboration briefed that the European Virus Bioinformatics center curates a list of bioinformatics tools specifically for coronaviruses. On the other way ELIXIR provides a range of services to study SARS-CoV-2, in particular, the European Galaxy server for data-intensive research that provides access to scientific tools and training materials to guide users through COVID-19 data analysis.

To deal with the Covid19 period and beyond, bioinformatics and artificial intelligence (AI) were found to be effectively useful. If scientists have been able to uncover numerous secrets about SARS-CoV-2 in such a short time, ranging from its identification to its origin, as well as it's functioning and spread, it is largely due to expanding biotechnology research with the help of artificial intelligence and bioinformatics tools.

Bioinformatics all over the world have been quick to respond to the COVID-19 pandemic by developing coronavirus-specific tools to further SARS-CoV-2 research and improve COVID-19 detection, comprehension, and treatment. This evaluation does not claim to be comprehensive, and additional tools will be developed considering the rapidly evolving research [9]. At the same time, Artificial intelligence (AI) has been implemented at multiple levels of the health care system to address the global health crisis [10]. SARS-CoV-2 and COVID-19 research covers a wide range of topics, including high-throughput technologies like Next-Generation Sequencing for detecting the SARS-CoV-2 genome, databases storing SARS-CoV-2 genomes and variants, bioinformatics software tools and databases for analysing and storing hostvirus interactions (HVI).

Another huge problem that researchers and decisionmakers have to deal with is the ever-increasing volume of the data, known as big data, which challenges them in the process of fighting against the virus. This justifies how and to what extent Artificial Intelligence (AI) could be crucial in developing and upgrading health care systems on a global scale [11]. Unprecedented amount of data derived from public health surveillance, real-time epidemic outbreak monitoring, trend now casting/forecasting, and regular situation briefing and updating, molecular and computational techniques and information and communication technologies (ICTs) [12,13]. The main advantage of these AI-based platforms is to accelerate the process of diagnosis and treatment of the COVID-19 disease. The most recent related publications and medical reports were investigated with the purpose of choosing ate reaching a reliable Artificial Neural Networkbased tool for challenges associated with COVID-19 [14]. The potential research areas of bioinformatics and AI, which have been well established in combating COVID-19 disease, having much potential in rapid virology research and prevention of diseases in near future, are highlighted below.

Role of Bioinformatics Resources in SARS-CoV-2 Research

SARS-CoV-2 Sequencing

From the beginning of the pandemic, bioinformatics proved its worth. Following the discovery of the first virusinfected individuals in December 2019, Chinese scientists set out to sequence the genome the genetic material made up of RNA, which is a lengthy chain of nucleotides of the novel pathogen using samples obtained from these patients. Even though this operation was carried out by biologists, bioinformatics methods were used to generate the complete sequence. The SARS-CoV-2 genome, which contains roughly 30,000 nucleotides, was thus exposed in record time only twelve days. This was made possible by breakthroughs in algorithms over the last 10 years, as well as open-source access to software programmes and global genomic data sharing. This tendency began in the 2010s, particularly during the Ebola outbreak, but has now become the norm with Covid-19 [15].

Databases for Bioinformatics

Scientists experimentally determined the sequence of the SARS-CoV-2 virus shortly after its discovery in Wuhan, China, in December 2019, and deposited it in a public database so that anyone can access it and work on it. Bioinformatics took the sequence from the database and began analysing it to extract important information about the virus, as this is the first stage in developing a medication to combat COVID-19. The SARS-sequence CoV-2 was compared to those of other viruses, particularly other coronaviruses, and it was discovered that it had sequence similarities with SARS-CoV, the virus that caused the earlier SARS outbreak in 2003. Furthermore, the SARS-CoV-2 sequence was discovered to be remarkably similar to a coronavirus identified in bats, leading to the conclusion that the virus originated in bats [5]. Following mutations or alterations in its genome, the virus migrated from bats to humans via a pangolin intermediaryall this information was found by examining viral sequences. demonstrating the importance of Bioinformatics once more Baruah C, et al. [5]; Baruah C, et al. [16].

Vaccine Development

Because the pathogen's whole genomic sequence has been available since December 2019, COVID-19 is a great candidate for this method. All open reading frames (ORFs) in the sequences are identified using four computational algorithms (ORFfinder, GetOrf, etc.). The antigens discovered could then be mapped and evaluated for pathogen expression (i.e., COVID-19) and immunogenicity during infection. For COVID-19 vaccination candidate (VC) selection, a detailed investigation of T-cell and B-cell epitope prediction is preferred. The immune system is divided into two types: Humoral and cellular. Bioinformatics databases such as the Immune Epitope Database (IEDB) are in use to identify B-cell epitopes for Humoral responses. Antigens that could be detected by major histocompatibility complex (MHC) molecules found in T cells are searched for in databases for cellular responses. Following that, in vitro and in vivo assays are used to validate the presence of VCs. As a result, immune informatics could well be utilised for better understanding on the pathophysiology, diagnostics, immune system response, and vaccine development of infectious diseases Jin C, et al. [17].

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Establishing the Virus's Ancestors

Once the virus's genome had been discovered, bioinformatics once again has been in assistance in extracting useful information, this time concerning the virus's origin. By comparing the new genetic material to that of other known coronaviruses, the researchers discovered that SARS-CoV-2 was more related to diseases found in bats than to the human SARS and MERS viruses that caused outbreaks in 2003 and 2012, respectively. This clearly shows that SARS-CoV-2 originated in these mammals, with another host animal serving as a link between them and humans. The researchers were able to identify the key proteins essential for the virus to function -SARS-CoV-2, like other viruses, requires a host cell to reproduce and spread and in particular, those involved in infecting human cells. They include the well-known Spike protein, which recognises cell receptors before penetrating the host and is now the focus of biologists' attention because it is the target of the already available Covid-19 vaccines Robson B, et al. [18].

COVID-19 Portals at EBI and NCBI

Researchers have well been able to upload, access, and analyse COVID-19-related reference data and, specialty datasets using the COVID-19 Portal. In the first instance, all COVID-19 data stored at EMBL-EBI is being gathered onto a dedicated page on the Pathogen Portal as the COVID-19 Portal, which is being created. An initial version of the COVID-19 Portal is expected to go live in April, 2020, according to EMBL-EBI. At the same time, NCBI Virus community portal for viral sequence data from its archives such as RefSeq, GenBank, and others have been instituted.

Disease Map for COVID-19

Many research organizations have collaborated to create a COVID-19 disease map by sharing information and best practices. The goal is to create a map of process specific to the SARS-CoV-2 virus that focuses on host-pathogen interactions.

VADR (Validation and Annotation of the SARS-CoV-2 Genome)

Based on models derived from reference sequences, VADR validates and annotates viral sequences [19]. A coronavirus models based on NCBI RefSeq entries has been made available for evaluating coronavirus sequences, including one for SARS-CoV-2 (NC 045512.2). VADR maps the RefSeq characteristics, which include protein coding sequences (CDS), genes, mature peptides (mat peptides), and structural RNA (stem loop), by computing an alignment of each input sequence to the RefSeq. A planned ribosomal frameshift occurs in the ORF1ab polyprotein CDS, which VADR can correctly annotate. Since March 2020, GenBank has been using the programme to screen and annotate incoming SARS-CoV-2 sequence submissions. It recognises and outputs information regarding more than 40 types of sequence issues, such as early stop codons in CDS. VADR (v1.1) now adds heuristics for faster annotation and handling of ambiguous N nucleotide stretches that were added expressly for the SARS-CoV-2 study.

Next Strain

Next strain is an open-source project that uses pathogen genome data to advance science and public health. They offer an always-updated perspective on publicly available data, as well as advanced analytics and visualisations that highlight pathogen evolution and epidemic propagation.

Collection of COVID-19 Pathways

Wiki Pathways is a library of biological pathways created and maintained by scientists for the scientists. During the current COVID-19 crisis, this unique subset of disease pathways is being highlighted. Another example is **CoV-Hipathia**, which is an online application for analysis and interpretation of the Covid-19 pathway this web application uses a mechanistic model of human signalling to interpret the effects of simultaneous changes in gene expression levels and/or genetic mutations in signalling pathways.

Mechanisms of Molecular Action are Being Modelled

Despite its importance, genetic data alone is insufficient to understand how the virus works, once it has entered the human body. To combat the disease, biologists must be able to define the molecular mechanisms at work in great detail. They use structural bioinformatics, a subfield of bioinformatics, to do this. Scientists hope to discover the three-dimensional structure of molecules and attempted to understand how it impacts their interactions using computational simulations that can mimic all of the actors engaged at the atomic scale Baruah C, et al. [5]; Baruah C, et al. [16]. In the case of SARS-CoV-2, such models have aided experiments (crystallography, electron cryomicroscopy, and so on) aimed at determining the structure of the Spike protein and elucidating its docking dynamics with a host cell. This proved to be critical for vaccine development.

Role of Artificial Intelligence (AI) in SARS-CoV-2 Research

Prediction and Tracking with AI

The SARS-CoV-2 pandemic has led to one of the most critical and boundless waves of publications in the history

of modern science. The necessity to find and pursue relevant information and quantify its quality is broadly acknowledged. Modern information retrieval techniques combined with artificial intelligence (AI) appear as one of the key strategies for COVID-19 living evidence management. A novel, automated search platform, called Risklick AI, which aims to automatically gather COVID-19 scientific evidence and enables scientists, policy makers, and healthcare professionals to find the most relevant information tailored to their question of interest in real time. Risklick AI by this time has well been able to determine COVID-19 references more effectively and efficieantly, both in terms of precision and recall, compared to the baseline platforms. Hence, Risklick AI could become a useful alternative assistant to scientists fighting the COVID-19 pandemic Haas Q, et al. [20]. By extracting information from social media platforms, calls, and news sites, AI might well be used to forecast the spread of viruses and construct early warning systems, as well as provide important information about sensitive regions and predict morbidity and mortality. Using machine learning (ML), Bluedot discovered a cluster of pneumonia patients and projected the COVID-19 outbreak's outbreak and geographic location based on existing data. Health Map compiles publicly available COVID-19 data and makes it easily accessible to aid in the effective tracking of the virus's transmission. The usefulness of AI in identifying and forecasting COVID-19 outbreaks using multitudinal and multimodal data has recently been highlighted.

Contact Tracking with Artificial Intelligence

In COVID-19, AI can supplement mobile health applications in which smart devices such as watches, phones, cameras, and a variety of wearable devices are used for diagnosis, contact tracking, and efficient monitoring. Telemedicine applications like AI4COVID-19, which rely on audio recording samples of 2 s cough, could be deployed as well as the use of artificial intelligence in the monitoring of COVID-19 instances. In clinical contexts, AI approaches are used to monitor patients and anticipate therapy outcomes. AI may give essential information for resource allocation and decision-making in the Intensive Care Unit (ICU) by prioritising the requirement for ventilators and respiratory assistance based on data generated from vital statistics and clinical indicators. AI can also be utilised to forecast recovery or mortality in COVID-19, as well as to offer daily updates, storage and trend analysis, and therapy tracking.

AI in the Early Stages of Diagnosis

COVID-19 instances were detected and quantified using AI from chest x-ray and CT scan pictures [21]. The COVID-19 detection neural network (COVNet) was built by researchers to distinguish between COVID-19 and community-acquired pneumonia using visual 2D and 3D data collected from a volumetric chest CT image. Further Multi-Objective Differential Evolution and convolutional neural networks to construct a unique deep learning model for COVID-19 diagnosis using a chest CT image has recently been introduced. COVID-ResNet, which used an automated and discriminative learning rate as well as progressive picture resizing to diagnose COVID-19, outperformed COVID-Net. Shi F, et al. [21] employed AI-based classifiers to predict the outcome of COVID-19 RT-PCR results using 16 simple characteristics extracted from the full blood profile. This could help reduce the number of RT-PCR tests in resourceconstrained environments.

Vaccine Development with Artificial Intelligence

Never before in human history has there been such a race to produce a vaccine against a virus. By utilising the power of AI, the velocity of discovery can be greatly enhanced [22]. Using the Vaxign reverse vaccinology-machine learning platform and supervised classification models, Ong E, et al. [2] identified probable COVID-19 vaccine candidates.

Covidex: Machine Learning-Based Alignment-Free Subtyping

Viral subtypes, also known as clades, are groups of isolates from a given species' worldwide population. Subtyping is important in virus epidemiology, evolution, and pathogenesis research. The input data must be aligned to a set of pre-defined subtype reference sequences in most subtype classification methods. These approaches can be computationally expensive, especially for lengthy sequences like SARS-CoV-2 (which has a genome size of 30 kb). Machine learning algorithms for virus subtyping may be employed to address this issue. Covidex is an open-source machine learning subtyping tool that does not require alignment.

Design of Pharmaceuticals

It is critical to develop COVID-19 therapeutic and immunisation measures to reduce the pandemic threat. The key to discovering possible therapeutic candidates for clinical trials is to understand the molecular pathways behind the disease's development. PPIs (viral-host proteinprotein interactions) are important during viral infection and have therapeutic potential. A screening of known medications and PPIs, referred to as drug repurposing, is usually cheaper and faster than creating drugs from scratch to identify new therapies [23]. This is especially true for SARS-CoV-2, as it belongs to a viral genus that has been extensively investigated. As a result, we may extrapolate data and prospective therapeutic targets from other beta coronaviruses, particularly SARS-CoV-1. The databases can store information on virus-host PPIs (see VirHostNet, CoVex) and virus-drug interactions (see CORDITE, CoVex), as well as information on other viruses and medications, to infer probable PPIs for SARS-CoV-2 (see CoVex, P-HIPSTer).

Corona Virus Explorer (CoVex)

CoVex is a network and systems medicine web platform that combines SARS-CoV-2 and SARS-CoV-1 experimental virus-human protein interactions, human protein-protein interactions, and drug-protein interactions into a large-scale interactome. Using numerous state-of-the-art graph analysis algorithms specifically adapted to the network medicine environment, it allows scientific and clinical researchers to anticipate novel drug targets as well as drug repurposing prospects. Expert knowledge of virus replication, immunerelated biological processes, and medication mechanisms can be used to assemble a set of host or viral proteins in this case [23].

Artificial Intelligence in Genomics

An ontology-based side effect prediction framework and an Artificial Neural Network to evaluate the side effects of Traditional Chinese Medicines for the treatment of SARS-CoV-2 have been reported Uddin M, et al. [19]; Abd Alrazaq A, et al. [24].

Identifying the Source of the Epidemic

These genealogical trees have also helped to fill in the gaps in the pandemic's history, country by country. In France, for example, a study of every genetic sequence accessible in March 2020 by scientists, including Alizon, revealed that they all descended from a single common ancestor originating from the early days of the outbreak in China. The fact that many viral lineages from that country were discovered in France shows that multiple virus "imports" contributed to the first wave of the outbreak. This number has been estimated to reach over a thousand in the United Kingdom, where many more sequences are available. Boston, in the United States, is another example, this time on the scale of a city. According to American experts, an international trade conference in February 2020 was a "super spreader" event that, in their estimation, resulted in more than 100,000 contaminations around the world over the next nine months. These insights are critical in determining what causes such catastrophes and how to avoid them in the future. "Phylodynamics" is an invaluable tool for monitoring an epidemic, especially because the data it uses has the advantage of minimising certain analytical biases, such as the number of new cases by time unit [25]. The researcher hopes to go even further with his team by merging genomic and traditional epidemiological data, considerably increasing total viral monitoring.

Keeping Track of the Virus's Progress

In addition to identifying the virus's origin and biology, genomic data can also be used to retrace the spread of an epidemic. "During a period of infection, the regular accumulation of mutations in the genomes of viruses on average one or two each month can be utilised as a kind of 'molecular clock' [26]. When people are infected with similar viruses, it suggests they are near the transmission chain. "Tracing the evolution of an epidemic across time and geography is achievable by comparing the genetic material of viruses in infected patients and using information on the dates and sites of sampling," explains Samuel Alizon of the MIVEGEC laboratory. In the context of Covid-19, the nascent discipline of phylodynamics is rapidly expanding.

In practice, bioinformatics experts employ genomic data to create a phylogenetic tree, or a family tree, that connects the viruses sequenced in various infections. They do it by employing the statistical concept of greatest probability, which states that the tree created best describes the relationships between the sequences given. As institutions and organisations such as the Canadian Institutes of Health Research (CIHR) increase funding for 49 additional COVID-19 research projects, and the Innovative Genomics Institute "pivots from genome editing research to an all-out effort to slow the spread of COVID-19," bioinformatics is taking the lead in the fight against the virus. According to The History of Vaccines, vaccine development is "a long, intricate process that sometimes takes 10-15 years." Granted, a significant portion of that time is spent complying with legal safety regulations, but the typical discovery process involved in generating the vaccine is still lengthy. According to the COVID-19 Vaccination Tracker, over 30 vaccine options are being investigated at the same time. Despite this, "experts think it could take between 12-18 months" to develop a vaccine that can successfully and safely contain the epidemic.

Conclusion

The global spread of COVID-19 poses a significant challenge for people to overcome. The most advanced and effective technique in biomedical research has been proven to be advances in bioinformatics and artificial intelligence-based techniques. This was proven by highthroughput screening and precise data processing. In the current pandemic situation, computational approaches have been successfully used from the preliminary stage of viral sample identification to the end stage of drug design by discovering novel information on SARS-CoV-2 genomic content, variations, diversity within the species, and predicting potential drug/vaccine candidates against viral genes in a very short period of time. The successful adoption of bioinformatics and AI approaches to SARS-CoV-2 amid the current economic downturn is a significant achievement for the scientific community.

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