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Chapter 17

Machine learning applications for COVID-19: a state-of-the-art review

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1. Introduction

The field of machine learning has made tremendous progress over the past decade. Improved deep learning algorithms coupled with increased computational capacity have catalyzed the growth of the field into the stratosphere. As a result, machine learning has been used in a diverse array of applications. Arguably the most crucial application of machine learning has been in the fight against the COVID-19 pandemic. Researchers have aggressively—and often successfully—pursued a number of different avenues using machine learning to combat COVID-19. A range of machine learning applications have been developed to tackle various issues related to the virus. In this chapter, we present the latest results and achievements of the machine learning community in the battle against this global pandemic. In contrast to other existing surveys on the subject we provide a general overview that is nuanced enough to provide a substantial insight. Our survey includes preprint works to ensure the most up-to-date coverage of the topics. The current applications of machine learning in the area of COVID-19 can be divided into four groups:

- forecasting
- medical diagnostics
- drug development
- contact tracing

Deep learning algorithms have been successfully deployed to forecast the number of new infections. Recurrent neural networks have shown superior performance in time-series forecasting over traditional approaches such as autoregressive integrated moving average (ARIMA) models. Researchers have used recurrent networks, and their variant long short-term memory networks, to successfully model the spread of the infection and predict the future number of infections in population. Arguably the most important application of machine learning is in the field of medical diagnostics that is made possible by the advances in computer vision. Machine learning has achieved near-human-level accuracy in many image recognition tasks. Therefore, it is no surprise that image recognition software is successfully being used to detect signs of COVID-19 in patient chest X-ray images. In many parts of the world where an effective clinical testing procedure is not available or unaffordable, chest X-ray images and CT scans provide the only option to diagnose the virus. Studies have shown that deep learning approaches can diagnose COVID-19 based on chest X-ray images with over 99% accuracy. Smart contact tracing using artificial intelligence has helped authorities locate potentially infected persons. A number of software solutions based on artificial intelligence are currently in use to trace the spread of the virus. Machine learning has been used to help guide researchers to new discoveries in pharmacology. In particular, variational autoencoders have the ability to analyze perturbations in chemical composition that can lead to possible new medicines. Applying autoencoders to the existing flu vaccines can help identify potential avenues to creating a COVID-19 vaccine.
The challenge to fight off the global pandemic and help humanity has spurred researchers across numerous disciplines. In an effort to accelerate scientific research into COVID-19 the publishing community has made all the related publications freely available to the public. As a result, we have been able to access and assess all the current research and present our survey to the readers. Our goal is to provide a quick, but sufficiently detailed, overview of the current state of the art in machine learning research applied to COVID-19. We hope our survey will supply the reader with the necessary information to facilitate a deeper investigation into the topic.

The paper is structured as follows. In Section 2, we discuss the use of machine learning in forecasting the number of new infections. Section 3 discusses the use of deep learning in the detection and diagnosis of the infection. Section 4 contains information about the use of machine learning in drug discovery and development. Section 5 discusses the current research related to the application of machine learning for contact tracing. Finally, Section 6 concludes the chapter with a few closing remarks.

2. Forecasting

Forecasting the number of infections is critical for proper planning and allocation of resources. Modern machine learning (ML) algorithms such as long short-term memory (LSTM) networks have been shown to outperform the traditional time series models such as ARIMA and Generalized AutoRegressive Conditional Heteroskedasticity (GARCH). As a result, LSTMs have been used in various applications involving time series projections [16,18]. Several countries employ ML-based software to estimate the number of future infections and the trajectory of the infected population. In this subsection, we provide an overview of the latest advances in ML related to forecasting the number of COVID-19 infections. The results of our survey are summarized in Table 17.1 and a more detailed discussion follows below.

A comparative study of ML-based algorithms for COVID-19 forecasting was carried out in Ref. [7]. The authors analyzed a number of evolutionary algorithms such as genetic algorithm, particle swarm optimization, and gray wolf optimizer as well as ML algorithms such as multilayer perceptron (MLP) and adaptive network-based fuzzy inference system (ANFIS). The models were evaluated on the basis of their accuracy for different prediction lead times. The authors employed data from five countries in their study experiments and revealed that MLP and ANFIS algorithms produce the best results, achieving a correlation level of 0.999. A novel approach from Google Research that combines temporal and spatial data is proposed in Ref. [20]. Using graph neural networks and Google mobility data the authors uncovered the rich interactions between time and space that is often present in the spread of a pandemic. Numerical experiments demonstrate the power of mobility data with the GNN framework. In Ref. [29], the authors employed an ensemble neural network to predict the number of confirmed cases and deaths in Mexico. The proposed ensemble network (MNNF) consists of three modules: nonlinear, autoregressive, and function-fitting neural networks. The module predictions are combined via a fuzzy integrator—designed to handle uncertainty—into a single output. The method was tested on data from Mexico. The authors carried out experiments to predict the number of confirmed cases and deaths 10 days ahead. The results revealed that the MNNF method outperforms single neural network models. The authors in Ref. [9] tested three LSTM-based models to forecast the number of infected individuals for 32 states in India. The tested models include stacked, convolutional, and bidirectional LSTM neural networks. The predictions were made one day and one week ahead. The results show that the bidirectional LSTM produces the optimal results. Several ML models are compared in Ref. [40] to forecast confirmed cases in Brazil and the United States. The models under consideration include Bayesian neural network, cubist regression, kNN, random forest, and SVR. In addition, variational mode decomposition (VMD) was applied as a preprocessing step. The authors also considered exogenous variables such as temperature and precipitation. Numerical experiments produce mixed results with no clear favorite. It can only be noted that VMD improves model performance when the prediction horizon is 6 days ahead. The authors in Ref. [36] compared statistical and ML approaches to time series forecasting. In particular, they studied ARIMA, support vector regression (SVR), and LSTM models to forecast the numbers of infections, deaths, and recoveries. The model input consisted of the data from the previous 110 days. The model was used to predict infections for the next 48 days. The study was based on data from 10 countries. The results showed that LSTM models generally outperform ARIMA and SVR. Machine learning approaches do not always outperform traditional methods. In Ref. [35], the authors compared classic statistical methods to SVR to predict the number of positive cases, death rate, and recovery rate. The study covers a large number of countries. The results showed that statistical models outperform SVR. In Ref. [14], the authors applied deep learning to forecast the number of infections and deaths regionally and worldwide. The LSTM models used the observed previous 3 days of data to forecast 10 days ahead. In their analysis the authors considered Middle East, Europe, China, and worldwide data. The results showed that the forecasts achieved a 1.5% root mean square error (RMSE).
## Table 17.1: ML-based research studies in COVID-19 forecasting.

| Study            | Objective                                      | Methodology                                                                 | Data                                                                 | Results                                                                                     |
|------------------|------------------------------------------------|-----------------------------------------------------------------------------|----------------------------------------------------------------------|---------------------------------------------------------------------------------------------|
| Kapoor et al. (2020) [20] | Forecast daily new cases in the US | A spatiotemporal graph neural network is used to learn the complex interactions between the time and mobility data. The model is implemented via GNN framework | NYT COVID-19 dataset and the Google mobility dataset/reports. The data include positive cases in the US over the period of Jan–Apr 2020 | GNN model achieves a correlation of 0.998                                                   |
| Ardabili et al. (2020) [7] | Comparative study of ML forecasting models | Compared GA, PSO, GWO ANFIS, and MLP approaches and their accuracy for different lead-times | Worldometer. Number of COVID-19 cases for five countries over the period of Jan–Mar, 2020 | ANFIS and MLP produce the best results with a correlation of 0.999                           |
| Melin et al. (2020) [29] | Make up to 10-day ahead predictions of number of confirmed cases and deaths | Ensemble of neural networks consisting of three modules: two nonlinear autoregressive networks (NAR) with different parameters and one function fitting network (FITNET). The output of the modules is combined via a fuzzy integrator | Mexico government (coronavirus-gob.mx). Confirmed cases of COVID-19 and related death cases in Mexico. The data on the state and country level over a 110-day period | %RMSE predicted confirmed cases on the country level 0.0808; %RMSE for the states ranges from 0.2157 to 0.0914; %RMSE for the states ranges from 0.0175 to 0.2094 |
| Arora et al. (2020) [9] | Predict the number of next day (and week) positive cases. | Three LSTM-based models stacked, convolutional, and bidirectional LSTM, are tested | Ministry of Health and family welfare (India). Number of positive cases in 32 states and territories in India over the period of Mar 14, 2020 to May 14, 2020 | Average MAPE for stacked, convolutional, and bidirectional LSTM model are 5.05%, 4.81%, and 3.22%, respectively |
| da Silva et al. (2020) [40] | Predict the number of new cases 1, 3, and 6 days ahead | Various ML models—Bayesian neural network, cubist regression, kNN, random forest, and SVR—are considered. In addition, variational mode decomposition (VMD) preprocessing is applied. Exogenous input variables—temperature and precipitation—are also considered | John Hopkins University repository and Brazilian State Health offices API. Number of daily positive cases for five states in the US and Brazil until Apr 28, 2020 | Mixed results with different models achieving the best outcomes on various subsets of data. The best models achieved an out of sample forecasting error of 3% |
| Shahid et al. (2020) [36] | Predict the number of positive, death, and recovery cases | ARIMA, SVR, and LSTM models are compared. The models are applied to data from 10 countries | China Data lab, 2020, “World COVID-19 Daily Cases.” Number of confirmed, death, and recovery cases over the period of Jan 22, 2020 to Jun 27, 2020 | Mixed results, but in general LSTM appears to produce better results. For instance, LSTM has the lowest MAE values for confirmed cases and deaths as 2.0463 and 0.0095, respectively |
| Rustam et al. (2020) [35] | Predictions for the next 10 days based on the data from previous 56 days | Linear regression, LASSO, support vector regression, and exponential smoothing (ES) are used. The predictions are made for infection, death, and recovery rates | John Hopkins University repository. Number of confirmed, death, and recovery cases worldwide over the period of Jan 22, 2020 to Mar 27, 2020 | ES achieves the best results in death rate prediction with $R^2 = 0.98$. LASSO achieves the best results in confirmed rate prediction with $R^2 = 0.98$ |
| Direkoglu et al. (2020) [14] | Use previous 3 days to forecast the next 10 days | LSTM model is used to forecast the number of new cases and deaths regionally and worldwide | WHO, CCDCP, and worldometer. Number of confirmed, death, and recovery cases worldwide over the period until Apr 10, 2020 | The trained LSTM model achieves 1.5% RMSE |
3. Medical diagnostics

Diagnosing COVID-19 infection is a key first step to fighting the virus. The rapid spread of the disease across the globe has made diagnosis of the disease at early stages not only important for the individual patient but also for preventing community spread of the disease. Polymerase chain reaction (PCR) tests that are currently employed to detect the presence of the COVID-19 virus require time and capital to administer. Despite recent improvements, PCR tests remain scarce and costly in developing countries and rural areas. PCR tests may further suffer from sample preparation and quality control which can lead to insufficient sensitivity [39]. Therefore, developing alternative approaches to testing is a vital research area. At present there are several ML applications that support the diagnostic process (Table 17.1). ML-based research studies in COVID-19 forecasting demonstrated capability to achieve high accuracy in image detection tasks. Consequently, applying deep learning and other ML techniques to X-ray and CT scan images has been an intensely researched area. In addition, detection approaches based on clinical data have also been tried and tested. Artificial intelligence (AI)-based methods augment the diagnosis process and accelerate the treatment of the disease. These models can assist the physicians and healthcare professionals not only during testing and treatment but also for planning and managing of resources [25]. The results of our survey on the current AI/ML research for COVID-19 diagnostics are summarized in Tables 17.2 and 17.3.

Imaging techniques such as X-rays and CT scans are widely used as diagnosis tools for many lung diseases including tuberculosis, lung cancer, and pneumonia viruses. CT scan images provide fast and detailed information about the pathology and prognosis of diseases. As a result, ML techniques are being increasingly integrated with imaging and computer vision methods for applications in disease diagnosis. The success of deep learning techniques in detecting and diagnosing various types of pneumonia has been already reported in the literature. The authors in Ref. [26] developed a robust model based on a three-dimensional convolutional neural network (CNN) framework to extract features from CT scan images and distinguish COVID-19 from community-acquired pneumonia. When diagnosing patients in early stages, AI models proved to be successful by integrating both CT scan imaging and clinical information [30]. Combining the output of a CNN model on CT scan images and the output of ML models such as SVM and random forests on clinical data the accuracy of diagnosis reaches the levels of human healthcare experts. CT scan imaging is the diagnostic tool predominantly used in treating pulmonary infections. It is also employed during the current outbreak by many countries in diagnosing COVID-19 patients—particularly at early stages. Further progress was made by Zhou et al. [48], who identified the importance of segmentation and proposed deep learning-based models to address these issues in ML-based diagnosis of COVID-19.

Despite the promising research results there remains a lot of room for growth of ML-based diagnostics. Production-ready applications that can be used in hospitals require further refinement. A great deal of research is yet to be conducted to improve their reliability. The main challenge in deploying the AI/ML models in COVID-19 is the generalization ability of these models, which is also prevalent in AI-based models in other applications. Another major bottleneck in implementing AI/ML-based solutions in healthcare is the availability of patient data samples of necessary size and quality to train the ML models. In some instances, although the data are available, the format and structure of the data pose another challenge. Integrating existing research solutions to practical applications and products is another challenge. Finally, it is vital to ensure that the studies and investigations conducted and reported during this pandemic and pressing times are technically, scientifically, and ethically correct.

A wide array of ML models has been deployed to try to diagnose instances of COVID-19. The list of models includes CNN, RNN, SVM, transfer learning, XGBoost, and others. Although these models demonstrate high performance and accuracy they possess limitations such as the lack of sufficient data to train the models, inability to generalize the results, etc. [48]. Despite the ongoing efforts to apply ML/AI in COVID-19 diagnostics, some members of the radiologist community have raised concerns regarding possible pitfalls. Laghi [24] cautioned that while AI/ML should be used for diagnosis of COVID-19, more objective and precise quantification is required in understanding the lung involvement of this disease. Wynants [44] reviewed the validity and usefulness of the various models published in the literature (Table 17.2) on diagnosis, prognosis, and risk prediction. Their analysis of over 145 models in 107 published documents showed that there is a high risk of bias. The results of these models are probabilistic and hence they are not recommended to be adopted for practical use. They call for more rigorous analysis of these models with proper methodological guidance and provision of the description of populations under study. They also warned that if the studies are unreliable, it would lead to harmful effects in diagnosis and prognosis of the disease. Based on a careful review of the existing literature on ML-based diagnostics for COVID-19 we conclude that the proposed models have significant potential. The existing models can be used as stepping stones for building more robust and resilient models that would assist healthcare professionals in diagnosis and decision-making. AI/ML researchers should learn from the
| Study                      | Objective                                                                 | Methodology                                                                                                                    | Data                                                                                                                                   | Results                                                                                                                                                                                                 |
|---------------------------|----------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Zhang et al. (2020) [46]  | Diagnose COVID-19 based on CT scans                                        | The proposed system consists of two segmentation models: one for lung lesion segmentation and another for diagnosis prediction. 3D convolutional blocks are used for the classification | A large database of 532,506 CT scan images of 4154 patients having COVID-19, common pneumonia, and normal controls          | Results are evaluated over the dice coefficient and pixel accuracy metrics. The system achieved an accuracy of 92.49%, sensitivity of 94.93%, and specificity of 91.13% |
| Apostolopoulos et al. (2020) [6] | Analyze the adoptability of CNN techniques for diagnosis of COVID-19 with the help of X-ray images | Transfer learning with CNN is used over the X-ray image data | An image dataset of 1427 X-ray images that include COVID-19-positive, common pneumonia, and normal conditions | The model achieved specificity of 96.46%, sensitivity of 98.66%, and accuracy of 96.78%. Results vary according to the severity of symptoms                                                                 |
| Zheng et al. (2020) [47]  | Detect COVID-19 via deep learning                                          | Deep CNN network with three stages: first stage with 3D convolution, batchnorm, and pooling layers; second stage has two 3D residual blocks; third stage is with progressive classifier which abstracts the information by 3D max pooling and output the probability of COVID-19. CT scan images were pre-processed by a simple 2D UNet to create 3D lung mask | 540 patients' chest CT scans are considered | The proposed model achieved sensitivity of 90.7%, specificity of 91.1%, and AUC of 97.5%                                                                                                                 |
| Sun et al. (2020) [42]    | Detect and classify COVID-19 from chest CT scan images                      | Deep forest algorithm based on adaptive feature selection. From the CT scan images, location-specific features are extracted. The trained deep forest model is used to reduce the redundancy of features and classify COVID-19 and community-acquired pneumonia | A dataset of 2522 chest scan images are considered | The proposed model achieved sensitivity of 93.05%, specificity of 89.95%, and accuracy of 96.35%                                                                                                          |
| Kasani et al. (2020) [21] | Automatically detect COVID-19 in X-ray and CT scan images                  | Compared the performance of a pool of deep learning-based different feature extraction models such as DenseNet, MobileNet, ResNet, InceptionV3, and NASNet. Features extracted from these models are fed to classification techniques such as decision trees, random forests, XGBoost, AdaBoost, bagging classifier, and light-GBM | A total of 137 images among which 117 are X-ray and 20 are chest CT scans images. These are COVID-19-positive patients' data and those of a similar number of healthy patients | PMobileNet and inception V3 with bagging classifier have provided the best classification performance with 99% for precision, recall, and F score. However the data are limited |
| Li et al. (2020) [26]      | Develop automatic ML framework to detect coronavirus with the help of chest CT scan images | Three-dimensional deep learning framework aimed to extract two-dimensional local features and three-dimensional global features. Then the features are submitted to a fully connected network with a softmax activation | T4352 CT scans collected from 3322 patients. Among these, 30% were for coronavirus, 40% for community-acquired pneumonia, and the remainder for non-pneumonia abnormalities | High specificity and sensitivity is achieved                                                                                                                                                                |
| Study                  | Objective                                                                 | Methodology                                                                                                                                  | Data                                                                                                                                   | Results                                                                                                                                  |
|-----------------------|---------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------|
| Nour et al. (2020)    | Detect the positive cases of COVID-19 automatically from chest X-ray images | A serial five convolutions layer network is designed to learn the model from the scratch. Optimization of the model parameters is made through Bayesian optimization. Using the learned model, deep feature vectors are extracted. For classification, SVMs based on RBF kernel, C4.5 decision tree, and k-nearest neighbor techniques are adopted | An open-access X-ray image database containing 2905 images is considered. The images belong to three classes: COVID-19, normal, and viral pneumonia | The proposed model with SVM classification achieved accuracy of 98.75%, sensitivity of 89.39%, specificity of 99.75%, and F-score of 95.75%. The main concern is that whether X-ray images are relevant for early diagnosis |
| Wang et al. (2020)    | Perform diagnosis and prognosis of COVID-19 using CT                      | Proposed a DenseNet-like structure with multiple stacks of convolution, ReLu activation, max pooling, and batch normalization operations       | CT scan images of 5372 patients among which 4106 patients’ data are used to pretrain the model and 1266 patients’ data to test and validate. Prognostics analysis is made with 471 patients who are tested as COVID-19 positive are considered. While considering the ROI, 3D bounding box of the entire lung is considered | Proposed model exhibited good performance with AUC of 90%, specificity of 89.93%, and sensitivity of 78.93%. The prognosis should be based on the severity of the symptoms |
| Mei et al. (2020)     | Design an AI model that can diagnose COVID-19 patients in the early stage by integrating CT scans, clinical symptoms, contact history, and testing | CNNs were deployed in two layers. The first CNN model is a slice selection CNN that selects the abnormal lung scans. The second CNN is used to diagnose and predict the likelihood of COVID. Further, patient details were fed to the ML model such as SVM/MLP/RF to classify COVID-19 positivity. The third output was obtained by integrating the result of diagnosis by the CNN model and patient’s clinical information to an MLP | CT scan image dataset of 905 patients. Further, clinical information details of these patients are also considered | Results of the proposed AI model that combined both CT images and clinical information during diagnosis are equivalent to the accuracy of human experts, particularly for early-stage cases |
| Burdick et al. (2020) | Predict the needs and requirements of ventilation during the diagnosis of COVID-19 patients | XGBoost classifier-based method which uses an ensemble learning technique to learn and classify low-risk or high-risk category patients | 197 patients with positive diagnosis of COVID-19 | The specificity and sensitivity results indicate that the model was able to identify and discriminate the patients who require ventilation support |
| Elaziz et al. (2020)  | Detect COVID-19 infection based on X-ray image                            | Feature extraction based on fractional multichannel exponent moments and feature selection based on modified manta-ray foraging optimization based on differential evolution are implemented in a multicore environment | 216 positive cases and 1675 negative cases of COVID-19. Another dataset with 219 and 1341 positive and negative cases, respectively | Significant gain in computational time. Accuracy of the method is proved to be better than other optimization methods |
experiences of this pandemic and focus on developing models in collaboration with healthcare professionals and medical experts. We note that the most important challenge is the availability of data to train the models as well as the treatment of the data. Resolving this issue could have a big impact on the robustness and generalization ability of models for practical applications.

4. Drug development

Machine learning algorithms are increasingly being used to search for new chemical combinations that can lead to effective medicine. Artificial intelligence and machine learning techniques have become an integral part of the pharmaceutical world. Integrating these techniques into the complex drug-developing pipeline has proven to be both cost-effective and less time-consuming. Machine learning techniques are particularly useful as they provide a set of tools that improve the process of drug discovery and development for specific situations with the help of available data that are reliable and of high quality. As a result, a large effort has been under way to apply AI/ML-based solutions in pharmacology. A summary of the survey of the current literature in the field is provided in Table 17.5. Several pharmaceutical companies have employed ML-based algorithms, such as artificial neural networks, support vector machines (SVMs), deep learning, and many others to develop various drugs and vaccines [34]. The authors in Ref. [34] provide a review of recently developed algorithms to design automated drug development pipelines consisting of drug discovery, drug testing, and drug repurposing. In drug discovery, the deep learning algorithm generative adversarial networks (GAN) is used to identify DNA sequences associated with specific functions and Bayesian optimization (BO) is used to produce proteins of interest with lower costs. In drug testing, sequential decision-making algorithms such as the Bayesian-based multi-armed bandit (MAB) algorithms are used to test several drug candidates and determine the best treatments. In drug repurposing, text mining methods and graph-based recommender systems are used to identify correlations and predict drug—disease interactions. The authors compiled a list of relevant data sets for drug development pipeline studies.

In 2019, the National Institute of Allergy and Infectious Diseases sponsored the first US clinical trial to develop a vaccine against SARS-CoV-2 using an AI-based model [5]. An AI program called Synthetic Chemist was created to generate trillions of synthetic compounds and another AI-based program called Search Algorithm for Ligands (SAM) was used to sift through the trillions of compounds and determine the most suitable candidates as vaccine adjuvants. With the fast spread of COVID-19, there has recently been a race in utilizing ML techniques and AI capabilities to develop an effective vaccine and antivirals.

The authors in Ref. [1] incorporated reverse vaccinology, bioinformatics, immunoinformatics, and deep learning strategies to build a computational framework for identifying probable vaccine candidates and constructing an epitope-based vaccine against COVID-19. The screening of viral proteome sequences resulted in short listing of Spike protein or Surface Glycoprotein of SARS-CoV-2 as a potential protein target that could be used to design the vaccine. The physicochemical properties of the protein were further examined using LSTMs and the results showed that the protein is the primary responsible agent for the pathophysiology of SARS-CoV-2. The authors proposed that their computational pipeline can be used to design an effective and safe vaccine against COVID-19. In Ref. [45], the authors used an “in-silico” analysis to design a potent multiple epitope peptide vaccine against SARS-CoV-2. MLP and SVM algorithms were used to screen for potential epitopes. The vaccine immunogenicity was enhanced using three potent adjuvants and its tertiary structure was predicted, refined, and validated using appropriate strategies. The results showed that the vaccine can interact effectively with toll-like receptors (TLR) 3, 5, and 8, and by using in silico cloning, it demonstrated a high-quality structure, high stability, and potential for expression in *Escherichia coli*. The authors in Ref. [33] surveyed the existing literature about COVID-19 and vaccine development. They used the Vaxign Reserve Vaccinology (VRV) tool and Vaxign-ML, a machine learning-based vaccine candidate prediction and analysis system, to predict and evaluate potential vaccine candidates for COVID-19. The results showed that in addition to the commonly used S protein, the nonstructural protein (nsp3) was found to be second highest in protective antigenicity. After further investigation of the sequence conservation and immunogenicity of the multidomain nsp3 protein, the authors concluded that nsp3 can be an effective and safe vaccine target against COVID-19.

For the development of drug treatment for COVID-19, the authors in Ref. [10] used a pretrained deep learning-based drug—target interaction model called Molecule Transformer-Drug Target Interaction (MTDTI) to predict any commercially available antiviral drugs that could be effective against SARS-CoV-2. The model was compared to a CNN-based model called DeepDTA and another two traditional machine learning-based algorithms, gradient boosting and regularized least-squares model, using various datasets. The MT-DTI showed the best performance in predicting the drug—target interactions and was able to identify various antiviral drugs such as redeliver, dolutegravir, efavirenz, and atazanavir which
could potentially be used in the treatment of SARS-CoV-2 infection. In Ref. [22], the authors used deep neural networks (DNNs) and established an AI platform to identify potential old drugs that could be used against SARS-CoV2. Different learning datasets consisting of compounds reported or proven active against SARS-CoV, SARS-CoV-2, human immunodeficiency virus (HIV), and influenza virus were generated and used to predict drugs potentially active against coronavirus from the marketed drugs. The predicted drugs were then tested and verified to serve as feedbacks to the AI platform for relearning and thus to generate a modified AI model. The implemented AI-based framework was able to identify eight drugs with activities against feline infectious peritonitis (FIP) coronavirus. The authors suggested that with prior use experiences in patients, these identified old drugs could potentially be proven to have anti-SARS-CoV-2 activity and hence be applied in fighting the COVID-19 pandemic. The authors in Ref. [23] analyzed over 10 million compounds using a machine learning pipeline in order to predict chemicals that interfere with SARS-CoV-2 targets. The pipeline involves selection of important physicochemical features for each target using recursive feature elimination algorithms, followed by fitting aggregated multiple SVM models and regularized random forest algorithm (regRF) to improve generalizability and then evaluating model performance using various computational validation methods. The authors concluded that their identified chemicals can accelerate testing of short-term and long-term treatment strategies for COVID-19. The importance of AI and machine learning (ML) techniques that can accelerate the discovery of a possible cure for COVID-19 is discussed in a recent review article [8]. One review article [19] focused on the recent advances of COVID-19 drug and vaccine development using artificial intelligence and discussed the potential of intelligent training for the discovery of COVID-19 therapeutics.

5. Contact tracing

Effective contact tracing is a major factor in a virus containment strategy [2]. In conventional contact tracing, a healthcare professional interviews the infected patient to trace and discover other individuals who may potentially be infected though contact with the patient. The main challenge of the conventional approach is the difficulty for an individual in recalling all their contacts. In addition, the process requires the availability of specialized clinicians using their experience and other resources [12]. Recent technological improvements have allowed the contact tracing process to be optimized with less human intervention in an intelligent approach known as digital proximity (DP) contact tracing. The DP approach utilizes network technologies to identify and locate individuals who could be potentially infected through contact.

With the widespread availability of computing networks and mobile applications—and their associated technologies including smartphones, smartwatches, and others—most of the technology-based contact tracing systems are built into mobile platforms [4,28]. These systems, named digital contact tracing (DCT), enable a registered user’s exposure to be evaluated through wireless signals such as Bluetooth Low Energy. Alternative technology-based tracing systems that are nonmobile and application-based utilize tracking information collected from a variety of sources such as banking transactions, security camera footage, GPS data from vehicles, mobile phones, and others to estimate the proximity of an individual to an infected person.

Artificial intelligence and machine learning—in particular deep learning algorithms—have been successfully used in medical diagnosis and screening systems due to their exceptional learning capabilities. In the context of DCT systems, these technologies can be incorporated to aid the decision-making process and improve the detection accuracy of contact tracing. Concretely, the data collected from registered users such as their daily tracks and geo locations in the DCT system are explored by the ML algorithm within digital platforms to provide medical professionals and government officials with useful insights. Artificial intelligence and machine learning applications are currently utilized through the entire life cycle of COVID-19 starting from detection to mitigation [25]. In contact tracing, a virtual AI agent is an alternative to a health professional in the case of classical contact tracing. The virtual AI agent with natural language capabilities can collect the information previously gathered by a health professional. In DCT systems, Bluetooth technology is widely employed as a proximity detector for COVID cases. However, the performance of Bluetooth-based contact tracing apps may be affected by changing the signal intensity, which can be exhibited by different mobile devices, mobile positions, body positions, and physical barriers [49]. Generic wireless multipath effects and shadowing are persistent issues which can lead to false-positive and false-negative identification (Table 17.4) To improve the proximity detection accuracy in DCT systems, ML techniques can be used to analyze the Bluetooth signal and other phone sensor data.

Recently, a two-stage classifier was proposed that utilizes vanilla neural network to extract features from a signal emanating from different sources [17]. Employing a deep learning technique directly on a smartphone involves high computational cost and power consumption. Therefore, during the first stage, raw data from different sources are converted
| Study                          | Objective                                                                 | Methodology                                                                                                                                                                                                 | Data                                                                                                           | Results                                                                                                                                                                                                 |
|-------------------------------|---------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Ahuja et al. (2020) [5]       | Vaccine development against COVID-19                                      | Deep neural network-based AI programs: Synthetic Chemist and Search Algorithm for ligands (SAM) are used                                                                                                     | COVID-19 Open Research Dataset (CORD-19)                                                                       | New approaches combining integrative medicine with AI models are emerging in the recent race to utilize ML techniques and AI capabilities to develop an effective vaccine against COVID-19                              |
| Abbasi et al. (2020) [1]      | Identify a suitable vaccine candidate and construct an epitope-based vaccine against COVID-19 | A computational framework using reverse vaccinology, bioinformatics, immunoinformatics, and AI-based strategies                                                                                              | NCBI database in FASTA format. Crystal structures of human alleles: Protein Data Bank                          | Spike protein (surface glycoprotein), B-cell, and T-cell epitopes were predicted for the construction of an epitope-based vaccine                                                                     |
| Yazdani et al. (2020) [45]    | Develop a multiepitope peptide vaccine against SARS-CoV-2                 | A variety of ML methods including ANN, SVM, BepiPred, ANTIGENpro, and VaxiJen are employed                                                                                                                 | NCBI database in FASTA format IEBD database                                                                   | Designed vaccine construct consists of several immunodominant epitopes has high antigenic capacity and induces humoral and cellular immune responses against SARS-CoV-2                                           |
| Ong et al. (2020) [33]        | Predict protein candidates for vaccine against COVID-19                  | Vaxign-RV and Vaxign-ML strategies are used. The sequence conservation and immunogenicity of the predicted protein were further investigated                                                                  | NCBI and UniProt databases                                                                                   | S protein had highest protective antigenicity score. nsp3 protein—with the second highest antigenicity score—was predicted as an alternate vaccine candidate                                                |
| Beck et al. (2020) [10]       | Predict binding affinity values between commercially available antiviral drugs and target proteins | Deep learning-based MT-DTI was compared to DeepDTA, gradient boosting, and regularized least-squares model                                                                                                  | DrugBank, Drug Target Common (DTC), BindingDB, and NCBI databases                                            | MT-DTI performance best compared to DeepDTA and ML-based algorithms (SimBoost and KronRLS). Atazanavir is the best chemical compound against the SARS-CoV-2 3C-like protease                                      |
| Ke et al. (2020) [22]         | Identify preexisting drugs with antiviral activities                      | Deep learning-based AI system was established. The predicted drugs were tested in vitro for verification and the results were fed back to the AI system for relearning                                               | DrugBank: https://www.drugbank Database 1: SARS-COV, HIV, influenza, other drugs Database 2: 210 inhibitors of the 3C-like protease of SARS-CoV | 8 marketed drugs: Vismodegib, gemcitabine, clofazimine, celecoxib, brequinar, convivaptan, bedaquiline, and volcapone were identified as potential candidates against COVID-19                                  |
| Kowalewski and Ray (2020) [23]| Identify chemicals that interfere with SARS-CoV-2 targets.               | A machine learning drug discovery pipeline consisting of multiple support vector machine (SVM) models and random forest algorithm (RFA) was developed                                                    | NUNII, DrugBank, therapeutic targets and bioassay database, ZINC                                              | SVM model with the RBF kernel outperformed regularized random forest or performed comparably                                                                                                           |
| Keshavarzi et al. (2020) [8]  | Review of ML-based drug development                                       | A multifaceted and comprehensive investigation of existing literature of AI-based approaches (SUMMIT, GAN, RF, SVM, RFE, LSTM) used for COVID-19 drug and vaccine development. The results were used to create a database: CoronaDB-AI | Complete toxicity dataset from distinct databases, including ToxCast and Tox21. Comprehensive epitope-based dataset | SML-aided molecular docking is one of the most prevalent approaches for virtual screening. 3CLpro is the most popular target for virtual screening. Spike protein has been the most popular candidate for virtual vaccine discovery |
into fixed-length vectors and stored in the database. In the second stage, the vanilla deep learning algorithm is applied to
detect proximity [17]. A similar project under the TC4TL challenge compares several deep learning models including
Conv 1d [27], support vector machines [38], and decision tree-based algorithms [13] to evaluate the accuracy of Bluetooth-
Based distance measurement [31,37]. The performance of different techniques is measured based on the lowest normalized
decision cost function (NDCF) which represents proximity detection performance considering the combination of false
negatives and false positives. The results show that the Conv 1d network has the lowest NDCF.

It is evident that the performance of classification algorithms varies widely based on proximity thresholds. For example,
Song [41] reported that when considering two people 6 feet apart in classifying Bluetooth beacon RSSI values, a Gaussian
support vector machine classifier yielded better accuracy than a decision tree classifier. For validation, each experiment was
conducted by placing two Raspberry Pi’s 6 feet apart and measuring the RSSI values.

An AI-based contact tracing app named COVI developed in Canada leverages probabilistic risk levels to profile an
individual’s infection risk level [3]. COVI uses the advantages of ML algorithms to optimize and automate the integration
of pseudonymized user data in assessing the risk levels. An a priori version of an epidemiological model-based simulated
dataset is used to pretrain the ML models. Upon the collection of real data through an app, the simulator parameters are
tuned to match with real data. The impact of ML in the COVI app is observed by using the ML predictor inside the
simulator to influence the behavior of the agent in recommending the risk levels. The contact tracing application can be
used to predict the lockdown area based on places visited by an infected patient. In Ref. [28] the authors proposed a K-
means clustering algorithm with DASV seeding to predict the lockdown area. The proposed method has been tested in
Denver, United States, and successfully identified the area to be locked down as users walking in the area approach each
other very frequently. Despite the significant advantages of using DCT systems, there are issues related to data privacy and
use. However, these are beyond the scope of this review chapter.

6. Conclusion

Machine learning has become a potent tool in many applications. In particular, it has recently been employed in the
battle against COVID-19. There exists a growing body of literature that is dedicated to the subject. The decision by the
major publishers to make all COVID-19-related research publicly available has improved information
flow. In this
chapter, we attempted to provide an overview of the rapidly increasing corpus of research in machine learning related to
COVID-19. We discuss the state-of-the-art research including the material on research archives. In particular, we
covered four major areas of ML research related to COVID-19: forecasting, medical diagnostics, drug development, and
contact tracing.

Our survey revealed the following key observations. In forecasting, recurrent neural network such as LSTMs have been
used to predict the future infection and death rates. Many studies are focused on the North American region, but also other
countries including Brazil and China (Table 17.5). The best models achieve a correlation of 0.999. In medical diagnostics,
deep learning models that have previously shown success in other domains are being deployed to detect the presence of
the infection based on CT scans and X-rays. The best models achieve an accuracy rate of 99%. In drug discovery, a variety of
algorithms are being used to develop new vaccines against the infection. However, the majority of these studies are still in
the initial stage. In contact tracing, AI-based applications are utilized to identify and locate potential virus carriers, though
with limited success.

Despite the tremendous progress, the current machine learning approaches suffer from two major drawbacks. First,
the underlying algorithms have not yet reached the level of human reasoning. The deep learning models such as CNNs,
LSTMs, Transformer, and others remain imperfect and cannot consistently outperform a human expert. Second, the
lack of data hinders the training and development of the models. Patient data are notoriously difficult to obtain. Since
deep learning models rely on an abundance of data, the lack of thereof results in suboptimal generalization
performance.

Our main recommendation based on the extensive survey of current literature is the involvement of government
agencies to facilitate procurement of COVID-19-related data. Public institutions and government agencies can play a key
role in obtaining and disseminating data from hospitals to researchers. Since machine learning algorithms rely heavily on
large amounts of data their availability could drastically improve results.
### TABLE 17.5 ML-based research studies in contact tracing.

| Study                      | Objective                                             | Methodology                                                                 | Data                                                                 | Results                                                                 |
|----------------------------|-------------------------------------------------------|-----------------------------------------------------------------------------|----------------------------------------------------------------------|------------------------------------------------------------------------|
| He andand Printz (2020)    | Detect proximity of individuals                       | A two-stage classifier that utilizes vanilla neural network to extract features from a signal emanating from different sources | National Institute of standards and Technology (NIST) COVID-19 data repository ([https://covid19-data.nist.gov](https://covid19-data.nist.gov)) | No comparison, however, it shows the variation of different phone carriage states and prediction accuracy |
| Shankar et al. (2020)      | Comparative study to evaluate the accuracy of Bluetooth-based distance measurement | Deep learning, SVM, and decision tree-based classification models are compared | MIT PACT RangeAngle data set [https://mitll.github.io/PACT/datasets.html](https://mitll.github.io/PACT/datasets.html) and MITRE COVID-19 synthetic data set | Conv 1d exhibits on average 90% better performance than other classification models |
| Song, (2020)               | Comparative study of different algorithms to determine the proximity within 6 feet | Various ML algorithms are tested in classification of bluetooth beacon RSSI values | piPact, Beaver Works summer Institute, July 2020, [https://beaverworks.ll.mit.edu/CMShw/pipact](https://beaverworks.ll.mit.edu/CMShw/pipact) | Gaussian SVM shows better performance than logistic regression, k-nearest neighbors, and decision tree-based classifier with training, validation, and testing accuracy of 76.12%, 72.60%, and 79.67%, respectively |
| Alsdurf et al. (2020)      | Capture the dependencies across the whole history of the user | Transformer deep learning architecture is used as the base algorithm         | Simulated dataset based on epidemiological model                       | ML-based risk prediction could reduce the reproduction number compared to standard digital contact tracing applications |
| Maghdid et al. (2020)      | Predict the lockdown area based on people movement    | K-nearest unsupervised machine learning algorithm is used for prediction     | Android-based smartphone application for user data collection          | Used a threshold of 5 meters as the proposed protocol to predict the lockdown area |

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