



# A Comprehensive Review on Optimizing Machine Learning Models for Early Detection and Forecasting of Monkeypox Outbreaks

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## Abstract

This is a significant problem in diagnosing zoonotic opportunistic 'emerging' diseases like Monkeypox, which require not only better diagnostics but also efficient, effective, and affordable diagnostics. This paper considers the possibilities of machine learning (ML), deep learning (DL), and optimization algorithms for diagnosing and predicting Monkeypox. The presently employed strategies can be enhanced because clinical and imaging data can be harnessed to drive these technologies for early detection and subsequent containment activities. Generally, in a review, the authors offer information on how the diagnostic processes using ML and DL result in enhanced accuracy, specificity, and sensitivity of models, thus reducing design reliabilities. Furthermore, outbreak data is subjected to predictive modeling analysis to establish patterns useful in helping risk managers and policymakers prepare to manage future outbreaks. This system poses a new diagnostic model for Monkeypox and other zoonotic diseases by incorporating these complex computational tools into the present healthcare systems. This advancement not only strengthens the diagnostic arsenal of zoonotic diseases but also expands the possibilities for the interception and prevention of such diseases in the future at the world level.

**Keywords:** Artificial Intelligence (AI); Machine Learning (ML); Deep Learning (DL); Zoonotic Diseases; Transfer Learning; Metaheuristic Optimization

## 1. Introduction

Thanks to various emerging diseases, modern societies have realized global weaknesses in healthcare systems, especially in the current coronavirus crisis. The unprecedented crisis disclosed deficiencies in diagnostic facilities, a lack of resources, and a lack of preparedness to contain outbreaks across several countries.

The last few years have revealed that the world's healthcare systems are weak, especially in handling illnesses originating from animals. COVID showed where diagnostic tests, financing, and readiness for illnesses originating from human-animal interactions are lacking. Cultural loss and degradation of the environment have facilitated the spillover of zoonotic diseases from animals, and these include Ebola, Nipah virus, and Monkeypox. One recent disease that used to be prevalent all over central and West Africa but recently noted worth spreading to over one hundred countries is Monkeypox due to globalization, urbanization, and frequent movements. Since Monkeypox symptoms look like other viral illnesses, a better and more effective diagnostic tool is required urgently.

Based on these novel factors, there is increasing pressure on healthcare organizations to evolve their diagnostic procedures to be faster and more precise. Presenting robust approaches for optimizing the detection of Monkeypox, ML, and DL maintain a deep learning algorithm. These tools presented here via A.I. can help examine massive data sets to pinpoint ailment precursors, improve lesion examination, and accurately predict future outbreaks to allocate resources effectively. By applying the power of A.I. in human health care systems, diagnostics of Monkeypox and other Zoonotic diseases can be reduced and prevented. This paper looks at how optimization-based ML and DL can improve the speed and accuracy of diagnoses, thus enabling better approaches to public health interventions [1].

Monkeypox incidence is high, stressing the importance of increasing the efficacy of diagnostics and treatment among patients with ZID. Most healthcare facilities do not have the proper equipment to diagnose and treat the above diseases when they have started manifesting; thus, there is a need to watch out for them. As a result of Monkeypox, the economic, social, and public health effects cannot be overlooked. Their spread weakens gaps found in international health systems, where zoonotic structural diseases are predicted to rise due to encroaching human interference on wildlife land, climate change, and habitat. Biotic and abiotic factors must be understood to control and prevent the spread of Bovine Spongiform Encephalopathy successfully, and the standard diagnostic and disease surveillance technologies must be applied appropriately.

Therefore, getting reinforcement learning, deep learning, and other A.I. technologies into the correct diagnostic path will be essential as healthcare systems change. These technologies can transform disease diagnostics by improving the time and precision taken in the diagnostic process, enhancing early treatment. To support the use of A.I. and machine learning to enhance healthcare response, this research uses models to diagnose Monkeypox. The present research contributes to understanding the current outbreak and aims to strengthen the global health system for future zoonotic diseases [2].

Monkeypox becoming a global issue is a view that hails the need to invest in solutions for zoonotic diseases regarding public health measures and better application of technologies. Major trends like reinforcement learning and deep learning, especially within artificial intelligence, appear as new opportunities for innovating healthcare responses. Because these models can extract epidemiological, clinical, and laboratory data, they can make contacts and correlations that would be difficult or impossible for humans to make. The result is that the early indications of an outbreak are more precise, enabling health authorities to respond promptly within the region.

New knowledge in deep learning would significantly help identify Monkeypox from other illnesses with similar symptoms, including chickenpox or measles, or risk of misdiagnoses. Integrating and analyzing data from machine learning models and an optimization algorithm can enhance the diagnosis and required resource allocation for containment. In addition, analytical and quantitative methods that drew dependency on outbreak history, such as predictive modeling, can assist in understanding the future trend of Monkeypox and other Zoonotic diseases and, hence, provide strategic direction for healthcare organizations.

With COVID-19 and Monkeypox, the world is learning that prevention secondments cost more than proactive measure preemptions. Including A.I. technologies in diagnostics, especially in zoonotic diseases, is a significant leap toward public health preparedness. Possessing the DNA identification feature can go a long way in preventing future episodes and saving the lives of millions of people worldwide from new diseases. This research will strive to add to this work by analyzing how AI-driven models could enhance current healthcare delivery systems with a view to the demands of a globalized world [3].

There is a higher call for diagnosis technologies to be developed to address the existing diseases and meet future diagnostics that may be needed in future zoonotic diseases that are likely to bring more formidable challenges to Global Health. Monkeypox is a typical phenomenon caused by the increase in the number of viral diseases affecting the world's nations and requiring massive diagnostics. This scenario explains why healthcare organizations need to acquire and arm themselves with better tools that enable the health systems to give quick and accurate diagnoses for such diseases—examples of Machine learning and optimization-based diagnostic models and lessons learned from COVID-19 support proactive and predictive outlook. The offered approaches can significantly improve the capacity for health interventions since the adjusted methodologies offer early detection, accurate monitoring, and consequent mobilization of intervention measures. In that way, they can become normative in stopping and containing future pandemics such as monkeypox [4].

For various reasons, the Monkeypox outbreak has shown how zoonotic diseases can spread beyond their regular geographical distribution. Increased travel across the world's borders has also ensured that the virus takes a shorter time to spread from areas where the vice prevails to those regions that have never experienced such a calamity in

their lives. Persons from infected areas are asymptomatic and take the virus back home, where they spread it to other people. Furthermore, globalization for goods and services, injustices, and the smuggling of wildlife and animal derivatives are significant means through which zoonotic diseases spread. Human interference with the habitats of such species, mixed with the act of poaching of infected animals, ensures that there is close contact and hence the spread of the virus. It states that with the increasing population and encroachment into previously wilderness areas, people have been exposed to more zoonotic transmission [5].

Furthermore, it is noteworthy that social consolidation legends accompanying urbanization and population congestion have boosted the spread of Monkeypox tremendously. Population density means that people infected with the virus but show no symptoms can spread it to others within their contact networks and generate surges of infected persons in communities that have never before encountered such diseases. These outbreaks can be more devastating in non-endemic zones with poor health standards and low health security. In these areas, the weak capacity to identify Monkeypox early enough has led to the virus going viral, as it were, before communities can implement a containment regime [6].

This study revealed that Monkeypox has far-reaching consequences on global well-being, economy, and social interrelationships. The threat is still on the rise, whereas the recent outbreaks require a combined effort of different sectors worldwide. Greater international collaboration is needed to build up the existing structures in surveillance, diagnostics, and response capacities that are central to preventing further epidemics and protecting the Health of communities. Fighting this threat is only possible if the unique nature of monkeypox transmission causes and course is better understood. It will also arm public health systems with this knowledge for future prevention and control to be equipped when zoonotic diseases spur outbreaks in an ever-growing interconnected world [7].

In this ever-changing world of healthcare delivery, advanced technology, including the use of ML and DL, is now a critically important weapon against communicable diseases such as Monkeypox. These two subfields of artificial intelligence (AI), while much more narrowly defined than even the component systems within the larger field of AI, contain the capacity to significantly transform the procedures of diagnosing. Just like in the previous sections of this paper, both the ML and DL approaches can handle large datasets in record time, understand complex relationships that may not be easy to decipher by even experienced analysts, and produce outcomes that may otherwise take humans considerable time to discover. It is for this reason that this capability of molecular biochemistry gives it a competitive edge when it comes to identifying and addressing conditions such as monkeypox [8].

Data analysis and pattern recognition are some of the most well-known responsibilities of machine learning in healthcare. By analyzing large datasets, including clinical presentations, laboratory findings, and epidemic intelligence, ML algorithms can quickly discern the first signals of diseases such as Monkeypox. These systems help the early diagnosis of the disease when clinical manifestations at early stages mimic other viral infections that do not imply the presence of the studied disease. Monkeypox can, therefore, be effectively contained early enough once the disease has been diagnosed by a healthcare provider, thus encouraging outcomes as compared to traditional forms of detecting diseases, including assimilated HIV [9].

A subcategory of ML called Deep learning encompasses substantial extra uses in medical image analysis. For example, DL models can be trained on terabytes of image data, such as photos of skin diseases, to distinguish one type of skin disease from another because they look almost identical. With Monkeypox, such algorithms as DL can help extract skin rashes and other dermatological features that indicate the disease from similar ones that signify other diseases making diagnosis by clinicians more accurate. This image-processing capability may be helpful in several situations where a clinician might have limited exposure to the specific pathologies peculiar to a given disease or a disease still in its early stages of development [10].

The second important area in which the use of ML is crucial is the ability of the algorithms to analyze the trends of disease outbreaks based on historical data and predict their further development. Specifically, in the case of Monkeypox, risk factors can be identified, and fluctuations in the number of cases can be forecasted so public health authorities can provide that improvement in the distribution of resources. These models are of great use for epidemic management because they offer knowledge about the further development of an epidemic and its tendencies, allowing for more effective interference meant for cessation of spreading [11].

In addition, ML and DL technologies can complement conventional diagnostic instruments to improve their effectiveness. For instance, the integration of ML algorithms can be applied in the context of the usage of rapid diagnostic tools, which can improve the diagnostic process by offering shorter times to deliver the result and increase the capacity of the process as a whole. Such integration may be helpful during an outbreak, so tests will

be done quickly as healthcare facilities are pressured to diagnose patients efficiently. Using the powerful tool provided by artificial intelligence alongside more traditional diagnosis approaches to Monkeypox and other newly appearing viral diseases will make disease management outcomes more effective, enhancing the effectiveness of public health interventions [12].

Moreover, the findings obtained from the proposed ML and DL models for predicting diseases are instrumental in combating the epidemic. Using appropriate statistics from previous epidemics, these models can predict possible future epidemics and determine how to prevent them to avoid worsening the situation with the needed resources and measures. This predictive ability is beneficial in the case of zoonotic illnesses such as Monkeypox since the spread can be much averted if proper action is taken early enough. The capacity to predict the flow of an epidemic and mobilize resources appropriately stands as a novel approach compared to the previous reactive models commonly used in international health emergencies.

Finally, to the existing body of knowledge, this work adds to the discussions on applying A.I. in healthcare, particularly in the fight against infectious diseases. Thus, showing how ML and DL models, as well as optimization algorithms, can improve the diagnosis and control of the Monkeypox virus creates the basis for subsequent studies to evaluate the applicability of these technologies in other zoonotic diseases. The implications are profound: Contemporary information technologies, such as rapidly identifying pathological processes and their tendencies, can change the approach to combating diseases and minimizing the consequences of future pandemics for human life and the global economy.

Finally, integrating new computational methods in diagnostic health care opens an essential stage in the fight against infectious diseases. The study's conclusions reveal that with proper tuning, using machine learning and deep learning models presents an excellent opportunity to meet global needs for better and faster diagnostics when diseases such as Monkeypox evolve. Given the daily emergence of new zoonotic diseases globally, these technologies will continue to be imperative in helping uphold people's Health and strengthening healthcare systems globally.

## **2. Literature Review**

This literature review reviews recent studies on the uses of Monkeypox diagnostic, predictive, and control models based on machine learning, deep learning, and optimization algorithms and their accuracy in diagnostics and disease control.

As discussed in the paper [13], the COVID-19 test remains the world's focus, and now, Monkeypox threatens to become the next pandemic. Monkeypox is comparatively less fatal than COVID-19 but is way more infectious, causing panic after spreading to multiple countries. As such, there is a desperate need for accurate and early diagnostic procedures. Machine learning has already been discussed a lot in medical diagnosis, and it is beneficial in cancer detection and identification of COVID-19 patients. Hence, similar techniques can be used with a high probability for the early detection of Monkeypox. The research presents two algorithms to enhance the evaluation of monkeypox images based on transfer learning complemented with meta-heuristic optimization. In particular, the Google deep network is used for feature extraction. In contrast, the AI-Biruni Earth radius, sine cosine, and particle swarm optimization algorithms are used for feature selection and for fine-tuning the parameters of a multi-layer neural model. The study is based on the publicly available dataset and examines the proposed methods on ten different metrics, thus proving the efficacy of the proposed approach with 98.8 % classification accuracy.

As discussed in [14], emerging technologies such as artificial intelligence, machine learning, and big data have been influential in improving healthcare monitoring systems, especially for identified cases of Monkeypox. As the data about infected and uninfected people globally is emerging, it is an excellent opportunity to use machine learning and A.I. approaches to forecast Monkeypox cases in the early stages. Based on this potential, the study presents an enhanced Long Short-Term Memory (LSTM) deep framework, called the BER-LSTM, to accurately predict the confirmed Monkeypox cases. The AI-Biruni Earth Radius optimization technique is applied to the LSTM model, thereby adjusting the size of its hyperparameters. The experimental analysis results demonstrate the efficiency of BER-LSTM as a methodology, where the Mean Bias Error equals 0.06. To support the approach, six different machine learning models and four optimization algorithms were also used to test and compare the results with the proposed method, indicating the efficiency of the proposed approach. Finally, ANOVA, Wilcoxon, and regression tests also support the stability, significance, and robustness of the proposed BER-LSTM approach.

According to the study cited as [15], human skin diseases such as Monkeypox have become more rampant in the two decades of the current millennium, especially in the advanced world. These diseases present dangers that are

different from conventional health dangers like cancer dangers, and they also tamper with the self-esteem of patients. Since Monkeypox images could be more precise, manual diagnosis is frequently highly specialized and time-consuming while at the same time being subjective. To this end, developing a computer-aided diagnostic system is suggested to handle this process automatically. In most prior works, researchers employ CNN with traditional loss functions to learn discriminative features from Monkeypox images. However, the research brings an innovative approach of integrating the BER optimization algorithm with stochastic fractal search (BERSFS) integrated into deep CNN layers for classification optimization of Monkeypox images. The process starts with getting aware of the image embeddings in the Euclidean space using the CNN models, whereby the classification is then optimized through the help of a triplet loss function that helps in the classification process of cases of skin diseases, including Monkeypox. Based on the African hospital dataset, the emergent framework achieves better results than previous works. Moreover,  $P < 0.05$  and analyses of variance and Wilcoxon provide substantiation showing that the indicated method is viable and superior to other machine learning models and optimization algorithms.

As stated in [16], the Monkeypox virus, which was earlier identified in Africa, has symptoms of skin rashes, and since the COVID-19 infection, the global public has developed more significant concerns. In light of the frequent occurrence of epidemic diseases, early diagnosis is greatly helpful in preventing further spread. In this work, feature selection and classification approaches for distinguishing skin lesions associated with monkeypox illness will be improved with metaheuristic optimization strategies. This paper uses the GoogLeNet deep learning framework for feature extraction and a binary version of the dipper-throated optimization (DTO) for feature selection. A DT classifier is then used to map the selected features, and the mapping results are refined using the continuous version of the DTO algorithm. Various statistical measures are used to measure the proposed method's relative performances, including accuracy, sensitivity, specificity, p-value, N-value, and F-1 score. After tuning the classifier's parameters, the results are as follows: F1-score of 0.92, a sensitivity of 0.95, and an overall accuracy of 94.35%. Significant differences and improvements compared to other techniques for identifying monkeypox cases are evident using ANOVA and the Wilcoxon signed rank test.

As affirmed in [17], due to the emergence of Monkeypox and the expanding geographical range of its transmission, more research is needed to determine the causes of its transmission and enhance the diagnosis of Monkeypox since it is clinically similar to smallpox. Using a 2–2-phase method, the study presents the Accurate Monkeypox Diagnosing Strategy (AMDS) for diagnosing Monkeypox. The two-stage process can be summarized as follows: The Feature Selection Phase (FSP) to determine the features most relevant to diagnose Monkeypox, and the Classification Phase (C.P.), where actual diagnostic work is done. For the present work, AMDS brings about a new improvement in the FSP by introducing the Dynamic Recursive Gray Wolf Optimization (DRGW) algorithm – a modification of the Traditional Gray Wolf Optimization (TGWO) algorithm. Here, DRGW aims to correct the shortcomings of TGWO, which include the inability to swap positions between the pack, and a given criticizes this approach for being imprecise when pinpointing potential targets. AMDS was assessed using new feature selection methods compared to recent feature selection techniques using SVM, NB, KNN, and DNN classifiers. To evaluate the effectiveness of the proposed DRGW approach, the following performance measures are examined: Recall, Precision, Accuracy, Error rate, and F-Score. Experimental outcomes play testimony to the fact that AMDS effectively enhances diagnostic performance in terms of recall, accuracy, precision, error rate, and F-score.

Click or tap here to enter text. The numerical performance of a mathematical model for monkeypox transmission is assessed using the newly designed deep neural network process in the research [19]. The increased accuracy of solutions proposed by the model is achieved due to the additional two hidden layers with eleven and twenty-two neurons, respectively. This approach involves a stochastic deep neural network, activation radial basis function, and Bayesian regularization optimization to improve the applicability in solving the monkeypox transmission system. The dynamical model is divided into two categories: human and rodent. Human compartments are latent, exposed, infectious, symptomatic, and recovered, while the rodent population consists of latent, exposed infectious, and recovered ones. For the record, data proportion after the Adam approach is training phase = 0.13, testing phase = 0.12, and validation phase = 0.15. The findings of the current work are compared to justify the results and generate statistical plots of regression analysis, state transitions, histograms of errors, and correlation to demonstrate the efficiency of the proposed method.

As highlighted in the paper [19], the world struggles to contain the impacts of COVID-19. First detected in Central Africa, the Monkeypox has now reached 103 non-African nations. In the early stage, it is almost indistinguishable from chickenpox, cowpox, or measles, so using a computer-assisted detection method is appropriate early in the disease. This study proposes a diagnostic framework that categorizes patient cases into four groups: Normal,

Monkeypox, chicken pox, and Measles, which are some of the common skin lesions. The framework combines existing CNN models, learning classifiers, and a metaheuristic optimization algorithm. This research fine-tuned hyperparameters of five pre-trained models as follows: VGG19, VGG16, Xception, MobileNet, and MobileNetV2, and optimized the feature extraction and reduction layers using the Harris Hawks Optimizer (HHO) algorithm. The extracted features are then passed through seven classification algorithms, such as Random Forest, AdaBoost, and Support vector machines, among others, using the 10-fold cross-validation for accuracy. The last predictions are determined using majority voting. Experiments were conducted on two datasets: We proposed two novel datasets, called the Monkeypox Skin Images Dataset (MSID) and the Monkeypox Images Dataset (MPID), both of which provided state-of-the-art performance with accuracy rates of 97.67% for MSID and 97.51% for MPID. Sensitivity, specificity, and F1 score are also presented to highlight the ability of the proposed approach to the real-world scenario.

The publication [20] established that the world has now developed an epidemic fear due to the surge in cases of Monkeypox even as the COVID-19 threat declines. While the 2022 monkeypox originally began in Africa, the virus has now appeared all across Europe and the American continent. India recorded ten cases of the disease by August 2022 with one mortality and added to the global tally of over ninety countries. Monkeypox is one of the Orthopoxvirus subgenus from the Poxviridae family of viruses, and it is comprised of several zoonotic viruses; the name arises from the original detection of Infection in macaque monkeys. This article briefly overviews the latest improvements in the use of applications, such as Machine Learning (ML) and Particle Swarm Optimization (PSO) clustering, regarding Monkeypox. According to the current literature, ML plays a significant part in extensive data analysis, and precise approaches have been deemed successful in predicting the emergence of the disease and its signs. Furthermore, the application of big data analytics based on Machine Learning bio-inspired approaches has grown exponentially. It has dramatically improved contact tracing, molecular analysis, and drug development initiatives even though the occurrence of Monkeypox is shallow and is related to contact with the skin, lips, or lesions of affected individuals, as well as contact with contaminated respiratory droplets in half of the cases.

As documented in the paper [21], MPXV, a member of the Orthopoxvirus genus, is a zoonotic virus that primarily circulates in central and western Africa and causes smallpox-like disease that can be fatal in up to 15% of affected human beings. After the smallpox vaccine discontinuation in 1980, human MPXV infection rates have risen sharply in the Democratic Republic of the Congo, with reported rates as much as 20 times higher. This is evident in the recent Mpox virus, where the most significant chunk of the cases were recorded in areas that were not endemic to the virus. Specificity of epidemiologic reporting is essential since an antibody response to vaccination with OPXV and recent OPXV or MPXV infection is unlikely to be distinguishable due to protein conservation. To this end, a peptide fiction was formulated based on MPXV-specific peptides sequenced for exposure detection to increase the sensitivity and propriety of the testifying antibodies. A comparative immunogenic protein analysis found that an array of proteins specific to OPXV can be spotted in MPXV. To assess the performance of these peptides, cross-sectional ELISA against confirmed Mpox outbreak sera, vaccinee sera, and smallpox sera obtained before eradication was conducted. Compared to sympathectomy, the peptide combination had ~86% sensitivity and ~90% specificity; moreover, the assay was validated in a serosurvey by testing specimens collected from a region in Ghana linked to MPXV-infected rodents imported into the United States in 2003.

Monkeypox has been recognized in the studies detailed in [22] as a zoonotic emerging viral disease, similar to smallpox but less severe in most cases. In addition to recent concerns related to COVID-19, Monkeypox is an additional threat. This article introduces a new mathematical model for simulations and considerations of several epidemic parameters and provides optimal approaches for controlling the current epidemic. An issue of central interest pertains to the viral load in the environment about disease spread. The model first includes constant control measures and then examines fundamental mathematical characteristics, including equilibrium, stability, and reproductive number. Model parameters are then estimated with identified reported monkeypox cases in the USA during the 2022 outbreak, applying the nonlinear least squares method. The sensitivity analysis is normalized, formulating an optimal control problem with six control variables. Computer simulation shows that the combined use of all the identified measures is an optimal approach to limiting the spread of the Infection. The authors of these studies expect that these findings might help control the future occurrence of Monkeypox.

To the best of our knowledge [23], Monkeypox (MPX) is a newly identified infectious disease, and different strategies have been discussed in the literature to model the pattern of spread and propose control interventions. This paper concerns the MPX dynamics and appropriate interventions by evaluating the optimal interventions using a new epidemic model. This is done by considering both constant and time-dependent control measures with parameters estimated from actual MPX cases during the 2022 outbreak in the USA. Nonlinear least squares are

then used to parameterize the model, and a detailed sensitivity analysis is then conducted on the thus-derived model. Sensitivity indices are then used to algorithmically alter the model for four time-dependent control variables to be included. Optimization, in this case, is done under Pontryagin's maximum principle. The effectiveness of four types of control: single, couple, triple, and quadruple interventions is explored. The findings shown in the present study reveal that the use of the quadruple intervention, whereby all the control measures are implemented in unison, offers the best chances of controlling MPX in the general populace.

In the study mentioned earlier, the repellent [24] human monkeypox cases have increased recently as the world bounces back from the COVID-19 pandemic. Due to the nature of the symptoms, one needs to predict and accurately diagnose Monkeypox from chickenpox or measles. Here, the authors present a new deep learning-based method of predicting human Monkeypox based on image analysis. The data is gathered from the Monkeypox Skin Lesion Dataset, and then image manipulation techniques are applied, including resizing, normalization, and data expansion. In this case, the CBAM is used for feature extraction because it effectively combines channel and spatial attention. At the same time, the MRBM performs the final prediction because incorporating E.O. into the RBM enhances its capacity for minimizing error. Performance enhancement of the proposed MRBM-EO model is evident, with 43.75% better RMSE and 10.90% higher accuracy against the tested models such as PSO-SVM, Xception-CBAM-Dense, ShuffleNet, and RBM.

As explained in the methods section of this paper [25], the authors present and mathematically study a compartmental model describing monkeypox dynamics with quarantine and isolation measures. The proposed model is a 7-dimensional system of ordinary differential equations for how Monkeypox spreads between humans and rodents. The positivity and boundedness of the solutions are used to prove that the model is mathematically well-posed. Applying the next-generation matrix method, the primary reproduction number  $(R_0)$  is obtained and subsequently used to analyze the stability of the monkeypox-free equilibrium. This work also shows that backward bifurcation occurs in the presence of a fraction of quarantined exposed individuals if  $(R_0 < 1)$ , and using center manifold theory, we exclude this bifurcation in some situations. Global attractivity of the monkeypox-free steady state is demonstrated using the Lyapunov function approach; more so, a sensitivity analysis of parameters helpful in designing control measures for Monkeypox is achieved. Simulation results support the importance of quarantine and isolation measures, minimizing the direct contact between people, and interpersonal and interspecific contact with rodents to achieve a monkeypox-free state.

Writing in [26], the authors suggest that this work will involve deep learning strategies, particularly the Convolutional Neural Networks (CNNs) methodology for identifying monkeypox skin lesion patterns that are challenging to distinguish with the naked eye. When the proposed CNN model was optimized with GWO, there was a significant improvement in all quantitative measures, such as accuracy, precision, recall, F1-score, and AUC, compared with the baseline model. The optimized CNN hence got a better accuracy of 95.3%, which showed the model's enhanced ability in training to differentiate the positive and the negative ones. Such an approach may enhance the productivity of the monkeypox diagnostic process and increase diagnostic accuracy, especially in a limited-resource environment, resulting in better patient outcomes. Further, it has the potential to play a significant role in managing monkeypox vectors and, hence, the control of the disease in the general population. The work gives a new, efficient approach to diagnosing Monkeypox, which has excellent possibilities for practical use.

As described in Section [27], this work describes the application of the ML method known as PSO towards the prediction and identification of Monkeypox and other skin diseases through image analysis. To improve the accuracy of monkeypox diagnosis, the current study focuses on exploiting inherent characteristics of PSO, including exploration and exploitation. In addition to Monkeypox, the pictures incorporated in the study are those of chickenpox, smallpox, cowpox, measles, tomato flu, and normal skin. The images were obtained from the International Skin Imaging Collaboration (ISIC) for the experiments. PSOMPX was then compared with four pre-trained deep learning models, VGG16, ResNet50, InceptionV3, and the Ensemble model, using performance metrics of accuracy, precision, recall, and F1 score. The experiments revealed that the developed model, PSOMPX, can better diagnose Monkeypox and other skin diseases than other models.

The Human Monkeypox Detection (HMD) strategy is presented in the current research [28] as an identification protocol to enable the early detection of monkeypox patients. The HMD strategy consists of two primary phases: the first is called the Selection Phase (S.P.), and the second is called the Detection Phase (D.P.). The selection phase utilizes the IBCO algorithm, an enhanced binary chop optimization algorithm, a hybrid filter and a wrapper feature selection model. This phase seeks to determine which monkeypox features are most important in the dataset. When in the Detection Phase, an Ensemble Diagnosis (E.D.) model is developed on the selected features to produce effective and efficient detection. The E.D. model in this study combines three diagnostic WNB, WKNN, and DL

algorithms based on weighted voting. To find the weighted values for WKNN, the Grey Wolf Optimization (GWO) algorithm is applied, whereas, for WNB, weighted values are determined by employing feature impact on classification categories. It was shown that IBCO is better than other feature selection methods, and E.D. is better than the other modern diagnostic tools. The proposed HMD strategy provided excellent performance rates with held-out accuracy and precision of 98.48%, hold-out recall of 91.1%, and micro-average precision and macro-average recall of 88.91%. Also, the strategy gave better implementation time for the results, implying the practical application of the strategy in real diagnostic work.

As described in [29], this work describes Monkeypox's epidemiology, showing the contribution of contaminated surfaces through a deterministic mathematical model. The work starts with basic reproduction numbers and conducts the stability analysis of disease-free and endemic stable states. Consequently, the main analytical results indicate a forward bifurcation at the critical level of the primary reproduction number equal to unity that may reflect a possibility of the disease spread. In particular, backward bifurcation is not observed, which indicates that the primary reproduction number is the only measure of the existence of an endemic state in this model. A detailed description and improvement of the disease transmission and control, as well as a sensitivity analysis of the main parameters influencing the occurrence of Monkeypox, is done. Subsequently, previous work modifies the model into an optimal control problem, enabling the development of intervention methods. The effect of these control measures has been shown through numerical simulations, where contaminated surfaces are described as significantly influencing the transmission process. This work adds a wealth of knowledge to modeling monkeypox infection, particularly advocating for a precise approach in the case of outbreaks. **PUBLIC HEALTH IMPLICATIONS:** The knowledge generated from this work can help develop effective prevention measures to control Monkeypox and other communicable diseases.

To address the research presented in [30], the first increase in monkeypox cases in non-endemic countries in May 2022 for developing a dual-target monkeypox virus test based on adaptations of two previous publications of quantitative PCR assays. These assays have been designed to be compatible with the high-throughput PCR equipment that forms the basis of current SARS-CoV-2 testing. The ability of the test to analyze was also evaluated by the researchers through serial dilutions of quantified monkeypox virus reference material, with the lower threshold being evaluated at 4.795 copies/mL (95% CI 3.6–8.6). Finally, the performance of the assay was compared to an oc2500 commercial manual orthopoxvirus research-use-only PCR kit, thus providing a valid comparison with another reliable PCR assay for detecting orthopoxviruses in clinical swab samples; the percentage concordance obtained was 100% on 11 positive samples and 100% on 56 negative samples. The work also emphasizes the utility of large-capacity and timely PCR testing for monitoring and containment of monkeypox cases, indicating the efficiency of this modified two-target method for large-scale molecular diagnostic.

As described in the paper [31], the present work aims to describe the dynamics of monkeypox infection spread and analyze the results of the mathematical modeling of the outbreak in the USA, which was most affected in 2022. The model under consideration is a nonlinear differential equations model with constant control actions. The human world is divided into four classes, while the animal one is divided into three subclasses. An extensive theoretical review of the model and stability assessment of the equilibrium states are demonstrated. Model parameters are derived based on the historical data on cumulative monkeypox cases in the United States and some demographics from the U.S. population. Thus, the study also analyses the effects of the different parameters on the primary reproduction number ( $R_0$ ) to identify crucial interventions. Using optimization theory, the study identifies the qualitative preventive measures that can reduce the infection rate and benefit health authorities interested in designing efficient measures to prevent the spread of Infection.

The works discussed in the study mentioned [32] studied the relationship of the monkeypox virus to skin lesions and, more specifically, the identification of these lesions during a pandemic. Their approach focuses on improving feature selection and classification algorithms using metaheuristic optimization. For this reason, GoogleNet was deployed for feature extraction, while the Dynamic Binary version of the Al-Biruni earth radius optimization (DBER) algorithm was used for feature selection. After the feature selection, the classification model implemented was the CNN, and the parameters of the CNN were then fine-tuned using the DBERc algorithm. A specificity of 0.990 and sensitivity of 0.994 where other statistics also aced a P-value of 0.908, an R-value of 0.998, and an F1-score of 0.992 were all used to measure performance. The authors also used a combination of feature selection utilizing a filter approach and CNN classification that gave high accuracy for detecting skin lesions caused by Monkeypox with 0.992 accuracy overall.

Table 1 includes a summary of numerous studies. The table also reveals various approaches, such as deep learning, machine learning, and mathematical models that have been adopted to improve the identification and prevention of Monkeypox. Research methods included using transfer learning with Google Net, LSTM frameworks, CNN models, AI-Biruni Earth Radius Optimization, Harris Hawks Optimizer, and Particle Swarm Optimization. Such approaches were applied to datasets comprising dermatoscopic images of the human skin to clinical samples of swabs, and the results showed high values in performance criteria of classification accuracy at the level of 98% or more, increased recall and precision, and decreased error rate. Moreover, mathematical models examined controlling and intervening in the transmission of Monkeypox, particularly in the recent occurrences in 2022, with several models highlighting the importance of quarantine, isolation, and multiple interventions. In summary, the existing literature reveals high success rates in enhancing monkeypox diagnostics and epidemiological management by applying modern computational methods.

**Table 1:** Summary of Literature Review

Study Reference	Key Focus	Methods/Algorithms	Dataset	Results/Performance
[1] A. A. Abdelhamid et al. (2022)	Classification of monkeypox images	GoogleNet for feature extraction, AI-Biruni Earth Radius Optimization for parameter tuning	Public dataset	98.8% classification accuracy
[2] M. M. Eid et al. (2022)	Forecasting monkeypox cases	Enhanced LSTM framework (BER-LSTM) with AI-Biruni Earth Radius optimization	Global Emerging Data on Monkeypox	Mean Bias Error of 0.06, improved prediction accuracy
[3] D. S. Khafaga et al. (2022)	Automated classification of monkeypox images	BER optimization with stochastic fractal search (BERSFS) in deep CNN	African hospital dataset	P<0.05, improved classification accuracy
[4] A. H. Alharbi et al. (2023)	Early diagnosis of Monkeypox	Google for feature extraction, binary dipper-throated optimization (DTO)	Skin lesion dataset	Accuracy of 94.35%, F1-score of 0.92, sensitivity 0.95
[5] A. I. Saleh et al. (2024)	Diagnostic Framework for Monkeypox	Dynamic Recursive Gray Wolf Optimization (DRGW) algorithm	Various datasets using SVM, NB, KNN, and DNN classifiers	Enhanced accuracy, precision, recall, and F-score
[6] A. N. Akkilic et al. (2024)	Transmission Model for Monkeypox	Radial Basis Function with Bayesian regularization optimization in deep neural networks	Human and rodent population data	Model with improved accuracy, regression, and error minimization
[7] M. Harris et al. (2022)	Diagnostic Framework for Monkeypox	Pre-trained CNN models with Harris Hawks Optimizer (HHO)	MSID and MPID datasets	Accuracy: 97.67% (MSID), 97.51% (MPID)
[8] A. K. Mandal et al. (2022)	Predicting emergence and signs of Monkeypox	Machine Learning with Particle Swarm Optimization (PSO) clustering	Global monkeypox case data	Significant improvements in disease prediction
[10] A. Alshehri and S. Ullah (2022)	Mathematical modeling of monkeypox spread	Nonlinear differential equations with constant control measures	USA monkeypox case data (2022)	Effective control of Infection spread using identified interventions

[11] Samreen et al. (2023)	Monkeypox infection control strategies	Nonlinear least squares, Pontryagin's maximum principle	2022 USA outbreak data	Quadruple interventions provided the best control measures
[12] D. Devarajan et al. (2024)	Predicting human Monkeypox	Modified Restricted Boltzmann Machine with Equilibrium Optimizer (MRBM-EO)	Monkeypox Skin Lesion Dataset	10.9% higher accuracy and 43.75% better RMSE against tested models
[13] O. J. Peter et al. (2023)	Monkeypox transmission dynamics	Compartmental model with quarantine and isolation	Human and rodent data	Quarantine and isolation measures are critical for controlling the spread
[14] E. H. I. Eliwa et al. (2023)	Identifying monkeypox lesions	Convolutional Neural Networks (CNN) with Grey Wolf Optimization (GWO)	Monkeypox skin lesion data	Accuracy improved to 95.3%, enhanced diagnostic productivity
[15] A. K. Mandal et al. (2024)	Image-based monkeypox diagnosis	Particle Swarm Optimization (PSO) and digital image analysis	ISIC skin image data	Outperformed VGG16, ResNet50, and InceptionV3 models
[16] A. I. Saleh and A. H. Rabie (2023)	Human monkeypox detection strategy	IBCO (Binary Chimp Optimization) and Ensemble Diagnosis model	Monkeypox datasets	Accuracy: 98.48%, Recall: 91.1%, practical diagnostic application
[17] A. H. Hassan et al. (2024)	Transmission via contaminated surfaces	Deterministic mathematical model with control measures	Contaminated surface data	Sensitivity analysis and control measures reduced transmission
[18] D. Nörz et al. (2022)	High-throughput monkeypox virus detection	Modified dual-target PCR assays	Clinical swab samples	100% accuracy in detecting positive and negative cases
[19] A. Alshehri and S. Ullah (2023)	Monkeypox infection dynamics and prevention	Nonlinear modeling with optimization theory	USA outbreak data (2022)	Qualitative measures identified to reduce infection rates
[20] A. H. Alharbi (2024)	Classification of monkeypox skin lesions	GoogleNet with Dynamic Binary Al-Biruni Earth Radius Optimization	Skin lesion datasets	Accuracy: 99.2%, Sensitivity: 99.4%, F1-score: 0.992

In Conclusion, the examined papers evidence a vast improvement in utilizing sophisticated computational methods, such as machine learning, deep learning, and optimization algorithms, in improving diagnosis, prognosis, and regulation of Monkeypox. Such methods have been immensely helpful in enhancing assessment reliability, forecasting case incidence, and enhancing interventional measures. With synergistic employment of various data sources and the emergence of new algorithms, scientists have recorded high levels of classification rate, improved disease diagnosis, and control of spread, among others. These technologies supplement critical interventions in future public health campaigns, contributing to the containment of Monkeypox and other I.D. outbreaks.

### 3. Conclusion

Monkeypox remains a critical concern because the disease keeps resurging in endemic zones and other new regions, hence requiring better diagnostics and prognosis models. This review highlights the possible application of machine learning (ML), deep learning (DL), and optimization algorithm approaches for early diagnosis and

prognosis of Monkeypox. These devices and techniques facilitate the analysis of clinical and image data, enhancing the throughput for diagnosis compared to conventional methods. The effectiveness of methods such as ML and DL also leads to faster diagnosis and the ability to predict future trends, which is critical in guiding future responses and resource allocation during epidemics.

Combined with prefabricated ML and DL categories, metaheuristic optimization algorithms strengthen the ability to distinguish Monkeypox from similar emerging diseases. This enhancement is extremely important for expanding the diagnostic accuracy of clinical diagnoses and diagnostic tests. Since artificial intelligence is gradually imposed in healthcare facilities, it is impossible to do without these computing methods to quickly identify Monkeypox and other zoonotic diseases.

As such, more subsequent research should focus on improving these algorithms and extending their applicability to other upcoming EIDs. In this way, resource utilization efficiency will be optimized for the health systems of the entire world, and population protection during further pandemics will increase manifold. The development of these technologies also holds promises for the future, not only for immediate public health responses but also to help build a much more responsive system for all new threats in the globalized world.

## References

- [1] J. Otte and U. Pica-Ciamarra, "Emerging infectious zoonotic diseases: The neglected role of food animals," *One Health*, vol. 13, p. 100323, Dec. 2021, doi: 10.1016/J.ONEHLT.2021.100323.
- [2] M. Shafaati and M. Zandi, "State-of-the-art on monkeypox virus: an emerging zoonotic disease," *Infection*, vol. 50, no. 6, pp. 1425–1430, Dec. 2022, doi: 10.1007/S15010-022-01935-3/METRICS.
- [3] S. K. Towfek, N. Khodadadi, L. Abualigah, and F. H. Rizk, "AI in Higher Education: Insights from Student Surveys and Predictive Analytics using PSO-Guided WOA and Linear Regression," *Journal of Artificial Intelligence in Engineering Practice*, vol. 1, no. 1, pp. 1–17, Apr. 2024, doi: 10.21608/JAIEP.2024.354003.
- [4] A. M. Zaki, A. A. Abdelhamid, A. Ibrahim, M. M. Eid, and E. S. M. El-Kenawy, "Enhancing K-Nearest Neighbors Algorithm in Wireless Sensor Networks through Stochastic Fractal Search and Particle Swarm Optimization," *Journal of Cybersecurity and Information Management*, vol. 13, no. 1, pp. 76–84, 2024, doi: 10.54216/JCIM.130108.
- [5] E. Alakunle, U. Moens, G. Nchinda, and M. I. Okeke, "Monkeypox virus in Nigeria: Infection biology, epidemiology, and evolution," *Viruses*, vol. 12, no. 11, Nov. 2020, doi: 10.3390/V12111257.
- [6] "The Importance of the One Health Approach in Tackling Emerging and Re-emerging Zoonotic Epidemics and Pandemics".
- [7] N. Kobayashi, "Impact of Emerging, Re-Emerging and Zoonotic Viral Infectious Diseases, in a Virologist's Perspective," *Open Virol J*, vol. 12, no. 1, pp. 131–133, Sep. 2018, doi: 10.2174/1874357901812010131.
- [8] A. N. Akkilic, Z. Sabir, S. A. Bhat, and H. Bulut, "A radial basis deep neural network process using the Bayesian regularization optimization for the monkeypox transmission model," *Expert Syst Appl*, vol. 235, Jan. 2024, doi: 10.1016/J.ESWA.2023.121257.
- [9] N. Haider et al., "COVID-19—Zoonosis or Emerging Infectious Disease?," *Front Public Health*, vol. 8, p. 596944, Nov. 2020, doi: 10.3389/FPUBH.2020.596944.
- [10] D. S. Khafaga et al., "An AI-Biruni Earth Radius Optimization-Based Deep Convolutional Neural Network for Classifying Monkeypox Disease," *Diagnostics (Basel)*, vol. 12, no. 11, Nov. 2022, doi: 10.3390/DIAGNOSTICS12112892.
- [11] M. Shafaati and M. Zandi, "State-of-the-art on monkeypox virus: an emerging zoonotic disease," *Infection*, vol. 50, no. 6, pp. 1425–1430, Dec. 2022, doi: 10.1007/S15010-022-01935-3.
- [12] D. S. Khafaga et al., "An AI-Biruni Earth Radius Optimization-Based Deep Convolutional Neural Network for Classifying Monkeypox Disease," *Diagnostics*, vol. 12, no. 11, pp. 2892–2892, Nov. 2022, doi: 10.3390/DIAGNOSTICS12112892.
- [13] A. A. Abdelhamid et al., "Classification of Monkeypox Images Based on Transfer Learning and the AI-Biruni Earth Radius Optimization Algorithm," *Mathematics 2022*, Vol. 10, Page 3614, vol. 10, no. 19, p. 3614, Oct. 2022, doi: 10.3390/MATH10193614.
- [14] M. M. Eid et al., "Meta-Heuristic Optimization of LSTM-Based Deep Network for Boosting the Prediction of Monkeypox Cases," *Mathematics 2022*, Vol. 10, Page 3845, vol. 10, no. 20, p. 3845, Oct. 2022, doi: 10.3390/MATH10203845.

- [15] D. S. Khafaga et al., "An Al-Biruni Earth Radius Optimization-Based Deep Convolutional Neural Network for Classifying Monkeypox Disease," *Diagnostics* 2022, Vol. 12, Page 2892, vol. 12, no. 11, p. 2892, Nov. 2022, doi: 10.3390/DIAGNOSTICS12112892.
- [16] A. H. Alharbi et al., "Diagnosis of Monkeypox Disease Using Transfer Learning and Binary Advanced Dipper Throated Optimization Algorithm," *Biomimetics* 2023, Vol. 8, Page 313, vol. 8, no. 3, p. 313, Jul. 2023, doi: 10.3390/BIOMIMETICS8030313.
- [17] A. I. Saleh and S. A. Hussien, "Monkeypox diagnosis based on Dynamic Recursive Gray wolf (DRGW) optimization," *Biomed Signal Process Control*, vol. 87, p. 105483, Jan. 2024, doi: 10.1016/J.BSPC.2023.105483.
- [18] A. N. Akkiliç, Z. Sabir, S. A. Bhat, and H. Bulut, "A radial basis deep neural network process using the Bayesian regularization optimization for the monkeypox transmission model," *Expert Syst Appl*, vol. 235, p. 121257, Jan. 2024, doi: 10.1016/J.ESWA.2023.121257.
- [19] M. Harris Hawks Optimizer Algorithm Electronics and S. Ateeq Almutairi, "DL-MDF-OH2: Optimized Deep Learning-Based Monkeypox Diagnostic Framework Using the Metaheuristic Harris Hawks Optimizer Algorithm," *Electronics* 2022, Vol. 11, Page 4077, vol. 11, no. 24, p. 4077, Dec. 2022, doi: 10.3390/ELECTRONICS11244077.
- [20] A. K. Mandal, P. K. D. Sarma, and S. Dehuri, "Machine Learning Approaches and Particle Swarm Optimization Based Clustering for the Human Monkeypox Viruses: A Study," *Communications in Computer and Information Science*, vol. 1737 CCIS, pp. 313–332, 2022, doi: 10.1007/978-3-031-23233-6\_24/TABLES/5.
- [21] T. Y. Taha et al., "Design and Optimization of a Monkeypox virus Specific Serological Assay," *Pathogens*, vol. 12, no. 3, p. 396, Mar. 2023, doi: 10.3390/PATHOGENS12030396/S1.
- [22] A. Alshehri and S. Ullah, "Optimal control analysis of Monkeypox disease with the impact of environmental transmission," 2022, doi: 10.3934/math.2023865.
- [23] Samreen, S. Ullah, R. Nawaz, and A. Alshehri, "Mathematical modeling of monkeypox infection with optimized preventive control analysis: a case study with 2022 outbreak," *The European Physical Journal Plus* 2023 138:8, vol. 138, no. 8, pp. 1–34, Aug. 2023, doi: 10.1140/EPJP/S13360-023-04305-6.
- [24] D. Devarajan, P. Dhana lakshmi, S. Krishnaveni, and S. Senthilkumar, "Human monkeypox disease prediction using novel modified restricted Boltzmann machine-based equilibrium optimizer," *Scientific Reports* 2024 14:1, vol. 14, no. 1, pp. 1–20, Jul. 2024, doi: 10.1038/s41598-024-68836-3.
- [25] O. J. Peter, A. Abidemi, M. M. Ojo, and T. A. Ayoola, "Mathematical model and analysis of monkeypox with control strategies," *The European Physical Journal Plus* 2023 138:3, vol. 138, no. 3, pp. 1–20, Mar. 2023, doi: 10.1140/EPJP/S13360-023-03865-X.
- [26] E. H. I. Eliwa, A. M. El Koshiry, T. Abd El-Hafeez, and H. M. Farghaly, "Utilizing convolutional neural networks to classify monkeypox skin lesions," *Scientific Reports* 2023 13:1, vol. 13, no. 1, pp. 1–20, Sep. 2023, doi: 10.1038/s41598-023-41545-z.
- [27] A. K. Mandal, P. Kumar, and D. Sarma, "USAGE OF PARTICLE SWARM OPTIMIZATION IN DIGITAL IMAGES SELECTION FOR MONKEYPOX VIRUS PREDICTION AND DIAGNOSIS," *Malaysian Journal of Computer Science*, vol. 37, no. 2, pp. 124–138, Apr. 2024, doi: 10.22452/MJCS.VOL37NO2.2.
- [28] A. I. Saleh and A. H. Rabie, "Human monkeypox diagnose (HMD) strategy based on data mining and artificial intelligence techniques," *Comput Biol Med*, vol. 152, p. 106383, Jan. 2023, doi: 10.1016/J.COMPBIOMED.2022.106383.
- [29] A. H. Hassan, D. Aldila, and M. H. Noor Aziz, "Optimal control and stability analysis of monkeypox transmission dynamics with the impact of contaminated surfaces," *Front Appl Math Stat*, vol. 10, p. 1372579, Mar. 2024, doi: 10.3389/FAMS.2024.1372579/BIBTEX.
- [30] D. Nörz et al., "Rapid Adaptation of Established High-Throughput Molecular Testing Infrastructure for Monkeypox Virus Detection," *Emerg Infect Dis*, vol. 28, no. 9, p. 1765, Sep. 2022, doi: 10.3201/EID2809.220917.
- [31] A. Alshehri and S. Ullah, "Mathematical analysis of monkeypox infection with optimal control analysis: A case study with a new outbreak in the United States," *Math Methods Appl Sci*, 2023, doi: 10.1002/MMA.9505.
- [32] A. H. Alharbi, "Classification of monkeypox images using Al-Biruni earth radius optimization with deep convolutional neural network," *AIP Adv*, vol. 14, no. 6, p. 65133, Jun. 2024, doi: 10.1063/5.0213963/3299108.