

Artificial Intelligence in Biological Sciences

Subjects: Biophysics

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Artificial intelligence (AI), currently a cutting-edge concept, has the potential to improve the quality of life of human beings. The fields of AI and biological research are becoming more intertwined, and methods for extracting and applying the information stored in live organisms are constantly being refined. As the field of AI matures with more trained algorithms, the potential of its application in epidemiology, the study of host–pathogen interactions and drug designing widens. AI is now being applied in several fields of drug discovery, customized medicine, gene editing, radiography, image processing and medication management. More precise diagnosis and cost-effective treatment will be possible in the near future due to the application of AI-based technologies. In the field of agriculture, farmers have reduced waste, increased output and decreased the amount of time it takes to bring their goods to market due to the application of advanced AI-based approaches. Moreover, with the use of AI through machine learning (ML) and deep-learning-based smart programs, one can modify the metabolic pathways of living systems to obtain the best possible outputs with the minimal inputs. Such efforts can improve the industrial strains of microbial species to maximize the yield in the bio-based industrial setup.

Keywords: artificial intelligence ; biotechnology ; agriculture

1. Artificial Intelligence (AI) in Medical Science

Medical science and biotechnology advancements have opened new avenues for developing medications and antibiotics. AI has enormous potential for widespread applications in the pharmaceutical industry. With AI, novel therapeutic molecules based on known target structures can be discovered ^[1]. A branch of AI known as ML is commonly employed in disease diagnosis since it leverages the outcomes of diagnostic testing to improve the accuracy of results ^[2]. AI allows researchers to manage challenging issues, including quantitative and predictive epidemiology, precision-based medicines and host–pathogen interactions ^[3]. AI can help in disease detection and diagnosis and make computer code more accessible to non-technical individuals ^[4]. Predictive epidemiology, individual-based precision medicine and the analysis of host–pathogen interactions are examples of research areas that could benefit from machine and deep learning breakthroughs ^[5]. These approaches aid with disease diagnosis and individual case identification, more accurate forecasts and fewer mistakes, faster decision making and better risk analysis. The growing number of tissue biomarkers and the complexity of their evaluations significantly promote the use of AI-based techniques. These AI-based biomarkers help physicians in the prediction and analysis of the diagnosis, patient responses to the treatment and patient survival ^[6]. More realistic models of complex socio-biological systems are achievable because of knowledge representation and reasoning modelling ^[7]. ML-based methods can also be used to improve the efficiency and reliability of epidemiological models ^{[8][9]}. ML advances helped develop ten cellular parameters algorithmic program-based models that can accurately distinguish benign from malignant tumors ^[10].

It is important to take into account individual differences in genetics, ecology and lifestyle in precision medicine ^[11]. Medical practitioners recognize that the metabolic, physical, physiological and genetic makeup of an individual affects how their body responds to drugs in a certain way. Despite this, researchers are currently employing an umbrella approach that treats all patients, regardless of their varying conditions, with the same drug. However, due in large part to advances in AI, a new era of personalized medicine, in which pharmaceuticals are tailored to the body's needs and adaptability, is evolving. Although the transition appears to be simple, it entails a significant amount of data collection, processing, maintenance and execution ^[12]. Moreover, millions of prediction analyses will be included in the process to identify the best therapeutic candidate molecules for a particular case. Using this strategy, physicians and clinicians may better predict which disease treatment and preventative strategies will be most effective for particular patient groups. Researchers could use AI in DNA, RNA and protein studies to better visualize the effects of drug doses on living tissue over time and reorganize signaling networks during therapy ^{[13][14]}. Based on AI, IBM Watson assists in the creation of the appropriate treatment plan for a patient depending on the patient's medical history and personal data, including genetic makeup ^[15]. An AI-based system of personalized medicine will not only reduce treatment cost but also minimize the side effects of drugs in the patient ^[16]. In addition to saving time and improving patient care, AI can also simplify gene editing,

radiography and drug management planning procedure ^[17]. Furthermore, electronic health records (EHRs) can be improved with evidence-based clinical decision support systems ^{[11][18][19]}. AI involves massive processing capacity (supercomputers), algorithms that can learn at a phenomenal rate (deep learning) and a new strategy that utilizes physicians' cognitive talents. This technique can contribute to the development of innovative theoretical models of disease pathophysiology and can help forecast major adverse effects of prolonged medications ^[20]. In a recent study, an AI-based approach was found to be very beneficial for the early identification, diagnosis, prognosis and treatment of myopia ^[21]. In cardiology, dermatology and oncology, deep learning algorithms outperform physicians at least in the diagnosis of disease ^{[22][23][24]}. Evidently, computer algorithms can detect metastatic breast cancer in sentinel lymph node biopsies in full slide images with an accuracy rate of more than 91 percent, and this was raised to 99.5 percent when physician inputs were added ^[25]. One of the proven applications of AI in risk analysis is for diagnosing heart malfunctioning through cardiovascular imaging. It includes automated monitoring of any deviations from normal conditions based on image processing, myocardial function and the detection and analysis of coronary atherosclerotic plaques ^[26]. The YOLOV3 algorithm was used for AI-based medical image segmentation for 3D printing and naked eye 3D visualization to detect the prostate in T2-weighted MRI images (AIMIS3D) ^[26]. There are several variables that might be efficiently analyzed through AI, such as determining which conditions are resistant to certain antibiotics and not to others ^[27]. Such analysis can support physicians and significantly decrease unnecessary testing and costs in medical care.

It is important to underline the importance of combining these algorithms with medical expertise. New pharmaceutical compounds can be discovered via data analysis using AI, which reduces the need for clinical trials, allowing medications to be brought to market more quickly without compromising their safety ^[28]. Moreover, researchers may be able to forecast the onset of genetically predisposed diseases considerably earlier with the help of AI ^[17]. Patients will also be able to prevent and treat certain inherited diseases.

One of the applications of AI in the pharmaceutical industry is "Open Targets", which is a relatively new strategic effort to explore the relationship between drug targets and diseases, as well as how certain genes are linked to diseases ^[29]. SPIDER is another AI technique that is being designed to determine the role of natural products in drug discovery ^[30]. Furthermore, quantitative structure–activity relationship (QSAR) studies are particularly useful in creating novel effective medications in a very short period of time using a computer simulation tool ^[31]. A QSAR model based on a radial basis function (RBF) artificial neural network (ANN) model that was trained using particle swarm optimization (PSO) technique was used in a recent study to predict the pKa values of 74 different types of drugs ^[31]. Natural language processing (NLP), ML, and robotic process automation are clearly the three key areas of advancement for AI in the field of medicine ^{[32][33]}. Natural Language Processing has recently been used to enhance colonoscopy analysis, improving accurate detection of adenoma and polyps ^[34]. Additionally, an ML approach may be used to predict diseases such as atrial fibrillation and urinary tract infections in certain patient groups by using models such as support vector machine (SVM) based on clinical features of the disease ^{[35][36][37]}. Similar initiatives have been utilized to improve heart disease prognosis using a heart-murmur-detecting technology ^[38]. The FDA has already approved up to 29 AI-based medical devices and algorithms in various fields of medical sciences ^[39].

The first AI-based model approved by the FDA in the healthcare sector was a diagnostic model based on an autonomous AI system, IDx-DR. This model was successfully used in to detect diabetic retinopathy with sensitivity, specificity and imageability of 87.2%, 90.7% and 96.1%, respectively, in a sample size of 819 subjects over 10 primary care units in the United States. The model was trained with a diversified sample dataset consisting of individuals of different ages, races and sex, thus minimizing the chances of errors in different groups ^[40]. Several randomized clinical trials (RCTs) have also been performed to test the efficacy and safety of AI and ML models in clinical practice. In an RCT (Registration number: ChiCTR-DDD-17012221), the impact of a deep-learning-based automated polyp identification algorithm on polyp detection accuracy and adenoma detection rates (ADRs) was evaluated. In this RCT, successive patients were randomly assigned to go through colonoscopy either with or without the help of the automated polyp identification model that provided a simultaneous optical notification and sound alert upon polyp discovery. Results obtained from patients who have undergone the automated AI-based detection system outperformed the control cohorts of ADR and the average amount of adenoma and polyps detected per coloscopy. This automated technology can thus be pertinent in treatment regimens and routine practices for improved identification of colon polyps due to its great sensitivity, high precision and stable outcomes ^[41]. The introduction of AI systems in medical decision making has also resulted in the cost-effectiveness of complete medical treatment. In a study, the use of a procalcitonin-based decision algorithm (PCTDA) for hospitalized sepsis and lower respiratory tract infection patients led to a shortened duration of stay, lowered antibiotic administration, lesser artificial ventilation periods and decreased number of patients with infections and antibiotic resistance. On average, PCTDA-based treatment brought about a 49% and 23% decrease in overall expenses from conventional treatment for sepsis and lower respiratory tract infections, respectively ^[42]. The pharmaceutical industry will better grasp genetic information with improved AI and ML skills. Evidently, when integrated with ML and NLP, robotic process automation has

significant applications and has the potential to reshape medical science in the near future ^[43]. Despite the tremendous advancements researchers have observed, there is still a lot of work to be done before AI-based therapy becomes a reality.

2. AI in Agricultural Biotechnology

Face recognition ^[44], cancer prediction in tissue ^[45] and metabolic flux analysis ^[46] are just a few examples of significant advances made with AI approaches, and there is a potential to achieve a similar revolution in the agricultural field. According to a report published by the United Nations' Food and Agriculture Organization (FAO), the world's population will reach more than 9 billion by 2050 ^[47]. Population expansion will eventually put a strain on the agriculture sector's ability to provide food. In order to feed the world's growing population and advance the nation's economy, agriculture is essential ^[48]. It is a significant source of revenue for a number of countries, including India.

Agriculture occupies around 38% of the planet's total land surface ^[47]. The majority of agricultural activities are now manual, and agriculture may significantly benefit from automation in terms of obtained yield and invested inputs. The implementation of technological breakthroughs in agriculture may contribute to the change in rural economies and villagers' livelihoods ^{[49][50]}. Agricultural techniques are generally designed to overcome a variety of obstacles, including pest infestation, inefficient use of pesticides and fertilizers, weeds, drought and a lack of an adequate irrigation system, inefficient harvesting, storage and finally marketing. The agricultural sector could be transformed by AI intervention in the areas of soil management, water requirement assessment, precise mapping of fertilizer need, pesticide, insecticide, herbicide need, yield prediction and overall crop management ^{[51][52][53]}. With the advancement of AI-based technology, drones and robots are being used to improve real-time monitoring of crops, harvesting and subsequent processing ^[54]. AI and ML techniques are currently being used by biotechnology companies to design and train autonomous robots capable of performing key agricultural activities such as crop harvesting at a much faster rate than traditional methods ^[51]. The data collected by drones are processed and evaluated using deep learning and computer vision techniques ^[55]. Machine learning approaches assist in the access and forecast of a wide range of environmental variables that influence agricultural output, such as weather fluctuations and the arrival of the monsoon in India ^{[51][56][57]}. As mentioned elsewhere, AI-based solutions in the agricultural industry help to improve efficiency and control numerous aspects such as crop yield, soil profile, crop irrigation, content sensing, weeding and crop monitoring ^{[51][58]}.

Traditional and older morphological characteristic inspection is time-consuming, error-prone and costly. The machine vision method might be easily applied in agricultural practices, which can speed up and simplify the procedure while being more precise and accurate ^[55]. Identification and selection of improved varieties may speed up and make the process easier by using automated non-invasive, rapid scoring of various plant features through high-throughput phenotyping methods ^[59]. Due to the tools of AI and IoT, swarm intelligence and drone technology can now be employed for several agricultural activities ^[60]. Recent developments in DL- and ML-based algorithm design to estimate the price of agricultural products may enable farmers to receive a higher return on their labor and investment ^[61]. For effective irrigation, artificial neural networks, fuzzy logic and meta-heuristic algorithms have recently been developed ^{[62][63]}. According to a recent study, convolutional neural network (CNN), which takes into account several environmental variables, is one of the most trustworthy ML algorithms to estimate soybean and maize yields ^[64]. Recent advances in AI-based biosensors for early disease detection in crop plants, even in asymptomatic plants, have the potential to greatly minimize product loss caused by biotic stressors ^[65]. AI-based drone technologies such as EfficientNetV2, which are designed to detect and classify plant diseases with accuracy and precision of 99.99% and 99.63%, respectively, are one of the promising automated technologies for the monitoring of plant health in a time-saving and cost-effective manner ^[66]. For the detection of bacterial spot disease in plants, a hybrid AI model based on convolutional autoencoder (CAE) and CNN has also achieved 99.35% and 99.38% in the training and testing periods, respectively, ^[67].

The use of AI may make it simpler to identify potential targets in big genome data for genetic manipulation and design effective synthetic promoters in efforts to improve agronomic traits in plants ^{[68][69]}. The growing necessities for smart agriculture have resulted in substantial advancements in the area of AI-based agricultural forecasting and prediction, which has improved crop productivity to a great extent ^[55]. A similar attempt was made in a recent study where image datasets were analyzed by employing AI algorithms, namely ANN and genetic algorithm (GA)-based platforms, for the prediction of crop yield in an optimized manner ^[70]. During the training period, the model obtained a maximum validation accuracy of 98.19%, whereas a maximum accuracy of 97.75% was yielded during the test period ^[70]. This model worked effectively under limited resource restrictions and less data, producing optimal results ^[70]. In another significant study, a new methodology for predicting agricultural yield in greenhouse crops employing recurrent neural network (RNN) and temporal convolutional network (TCN) algorithms was proposed ^[71]. Based on previous environmental and production

data, this approach can be utilized to estimate greenhouse crop yields more accurately than its standard ML and deep learning peers [71].

Furthermore, this experimental investigation has also demonstrated the crucial importance of previous yield datasets in correctly predicting future crop productivity [71][72]. Several million individuals in developing nations have benefited from the green revolution by preventing and combining high-yield crops, synthetic fertilizers and water. However, owing to widespread misuse of herbicides, pesticides and fertilizers, the green revolution could not be considered fully “green”. Certain approaches for high-yielding crops typically need a large amount of agro-chemicals and water [73]. AI-based approaches are being developed to reduce the reliance on noxious agro-chemicals and to attain a state of sustainability in agriculture [41]. For optimizing agricultural resources, a remote sensing assisted control system (RSCS) has been developed [74]. This methodology makes use of AL and ML technology to improve environmental sustainability while fostering novel agricultural product development planning. When analyzed with other techniques, the findings revealed that the RSCS demonstrated the highest precision, performance, data transfer rate, productivity, irrigation management and carbon dioxide release ratio of 95.1, 96.35, 92.3, 94.2, 94.7 and 21.5%, respectively, [74]. Thus, AI models have the potential to manage agricultural products and productivity in a “green” manner. In another study, an AI and machine vision-based smart sprayer was developed to spray herbicides specifically to weed targets, thus reducing weedicide overuse and environmental contamination. This sophisticated technology combined a cutting-edge weed detection concept, a unique rapid and precise spraying method and a weed mapping model with 71% and 78% precision and recall, respectively, [75]. Due to limited collecting techniques and a lack of integration of diverse data sources, data gathering from agricultural regions linked to soil hydration, crop quality or insect infestations frequently depend on manual analysis.

Meanwhile, as the industry becomes more digital, the combination of remote sensing for computerized screening and analytical techniques with datasets for soil studies, weather predictions, etc., and sophisticated AI models is reducing the need for agrochemicals [55]. In this regard, the substantial NaLamKI action plan that seeks to create AI-based open access software that could greatly help the agricultural industry has received funding from the German government. This plan seeks to develop datasets by combining information from different sensors in order to optimize different farming practices with the help of AI and ML technologies [55][76]. Similar governmental initiatives are required in large numbers to make farmers adapt AI on a greater scale.

In agriculture, integrating precise image-based features with omics data may aid in finding critical traits involved in stress tolerance and acclimatization mechanisms [77], as well as contribute to the development of climate-resilient crops. Farmers will be able to generate more output with less input, increase the quality of their output and ensure a faster time to market for their harvested crops owing to AI-based technology adaptation [55]. Although first-generation AI can be employed in the surveyance and classification of omics data, it is tailored for the handling of specific problems related to single-omics datasets without integrating data from other modalities [55][78]. In agricultural biotechnology, next-generation AI is fundamentally envisioned to dynamically ameliorate and handle large multi-omics datasets in addition to predicting the breeding value of complex traits across different environmental conditions [78].

3. AI and Industrial Biotechnology

Industrial biotechnology, sometimes known as white biotechnology, is the modern application of biotechnology to the sustainable processing and manufacturing of commodities, chemicals and fuels from renewable sources using live cells and their enzymes. The demand for industrial chemicals, medicines, food-grade chemicals and other biochemistry-related raw materials has increased dramatically over the previous decade [79]. ML and AI-based technologies may aid in the design of novel pharmaceuticals and the identification of their efficacy and adverse effects before their actual production, drastically reducing the time spent bringing a drug from the lab to the market for ordinary people [28]. Microorganisms and plant/animal cells are used in biotechnological processing to make products in a variety of sectors, including drugs, pharmaceuticals, food and feed, disinfectants, pulp and textiles. In order to detect outages, optimize machinery for efficient manufacture and improve product quality, the Internet of things, ML and AI could be used effectively [80]. AI-based computer models are becoming increasingly widespread, and robotics and machine learning could be used to develop the best optimum growth conditions for the strains, as well as the degree to which valuable products can be obtained. For instance, AI or response surface methodologies (RSM) -based approaches have been used in the high-level production of amylases from *Rhizopus microsporous*, using various agro-industrial wastes for optimal experimentation designs [81]. Similarly, AI algorithms such as artificial neural networks (ANN) and genetic algorithms (GA) have been integrated for the optimization of fermentation media to produce glucansucrase from *Leuconostoc dextranicum*. A 6% rise in glucansucrase activity was predicted by the integrated ANN-GA model over a regression-based prediction approach [82]. The application of the integrated ANN-GA model for the optimization of cellulase production by *Trichoderma stromaticum* under solid-state

fermentation has been reported recently, and a 31.58-fold increase in cellulase production was achieved after optimization with the AI model [83].

AI-based technologies have also been used to scale up and optimize bioprocesses for enzyme production on pilot scales. A low-cost method for increasing the synthesis of extracellular laccase from *Staphylococcus arlettae* utilizing tea waste was performed in a study. RSM and ANN coupled with GA were two consecutive statistical methods that were employed to increase enzyme production and resulted in a sixteen-times rise in enzyme yield. Moreover, a pilot scale bioprocess was established utilizing the ideal parameters identified by GA, namely tea waste (2.5%) NaCl (4.95 mM), L-DOPA (5.65 mM) and 37°C temperature, which improved the enzyme production by 72 times [84]. Furthermore, some AI models based on the fuzzy expert system are also capable of monitoring wastewater treatment plants on a pilot scale [85].

Biofuel is one of the most important bioproducts for which the industrial production process can be enhanced using ML and AI for maximum output. In the bioenergy sector, AI-based approaches have been used to predict biomass feedstock properties, bioenergy end-uses, and bioenergy supply chains and have developed an integrated ANN-Taguchi method model for the prediction and maximization of biofuel production via torrefaction and pyrolysis [86][87]. Optimization and design of experimental factors were performed using the Taguchi method which led to the attainment of maximum biofuel yield up to 99.42%, whereas ANN showed linear regression prediction of 0.9999 for biochar and 0.9998 for bio-oils.

Integrated ANN-GA models have been used in the modeling and optimization of the methanolysis process of waste peanut shells for the generation of biofuels. Biofuel yield optimized by the RSM model was 16.49%, whereas that of the ANN-GA model was reported to be 17.61%. This shows that integrated ANN-GA has better optimization potential than the RSM model alone [88]. ML-based bioprocess models have also been constructed with the help of AI-based methods such as ANN, CNN, (long short-term memory networks) LSTMs, kNNs (k-nearest neighbors) and RF (random forests) for predicting the accumulation of carbohydrates in cyanobacteria biomass cultivated in wastewater for biofuel production. The finest results for approximation of system dynamics were achieved with a 1D-CNN with a mean square error of 0.0028 [89]. Textiles, new chemicals and biodegradable biopolymer synthesis could all benefit from similar processes [90]. Furthermore, it may be used to assist in the development of synthesis techniques for such biochemicals that produce the highest yield with the least amount of input. Additionally, AI could assist in real-time forecasting of market demand for medications or chemicals. AI and ML have also helped in the production of metabolites. Systems metabolic engineering is a process that helps in the rapid production of high-performing microbial strains for the long-term production of chemicals and minerals. The increasing availability of bio big data, such as omics data, has resulted in an application for ML techniques across various stages of systems metabolic engineering, such as host strain selection, metabolic pathway reconstruction, metabolic flux optimization and fermentation [91]. Various machine learning algorithms, including deep learning, have facilitated in optimizing the bioprocess parameters and exploring a larger metabolic space that is linked to the biosynthesis of a target bioproduct [92]. This trend is also influencing biotechnology businesses to adopt ML techniques more frequently in the creation of their production systems and platform technologies [93]. In the brewery industry, AI has demonstrated promising potential to overcome fundamental shortcomings and enhance production through knowledge accumulation and automated control. In a study, AI models were constructed using aroma profiles and spectroscopic data obtained from commercial alcohol for assessing the quality traits and aroma of beer. The intelligent models resulted in highly accurate predictions for six major beer aromas [94]. Smart e-nose technologies based on ANN models have also been developed to assess the presence of different chemicals such as ethanol, methane, carbon monoxide, hydrogen sulfide, ammonia, and so forth in beer [95]. A study was involved in the development of a computer program that simulated the operation of a highly customizable three-layer feed-forward multilayer perception neural network, which using data from prior experiments, could forecast changes in the parameters of white wine alcoholic fermentation. This provided a befitting approach for the digitalization of brewing processes, thus enabling it to be acclimatized to other intelligent and knowledge-based frameworks [96]. Another study led to the development of an innovative knowledge-based approach for controlling the batch fermentation of alcohol employed in making white wine. The primary sources of information used in developing the AI model were different case studies and experimental results, as well as the knowledge obtained from brewery experts regarding different parameters related to optimization and control of the overall process. Using the monitoring, regulation and data acquisition software of the fermentation bioreactor, an application for automated process control was developed [97]. The further incorporation of control systems, processes and innovative advancements can be greatly facilitated by such kinds of AI models, thus supporting sustainable development.

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