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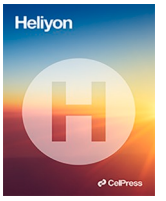

Review article

Systematic approaches to machine learning models for predicting pesticide toxicity

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ABSTRACT

Pesticides play an important role in modern agriculture by protecting crops from pests and diseases. However, the negative consequences of pesticides, such as environmental contamination and adverse effects on human and ecological health, underscore the importance of accurate toxicity predictions. To address this issue, artificial intelligence models have emerged as valuable methods for predicting the toxicity of organic compounds. In this review article, we explore the application of machine learning (ML) for pesticide toxicity prediction. This review provides a detailed summary of recent developments, prediction models, and datasets used for pesticide toxicity prediction. In this analysis, we compared the results of several algorithms that predict the harmfulness of various classes of pesticides. Furthermore, this review article identified emerging trends and areas for future direction, showcasing the transformative potential of machine learning in promoting safer pesticide usage and sustainable agriculture.

1. Introduction

Over hundreds of years, agriculture has been vital to the growth and prosperity of every civilization. Agricultural operations affect people's ability to meet their dietary needs for healthy energy sources. The agricultural applications are shown in Fig. 1 [1–3]. Plant protection focuses [4,5] on promoting integrated pest management, ensuring that high-quality pesticides are readily available to protect crops from pests and diseases [6], and simplifying quarantine procedures so that innovative, high-yielding processes can be implemented more quickly. Furthermore, pesticide use may have unintended consequences on human health and the environment. Acute intoxication can occur owing to the incorrect use of certain pesticides; in certain circumstances, serious health effects can result from prolonged to minimal risk [7–12].

In agriculture, pesticides are chemical substances used to eradicate, remove, or suppress parasites and bacteria [13–16]. Pesticides are frequently classified according to the organisms in which they act [17]. Pesticides are classified into three major categories: herbicides, insecticides, and fungicides Fig. 2 [14]. There are also multiple subdivisions for each class, each with significantly different toxicological [18–20] and chemical characteristics from the others [14].

Pesticides are the most commonly used pesticides in agriculture, accounting for 75% of total pesticide use [21–25]. Some commonly used commercial pesticides are shown in Fig. 3.

However, pesticides are highly beneficial to plant growth and protection. However, pesticides can have adverse effects on the

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environment because of their toxicity [26–29]. Humans are usually exposed to pesticides and their residues in food and drinking water. Constant exposure to pesticides poses a threat to human health, as these chemicals have been found to be toxic. Exposure to pesticides can lead to various health issues in the reproductive system, fetal development, and an increased risk of cancer and asthma [7,11,25, 30]. Moreover, the accumulation and persistence of pesticides in the environment makes them a chronic threat to human health [30–32].

Modern computer science has prioritized the development of artificial intelligence (AI). AI is growing rapidly because it can address problems that humans and conventional computing systems cannot [33–36]. Approximately 30.7% of the world's agricultural land is used for farming [37]. There are several challenges from planting to harvesting. Pest and disease infestation, inadequate chemical application, poor drainage and irrigation, weed management, and yield estimation are major issues [1,35]. From 2020 to 2026, agricultural AI spending is expected to increase by 25.5% [38]. AI may change how agri-firms compete in the food supply chain [39, 40]. Planned initiatives to promote technology and inspire businesses and farmers to exploit the benefits of AI will anticipate greater production levels, reduced pesticide use, and lower environmental impact [1,37]. AI will solve society's biggest issues [41], such as the need to generate more while reducing environmental damage and the labor crisis. Precision agriculture and smart farming can employ AI to help farmers produce more food and advance their industries [33].

ML can be used to predict the toxicity of pesticides and assess their potential risk to human health [28,42–44]. These methods can analyze a wide range of data, such as chemical properties and molecular structures, to identify the patterns and relationships between pesticides and their toxicity levels. Using ML, researchers can create predictive models to accurate pesticide toxicity and identify high-risk chemicals [45–48]. In this review, we investigated the ML approach for predicting pesticide toxicity.

2. Methods

2.1. Screening of articles using search engine

We searched the literature describing pesticide predictions. We used the Scopus search engine. To mitigate redundancy, we conducted a comprehensive search of systematic reviews and meta-analyses of pesticide toxicity. To gain insight into the present extent of the issue, a comprehensive examination of papers published from 2014 to 2023 was conducted. The search terms employed to locate relevant studies were "pesticide toxicity predictions ". The primary author, Anandhi, and the corresponding author, Iyapparaja, conducted individual searches for relevant papers. Any discrepancies in their findings were handled through conversation, and data extraction was performed using Microsoft Excel.

2.2. Query for study

- To what extent is pesticide toxic?
- How can pesticide toxicity be predicted?
- Which algorithm is best for predicting pesticide toxicity?

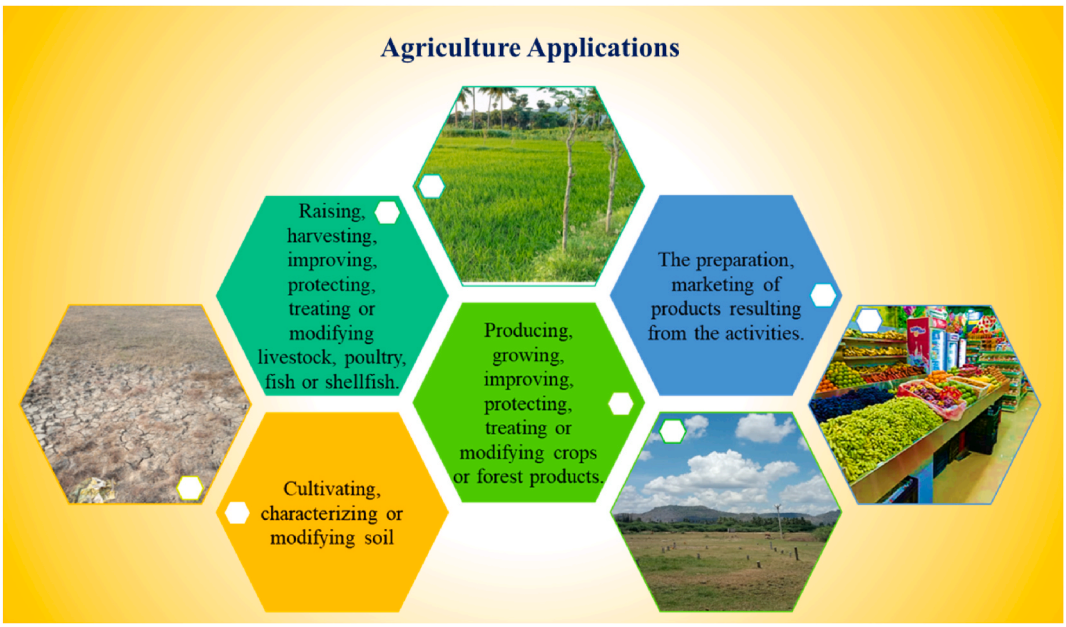

Fig. 1. *Agriculture application in the field developments* [1].

2.3. Research objectives

- ➢ To determine the potential health effects of pesticide exposure and how the incorporation of ML could be used to make these predictions.
- ➢ Use ML models to determine which pesticides are safe to use and which ones need to be limited.

2.4. Criteria for inclusion and exclusion

We framed three criteria for this review. They are us follows.

1.We concentrated on peer-reviewed publications between 2014 and 2023.
2.All articles related to pesticide toxicity were considered.
3. In addition, papers related to machine learning were included.

Apart from all three criteria, the remaining criteria were excluded.

3. Results and discussion

3.1. Exploration of articles

A total of 418 publications were examined, it was found that ninety of them were focused on insecticides related research. Among them, 157 articles were dedicated to herbicide studies, 47 articles were centered on fungicide investigations, and the remaining 124 articles covered diverse chemicals. The collection of 124 publications pertains to a wide range of topics, including pesticides, binary pesticides, biocides, agrochemical hazardous components, polycyclic aromatic hydrocarbons, and endocrine-disrupting compounds. Moreover, an extensive search was conducted within these papers utilizing the phrase "machine learning." A total of sixty-eight articles were identified, with 24 classified as insecticides, 21 as herbicides, and 12 as fungicides. Data extraction was performed using Microsoft Excel. The method for selecting articles is outlined in the flow diagram in Fig. 4.

3.2. Pesticides in agriculture

Pesticides play a crucial role in agriculture owing to their unique ability to kill pests [2,33,49]. Pesticide use on farmland has resulted in higher crop yields, which help in one-third of global food productivity, making them extremely important. Pesticide use on farmlands results in higher crop yields. Pesticides usually penetrate plants through three routes: surface penetration, root absorption, and tuber diffusion. This results in the detection of pesticides in the plants after harvest [25,48,50]. This leads to pesticide residues in soils, grasses, microorganisms, and crops that may persist in farm products, contributing to overall pesticide consumption through the diet [17]. Because of these contaminants, pesticide metabolites in farmed dairy products such as beef and milk have increased dramatically. Pesticide residue levels in high-fat livestock products can be biomagnified, resulting in greater health risks to humans and other living things [9,51]. These pesticides also affect non-target organisms such as rats, mice [52,53], honeybees [54,55], fish [24,56], earthworms [57,58], and other insects and worms [59]. Hence, there is growing concern about the potential risks of pesticides to consumers, and public safety has grown in recent years. Hence, ecological engineers, on the other hand, need to look for harmful toxins in the environment and produce new ways to break down toxic and dangerous pesticide waste into harmless, non-hazardous metabolites or compounds so that the former does not harm the environment [60]. In addition, researchers have targeted pesticide

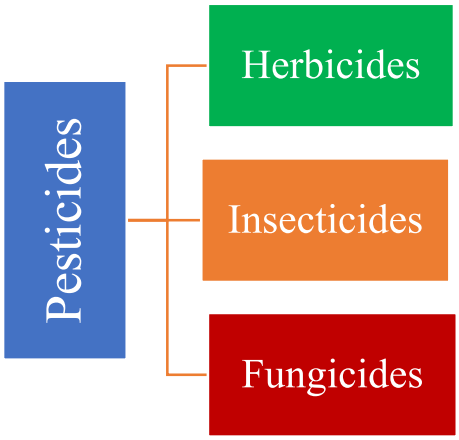

Fig. 2. – *Classifications of pesticides* [14].

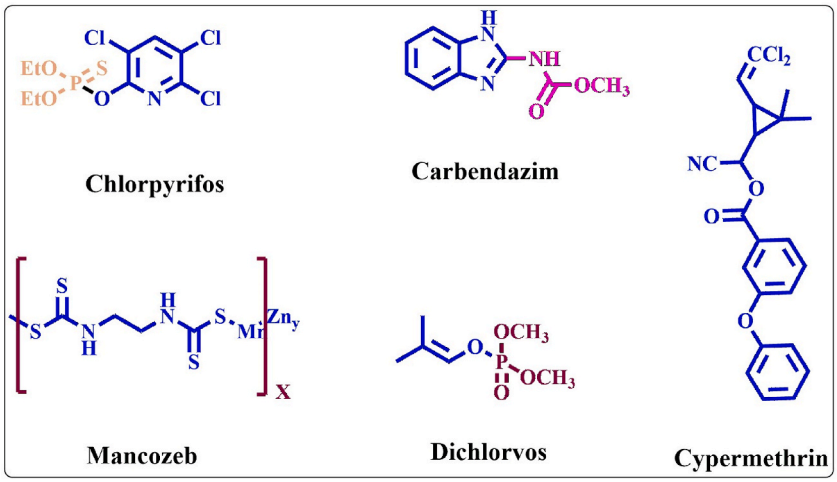

Fig. 3. Common pesticides.

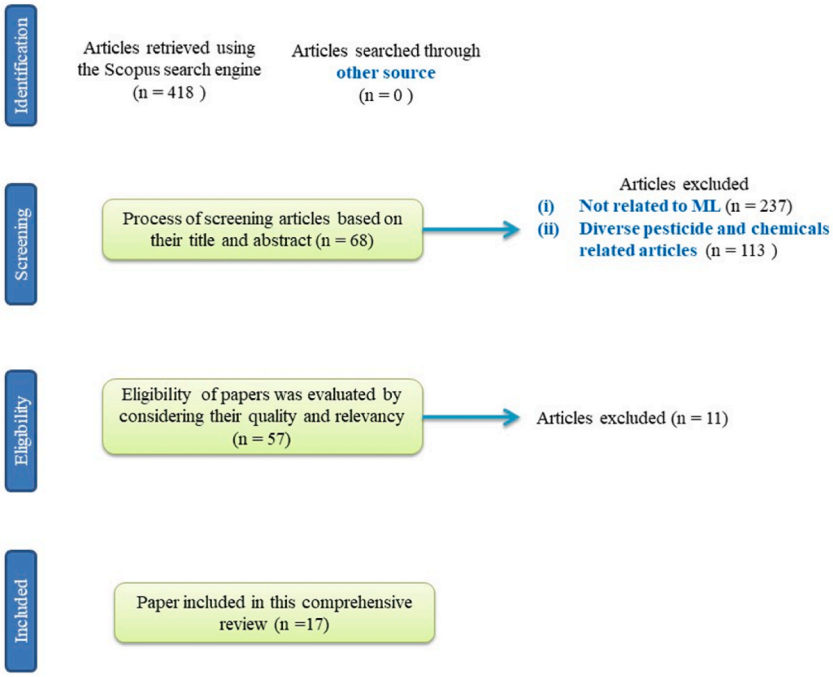

Fig. 4. Study selection process workflow.

residues in the environment, particularly in dietary products.

3.3. *Toxicity of pesticides*

Pesticides have complex chemistry and the potential to create medical consequences. This has led researchers to conduct comprehensive studies to uncover the intricate mechanisms underlying toxicity, which lead to acute and chronic effects, bio-accumulation, and persistence in the environment. Much research has been carried out on pesticides worldwide owing to their interaction with the environment in complicated ways. Hence, scientists and environmentalists have been checking pesticide usage and regulatory aspects. Depending on the pesticide or a combination of pesticides to which a person or nation is exposed and the level of exposure, this type of impact can affect virtually every organ in the human body. Pesticides can cause both immediate and delayed toxicity as well as chronic toxicity [30]. In addition, some pesticides are developmentally toxic, whereas others are carcinogens or reproductively toxic when used at high concentrations. All pesticides interfere with the neural circuits of insects, which appear

structurally and functionally similar to those of vertebrates. As a result, pesticide toxicity is not species-specific, and humans are particularly vulnerable to the hazards of pesticide exposure. WHO analytical data have identified and listed 150 pesticides as hazardous and poisonous. These 150 pesticides were retained in the soil, sediment, and water. As a result, it becomes bioaccumulative and toxic to aquatic organisms. The WHO also stated that these pesticides are toxic to bees and affect ecosystem services. Atrazine, flupyrifurone, hexachlorobenzene, glyphosate, methomyl, and rotenone are the most well-known pesticides listed by WHO. Paraquat is another hazardous pesticide that has been banned in 60 countries. Paraquat affects muscles and the nervous system and leads to pathogenic diseases, movement control, and emotional limbic activity. Flupyradifurone, hexachlorobenzene, pirimicarb, imidacloprid, tebuconazole, epoxiconazole, isoproturon, and 1,3-dichloropropene are the most toxic to humans. Inhaling these chemicals leads to heart failure and lung scarring may even be fatal. Another pesticide commonly called is used on grasses, fruits, and vegetables. These pesticides attack the leaves and roots of weeds and affect the growth of the plants, causing cancer and killing them [95,96]. To overcome these drawbacks, researchers are currently developing new pesticides. Modern pesticides are more selective than older pesticides because of their selectivity for bugs, which have different metabolic rates.

In recent years, biopesticides or pesticides derived from biological sources such as plants, bacteria, and fungi have received increased attention [61]. Biopesticides, which are increasingly used in successful integrated pest management programs, have generally acceptable ecological and biological profiles. The most widely used microbial pesticides are *the Bacillus thuringiensis* subspecies and strains that act as insecticides. Although allergic reactions have been reported in humans, insecticides contain specific chemicals that are mostly found in animals. As a result, new ways to make safe pesticides and break down commercial pesticides are important [14].

Subsequently, ML became attractive in the field of agrotechnology [62]. ML algorithms can process large amounts of data and detect results and patterns based on the data. As the forecasting model improves over time, no external manipulation is required. Instead of direct human involvement, machines learn from the input about the characteristics that create a mathematical framework for estimates.

There are only a very few studies on the use of ML in the field of agricultural pesticide toxicity prediction, in Fig. 5, according to the most recent Scopus data base search term, "machine learning toxicity of pesticide prediction." The benefit of utilizing ML in this field is that there is a lack of research in this area. ML algorithms would make it feasible to anticipate pesticide toxicity more precisely and effectively, which would result in a decrease in the use of hazardous chemicals in agriculture. Moreover, ML can be used to identify novel pesticides that are less hazardous and more effective. Despite this, there are challenges in applying ML in this area, such as the requirement for enormous amounts of data and the difficulty of deciphering intricate models. Besides these difficulties, it is obvious that greater study on the use of ML in agricultural pesticide toxicity prediction is required. By doing so, we can develop an agriculture sector that is safer and more eco-friendly.

Here, we discuss the potential health effects of pesticide exposure and how ML can be used to make these predictions. Researchers and scientists can use these models to decide which pesticides are safe and which are limited. New compounds that may be detrimental to human health can be identified using ML, allowing preventive measures to be taken before exposure occurs. ML is an invaluable asset to safeguard both humans and ecosystems from the harmful effects of pesticides.

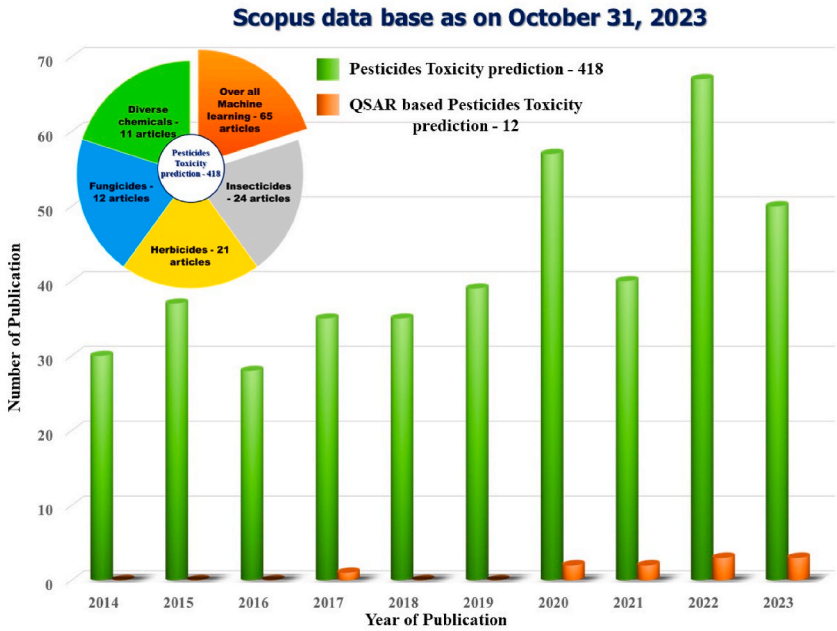

Fig. 5. Total number of publications related to the ML approach in pesticide toxicity prediction as per the Scopus database on October 31, 2023.

Table 1
Various methods of algorithms-based pesticides predictions.

S·NO	Year	Methods used[a]	Accuracy	Data sets	Features	Best model	Reference
1	2022	DT, DF, RF, k-NN, SVM, LDA, and LR	45%–61%	They take 29 chemicals chosen from a list of 275 chemicals data. They reported alternative approach to evaluate the potential reproductive toxicity of chemicals	They are using 500 iterations for the data sets to derive 5-fold cross and external validations for the data sets. To predict the toxicity	DT	[42]
2	2022	LVQ; RF, and SVML	95.7%	22 toxic organic compounds which includes herbicides, pesticides, and industrial chemicals	This approach allows them to thoroughly evaluate the performance of each family and reduce the chances of bias or overfitting. Additionally, by repeating the cross-validation process three times, they can ensure the robustness and reliability of their results	RF	[44]
3	2023	RF, ANN, and SVR	–	7858 compounds were chosen from a pool of 9403 chemicals. ToxCast Database of the US EPA	The study selected the chemical bonds (CBs) of 216 compounds using RF, outperforming ANN and SVF models. Human CBs of 7858 ToxCast chemicals were predicted, with food additives and pesticides being most active	RF	[81]
4	2014	PNN and GRNN	PNN – 96.65% GRNN – 95.57	The data set consists of 303 registered pesticides	PNN and regression GRNN-QSTR models predict pesticide toxicity classes on land, demonstrating high predictive power and reliability in noisy environments with large training data sets	PNN and GRNN	[82]
5	2014	DT, RF, NB, SL, LibSVM, and SMV	79.7%	105 chemicals and vehicle controls, representing 14 compound classes	These studies suggested that using microarrays and supervised ML for chemical toxicant prediction is practical and efficient, but selecting the right feature and classification algorithms is crucial	SVM	[83]
6	2021	ANN, DT, k-NN, NB, RF, and SVM	–	Dataset included 144 compounds with high toxicity, 32 compounds with moderate toxicity, and 500 compounds with nontoxicity, total (676) data	The study used nine molecular fingerprints to create 54 binary classification models for honeybee acute contact toxicity prediction, with the SVM algorithm and CDK extended fingerprint being the best models	SVM	[84]
7	2018	DL, RF, and SVM	0.76	Three different datasets were used: the HESS dataset, which included 503 data points, the combined dataset, which included 810 data points, and the ORAD dataset, which included 346 data points	The Hazard Evaluation Support System Integrated Platform dataset predicts 214 test chemicals with an accuracy of 0.76, sensitivity of 0.90, and AUC of 0.81, potentially aiding in toxicity prediction	SVM	[85]
8	2020	MLR, PLS, k-NN, DT, and RF	0.90	The dataset for classification-based models consists of 413 chemicals. Model based on regression: 113 chemicals.	Two models, a k-NN classification-based model and a k-NN regression-based model, were used as integrated tools for hierarchical workflows, providing the best predictions based on statistical parameters and demonstrating reliability and robustness	k-NN	[86]
9	2021	GA-MLR and BPANN	–	57 types of organophosphates data sets	The LD50 of organophosphates is predicted using ALOGP2, RDF030u, RDF065p, and GATS5m descriptors, with the BPANN approach providing the best results and good agreement with experimental data	BPANN	[87]
10	2018	k-NN, SVM, and LDA	90%	Pesticides, hydrocarbons, alkanes which includes 79 various aquatic data	With an RMSE of 0.793 for reference MoA labels, it was confirmed that the classification model was good at predicting MoA and figuring out toxicity using the Target Site Model	k-NN	[88]
11	2023	MLR, SVR, GA, and SVR	–	664 different pesticide was evaluated with regression based (QSAR) models.	These findings highlight the importance of considering multiple factors when assessing pesticide toxicity. Additionally, further research is needed to fully understand the mechanisms by which electronegativity, lipophilicity, and polarity influence pesticide toxicity	MLP	[89]
12	2020	LRMP and LDA	70%	207 pharmaceuticals and pesticides which were identified as steatotic or	The QSAR model predicts steatosis for 1600 food and feed-relevant substances	LDA	[90]

(*continued on next page*)

Table 1 (*continued*)

S·NO	Year	Methods used[a]	Accuracy	Data sets	Features	Best model	Reference
				non-steatotic from existing data from *in vivo* human and animal studies	in the EuroMix project, providing data for risk assessment calculations in the EuroMix Inventory		
13	2023	PLS, RR, SVM, and non-linear SVM	0.85	13 sets of duplicate mixtures correspond to 44 data points and respective 44 observed toxicity values.	By utilizing q-RASAR modelling, researchers can effectively assess the potential harm caused by binary mixtures on honeybees. This approach not only provides reliable predictions but also offers an accurate understanding of the toxicity risks associated with pesticide combinations	PLS	[91]
14	2014	PNN and GRNN	96.62%	Experimental toxicity data of 237 structurally diverse pesticides	These models can aid in the evaluation and risk assessment of new chemical pesticides, providing valuable information for decision-making processes. Additionally, their accuracy and reliability make them valuable tools for researchers and policymakers in the field of pesticide regulation	PNN and GRNN	[82]

[a] ML- Machine Learning; DT - Decision Tree; DF - Decision Forest; RF - Random Forest, k-NN - K-Nearest Neighbors; SVM - Support vector machine; LDA - Linear Discriminant Analysis; Linear regression; LVQ - Learning Vector Quantization; SVML - Support Vector Machines with a Linear kernel; ANN - Artificial Neural Network; SVR - Support Vector Regression; PNN - Probabilistic neural network; GRNN - Generalized Regression Neural Network; NB - Naïve Bayes; SL - Simple Logistic; LibSVM - two Support vector machine methods; DL - Deep learning; MLR - Multiple linear regression; PLS - Partial least squares; GA-MLR - Genetic algorithm multiple linear regression; BPANN – Back Propagation Artificial Neural Network; MLR - Multiple linear regression; GA - Genetic algorithm; LRMP - Logistic regression Multilayer perceptron; PLS - Partial Least Squares; RR - Ridge Regression; LSVM – Linear Support Vector Machine; PLS - Partial Least Squares; RR - Ridge Regression.

3.4. ML application of Pesticide prediction

Water contamination is a major concern in the manufacturing of pesticides. Sub-structural alarms were investigated, and predictive models that could be extremely useful in determining chemical aquatic toxicity were developed (Table 1). The author investigated pesticide aquatic toxicity using nine cellular handprints to describe pesticides [9] and used six machine learning algorithms to create two- and three-level classification models that could guess the harmful effects of pesticides on water. The algorithms used were Random Forest (RF), k-Nearest Neighbour (k-NN), Nave Bayes (NB), Classification Tree (CT), Artificial Neural Network (ANN), and Support Vector Machine (SVM). The binary models involved the development of local models encompassing 829 pesticides in rainbow trout (RT) and 151 pesticides in lepomis (LP). Additionally, global models were constructed using a broader dataset consisting of 1258 pesticides on RT, LP, and 278 distinct fish species. After studying fish species, the authors discovered that they influenced the accuracy of the local binary models. A total of 1258 pesticides were utilized to create robust ternary models based on their prediction abilities. ANN for RT and SVM for LP were the most accurate binary models, with fittings of 0.90 and 0.90, respectively. The SVM was the most efficient binary model, with a fitting of 0.89 and an efficiency of 0.81, which was slightly lower than that of the best comprehensive binary model. Many underlying alarms have also been discovered, including chloroalkenes, nitrobenzenes, and nitriles, which may have a significant relationship with the toxicity of pesticides. This research shows a simple way to determine how harmful pesticides are to aquatic life early in the hazard identification process.

In addition, ALogP and molecular weight (MW) were used to determine the distribution of the chemical space. The chemical spatial distribution diagrams for all pesticide training sets and the external validation set are shown by the LP and external validation sets, respectively, while the RT training samples are the external validation set in this plot. This information was obtained from chemical space analysis, which showed that the training set and the external validation set were formed in the same chemical space, indicating that this model is adequate [9].

The aim of this study was to determine whether training sets for toxic elements and relevant substances can improve the accuracy of the prediction results for toxic elements. In an earlier study on the minimum effective dosage (oral rat LD50), local class-based models were found to be more consistent than more complex models [63]. To improve the forecast accuracy, it has been discovered that information should be divided into pesticidal processes. An approach based on linear discriminant analysis (LDA) was used to assign indications for pesticides based on their mode of action, target species, or target organisms' mechanisms of activity arrangement, among other things. According to this study, LDA was able to forecast these signs with a fit of approximately 0.87. The toxicity of the compounds was determined using the QSAR model. Toxicities can be found using a global hierarchical clustering (HC) or unsupervised learning method that sorts data into groups based on molecular similarities. When comparing the global HC technique to LDA ($R^2 = 0.47$) at the same level of accuracy (0.94), it showed a significant improvement in prediction performance ($R^2 = 0.50$). The worst results were obtained using a linear model on the entire training sample ($R^2 = 0.38$), which suggests that grouping information to find toxicities might be a good idea in this case. Fig. 6 depicts the steps involved in creating the training and prediction sets. It is also true that clustering the dataset into subsets improves the prediction accuracy. The method used to divide the dataset into subgroups did not

influence the accuracy of the dataset prediction.

Considering the results of a study on the frontier of deep learning, viewpoints formed over three years of ML research and development were considered, as was the outcome of an agrochemical research and development period. How 'deep learning' is enabling rapid technological innovation in several scientific disciplines and how speculations about its ability to influence people's work and personal lives are a source of on-going debate were discussed [64]. However, using it as a "black box" tool without understanding its limitations is far too simple, especially when the data being used are not of high quality. In this article, the author attempts to place a subset of AI (deep learning) from a wide-ranging mechanical and cultural perspective by demonstrating how it connects to earlier types of AI, giving a comprehensive description of how it works, and examining some of the implementation challenges that have been encountered. Initially, it appears that digitalizing difficult work aimed at evaluating agribusiness effectiveness will have the greatest impact on agribusiness growth. However, to achieve this, significant contributions are required in both the generation of large, well-organized datasets to deal with the skills required for analyzing the forecast accuracy in natural settings. Deep learning is used to adapt existing ML techniques for pesticide exploration and design, but it is not yet possible to replace these techniques completely.

Fig. 7 depicts a straightforward example of how an expert system can be used to diagnose fungal illnesses in red chilli peppers. The identification label (for example, "probably Fusirium" or "probably Antraknosa") will be made as soon as sufficient data are available to make an accurate classification decision. This is how the system operates.

This study makes a significant contribution by demonstrating one of the most notable benefits of using in silico analysis to determine the bioactive ability of substances: it minimizes the amount of time and cost spent on experimental investigation as well as the associated expenses. According to the author, the rapid use of ML algorithms in the study and synthesis of chemicals with precise physicochemical properties for application is possible using ML algorithms [7]. According to the findings of this report, the ML algorithm assisted us in the production of three dihydroquinoline (DQ) compounds that can be used as pesticides. In this study, it was discovered that the tobacco mosaic virus (90% effective) and *Fusarium oxysporum* were effective against the developed compounds (78%). We determined whether there was a relationship between pesticide function and molecular structure using various spectroscopic techniques and single-crystal X-ray scattering to examine the proposed DQ compounds. The Orthorhombic and monoclinic crystals developed with supramolecular configurations were primarily supported by non-classical C–H and O–H bonds (C–HO). This led to the formation of dimers and chains during molecular packaging. We used density functional theory (DFT) to determine the frontier molecular orbitals (FMO) and molecular electrostatic potential (MEP) maps to examine the electronic features of the molecular conformations that were described. The established method can also be used to examine the toxicity of new pesticides that are being developed when there are no trial toxicity data.

The purpose of this study was to categorize basil seedlings according to the quantity of nitrogen fertilizer they received, using an olfactory machine (OM) and ML algorithms. Using the findings of this study, we can better understand the uniqueness of basil plants and their ability to protect themselves from overgrowth. Basil (*Ocimum basilicum*) is an aromatic plant belonging to the Lamiaceae family with a variety of medicinal properties, including pain relief [65]. The application of nitrogen fertilizers has a significant impact on basil growth. Fertilization with a high concentration of nitrogen has an impact on plant metabolism, particularly amino acid compounds and other nitrogen-based metabolic functions. Additionally, the use of nitrogen fertilizers causes an increase in the amount

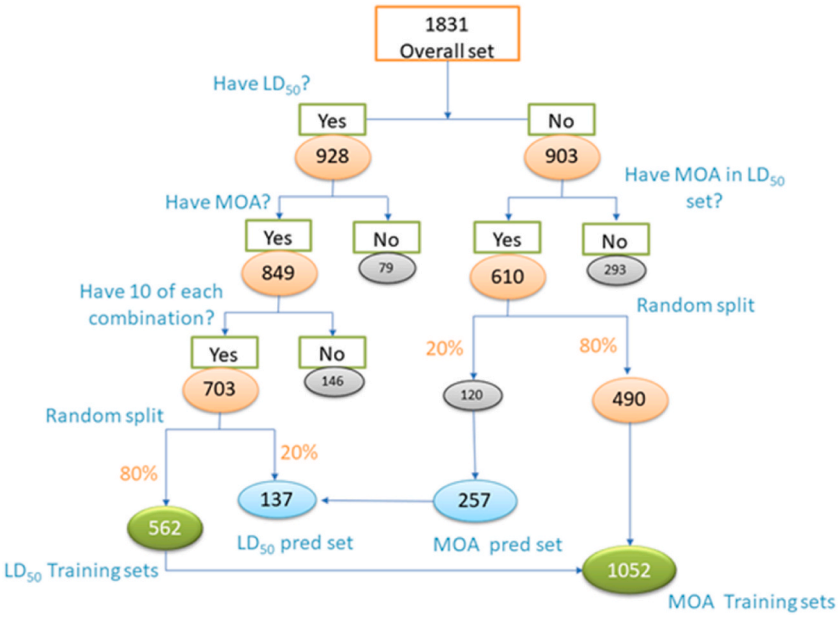

Fig. 6. - *Workflow for developing the training and prediction sets* [63].

Fig. 7. - *Putting deep learning in perspective for pest management scientists* [64].

of nitrate present in plant tissues, which is harmful to humans when consumed. A machine olfaction system was used in this study, which allowed researchers to identify basil plants established on the diverse amounts of N fertilizer that were applied to the plants (e-nose machine). The amount of urea fertilizer used (0, 50, 100, and 150 kg ha^{-1}) was investigated at four different levels. The relative humidity levels of the samples were nearly identical across the board. Several techniques were used to analyze the data, including principal component analysis (PCA), ANN, LDA, and QDA. The TGS822 sensor provided the most accurate categorization response. According to the PCA results, PC1 and PC2 accounted for 90% of data variation. Using linear and quadratic discriminant analyses, the data were divided into classes with a normal distribution (LDA and QDA). In this study, two techniques were used to divide the samples into 12 groups: LDA and QDA. Basil plant classification confusion matrices were developed using the LDA and QDA methods with accurate ordering rates of 95% and 97.78%, respectively, for the two approaches. As shown in LDA and QDA, E-nose signals were used to detect 12 different types of samples. The QDA method performed better than the LDA method in terms of accuracy. The precision, sensitivity, and specificity were all higher than 0.9891 for QDA, and the average values of the other parameters were lower than 0.9937 for QDA.

The widespread use of pesticides has led to an increase in the number of pest-resistant pests worldwide. Current approaches to weed resistance management include the identification of new phytotoxic compounds and herbicide modifications based on modes of action (MoA) prediction and characterization of structure-activity correlations and underpin herbicide classification according to their actions with herbicide selectivity. Usually, step-by-step evaluation-shows a program of computer simulations and herbicide equivalence values using net charge, relative polar surface area, number of H bonds, acceptors and donors, logP, and topological characteristics of the molecules together. This study also proposes an in silico sequential screening platform that can identify herbicide-like compounds from chemical registries or libraries, considering the probability and selectivity of weed species, in addition to a default mechanism of action added to this concept, as illustrated in Fig. 8. The screening cascade was tested by using a dataset of naturally occurring phytotoxic compounds. These findings may have useful implications for improving diversion programs for herbicides and other coastal herbicides compared to synthetic chemicals. This is particularly evident when molecules with novel reaction properties, unique structures, and buoyancy are obtained from natural sources, as opposed to synthetic materials.

The author developed an initial ethical system that incorporates, evaluates, and correlates the professional and procedural dimensions of food safety risk assessment [66]. Assessing food safety risks using MLTs and AI implementation principles identified in scholarly and regulatory papers is a system that can be expanded in the future. The use of vast amounts of data and ML techniques is changing the way food safety risk assessment (FSRA) is performed. As FSRA activities continue to be "dataficated" and probabilistic

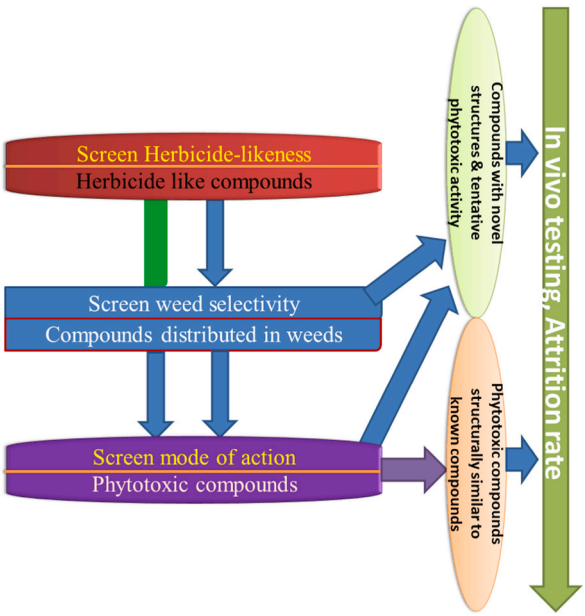

Fig. 8. - *Comprehensive ML based study of the chemical space of herbicides* [43].

models are increasingly integrated into their procedures, it is necessary to consider the advantages and disadvantages of these advancements in a balanced manner. Emerging methods of analysis have the potential to exacerbate the low level of trust in the EU's FSRA framework, which was addressed in 2019 through an EU-funded survey. The wide range of processed data raises interesting questions regarding how many different regulations work together with food safety laws.

Information security and the provision of personal data are combined with regulations required for the dissemination of scientific findings to the public. This work aims to provide recommendations on data authority and ownership issues that have arisen in the technical and legal sectors of FSRA to improve food safety. Consequently, a summary of the proposed amendments to food safety legislation and advancements in data collection, emerging concerns regarding the implementation of cutting-edge big data, and data examination methods are discussed in detail. A set of principle-based references is anticipated based on the application of high-level concepts to the field of FSRA using AI. Security, responsibility, equality, interpretability, and clarity (SAFETY) are some of the main points of the proposed set of recommendations. Confidentiality and security protection are used as meta-principles to guide the recommendations.

As previously reported, high-throughput phenotyping in *C. elegans* is an effective method for improving focused deconvolution in the development of anthelmintics and insecticides [67,68]. Hyperspectral imaging technology has made significant advancements in the field of food safety (FS). The use of hyperspectral imaging for non-destructive prediction of contamination was investigated using hyperspectral imaging. In this study, the application of a convolutional neural network (CNN) based on near-infrared hyperspectral data was proposed as a novel approach to overcome the problem of the low recognition rate of abamectin residue on the broccoli surface. In the convolutional neural network model, the maximum reliability was 84.9%, which was 10.1 points higher than the accuracy of the extreme learning machine model, which was based on a different technique. There is evidence that using a convolutional neural network, researchers can analyze hyperspectral data of low-concentration pesticide residues on broccoli surfaces, with residue concentrations ranging from 0.04 0.20 mg/kg. A specific path can be used to make pesticide residue detection and algorithms more efficient.

To achieve the goals of current therapies, new invertebrate-killing chemicals are required in the food and pharmaceutical industries. Insecticides and anthelmintics were discovered using genotyping tests [69]. However, determining the mechanism of action of these discoveries is critical in the discovery process and should not be omitted. To determine its mode of action, it is necessary to combine visible whole-organism signs with molecular and physiological information. In contrast, manual symptomology is time consuming and requires signs that are visible to the unaided eye to be effective. High-throughput imaging and numerical phenotyping were used to quantify the behavioral reactions of Caenorhabditis elegans. They then developed a classifier that accurately predicted the MoA for each of the typical modes of action, with an accuracy of 88% for a set of twenty-five different chemical compounds. Their approach was to categorize compounds within each mode of action to investigate substructures that are not represented by broad MoA labels. Images taken quickly and automated phenotyping could help refine mode-of-action categories and speed up finding new modes of action in the development of invertebrate products.

Furthermore, the most accurate RT prediction model was developed. We compared the effectiveness of several ML-based algorithms on different feature sets based on their ability to predict the response time (RT). Because of the increasing number of environmental pollutants detected using liquid chromatography combined with mass spectrometry in data mining, computational QSAR models are becoming increasingly popular in survival prediction models. The improved performance of the model was attained through the use of ML techniques, chemical characteristics, and sample data. They tested four methods on three datasets, with the training and test sets consisting of 321 and 77 pesticides, respectively, for several ML-based algorithms on different feature sets based on their ability to predict the response time (RT). Because of the increasing number of environmental pollutants detected using liquid chromatography combined with mass spectrometry in data mining, computational QSAR models are becoming increasingly popular in survival prediction models. The improved performance of the model was attained using ML techniques, chemical characteristics, and

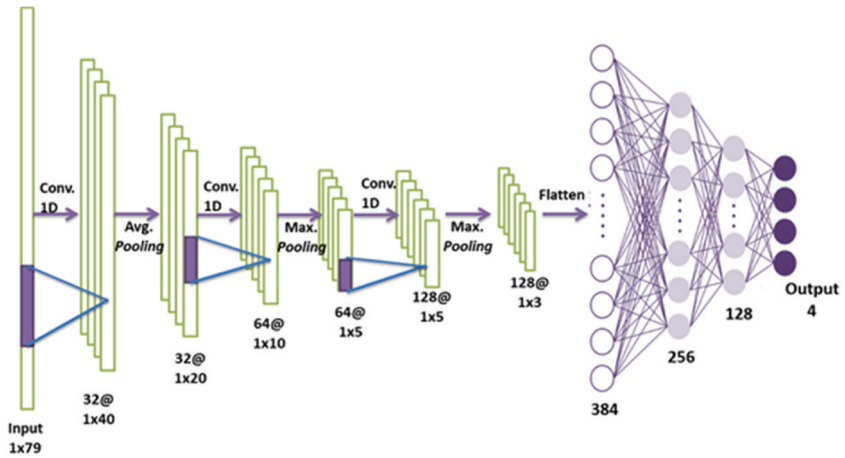

Fig. 9. - *One-dimensional CNN architecture* [71].

sample data. They tested four methods on three datasets, with training and test sets consisting of 321 and 77 pesticides, respectively. Various combinations of algorithms applied to different feature sets produce various results. Increasing the complexity of the chemical characteristics and the size of the training set are effective strategies for improving the results. The XGBoost, RF, and light GBM algorithms were used to generate excellent results on large-scale chemical descriptors (LSCD), whereas the Keras method was used to generate excellent results on fingerprints. These models produce similar results, with a DRT of 1.0 min correctly predicting at least 90% of the toxins in the testing dataset, among other things. According to the results of this study, the combined prediction technique based on the average outcomes of the four models outperformed any single model. Using this method, researchers were able to identify pesticides and pesticide transformation products in 120 strawberry samples collected as part of a nationwide food contamination survey. Standards have approved all 20 pesticides and 12 pesticide transformation products, as well as two transformation pesticide (bifenazate diazene and spirotetramat-enol) products, out of a total of 20 pesticides and 12 pesticide transformation products. When the in silico MS2 spectra were combined with other MS identification methods, they could be used for chemical identification [70].

The author collected 30 leaves of garlic chives (*Allium tuberosum*) captured in infrared hyperspectral imaging wetted with the detection and recognition of pesticide residues on garlic chive leaves using purified water, cyhalothrin, trichlorfon, phoxim, and mixtures of trichlorfon and phoxim, which are rapid, precise, and non-destructive [71]. The isolated forest approach removed outliers, enhanced the signal to noise ratio of hyperspectral images using modified median filtering This paper presents a DL model to be used for drug detection proposed killing bacterial residues in garlic chive leaves by one-dimensional (1D) CNN, outperforms spear Bayes, RF, and SVM. Fig. 9 shows the layered 1D CNN design. Input refers to the input level, which is responsible for receiving shortwave infrared signals for subsequent system processing. The character "conv" indicates the one-sided convolutional level. The goal of 1D is to extract features from input data. The pooling layer can compress the output data of the convolution layer, thus reducing guesswork and preventing overfitting.

In this experiment, the optimal pooling strategy was determined by combining the maximum pooling and average pooling of pooling levels. The fattening layer converts the results from the previous layer into a vector suitable for the next layer. Two hidden layers are used in the fully connected layer. During the model validation phase, enabling four neurons in the output layer results in four different outputs. The relative accuracies of the 1D CNN in the railway, development, and experimental groups were 0.985, 0.98, and 0.979, respectively. In the estimation of customer service characteristics, each of the four groups has an AUC above 0.99, indicating a better fit and variability of the DL model than the five classical classification models considered in terms of accuracy and variability for satisfactory prediction of pounding losses of 0.208, indicating the presence of pesticide residues The combination of hyperspectral imaging and DL shows great potential in detecting and identifying non-destructive pesticide residues in garlic chive leaves.

According to the Agricultural Census of India, the agricultural sector accounts for 64.5 percent of the country's population and 16–17% of the nation's GDP [25]. The agricultural sector, which is the backbone of our economy, is largely ignored, with little or no development occurring. For a country that is ranked as the world's second-largest producer of rice, it is critical to change and concentrate on how to improve agricultural methods to make the lives of farmers easier. The application of modern technology to agriculture is necessary in the modern era. The application of current agricultural technologies is critical. Hungry farmers who have struggled to provide food for their families do not have access to high-tech devices. Pesticides and fertilizers are critical components of agricultural production. It is possible to use pesticides and fertilizers to aid in preventing pests from damaging crops as well as the provision of additional nutrients necessary for a successful crop. Pesticides and fertilizers, on the other hand, can be extremely dangerous if they are not handled with care and caution. GPS and Internet of Things (IoT) technologies are used to figure out what kind of soil it is and how many herbicides and fertilizers to use in a cost-effective way after the research is done.

Pesticides and fertilizers, ML, and text prediction sequencing were investigated in 2021. The relationships between this approach

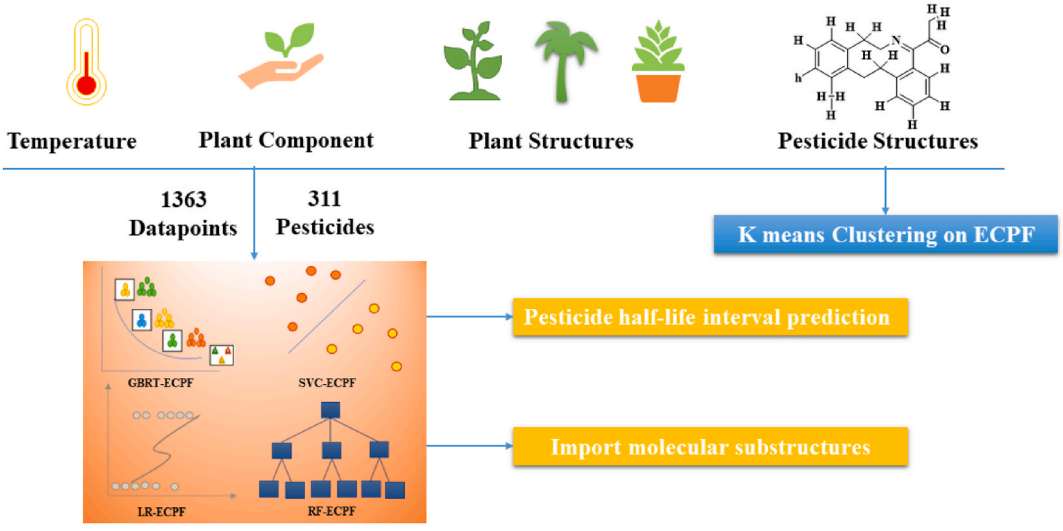

Fig. 10. *Workflow via ML models with the datasets* [23].

and ML, Text Processing (TP), the Random Forest Algorithm (RFA), and the Flutter Framework (FF) are the primary emphasis of this study. The authors attempt to explain ML, TP, RFA, and FF for the benefit of the readers. Following training using an ML technique, RFA can be used to estimate the harvest of four crops: wheat, maize, tomatoes, and potatoes. Several classifications and prediction subtrees were constructed with a random subset of predictors without chopping them down, and the forest was then averaged to produce a trained RF. The model was trained using a random sample of trees generated by bootstrapping source data. Predictor variables are scored based on how frequently they lead to accurate predictions, or the degree to which they reduce node contamination when used to make partitions. This scoring system ensured that only the most effective predictors were used in the final model, resulting in highly accurate predictions. Overall, the trained RF model is an essential tool for making accurate predictions based on complex data sets [72].

In 2022, ML algorithms were used to examine how long it would take for plants to recover from pesticide exposure. They used the 1363-point, 311-pesticide, 10-plant, 4-component-class dataset of the pesticide dissipation half-lives (Fig. 10). Owing to the large differences in the empirical data, new estimates of the dissipation half-life interval were offered. The authors used ECFP, temperature, plant type, and plant component class to build models that could predict dissipation half-life intervals. These models were then tested using GBR, RF, SVC, and LR ML models. When compared to various other ML models, including LR-ECFP, F1-microbinary = 0.662 0.009, and GBRT-ECFP F1-microbinary score = 0.698 0.010 had the best model performance for binary classification, with a score value. Correlation-based feature evaluation revealed that the molecular substructures of the aromatic rings, carbonyl groups, organophosphates, =C–H, and heterocyclic N-atoms were successful in relation to the pesticide disintegration half-lives. This research lends credence to the idea that ML models can be useful for determining how pesticides would behave in the natural world when applied to crops [23].

Deep learning has been used to detect pesticide usage on farms that grow crops, such as cucumbers, tomatoes, cabbage, and tangerines. They use readily available surveillance footage or cameras, as shown in Fig. 11. This information could provide essential data for encouraging the safe use of vegetables and pesticides by consumers, as well as enabling authorities to promptly analyze the nutritional value of agricultural goods. They designed PesViT as the primary model, which is based on end-to-end neural model optimization in mobile ViT employing Ghost blocks [73]. They then used momentum contrast methodology in conjunction with a contrastive self-supervised learning method (SSL-MoCo).

This technique employs unmarked sets of data with the necessary modifications to the hyperparameters to achieve the most accurate and fast outputs. Using the latest information collected from farms at different times of the day, the model achieved an efficiency of 95.36%, which was higher than the 91.25% achieved by the original Mobile ViT and 88.75% achieved by MobileNetV2. Particularly encouraging for the model's potential for wide-scale implementation is the fact that the experimental construct runs well, even on systems with modest hardware. Overall, this model represents a significant step forward in the development of precision agriculture tools that can help farmers optimize their yields while minimizing waste and environmental impact.

In 2023, image processing for deep learning approaches was used to forecast insect detection for leaf diseases and to prescribe pesticides. Leaf condition can predict the size and quality of a harvest month in advance, making it an important factor in agricultural and plant science. Disease classification, pesticide suggestions, and pre-processing of leaf pictures from a plant village dataset are all proposed here using a Deep Neural Network (DNN) approach [6]. The dataset was extended by geometrically manipulating plant leaf images and then splitting them into test and training data, as shown in Fig. 12. Subsequently, Convolutional Neural Network (CNN)-type ResNet-50 models were trained on the massive ImageNet image dataset. Using the concept of transfer learning, this study applied database design rules that were previously learned to a smaller model picture dataset of plant infections. The goal is to create a model that can identify diseases in leaves, pests, and suggest the correct pesticides. This technique has been used to test several sick leaves. Experiments showed that the accuracy and efficiency of plant sprig image detection can be improved by applying a transfer-learning-based CNN approach. It can quickly and accurately identify agricultural illnesses, reduce pesticide and fertilizer application, and boost both crop quality and production.

A portable NIR spectroscopy machine learning method was investigated for the detection of chlorpyrifos residues in pesticide-resistant bok choi (Brassica rapa subsp. chinensis). Vegetable pesticides and bacterial sprays pose potential health hazards to users. To identify chlorpyrifos residues in Bok Choi, researchers used a combination of NIR spectroscopy and ML algorithms. These

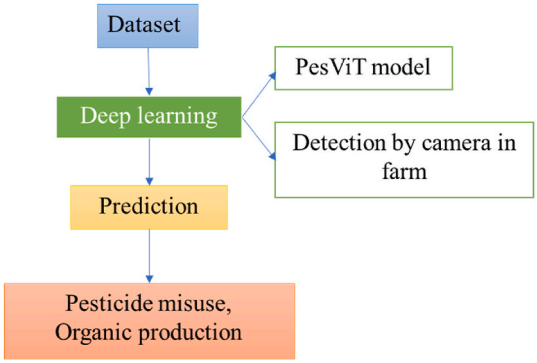

Fig. 11. *Pesticide monitoring in deep learning method using cameras* [73].

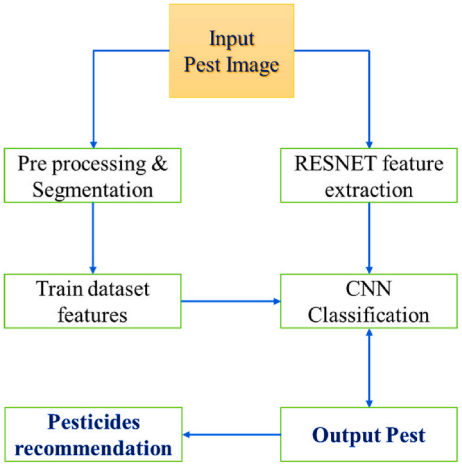

Fig. 12. - *Proposed block diagram for Convolutional Neural Network (CNN)* [74].

algorithms include the sufficient component artificial neural networks (PC-ANN), partial least-squares discriminant analysis (PLS-DA), and support vector machines (SVM). A total of 120 bok choi samples were obtained from two small conservatories that developed cultivation of internal individuals [46]. Sixty samples were allocated to each of the two treatment groups: pesticide and non-pesticide groups. Chlorpyrifos (2 mL/L), containing 40% EC residue, was added to the vegetables before irrigation. A compact one-dimensional computer was connected to a commercially available handheld NIR spectrometer with a wavelength range of 908–1676 nm. Ultraviolet light spectrophotometry was used to detect the presence of antimicrobial compounds in Bok Choi, the researchers used ultraviolet (UV) light spectrophotometry was used. By applying SVM and PC-ANN to the raw data spectra, the model that achieved the highest accuracy correctly classified each model in the measurement set according to its chlorpyrifos residue concentration. In the analysis of an unknown dataset, 40 samples were collected, so after the sample achieved 100 % success, F1-victory. The researchers found that the proposed portable NIR spectrometer, combined with ML algorithms (PLS-DA, SVM, and PC-ANN), could detect chlorpyrifos [46].

The use of portable NIR spectroscopy in conjunction with an ML technique for the nondestructive detection of pesticide residues (chlorpyrifos) in bok choi (Brassica rapa subsp. chinensis) has been studied. Vegetables sprayed with pesticides pose health risks to consumers. In this study, we used a combination of NIR spectroscopy and ML algorithms to detect the chlorpyrifos residues in bok choi. These algorithms include Partial Least-Squares Discrimination Analysis (PLS-DA), Support Vector Machines (SVM), Artificial Neural Networks (ANN), and Principal Component Artificial Neural Networks (PC-ANN). 120 bok choi samples were collected from two small greenhouses where they were grown in isolation [46]. There were 60 samples in each of the pesticide and non-pesticide treatment groups. Two milliliters per litre (mL/L) of chlorpyrifos 40% EC residue was added to the vegetables before they were sprayed. They interfaced a compact single-board computer with a commercially available handheld NIR spectrometer covering the range 908–1676 nm. Using ultraviolet (UV) spectrophotometry, they determined the presence of pesticides in bok choi. Using SVM and PC-ANN with raw data spectra, the most accurate model properly identified all the samples included in the calibration set based on their chlorpyrifos residue concentration. A satisfactory F1-score (100%) was obtained after testing the model on an unknown dataset consisting of 40 samples. Researchers have found that chlorpyrifos residues on bok choi could be detected using the suggested portable NIR spectrometer in conjunction with ML algorithms (PLS-DA, SVM, and PC-ANN) [46].

Because typical agricultural pest detection methods rely on manual selection of relevant feature sets, they are limited, ineffective, and time-consuming. To accurately identify 102 prevalent agricultural pest species, this study provides a cutting-edge crop pest recognition strategy based on deep Convolutional Neural Networks (CNN), as shown in Fig. 13. To obtain better accuracy even with a smaller pest dataset, the pre-trained model Mobile Net was retrained to take advantage of the knowledge learned from a larger and more generic dataset [74]. One hundred twenty-five distinct models were trained on the IP102 pest dataset. The best model was chosen after careful consideration of a wide range of models, the effects of several dataset splits, and hyperparameter adjustment. The model is then used in a flutter-based smartphone app that can classify pests using either the device's built-in camera or an image from the device's gallery, whether the user is connected to the Internet or not.

Toxicological predictions [75–77] based on ML algorithms use simulation tools to assess the potential dangers of substances and chemicals [78–80]. These models use the power of ML algorithms to analyze large datasets and identify patterns that might predict the toxicity of novel compounds. These algorithms can estimate the probable toxicity of a new chemical with high accuracy by training on past data. This method has the potential to significantly reduce the time and cost of traditional toxicological testing methods. Moreover, ML-based toxicity predictions can aid in identifying the possible dangers associated with chemical exposure in a variety of scenarios, including occupational and environmental exposure. Various reports are presented in Table 1. However, it should be noted that these models are not ideal and should be used in conjunction with traditional testing procedures to provide accurate and dependable results. As technology advances, ML-based toxicity predictions are anticipated to become an increasingly significant tool for ensuring the safety of chemicals and substances in various industries.

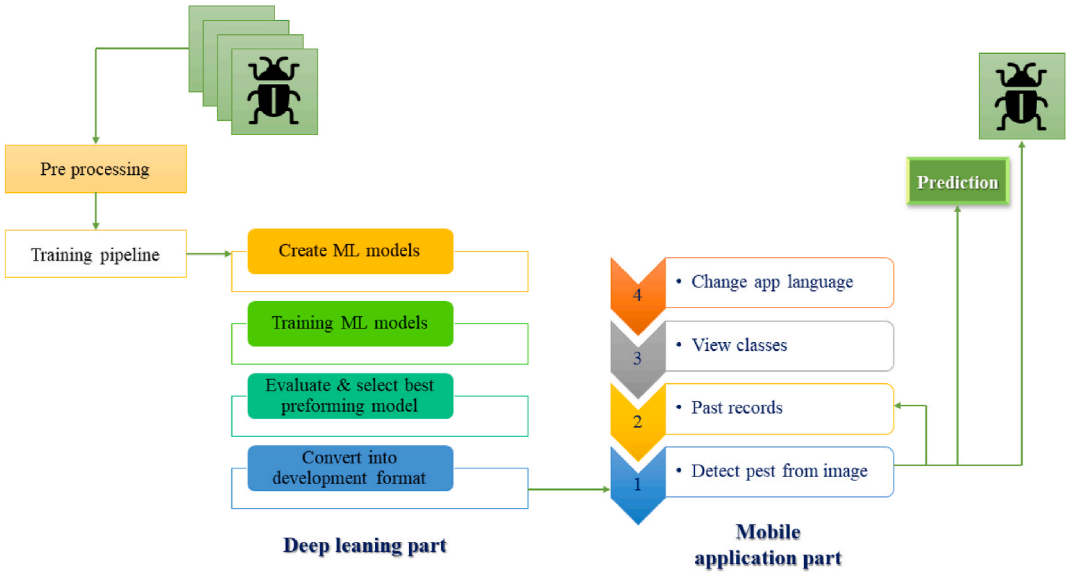

Fig. 13. *Block diagram for the ML model prediction* [74].

4. Conclusions and future prospective

In conclusion, the incorporation of ML algorithms into the field of pesticide toxicity prediction is a significant step towards addressing the complex difficulties associated with pesticide use in agriculture [92–94]. ML has emerged as a powerful ally that enables researchers, regulators, and stakeholders to make more informed decisions. Detecting and foreseeing pesticide toxicity in agricultural areas can greatly benefit from statistical insights and methods made available by ML. For toxicity prediction, it is recommended to use an SVM, k-NN, ANN, CNN, LDA, DQA, and RF, all of which are based on regression models. In the future, ML will be able to facilitate intermediate connections using mathematical techniques, such as the learning and optimization of moderating components based on input and output data alone. This will enable more precise and time-efficient pesticide toxicity predictions, thereby protecting both individuals and ecosystems from potential harm. ML can also help determine the most efficient and long-term strategies for pest management, thus decreasing the use of potentially dangerous pesticides. To ensure safe and responsible practices, it is essential to consider the ethical and social implications and consult specialists in the subject. As we progress, it is imperative to strike a balance between agricultural productivity and environmental preservation. ML models offer a valuable tool for achieving this equilibrium by guiding the judicious use of pesticides, minimizing risks to ecosystems and human health, and contributing to a more sustainable and responsible agricultural future.

4.1. *Consent to publish*

All authors consent to publish.

Data availability statement

Data included in article and referenced in article.

CRediT authorship contribution statement

Ganesan Anandhi: Writing – original draft, Formal analysis, Data curation, Conceptualization. **M. Iyapparaja:** Writing – review & editing, Supervision, Investigation.

Declaration of competing interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: M. Iyapparaja reports article publishing charges was provided by Vellore Institute of Technology. M. Iyapparaja reports a relationship with Vellore Institute of Technology that includes: employment. If there are other authors, they declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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