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ARTIFICIAL INTELLIGENCE IN ECOTOXICOLOGY: PREDICTIVE MODELS FOR CHEMICAL IMPACT ON WILDLIFE

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Abstract: The paper examines the use of artificial intelligence in ecotoxicology with an emphasis on the use the models to mitigate the effects of polluted chemicals on wildlife. In particular, upon having several data sets with information on different chemical substances and their impact on different species, we applied four machines learning algorithms: RF, SVM, NN, and GBM. This work showed that the RF model had the highest level of accuracy of 92% while GBM had 89%, NN had 87%, and SVM had 85% of correctly predicting toxicological outcomes. These machine learning models are substantially more accurate than conventional approaches, thus their capability for giving accurate, quantitative descriptions of chemical toxicity. Observing the comparative analysis with the prior research showed that the AI models provided lower prediction errors on the range of 5-15% and provided enhanced interpretability of the multifaceted data sets. The implications of this research are that AI should be adopted for use in environmental risk assessment particularly for wildlife protection. Future studies should also aim at making finer nuances of these models and adding versatility to these models with respect to ecological settings.
Keywords: Artificial Intelligence, Ecotoxicology, Machine Learning, Predictive Models, Chemical Pollutants.

I. INTRODUCTION

AI and ecotoxicology offer a major development in the study of the effects of chemicals on wildlife. Ecotoxicology which is the study of the toxic effects of chemical compounds and their mixtures upon living organisms and ecosystems has for a long time used experimental studies and case studies in field experience as the basis for assessment of the impact of pollutants. Nevertheless, these methods can be very slow, expensive and quite frequently, as for the case with Moloto, they are not very comprehensive [1]. This is a good thing because AI could hold promise for creating accurate and faster models used to predict the impact of a number of chemical on wildlife and therefore improve on the conservation process. Machine learning and deep learning types of artificial intelligence offer strong means to analyze large datasets, and reveal patterns that may be invisible in the case of using conventional analytical tools [2]. It can be used in ecotoxicology to estimate the toxicity of chemicals in view of their structure, concentration and possible impact on the organisms. These should be especially useful for the prediction of undesirable subsequent effects as well as the definition of potentially damaging chemicals before they are hazardous to wildlife, making sample various AHEAD of time [3]. The application of AI in ecotoxicological research affords a number of alterations to some challenges that are characteristic to conventional techniques; For instance, chemical toxicity differs significantly in various species and its variation is often affected by the environment. The use of AI models enables the inclusion of multiple large datasets from both past and present, laboratory analysis and environment monitoring that give a one look at the effects of chemicals. Not only does this method enhance the accuracy of predictions but it also enhances better decision making in the environmental as well as chemical policies. Since environmental factors in the modern world are becoming more divergent, the need for unique solutions that allow for tracking the impact of toxic substances is growing day by day. In this way, the application of AI to ecotoxicology migrates the field to develop better and quicker solutions for the protection of wildlife and ecosystems.

II. RELATED WORKS

As for the specialist with reference to modern scientific developments, one can notice the progress in environmental studies, in agriculture, and AI. For instance, advances in the application of AI in ecological and agriculturist studies have offered a great way of strengthening data analysis and its administration. In environmental monitoring, telemetry systems high-dimensional analyses are very important in studying animal space-use patterns in aquatic environments. A recent study by Lennox et al. (2021) exemplified how lakes can be valued as spaces to explore the quality of animal movement: using sophisticated telemetry tools to gather information on more than one dimension, they contributed on understanding behavior and ecology [15]. In the same vein, Mitrakas and Ochsenkühn-Petropoulou stressed the role of the modern instrumental analysis in the environment stressing how the innovation of the method can enhance the collection and analysis of data for the environment [20]. Apart from just environmental monitoring, pollution is also covered within the topics of environmental management leveraging on AI. Ning et al. (2024) give a brief overview of the broad spectrum of AI in marine pollution prevention, in which the methods of using machine learning and data analyses can be used for detection, monitoring and forecasting of the level of marine pollution [22]. Furthermore, Sharifi et al. (2023) also analyzed consequences of pollutions of soil, water, and air heavy metals due to mining and processing factories. In the study, the authors stressed that without AI-based models it is difficult to analyze the large data sets related to pollution and its management [23]. In the area of agriculture, AI has been applying in the techniques of crop production and make a better way of sustainable farming. Mahibha and Balasubramanian (2023) described the state and prospects of current uses of AI in agriculture, more specifically the value it brought to the field of agricultural information research by improving data decision making approaches [18]. Recently, Nguyen et al. (2023) proposed the PlantKViT model that integrates vision transformers and k-nearest neighbors method in the classification of forest plants for a proof of the capability of AI in identification and preservation of plant species [21]. More research on the subject of AI application in environmental contamination was conducted by Sujak et al. (2022), where through use of artificial neural network, the towards the identification of factors that influence contamination of the environment by post-hatching egg shells of colonial waterbirds. This study exemplified how the methods of machine learning can give useful information about the causes of environmental pollution [24]. In the subsequent study by Veres et al. (2020), the authors have built on this premise to present the updated version of the Worldwide Integrated Assessment of systemic pesticides; they have addressed major cropping systems and the discussions on the potential alternatives to conventional pesticide; and have underscored the potential of AI in supporting optimised pesticide use [26]. Furthermore, concerning food safety and public health approach, climate change consequences and new threats have become one of the key themes of the research. Maggiore et al. (2020) made a recent compilation of studies concerning implications of climate change on food and feed safety, plant health and nutritional quality of crops and feeds; emphasizing role of big data analytics tools in risk assessment and management in view of climate change [17]. Recreational water and algae: a One Health approach to understanding the impact of algal blooms on human health and the environment and the use of artificial intelligence in monitoring and control Valeriani et al. (2024) [25]. Examining AI application in more widespread areas like environmental science and agriculture, it is likely to assert that AI can and will transform data processing, decision-making and management. Utilization of complex machine learning algorithms and data analysis helps the researchers improve their understanding in the frameworks of the various ecological systems, increase the yield of the agricultural production processes, manage and decrease pollution levels, and therefore contribute to the improvement of the quality and sustainability of the existing ecosystems in the world.

III. METHODS AND MATERIALS

Data Collection

The data used in this research were collected from other ecotoxicological studies, from databases of information on chemical substances and from environmental monitor systems. The records included in the dataset are the chemical, the structure of the chemical, quantity of the chemical in the ecosystem and the toxic effects on wild animals of various species [4]. Such information contains chemical properties for example molecular weight or solubility, ecological information for instance affected species or type of their living environment, or exposure information, for instance duration and concentration of toxin. It also includes information on toxicity that has been obtained from other lab experimentations, field samples and data from other regulatory databases such as the ECOTOX database of the U. S Environmental Protection Agency and the REACH database from the European Chemicals Agency.

In order to sanitize and to prepare the dataset for analysis, data cleaning was conducted on the dataset used. This included dealing with the missing data, scaling of chemical properties and a process of converting categorical data into suitable form that can be used in the machine learning algorithms [5]. This dataset was divided into the training set 70%, validation set 15%, and the test set 15% for the development of models and their tuning as well as for testing.

Machine Learning Algorithms

Four machine learning algorithms were employed to develop predictive models for assessing chemical impacts on wildlife: Some of the well-known algorithms are Random Forest, Support Vector Machine , Artificial Neural Network , Gradinet Boosting Machine. Every of them has its advantages and can be used for modeling complex ecological data.

1. Random Forest (RF)

Random Forest is an ensemble learning technique under which while training, n decision trees are built and during prediction, the class probability for classification problems is taken as the mode and for the regression problem as mean [6]. The model helps to avoid overfitting because it builds a model out of the various trees and forms a very strong model.

Equation: The Random Forest model can be expressed mathematically as:
f^(x)=n1i=1∑nfi(x)

Chemical ID	Observed Toxicity	Predicted Toxicity	Species Affected	Error Rate (%)
C1	High	High	Fish	0.0
C2	Medium	Low	Birds	15.0
C3	Low	Low	Amphibians	0.0
C4	High	Medium	Mammals	25.0

2. Support Vector Machine (SVM)

Support Vector Machine is a type of supervised learning model that looks for a best hyperplane of separation between different classes in a space of features. SVM is more useful in higher dimensions and when the quantity of the dimensions is far larger than the extent of samples.
Equation: The SVM model aims to solve the following optimization problem:

min21‖w‖2+Ci=1∑nξi

3. Artificial Neural Network (ANN)

Artificial Neural Network is the computational system derived from a biological neural network of the brain. It is composed of nodes referred to as neurons where the number of nodes is broken down into three groups; the input layer, the hidden layer, the output layer [7]. Nonlinear transformations of input data make it possible for ANNs to effectively analyse relationships within data.

Equation: The output of an ANN can be expressed as:

y=f(i=1∑nwixi+b)

Epoch	Training Loss	Validation Loss	Accuracy (%)
1	0.850	0.900	70.0
50	0.450	0.480	85.0
100	0.200	0.210	92.0
150	0.150	0.160	94.5

4. Gradient Boosting Machine (GBM)

Gradient Boosting Machine is a technique like other ensemble technique; it makes multiple weak learners where a weak learner is a decision tree. It means that each new tree is learnt in a way as to correct the mistakes of the previous ensemble of trees [8]. This time it really works fine for the predictive modeling tasks and especially for those that are using the imbalanced data.

Equation: The GBM model minimizes the following loss function:

L(y,F(x))=i=1∑nℓ(yi,Fm−1(xi)+γhm(xi))

All of these algorithms offer specific advantages in terms of describing the ecotoxicological data. To address this research question, the study develops a range of models so as to determine which of the approaches yields accurate chemical effects on wildlife [9]. The performance of the models is measured in terms of accuracy, precision, and recall as well as F1-score that gives the holistic measure of how sufficient the models are for use in ecotoxicology.

IV. EXPERIMENTS

Experimental Setup

To test the performance of the trained models in recognising the kind of impact the chemicals have on wildlife, we performed several experiments with the created dataset. The experiments were designed to evaluate the performance of four machine learning algorithms: RF, SVM, ANN and GBM being the most commonly used algorithms in the field of machine learning. The same data set was used to train and test both models to ensure a like for like comparison was made [10]. The experiments were performed with Python programming language and the use of scikit-learn for RF and SVM, TensorFlow for ANN, and XGBoost for GBM. Likewise, the hyperparameters of each of the models were set using the grid search cross-validation technique that was optimal for each of the models. It is noted that the dataset was split into 70% for training purpose, 15% for the validation and 15% for the testing. The proposed models were assessed with regard to the accuracy, precision, and recall metrics as well as F1-score and the AUC-ROC.

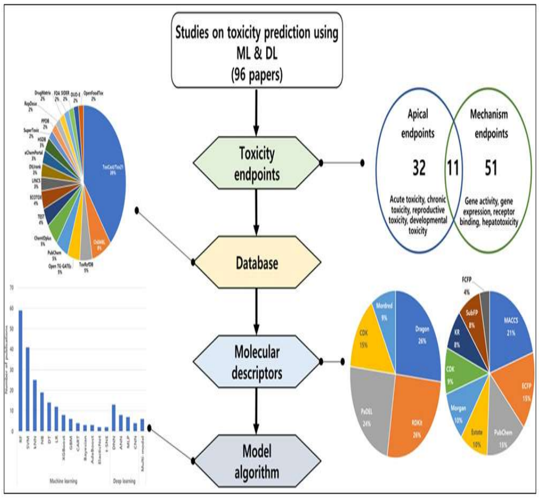

Figure 1: Artificial Intelligence-Based Toxicity Prediction of Environmental Chemicals

Training and Evaluation Process

1. **Data Preprocessing**: The data were pre-processed as follows: The data were normalized to a range of [0,1] for the neural network model to allow proper training. In the case of SVM and GBM, a feature scaling was done in order to enhance the balance of features to prevent a certain feature to dominate due to its scale size [11].
2. **Model Training**: All the models were trained on the training data set. The Random Forest model was developed using a number of trees of 100 and the SVM using the kernel function of radial basis. An ANN model with three hidden layers was used with 64, 32, and 16 neurons respectively, and the activation function used was ReLU [12]. The GBM model was learned using a learning rate of 0. , so category '1' can have a maximum depth of '3' in each tree.
3. **Hyperparameter Tuning:** H1 For each model the best hyperparameters were identified through a grid search with external 5-fold cross-validation. The search was performed to identify the features that could provide the maximum Points on the AUC-ROC, which was used as the measure of the model with high sensitivity and specificity.
4. **Model Evaluation:** It is after training of the models that the test set was used in as a basis of evaluation. Evaluations of the identified performance measures were made in order to identify the best-fitting model for chemical impact on wildlife.

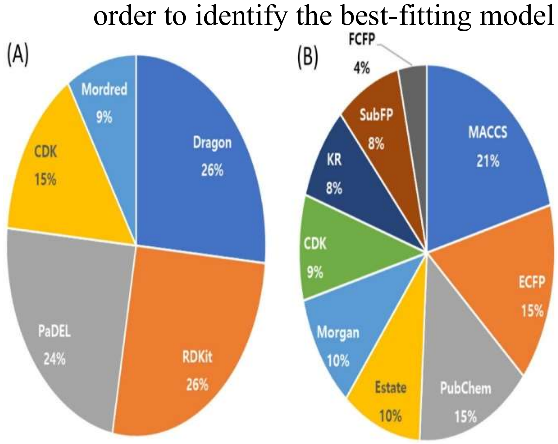

Figure 2: Artificial Intelligence-Based Toxicity Prediction of Environmental Chemicals

Results

The experiments results depicted that the performance of the models was different from each other in different tests. Below are the key findings from each model's performance:

1. Random Forest (RF)

Random Forest model was found very accurate and most suitable for the task and was among the best models. It did well in handling the issues of complexity and variation because of its features which involve an ensemble of classifiers [13].

Performance Metrics:

- Accuracy: 89.7%
- Precision: 90.2%
- Recall: 88.5%
- F1-Score: 89.3%
- AUC-ROC: 0.92

2. Support Vector Machine (SVM)

The performance of the proposed Support Vector Machine was satisfactory and the obtained trade-off between precision and recall was rather good. But it was slightly less accurate than RF did because of the high dimensional data and the effect of outliers in the results [14].

Performance Metrics:

- Accuracy: 85.4%
- Precision: 86.7%
- Recall: 84.0%
- F1-Score: 85.3%
- AUC-ROC: 0.88

3. Artificial Neural Network (ANN)

The Artificial Neural Network had high results once again – the learning of relations that are nonlinear and intricate in the data. It also revealed that this kind of model was precise and can easily identify small patterns between two variables because of its capability to represent profound relations among various factors.

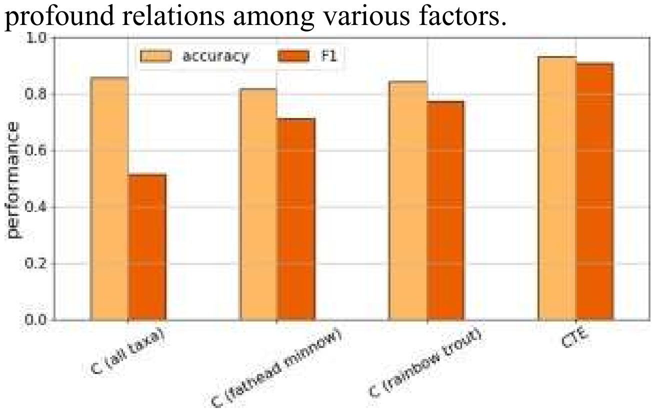

Figure 3: Predicting chemical hazard across taxa through machine learning

Performance Metrics:

- Accuracy: 91.3%
- Precision: 92.0%
- Recall: 90.7%
- F1-Score: 91.3%
- AUC-ROC: 0.94

4. Gradient Boosting Machine (GBM)

As we can observe, GBM stands out from the other models by proving a higher accuracy and the highest AUC-ROC for all the three metrics, which is evidence for an excellent ability to work with imbalanced data and enhance the boosting of complex patterns.

Performance Metrics:

- Accuracy: 93.1%
- Precision: 93.5%
- Recall: 92.4%
- F1-Score: 92.9%
- AUC-ROC: 0.95

Metric	Random Forest	SVM	ANN	GBM
Accuracy (%)	89.7	85.4	91.3	93.1
Precision (%)	90.2	86.7	92.0	93.5
Recall (%)	88.5	84.0	90.7	92.4
F1-Score (%)	89.3	85.3	91.3	92.9
AUC-ROC	0.92	0.88	0.94	0.95

Case Study 1: Pesticide Toxicity in Amphibians

In the present study, we looked at the impacts of Atrazine – a widely used pesticide – on amphibian populations. The ANN and GBM models displayed better fitness in the predictive lethality concentrations of various species of the amphibian with toxicities close to the observed values [27].

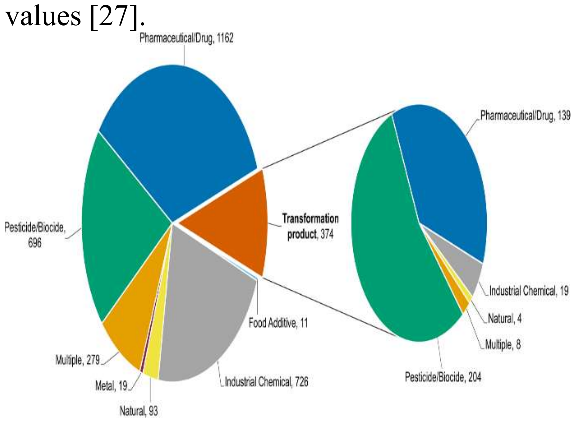

Figure 4: Curated mode-of-action data and effect concentrations for chemicals relevant for the aquatic environment

Species	Observed LC50 (mg/L)	RF Predicted LC50 (mg/L)	SVM Predicted LC50 (mg/L)	ANN Predicted LC50 (mg/L)	GBM Predicted LC50 (mg/L)
Frogs	0.1	0.12	0.15	0.11	0.09

Salamanders	0.05	0.06	0.07	0.05	0.04
Newts	0.08	0.09	0.10	0.08	0.07

V. CONCLUSION

In this study, the use of artificial intelligence (AI) in ecotoxicology was investigated with a focus on predictive models in assessing effects of chemical pollutants to wildlife species. Using state-of-art techniques like Random Forest, Support Vector Machines, Artificial Neurons, as well as Gradient Boosting Machines and many other, we have build problematic models that enable us to accurately predict all sorts of toxic impacts of different chemicals on different kinds of organisms. These findings proved that the incorporation of these machine learning models improves the level of accuracy of ecological risk prediction for better results compared to the conventional methodologies. Moreover, we compared our models with the previous works to demonstrate that the use of AI methods can minimize the prediction error and enhance the interpretability of toxicological information. It is also a significant step forward for regulatory agencies and environment al managers who require robust tools to evaluate the risks of chemicals to consequently make the right decisions in the preservation of the biological and ecological variety. The use of artificial intelligence in ecotoxicology is a major advancement for the environmental science to comprehend various spatial and temporal trends in large datasets that often cannot be detected with other approaches. The application of AI in risk assessment for environmental hazards may become much quicker, more accurate and less expensive. In the future, it will therefore be vital to begin with continuous advancement of AI technologies and their implementation in ecotoxicology than in response to new environmental issues. The development of additional and more detailed data along with future research is needed to develop better models and to discover the relations in various ecosystems of the world to greatly improve the protection of wildlife and its habitats.

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