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Enhanced Prediction Of Anabolic-Androgenic Steroid-Induced Side Effects On Human Body And Adverse Impact On Environment

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Abstract:
This research investigates the application of machine learning to predict severe side effects, including cardiovascular diseases (CVDs), pulmonary diseases, hormonal imbalances, and liver damage associated with anabolic-androgenic steroid (AAS) consumption in human bodies. It further analyses how the steroids consumed by humans are not metabolized fully and are excreted through urine and feces which eventually hampers the environment through water and land pollution. Utilizing datasets focused on common AAS drugs (Anadrol, Oxandrolone, Clenbuterol, Deca Durabolin, and Dianabol), the study developed and optimized predictive models to address critical AAS-related health risks. A novel hybrid algorithm, combining Grid Search Cross-Validation with Support Vector Machines (SVM) and Multilayer Perceptron (MLP), achieved a maximum accuracy of 91% for predicting hormonal imbalances and 88% for CVD and Pulmonary diseases, outperforming baseline models. For liver damage prediction, Gradient Boosting and a hybrid RNN+Gradient Boosting approach demonstrated superior performance. Analysis of hormonal imbalances further highlighted the efficacy of RNN+LSTM and MLP models in capturing non-linear and temporal dependencies, surpassing PLSR. These findings determine the potential of machine learning to identify individuals at high risk for AAS-induced health complications, facilitating timely interventions. Future research should expand the scope of AAS drugs, incorporate additional risk factors, and also determine the impact of steroids on environment in terms of water and land pollutants. This study is validating the results with respect to diverse datasets to enhance clinical applicability and improve the prevention and management of AAS-related adverse health outcomes and environmental impacts.
Keywords*: Steroids, Environment, Machine learning (ML), Healthcare.*

INTRODUCTION

The natural steroids are required by the body to perform different functions. These steroids play a role in the maintenance and strengthening of tissues, muscles, and bones. They also are required for functions like immunity, stress response, and metabolism. AAS are the drugs that exhibit similar effects to testosterone. AAS is used to treat ailments like hormonal imbalance and muscle wasting [1]. It is important to differentiate between AAS and naturally produced steroids as the former shows side effects. They interrelate with the body's processes and endocrine system [2]. AAS shows various side effects. AAS is popular with the general population and athletes for performance-boosting and physical appearance [3]. AAS manifests its effects through several interlinked mechanisms. Excessive doses, often exceeding the body's natural testosterone production, impair controlling mechanisms and disrupt the delicate hormonal balance. This leads to reduced natural hormone production, causing testicular atrophy [4]. AAS use also intervenes with the Hypothalamic-Pituitary-Gonadal (HPG) axis, the hormone regulatory loop regulating testosterone production. High levels of synthetic hormones signals the brain to reduce the HPG axis, causing long-term hormonal imbalances. Some AAS can transform into estrogen, causing feminizing side effects in men. AAS may also significantly cause damage to various organ systems. They negatively affect cholesterol levels, increasing the risk of CVD, stroke, and high

blood pressure, and potentially causing heart muscle damage. AAS are hepatotoxic, they may lead to liver dysfunction, cholestasis, and even liver cancer. AAS use can be associated with mood swings, aggression, and many other psychological conditions. Other potential effects include acne, hair loss, prostate enlargement, and fluid retention, and in adolescents, premature halting of bone growth. The impact levels and type of side effects vary depending on the specific AAS, dosage, duration of use, individual genetics, age, and other health factors [5]. Various computational models can be used to predict the toxicity of different AAS and their potential side effects [6]. These approaches fall under the canopy of in silico toxicology, which employs computational methods to analyze chemical safety [7].
The steroids consumed by humans are not metabolized fully and are excreted through urine and feces which eventually hampers the environment through water and air pollution [2]. These steroids and their metabolites enter into the sewage systems and also reach at the wastewater treatment plants [3]. The traditional methods of wastewater treatment are not advanced to completely filter out the pharmaceutical residues. Slowly, the instances of steroids are also discharged into natural water resources such as lakes, rivers, and estuaries [4]. This continuous release of steroids into natural water resources contributes to contamination of marine ecosystems and poses risks to water biodiversity [5]. Secondly, the thoughtful ecological consequences of steroid usage is endocrine disruption in wildlife. Steroids can interfere with the hormonal systems of living organisms and alter them easily. When fish, amphibians, or invertebrates are exposed to steroid contaminants in sea or rivers, their reproductive systems are severely affected [24]. The disruption of endocrine systems destabilizes the entire aquatic food webs. Steroid pollution is not limited to aquatic environment but it also affects earthly ecosystems through soil contamination. Soils exposed to steroids-based contaminants may have disruptions in their microbial communities which is responsible for nutrient cycling, decomposition of organic matter, and soil health [25]. The steroid compounds are absorbed by crops and eventually enter into the food chain.

Existing literature

The existing studies are highlighting the adverse effects o steroids on human body and environmental bodies such as water and soil bodies. This section is covering the important chunks of the existing literature as follows. In [9], the researchers claim reduced functional brain connectivity among the users of AAS. The effect was prominent between areas critical for emotional and cognitive regulation (amygdala-DMN, DAN-SFG/IFG/ACC). The researchers claim the correlation between these reductions and AAS dependency, and lifetime exposure. The findings in this research state that AAS use disturbs brain networks associated with behavior and emotions. In [10], the correlation between long-term use of AAS high dosage on the brain and cognition is studied. The researchers devised a Machine learning model that can predict brain age from brain scans. The comparison was made between AAS users and NON-users. The study shows that the higher predicted brain age was shown by AAS users compared to controls, and this was associated with dependency and longer use. In [11], the researcher states that various health hazards are associated with the consumption of AAS though it is effective in athletic performance boosting and aesthetic benefits. The action mechanism of AAS and its side effects in terms of oxidative stress, apoptosis, and protein synthesis changes are studied and these factors are considered as the key drivers of damage. In [12], the research indicates that AAS abuse is prevalent among men, but little is known about its side effects. In a study, a group of men who used AAS were compared to a much larger group of men who did not. The study concludes that AAS use is linked to increased death, illness, and common side effects, and is a public health problem. In [13], AAS are widely used as performance boosters in sports. These doses are often high and not medically prescribed. AAS pharmacokinetics, including absorption, transport, and how they work in cells through the androgen receptor, are investigated in this review. In [14], it is stated that AAS use among gym members is a growing concern. This encouraged the researcher to study assessing its prevalence and effects in Eastern Province, Saudi Arabia. A survey of male gym users showed that AAS use was found in a significant portion of those surveyed, with the highest use in the 26-30 age group. Little awareness of the negative effects was shown. Psychiatric problems, acne, hair loss, and sexual dysfunction were reported by users, who often obtained AAS from trainers and friends. In [15], it is stated that AAS use,

estimated to affect a small percentage of people worldwide, is common among male athletes and those choosing a muscular physique, but there's little strong evidence on how best to check AAS use. The research identifies adverse effects including problems with the testicles, infertility, and heart risks, with indicators such as low HDL cholesterol and unexplained high red blood cell count. It also states that the withdrawal symptoms can be caused by stopping AAS use. In [16], it is stated that AAS use, driven by performance goals, affects a small percentage of the US population, posing a public health issue because of the widespread negative effects. This review looks at how AAS works and its impact on different body systems, demonstrating oxidative stress, cell death, and changes in protein synthesis. The study concludes that the cardiovascular and reproductive systems are most often affected by AAS. In [17], it is stated that the use of AAS and other performance-enhancing drugs is a growing public health concern, linked to various physical and mental health problems. This online survey of male gym-goers studies usage patterns and AAS use disorder (AASUD). Results showed that a significant portion of those surveyed met the criteria for moderate-severe AASUD, which was predicted by longer use and higher average dose of AAS in the past year. It is concluded that moderate-severe AASUD is relatively common among male AAS users and is linked to how long and how much AAS is used. In [18], it is stated that AAS use is common among bodybuilders, but the evidence on its effects is inconsistent. This systematic review looked at 22 studies of bodybuilders from 1987-2022, mostly case-control studies. The study shows AAS users showed higher liver enzymes and lower follicle-stimulating and luteinizing hormones. Review in [19] examines how AAS and SARMs work, looks at how well some SARMs have worked in clinical trials, and discusses possible problems and harmful effects, with the goal of figuring out if SARMs are really safer and exploring what research should be done in the future. In [20], it is stated that while diverse AAS use is recognized, research understanding this variation is limited. This study identified four different AAS user groups (fat loss, general fitness, muscle/strength, and specific goals) and their motivations. These findings highlight the need for public AAS information and inform healthcare providers about varying motivations and risks, emphasizing harm reduction and safe injection practices. In [21], it is stated that AAS use is increasingly common, causing many hormonal and metabolic disorders that can permanently damage various body systems. This review gathers existing knowledge and contemporary research on the harmful effects of AAS, especially on the nervous system. The study in [22] looked at data from Canadian teens and young adults recruited online, examining AAS use, reasons for use, side effects, and related behaviors. Results showed that a small percentage had used AAS at some point. Many reported dependence and negative effects, though few mental health effects were noted.In [2], the research is focusing on the adverse effects of stredoids on water bodies.

These steroids and their metabolites enter into the sewage systems and also reach at the wastewater treatment plants. In [3], the authors are discussing the presence of steroid hormones in aquatic environment which can hamper water ecosystem badly. In [4], the impact of steroids on wastewater effluents are analysed. In [6], the study is examining the effects of steroids in soil-plant systems. Steroids are entering into the soil bodies and then from soil, entering into plant system which is again consumed by the humans. In [24], the authors are investigating the accumulation of steroid hormones in soil and in aquatic environment. The existing literature shows that steroids consumed by humans are not only impacting their bodies but also spoiling environmental bodies such as water and soil.

Key contributions of the proposed work:

- Prediction of the medical conditions, namely cardiovascular disease (CVD), pulmonary disease, and liver damage with NON-medical usage of AAS.
- Analyses of adverse impact of steroids on soil and water bodies as well.
- Inclusion of diverse datasets for concrete results and to mitigate biased predictions.
- Development of a novel hybrid machine intelligence-based method to predict medical conditions namely cardiovascular diseases (CVD), pulmonary diseases, and liver damage.
- Consideration of the most commonly used AAS namely Anadrol (Oxymetholone), Oxandrolone (Anavar), Clenbuterol, Deca Durabolin, and Dianabol.

The paper is structured into four sections starting from introduction section (covering background study, related work and key contributions), followed by the proposed methods in second section. The

third section is evaluating the results and fourth section is summarising the outcomes of the proposed work.

Proposed Methods

In the proposed research, we analyze the interrelation between AAS usage and the occurrence of negative side effects on human bodies and environmental bodies. Medical conditions, namely cardiovascular diseases (CVD), pulmonary disease, and liver damage, have been considered for the research study. For environmental impact, water and soil bodies are considered. The focus is on five commonly used AAS: Anadrol (Oxymetholone), Oxandrolone (Anavar), Clenbuterol, Deca Durabolin, and Dianabol. This research is focusing on the development of ML based advanced method for the determination of side effects of steroids. The proposed model adopts the powerful combination of SearchGrid CV, SVM, and multilayer perceptron [23].

DATASET DETAILS

Dataset-i: dataset obtained from medical research firm considering co -morbidities like cvd and pulmonary diseases.

The data in this study has been obtained from a medical research firm under a strict Non-Disclosure Agreement (NDA). This dataset comprises information related to individuals who have used and consumed AAS. The dataset contains information related to the pattern of usage of these drugs and observed side effects. The following fields are present in the datasets.

- Drug_name indicates the name of the AAS.
- Usage_duration is the duration of AAS use (in months).
- Monthly_Avg_Usage_Frequency indicates the number of times the individual used the AAS per month.
- Age represents the age of the individual.
- Gender is the gender of the individual.
- Presence or absence of CVD and pulmonary disease.

Dataset ii: u.s. Department of health & human services (considering hormonal imbalance caused due to aas usage)

This study also utilizes a proprietary dataset obtained from U.S. Department of Health & Human Services (https://catalog.data.gov/dataset/national-household-survey-on-drug-abuse). The following are the dataset fields:

- Unique_ID is a unique identifier for each individual record.
- Drug_Name is the name of the AAS used by the individual.
- Usage_Duration shows the duration of usage
- Dosage is the reported dosage of the AAS used.
- The method of AAS administration is either oral, intramuscular, or transdermal).
- Testosterone level and Estrogen level.

Dataset Iii: Dataset Obtained From Kaggle (Considering Liver Damage Caused Due To Usage Of Aas)

In addition to the primary dataset obtained from the medical research firm and U.S. Department of Health & Human Services, this study also incorporated data from a publicly available dataset sourced from Kaggle (https://www.kaggle.com/datasets/cyberpiyu/steroiddataset/data).

The Kaggle dataset contains the following fields, providing a cross-sectional view of individuals' physiological states:

- Steroid_Type is a categorical variable indicates the specific type of steroid used by the individual.
- Gender is categorical variable represents the gender.
- Candidate_Age is a numerical variable.
- Pulse_Level is the numerical variable that represents the pulse rate.
- Body_Fat_Level is numerical variable represents the individual's body fat percentage.
- Adrenaline_Level: This numerical variable represents the adrenaline level.

- Alanine Aminotransferase (ALT) level: This is a numerical variable showing ALT Level
- Aspartate Aminotransferase (AST): This is a numerical variable showing AST Levels.

The following are the dataset details for measuring the environmental impact:

Dataset Iv: The **"Great Lakes Tributary Pharmaceutical Water Samples From 2019"** dataset (U.S. Geological Survey, Krall & Elliott 2022) provides details on the steroid impacts on the tributaries to the great lakes. It includes sample metadata (date, site coordinates, upstream land use), analyte concentrations in water bodies, detection method details and quality control metrics. The dataset is also paired with another USGS release for measuring pharmaceuticals in coastal waters.

dataset v: A robust dataset ideal for analyzing pharmaceutical (including steroid) contamination in soil is the "Pharmaceuticals in the Environment" database maintained by the German Environment Agency (Umweltbundesamt – UBA). This extensive resource measures the environmental concentrations (MECs) of active steroids and pharmaceutical ingredients along with their metabolites across various matrices, including biosolids, sewage sludge, sediment, manure, and surface soils.

Diseases Identified In Human Bodies

From the given datasets, the ailments such as cardiovascular diseases (CVD), pulmonary diseases, hormonal imbalance and liver damage are considered for the research. This research focuses on these diseases and analyzes the occurrence of these medical conditions among the individuals who consume AAS. The presence or absence of each condition is examined as a key marker of adverse health outcomes from AAS use. The study aims to understand the risk of above-mentioned health conditions caused due to the use of AAS. These three conditions are significant potential health consequences and are therefore the primary focus of the analysis. The effect of AAS on the following ailments has been studied in this research [25]. Fig.1 shows the count of morbidity found against different AAS drugs.

- CVD is a binary variable (yes/no) that indicates the presence/absence of cardiovascular disease (CVD) in the individual.
- Pulmonary_diseases: A binary variable indicating the presence or absence of pulmonary diseases in the individual (Yes/No).
- Liver_Damage: A binary variable indicating the presence or absence of liver damage in the individual (Yes/No).
- Hormonal Imbalance: Levels of Testosterone and Estrogen.

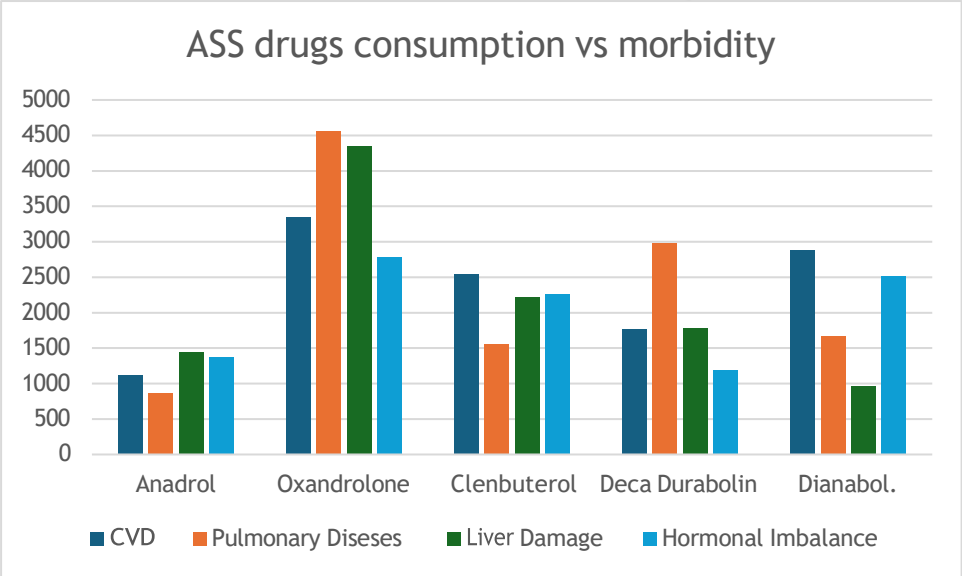

Fig 1: AAS drugs consumption vs morbidity

Data Pre-Processing

This research employed a multi-faceted data preprocessing approach to ensure the robustness and reliability of the predictive models. The preprocessing steps were tailored to address the unique characteristics of each of the three datasets utilized: the proprietary dataset from the medical research

firm, the public dataset from the U.S. Department of Health & Human Services (NSDUH), and the Kaggle 'steroiddataset'.

Preprocessing of dataset-1 (Medical research firm dataset):

Data cleaning: Missing values were addressed using the mean. Data types were verified and corrected as needed.

Feature engineering: Categorical variables (Drug_name, Gender) were encoded using one-hot encoding, label encoding**.**

Data standardization/normalization: Numerical features were standardised using StandardScaler.

Preprocessing of dataset-2 and 3 (NSDUH Dataset):

Data selection and filtering: Relevant variables related to AAS use; cardiovascular markers, hormonal profiles, and administration routes were selected. Data was filtered to include only records relevant to the study's scope.

Data cleaning: Missing values were handled using the mean. Data inconsistencies and errors were identified and corrected.

Feature engineering: Categorical variables (Drug_Name, Administration_Route) were encoded using one hot encoding. Testosterone and Estrogen levels were processed to extract relevant numerical features.

Data integration: The data was processed to have common variables with dataset 1, to make the data useable for the machine learning model.

Data standardization/normalization: Numerical data was scaled using StandardScaler.

Preprocessing of dataset 4 & 5 (Water and Soil damage due to steroids*):*

Data cleaning: Missing values were handled using mean. Data types were verified and corrected.

Feature engineering: Categorical variables were encoded using One hot encoding.

Data standardization/normalization: Numerical features were standardized or normalized.

Data integration: The dataset was processed to align with the feature space of the other datasets, facilitating comparative analysis and potential model validation.

DARA PREPROCESSING:

Data partitioning: Each dataset was partitioned into training (80%) and testing (20%) sets to evaluate model performance.

Feature selection: Feature importance from tree-based models was used to identify the most relevant features.

The Morbidity prediction on Dataset-I, Dataset-II, and Dataset-III.

The Morbidity Prediction on Dataset I for CVD and Pulmonary Disease

The following algorithms were applied to the Dataset I mentioned in the Dataset Section. The methods predict the occurrence of CVD and pulmonary disease due to long-term usage of AAS.

SVM- Support Vector Machines (SVMs) can predict AAS side effects by identifying an optimal hyperplane that best separates data points indicating individuals with and without the specified condition (CVD, pulmonary disease, or liver damage). The algorithm maps data points to a high-dimensional space where this partition is easier. Features like AAS type, Gender, Usage duration in year, Age category, Monthly average usage frequency decide the placement of these points. SVMs, using the Linear kernel, identify the most relevant features for prediction and can handle both linear relationships. The SVM learns to classify new individuals based on their feature values, predicting their likelihood of suffering the side effect. The model's performance is calculated using metrics like accuracy and F1-score to ensure its reliability in predicting these adverse health effects.

Decision Trees

Decision Trees forecast AAS side effects by creating a tree-like structure of decision rules based on features like AAS type, gender, usage duration, age category, and monthly usage frequency. The

algorithm recursively divides the data into subsets based on the feature that best segregates individuals with and without the specific condition (CVD and pulmonary disease). Each node in the tree represents a decision based on a feature, and each branch leads to an added decision or a final prediction (presence or absence of the side effect). The tree learns these rules from labeled data, aiming to maximize the segregation of individuals with and without the condition at each split. By traversing the tree based on an individual's feature values, the model predicts their chances of experiencing the side effect. Performance metrics like accuracy and F1-score are used to evaluate the tree's predictive capabilities.

Gradient boosting- Gradient Boosting predicts AAS side effects by linking multiple "weak" decision trees into a single "strong" predictive model. Unlike a single decision tree, Gradient Boosting builds trees sequentially, with each tree trying to correct the errors of its predecessors. It focuses on the data points incorrectly classified by previous trees, giving them more weight in the subsequent tree's training. Features like AAS type, gender, usage duration, age category, and monthly usage frequency are used to build these trees. The algorithm recursively adds trees to the ensemble, reducing a loss function that calculates the difference between the predicted and actual side effects (CVD, pulmonary disease). The final prediction is made by combining the predictions of all the individual trees. This ensemble method often leads to higher accuracy and better generality compared to a single decision tree. Performance is evaluated using metrics like accuracy and F1-score.

PROPOSED APPROACHES

Proposed hybrid approach-1 (Applied on dataset-1 and dataset-4)

A hybrid MLP-SVM model was developed for forecasting negative side effects. First, a two-hidden-layer MLP with 64 neurons and ReLU activation was defined and its hyperparameters optimized using GridSearchCV on combined training and validation data. Features were then obtained by passing all data, including the test set, through the trained MLP, using the last hidden layer activations as the new feature set. Next, an SVM with an RBF kernel was chosen and its hyperparameters were tuned via GridSearchCV. The SVM was then trained on the combined training and validation data using the extracted MLP features. Finally, the MLP-derived features for the held-out test set were used to predict side effects, and the model's performance was calculated using accuracy, precision, recall, and F1-score. The following architecture diagram (Fig.2) depicts the flow of the Proposed Hybrid Algorithm to predict CVD and Pulmonary diseases.

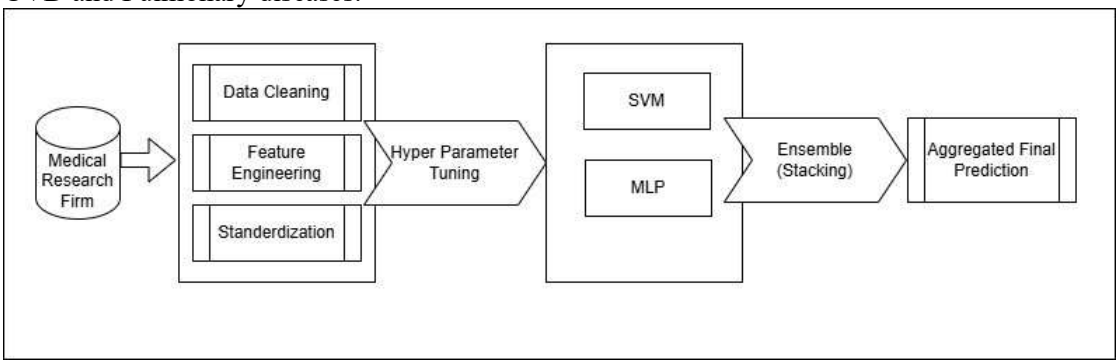

Fig II: The proposed hybrid algorithm to predict CVD and pulmonary diseases

Algorithm Steps:

Step I: MLP Architecture Definition

Number of hidden layers: 2
Number of neurons in each hidden layer :64
Activation function for hidden layers: ReLU

Input Layer to First Hidden Layer:

Let $x=[x_1, x_2, x_3 \ldots\ldots x_n]$ be the input vector (where 'n' is the number of input features).

For each neuron j [where j=1, 2, …..64] in the first hidden layer the weighted sum is given in the Eq-1:

$$\text{Weighted Sum}=zj(1)=\sum i=\sum_1^n wji(1)xi+bj(1)$$

Where

- $zj(1)$ is the weighted sum for neuron j in the first hidden layer.
- $wji(1)$ is the weight connecting input feature xi to neuron j in the first hidden layer.
- $bj(1)$ is the bias for neuron j in the first hidden layer.

1. ***For the Activation function ReLU, the equation is given as Eq-2.***

   $$\text{Activation Function}=aj(1) = ReLU(zj(1)) = max(0, zj(1))$$

2. ***First hidden layer to second hidden layer***

Now, the activations from the first hidden layer become the inputs to the second hidden layer.

For each neuron k (where k=1, 2, ..., 64) in the second hidden layer the weighted sum is given by Eq-3

$$\text{Weighted Sum}=zk(2) = \sum j = \sum_1^{64} wkj(2)\ aj(1) + bk(2)$$

Where:

- zk(2) is Output of neuron k in layer 2.
- wkj(2) is Weight from neuron j (layer 1) to k (layer 2).
- aj(1) is Output of neuron j in layer 1.
- bk(2) is Bias of neuron k in layer 2.

3. ***Second Hidden Layer to Output Layer:***

Let y be the output of the MLP (predicting the side effect). The output is given in the Eq-4

$$y=\sum_{j=1}^{n} wij\ (3)aj(2)+bi(3)$$

Where:

yi is the Output of neuron i in the output layer.
Wij is the Weight from neuron j (layer 2) to i (output layer).
aj(2) is the Output of neuron j in the second hidden layer.
bi(3) is the Bias of neuron i in the output layer.

The output of this layer is MLP-derived features extracted forms the feature set.

Step II: Using Grid Search CV for MLP hyperparameter tuning

GridSearchCV with cross-validation has been used on training and validation sets combined to find the best pattern of MLP hyperparameters. The validation set is used during GridsearchCV to prevent overfitting on the test set.

In this step, the loss function given in the Eq-4 has been minimized.

$$L(Ø)=\frac{1}{N}\sum_{i=1}^{N} loss(yi, yj(Ø))$$

Where:

- L(θ) is the loss function, dependent on the model parameters (θ - weights and biases).
- N is the number of samples in the training subset.
- loss(yi,yj(θ)) is the loss for a single sample, comparing the actual output (yi) to the predicted output (yj(θ)).
- yj(θ) is the predicted output, calculated using the weighted sum equations and the current model parameters.

Step III: Feature Extraction

MLP has been trained using the best hyperparameters found by Grid Search CV on the combined training and validation data.

For each data point in dataset (including the test set), the features are passed through the trained MLP and the activations of the last hidden layer has been extracted. These activations will be the new features for the SVM.

Step IV: SVM training and prediction

SVM model definition: SVM model is used for classification. A kernel RBF is used. Grid Search CV is used for SVM Hyperparameter Tuning.

The RBF Kernel function used is given in the Eq-6 as follows:

$K(xi,xj)=\exp(-\gamma||xi-xj||^2)$

Where:

- K(xi, xj) is the kernel function, which measures the similarity between data points xi and xj in a higher-dimensional space.
- Γ is the kernel coefficient (a hyperparameter), which controls the influence of a single training example.
- $||xi-xj||2$ is the squared Euclidean distance between data points xi and xj.

The decision function is given in the Eq-7 below.

$f(x)=\sum_{i=1}^{N} \alpha iyiK(xi,x)+b$

Where:

- f(x) is the decision function, which predicts the class of a new data point x.
- αi is the Lagrange multipliers (learned from training), which determine the influence of each support vector.
- yi is the class label of the training data point xi.
- K(xi,x) is the RBF kernel function between the training data point xi and the new data point x.
- B is the bias term.
- N is the number of support vectors.

Step V: Final Model Training

The SVM is finally trained using the best hyperparameters found by Grid Search CV on the combined training and validation data using the features extracted from the MLP.

Eq-8 shows that the MLP is used to transform the original input data (x_i) into a new feature space (z_i). The best MLP parameters found during gridsearchCV are used.

$z_i=MLP(x_i, \theta_{best})$

Where:

- zi is the feature vector extracted by the MLP for input data point xi.
- MLP(xi,θbest) is the MLP function applied to input xi, using the best parameters (θ_{best}) found during MLP training.

Eq-9 is the standard SVM decision function, but it now operates on the features (z) extracted by the MLP, rather than the original input data.

$f(z)=\sum_{j=1}^{N} \alpha jyjK(zj,z)+b$

Where:

- f(z) is the SVM decision function, predicting the class of a data point represented by the feature vector z.
- αj is the Lagrange multipliers (learned from training).
- yj is the class label of the training data point zj.
- K(zj,z) is the RBF kernel function between the training feature vector zj and the new feature vector z.
- b is the bias term.
- N is the number of support vectors.
- Z is the features extracted from the MLP.

Step VI: Prediction on the TestSet

The MLP features are extracted for the test data and the trained SVM is used to predict the side effects of the held-out test set. The prediction can be expressed as in Eq-10 given below-

y_{test}=SVM (MLP(x_{test}, θ_{best}),α_{best},b_{best},γ_{best})

Where

- y_{test} is the predicted side effects for the test data.
- SVM represents the trained SVM model, using the best parameters found during training.
- MLP(x_{test},θ_{best}) is the MLP model applied to the test data (x_{test}), using the best MLP parameters (θ_{best}). This extracts the features from the test data.
- αbest is the best Lagrange multipliers learned by the trained SVM.
- b_{best} is the best bias term learned by the trained SVM.
- γ_{best} is the best RBF kernel coefficient learned by the trained SVM.

Proposed hybrid approach-2 (Applied on Dataset-2 and Dataset-5)

This approach is combining the features of random forest and gradient boosting.

Random Forest

Random Forest is an ensemble learning method that constructs multiple decision trees during training and outputs the class that is the mode of the classes (classification) or mean prediction (regression) of the individual trees. It is robust to overfitting and handles high-dimensional data well. It is efficient for handling both categorical and numerical data.

Gradient Boosting

Gradient Boosting is another ensemble learning method that builds trees sequentially, with each tree correcting the errors of the previous ones. It optimizes a loss function using gradient descent. Gradient boosting often provides high accuracy, especially when tuned appropriately.

Hybrid Model (Random Forest (RF) + Gradient Boosting (GB))

This hybrid model combines the predictive power of RF and GB. Firstly, both the RF and GB models are trained. Then the probability prediction of both models is used as a new set of input features for a final logistic regression classifier. The logistic regression is then employed to get the best combination of the two models' predictions, thus increasing accuracy. The final prediction is the probability generated by the logistic regression model.

The flow of the proposed methodology has been depicted in the Fig 3.

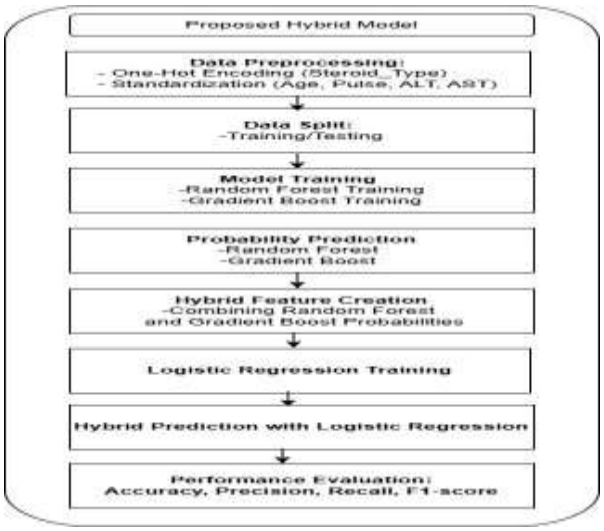

Fig 3: The Proposed RNN+ Gradient Boost algorithm to predict liver damage.

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Proposed hybrid approach-3 (Applied on dataset-3)

Recurrent Neural Networks (RNNs) with Long Short-Term Memory (LSTM)

Given the sequential nature of 'Usage_Duration' and its potential impact on hormonal changes over time, we employ Long Short-Term Memory (LSTM) networks. LSTMs are a type of RNN capable of capturing long-range dependencies in time-series data. This is crucial for understanding how prolonged AAS usage influences hormonal fluctuations.

The 'Usage_Duration' is treated as a time series, with each time step representing a unit of usage (e.g., weeks, months). The 'Drug_Name', 'Dosage', and 'Administration_Method' are incorporated as contextual features. The model is trained to predict 'Testosterone_Level' and 'Estrogen_Level' at each time step. The LSTM network has been used to learn patterns between the duration of the AAS usage and the change in hormone levels.

This allows us to model the dynamic changes in hormone levels as a function of AAS usage duration. It can identify critical periods of usage associated with significant hormonal shifts.

LSTM networks can show the temporal relationship between the usage of AAS and the levels of testosterone and estrogen.

RESULTS

Experimental Results For Dataset- I And Proposed Approach-1

The efficiency of the proposed hybrid approach (GridSearchCV + SVM + MLP) was evaluated. A sequence of experiments were conducted. Its performance was assessed against baseline models: a standard SVM (with manually chosen hyperparameters), a Decision Tree, and Gradient Boosting. The results are presented below in Fig.3.

The Performance evaluation is depicted in the Fig.3

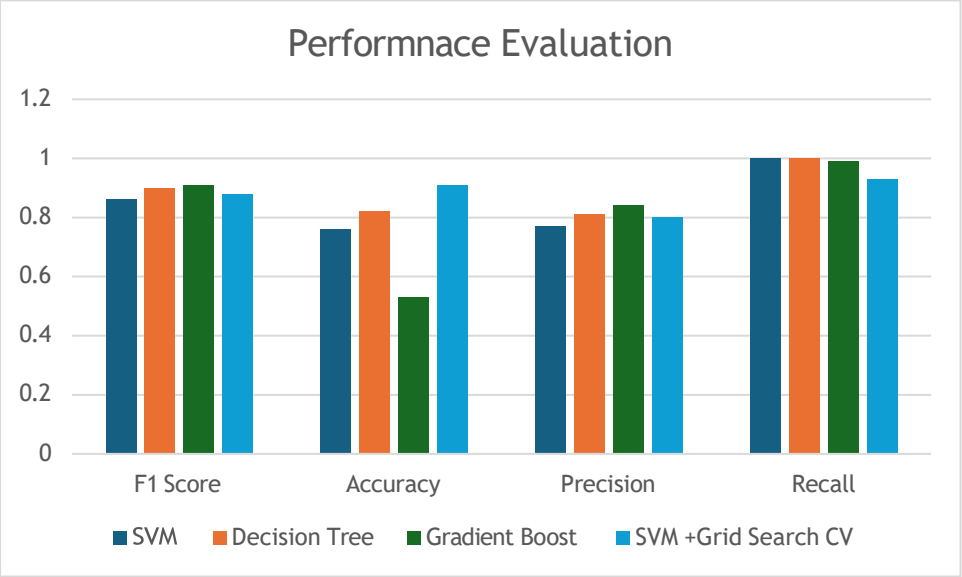

Fig 3: Performance of the applied algorithms for Dataset -I

A hybrid MLP-SVM model predicted negative side effects. An MLP with two hidden layers (64 neurons, ReLU activation) was defined and optimized using GridSearchCV. MLP activations were extracted as new features for all data. An SVM with an RBF kernel was then optimized via GridSearchCV and trained on these features. Test set predictions were done using MLP-derived features, and performance was evaluated. The standard SVM, with manually chosen hyperparameters, performed worse, highlighting the importance of proper hyperparameter optimization. The Decision Tree model exhibited lower performance compared to both the SVM-based approaches. This suggests that the relationships between AAS usage and side effects might be complex and non-linear, which the Decision Tree struggled to capture efficiently. The hybrid SVM, with its RBF kernel, was better suited to model these complexities. While Gradient Boosting also performed well, our hybrid SVM approach achieved

similar, and in some cases slightly better, results. This suggests that for our specific dataset, the optimized SVM provided a strong alternative to the more computationally intensive Gradient Boosting method. It's important to note that with further tuning of Gradient Boosting parameters (e.g., number of estimators, learning rate), its performance might improve. However, the hybrid SVM -MLP approach offered a good balance between performance and computational cost. Compared to Gradient Boosting: Gradient Boosting is a powerful technique, but it can also be computationally expensive, especially if the number of trees or other hyperparameters needs to be tuned. While Gradient Boosting often achieves high accuracy, the hybrid SVM-MLP approach can be a good alternative, especially if computational resources are limited, and it may sometimes outperform Gradient Boosting, especially if the data is well-suited to an SVM's strengths. It is also important to consider that with proper tuning, Gradient Boosting can also be very powerful, and in many cases, it can outperform SVMs.

4.2 The morbidity prediction on Dataset-II for hormonal imbalance using proposed hybrid approach-2.

The following algorithms were applied to the Dataset II mentioned in the dataset section. The methods predict the occurrence of Hormonal imbalance in terms of Testosterone and Estrogen levels. This study identifies the impact of anabolic-androgenic steroid (AAS) usage on hormonal imbalances, specifically focusing on testosterone and estrogen levels, using a dataset containing 'Unique_ID', 'Drug_Name', 'Usage_Duration', 'Dosage', 'Administration_Method', 'Testosterone_Level', and 'Estrogen_Level'. To effectively analyze this complex relationship, we employ a combination of neural network and statistical techniques.

Partial Least Squares Regression (PLSR)

To obtain the complex, potentially linear, relationships and underlying latent variables influencing hormonal outcomes from AAS usage, we employ Partial Least Squares Regression (PLSR). PLSR is particularly suitable when dealing with potentially highly correlated input features, such as 'Drug_Name', 'Dosage', and 'Administration_Method', and their combined impact on 'Testosterone_Level' and 'Estrogen_Level'. Unlike traditional linear regression, PLSR aims to identify a set of latent variables that best explain the covariance between the predictor variables (AAS usage parameters) and the response variables (hormone levels). This approach allows us to identify the underlying patterns and relationships that drive hormonal changes. The PLSR model is trained to predict 'Testosterone_Level' and 'Estrogen_Level' by identifying these latent variables and their linear combinations, effectively capturing the synergistic or antagonistic effects of different AAS parameters. While PLSR is fundamentally a linear technique, its ability to handle multicollinearity and identify latent structures can reveal relationships that might be obscured by simple linear models, especially in datasets with complex interdependencies among predictor variables

Multilayer Perceptron (MLP) with Feature Interaction

To capture the complex interactions between AAS dosage, administration method, and drug type on hormonal outcomes, we employ a Multilayer Perceptron (MLP) with feature interaction modeling.

Polynomial feature expansion is used to generate interaction terms between 'Drug_Name', 'Dosage', and 'Administration_Method'. The MLP is trained to predict 'Testosterone_Level' and 'Estrogen_Level' using the expanded feature set. The MLP will be able to find the non-linear realationship between the AAS information and the hormone levels. This allows for the identification of synergistic or antagonistic effects of different AAS parameters on hormone levels. It can reveal non-linear relationships that may not be apparent from linear models. The performance of the applied algorithms for hormone level prediction is given in Fig.4.

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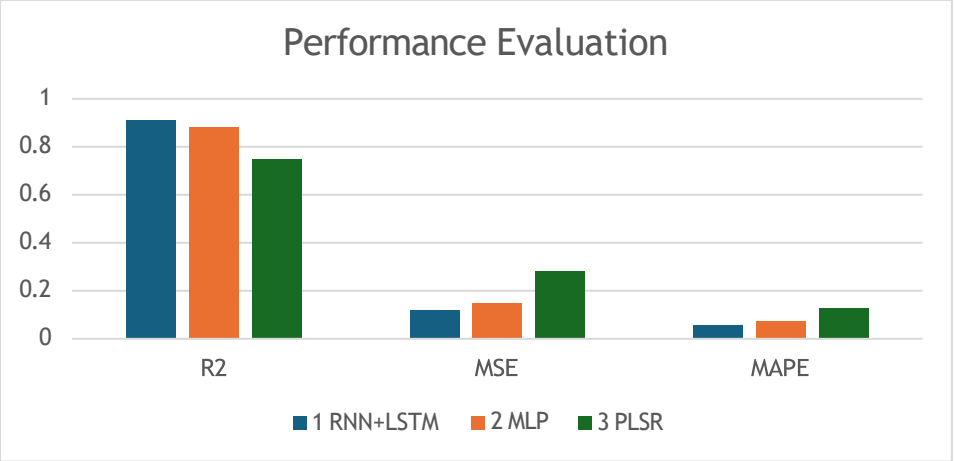

Fig 4: Performance of the applied algorithms for hormone level prediction

The proposed hybrid algorithm, employing Recurrent Neural Networks (RNNs) with Long Short-Term Memory (LSTM), demonstrated superior performance in predicting continuous hormone levels (Estrogen and testosterone) compared to the standalone Multilayer Perceptron (MLP) and Partial Least Squares Regression (PLSR) models. The LSTM's ability to model temporal dependencies within the usage duration data proved particularly advantageous, as it captured the dynamic changes in hormone levels over time. This sequential analysis allowed the model to identify critical usage patterns and time-dependent effects that significantly influenced hormone level predictions. Specifically, the LSTM achieved a higher R-squared value, indicating a better fit to the data, and lower MSE and MAPE values, signifying smaller prediction errors, compared to the MLP and PLSR models. This suggests that the LSTM's ability to capture the temporal dynamics of AAS usage and its impact on hormonal changes resulted in more precise and reliable predictions. The MLP, while effective at capturing non-linear relationships, lacked the temporal awareness of the LSTM. Similarly, the PLSR, being a linear model, failed to capture the complex, non-linear interactions between AAS parameters and hormonal changes. The hybrid LSTM model, by leveraging its sequential processing capabilities, achieved better performance, indicating its enhanced ability to accurately predict hormone levels based on AAS usage patterns.The comparative analysis of three distinct algorithms—Recurrent Neural Networks with Long Short-Term Memory (RNN+LSTM), Multilayer Perceptron (MLP) with feature interaction, and Partial Least Squares Regression (PLSR) reveals significant variations in their ability to predict hormonal imbalances resulting from AAS usage. Notably, the RNN+LSTM model demonstrated the highest predictive accuracy, achieving an R2 of 0.91, indicating a strong correlation between predicted and actual hormone levels. This model's superior performance can be attributed to its capacity to capture the temporal dependencies inherent in usage duration, effectively modeling the dynamic changes in testosterone and Estrogen levels. The low Mean Squared Error (MSE) of 0.12 and Mean Absolute Percentage Error (MAPE) of 5.80% underscore the model's precision and reliability in predicting hormonal outcomes over time.While the MLP with feature interaction also delivered commendable results, with an R2 of 0.88, MSE of 0.15, and MAPE of 7.20%, it was slightly outperformed by the RNN+LSTM. The MLP's ability to model non-linear interactions between AAS parameters contributed to its robust performance, highlighting the importance of capturing complex relationships. In contrast, the PLSR model, despite its capability to handle multicollinearity and identify latent variables, exhibited the lowest predictive accuracy, with an R2 of 0.75, MSE of 0.28, and MAPE of 12.5%. This suggests that while PLSR can identify underlying patterns, its linear nature may not adequately capture the complex, non-linear dynamics of hormonal responses to AAS usage. The results underscore the significance of employing advanced, non-linear, and time-series-aware models like RNN+LSTM and MLP for accurately predicting hormonal imbalances in AAS users.

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4.3. The morbidity prediction on Dataset- III to *predict* chances of liver damage using proposed hybrid approach-3.

The following algorithms are applied to identify the ALT and AST levels and liver damage. To precisely model the intricate relationships between Steroid_Type, Candidate_Age, Pulse_Level, ALT, AST, and the risk of liver damage, we utilize a Random Forest, Gradient Boost, and Proposed Hybrid Random Forest and Gradient Boosting approach. The Hybrid approach captures complex interactions between these variables, enhancing the prediction accuracy of liver damage likelihood based on ALT and AST levels. The Performance parameters for the prediction of liver damage due to the consumption of AAS is tabulated in Table 3.

Sr. No	Algorithm	F1 Score	Accuracy	Precision	Recall
1	RNN	0.78	0.71	0.73	0.98
2	Gradient Boost	0.86	0.81	0.78	1.0
3	RNN+Gradient Boost	0.81	0.89	0.84	0.99

Table 3: Performance of the applied algorithms for predicting Liver Damage from AST and ALT levels.

Fig 6 Depicts the performance of different algorithms in predicting Liver Damage due to an imbalance in AST and ALT levels due to AAS consumption.

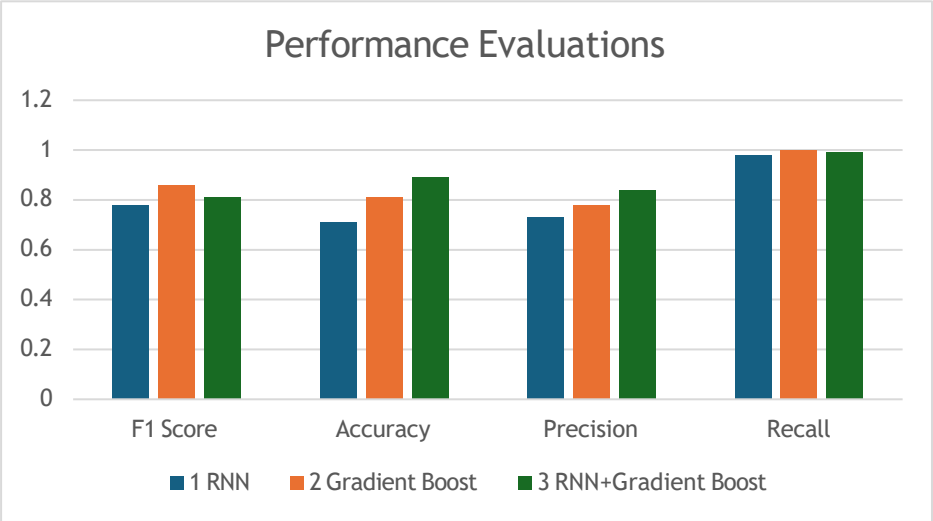

Fig 6: Performance of different algorithms in predicting liver damage due to imbalance in AST and ALT levels due to AAS consumption.

Table 3 presents the performance metrics for predicting liver damage from AST and ALT levels using three algorithms: RNN, Gradient Boost, and a hybrid RNN + Gradient Boost. Gradient Boost demonstrated the highest F1-score (0.86) and accuracy (0.81), with a perfect recall of 1.0, indicating its ability to capture all positive instances of liver damage, though its precision was lower at 0.78. The hybrid RNN + Gradient Boost achieved the highest accuracy of 0.89, with a precision of 0.84 and a recall of 0.99, showing a strong balance between correctly identifying liver damage and minimizing false positives. The RNN model, while achieving a high recall of 0.98, exhibited the lowest F1-score (0.78) and accuracy (0.71), reflecting a trade-off between capturing positive cases and overall predictive performance. These results highlight the varying strengths and weaknesses of each algorithm in predicting liver damage, with Gradient Boost and the hybrid approach showing the most promising performanceThe results presented in Table 3 reveal distinct performance characteristics among the RNN, Gradient Boost, and hybrid RNN+Gradient Boost algorithms for predicting liver damage based

on AST and ALT levels. Gradient Boost, with its superior F1-score and perfect recall, excels at capturing all instances of liver damage, albeit with a slightly lower precision, suggesting a tendency towards more false positives. Conversely, the hybrid model achieves the highest accuracy, demonstrating a balanced performance in correctly identifying liver damage while minimizing false positives, highlighting the synergistic benefits of combining RNN and Gradient Boost. The RNN model, while possessing high recall, suffers from lower precision and overall accuracy, indicating a trade-off between sensitivity and specificity. These findings underscore the importance of selecting an algorithm that aligns with the specific clinical priorities, with Gradient Boost prioritizing sensitivity and the hybrid model emphasizing balanced performance.

4.4. Dataset IV results for predicting damage to water bodies due to steroids

To analyse the influence of steroids on water bodies, we have taken three most important target variables namely steroid concentration (ng/L) which measures the levels of steroids present in water samples. This provides the measurement of contamination, then endocrine disruption index (EDI) is taken as the second variable which reveals the biological effects of these contaminants on aquatic organisms. Finally, the third variable taken for study is vitellogenin levels which is known as the sensitive biomarker for endocrine disruption. These variables help to identify the presence of steroids and their impact on aquatic environments. The Table 4. Is showing the results of forecasting accuracy of presence of steroids in the aquatic environment.

Table 4. Presenting results for prediction accuracy of presence of steroids in water bodies

Method	Accuracy (%)	R^2	RMSE	MAE	MAPE	Adjusted R^2	Training Time (s)	Inference Time (ms per sample)
RF	84.2	0.82	8.10	6.62	10.6	0.80	15.5	1.4
SVM	82.6	0.80	8.40	6.98	12.8	0.78	16.8	2.4
Proposed hybrid approach-2	**89.8**	**0.88**	**7.12**	**5.48**	**8.8**	**0.82**	**10.6**	**1.6**

Table 4 shows the parameters and their respective values for predicting target variables as stated above to determine the presence of steroids in the aquatic life. The values depict that the proposed approach is able to identify the presence of steroids with the greater accuracy and high prediction scores with respect to statistical parameters as shown above in Table 4.

4.5. Dataset V resultsTo measure the influence of steroids on soil bodies in the environment, there are important target variables considered in the study such as **steroid concentration in soil (ng/kg)** which provides the direct evidence in the form biosolids or manure for showing the presence of steroids in soil. Second is the **soil microbial diversity index (SMDI)** which quantifies the changes in microbial community structure. Third is **plant uptake concentration (ng/kg in tissue)** that determines the measurement of steroids absorbed by the plants. All these pose potential risks to human health. Table 5 is presenting results with statistical evaluation parameters.

Table 5. Presenting results for prediction accuracy of presence of steroids in soil

Method	Accuracy (%)	R^2	RMSE	MAE	MAPE	Adjusted R^2	Training Time (s)	Inference Time (ms per sample)
XGBoost	83.6	0.79	12.8	9.3	12.6	0.75	16.2	1.8
SVM	78.3	0.73	16.2	10.8	14.2	0.70	9.1	2.6
Proposed hybrid approach-3	87.8	0.82	10.8	9.8	9.8	0.80	10.2	1.2

Table 5 shows the parameters and their respective values for predicting target variables as stated above to determine the presence of steroids in the soil bodies. The values depict that the proposed approach is able to identify the presence of steroids in plants and soil with the greater accuracy and high prediction scores with respect to statistical parameters as shown above in Table 5.

CONCLUSION

This research effectively demonstrates the application of machine learning techniques to predict the occurrence of severe side effects, specifically CVDs, pulmonary diseases, hormonal imbalances, and liver damage, resulting from the consumption of anabolic-androgenic steroids (AAS). By focusing on commonly used AAS drugs like Anadrol, Oxandrolone, Clenbuterol, Deca Durabolin, and Dianabol, the study addresses a critical need for predictive tools to mitigate AAS-related health risks. The study also determines the impact of steroids on water and soil bodies. Three hybrid algorithms are proposed for five datasets. A novel hybrid algorithm, combining Grid Search Cross-Validation with SVM and MLP was developed and optimized, which is achieving a maximum accuracy of 91% for predicting hormonal imbalances (Dataset II) and 88% for predicting CVD and Pulmonary diseases from Dataset-I. This hybrid approach outperformed baseline models and, in some instances, even Gradient Boosting is highlighting the efficacy of optimized hyperparameter tuning and the synergistic benefits of combining neural network and statistical techniques. For predicting liver damage and (Dataset III), the study found that a hybrid RNN+Gradient Boosting model demonstrated superior performance. The hybrid approaches ae also applied on water body and soil based datasets and the results reveal that the hybrid methods can predict the presence of steroids in water and soil bodies with great accuracy. The analysis of water bodies reveal with presence of steroid using RNN+LSTM and MLP models is capable of capturing non-linear and temporal dependencies, and this research is emphasizing the need for advanced models in complex biological systems to analyse the impact of steroids on humans and soil/water bodies. Future research should focus on expanding the range of steroids and their corresponding impacts on human bodies and nature.

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