RESEARCH PAPER

An Intelligent Drug Detection and Classification Framework Using Machine Learning and Deep Learning

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ABSTRACT
Drug detection and classification are an important part of forensic science, public safety and chemical analysis. There are several ways in which drugs can be identified including chromatography, spectroscopy and chemical testing. This research looks to develop an intelligent methodology for detecting and classifying drugs using machine learning and deep learning. The project will use real world drug data to detect and classify drugs. This will be carried out by processing data, extracting features, training models and evaluating models. Once a dataset has been chosen the appropriate preprocessing steps will be taken to process the data. The data will then be classified using Support Vector Machine, Random Forest and neural networks. These models can be tested using accuracy, precision, recall, F1 score, specificity and confusion matrix. The main considerations will be looking at unbalanced classes, false positives, false negatives and generalisation of the models. An experimental analysis will be carried out to look at the advantages and disadvantages of the chosen methods. The aim of this project is to create a repeatable and efficient method for initial drug classification to help with research. The system can be used alongside confirmatory tests in a forensic lab. The results will show how effective and limitations of the system.

Keywords: *Drug Detection, Machine Learning, Deep Learning, Support Vector Machine, Random Forest, Substance Classification, Forensic Analysis.*
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1. INTRODUCTION

Drug detection and classification is a key aspect within Forensic science, Public Safety, Healthcare and Law Enforcements. Aiding investigations and analysis within a lab can be achieved using the ability to identify unknown substances. Traditionally chemical analysis, Chromatography, Infrared Spectroscopy and Raman Spectroscopy can be used to detect drugs[3]. However, this may require specialist equipment and skilled personnel to prepare samples for analysis. Intelligent detection systems can help with initial analysis. Recent developments in Machine Learning and Deep Learning methods have enabled automated classification of data. Using Machine Learning algorithms such as Support Vector Machine (SVM) and Random Forest models can be trained to detect patterns within structured data and extracted features[1]. Deep Learning models can be trained to identify complex characteristics from accurate input data. This will depend on the quality of data, number of classes, pre-processing and experimental design. This research will propose an intelligent drug detection and classification system. The selected Machine Learning and Deep Learning techniques will be implemented and evaluated using a validated data set. Data pre-processing, feature representation, training, hyperparameter tuning and evaluation will be carried out[2]. Analysis will be conducted using the accuracy, precision, recall, F1-score and confusion matrix of the classifiers. False positives and negatives will be considered along with how well it generalises to new samples. The aim of this research is to create an intelligent and repeatable framework that will allow comparison of initial classifications of substances. This should aid research and screening however will not replace confirmation analysis within a forensic lab.

2. LITERATURE REVIEW

Recent studies have looked into the application of machine learning and deep learning techniques for the detection and classification of drugs using spectroscopy and image processing[4]. One study looked into the application of handheld near infrared spectroscopy and machine learning for fast detection of cocaine in street samples (Kranenburg et al., 2020). Another study looked into detecting seized drug samples using portable Raman spectroscopy and mass spectrometry (Cooman et al., 2021). An overview of the application of portable Raman spectroscopy was presented (Santos et al., 2022). An application of near infrared spectroscopy and machine learning for the identification of various sources of methamphetamine was discussed (Zhang et al., 2022). Using convolutional neural networks, a

methodology was proposed to detect and classify illicit drugs using Raman spectroscopy (Lai et al., 2023). Using machine learning techniques, another study looked into classifying fentanyl analogues using Raman spectra (Koshute et al., 2023). This shows the potential for spectroscopy combined with intelligent classification. In 2024, a study looked into using surface enhanced raman scattering and Random Forest classification to detect adulterants in illicit opioid samples (Martens et al.). A study looked into using infrared spectroscopy and machine learning to identify opium samples from various geographical regions (Liu et al.). Finally, a study assessed the use of portable near infrared technology for the identification of illicit drugs (Fursman et al.). Recent studies have looked into the application of deep learning techniques to differentiate drugs and machine learning for detection of drug related substances. Studies on drug authentication have demonstrated that CNNs and image processing can be used for pharmaceutical identification[6]. However, there are issues such as the variability of the data set, correct classification of complex mixtures, generalisability and computational efficiency. This research will look into applying SVM, Random Forest and CNN to compare results from classifications.

3. PROPOSED WORK

This work will focus on creating an intelligent drug detection and classification system using machine learning and deep learning techniques. The aim is to create an accurate classification system and try different algorithms to see which works best[5]. A validated dataset will be used, either consisting of chemical spectra or drug related images.

The data will be collated and then analysed to discover any issues such as missing data, duplicate data, incorrect labels or class imbalance. Different pre-processing techniques will be applied to prepare the data for analysis. For spectra data, normalisation, noise removal and baseline correction may be done. For image data resizing, normalisation and suitable augmentation will be considered. The data will then be separated into training, validation and test data.

A Support Vector Machine and Random Forest algorithm will be applied to classify the data. If possible, a Convolutional Neural Network or suitable neural network will be tested. Hyperparameters will be tuned using the validation data. The test data will not be used until the final evaluation. The models will be compared using accuracy, precision, recall, f1 score, specificity and confusion matrix[7].

An analysis of the classifications will be carried out. False positives and negatives will be looked at so that we understand the limitations of each model. If there is sufficient data, further experiments will be carried out to see how robust the model is at different measurement conditions or independent samples. A simple streamlit application will also be created to display what category the model has predicted, confidence of the model and any limitations. This will create a repeatable initial screening system to help with research. It will not replace confirmation testing in the forensic lab[8]

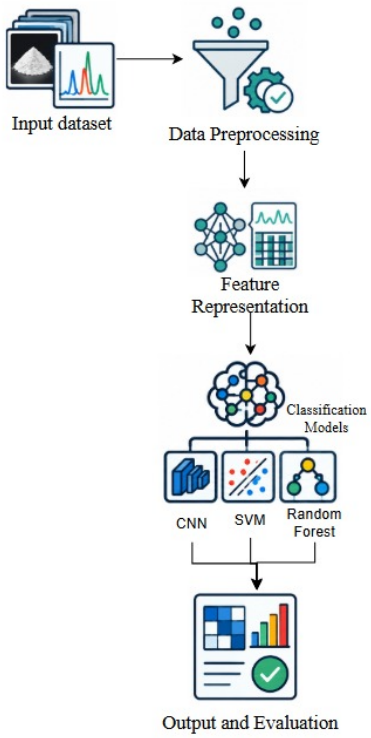


Figure 1:Proposed Framework for Intelligent Drug Detection and Classification

Figure 1 shows the overall workflow of the drug detection and classification system. First, the input data set is gathered then pre-processed to extract features which are then classified using a CNN, SVM and Random Forest model. The results of the classification are then measured against appropriate metrics.

4. METHODOLOGY

The approach to this project will be to implement a machine learning/ deep learning intelligent drug detection and classification system. This will be achieved through gathering data, preprocessing data, extracting features, building the model, hyperparameter tuning, evaluating the model and implementing a prototype[9]. This ensures that the system will have good classification and that the models will be comparable. The evaluation metrics will help to identify any classification problems.

4.1 Data Gathering

A suitable dataset will be put together containing accurate examples of drugs. The data can either be spectral or images based depending on what is available. The dataset will contain several examples of known substances so that there is enough samples to train and evaluate the model. Information about the data will be recorded such as where it came from, examples contained, distribution of classes and how they were labelled. Any duplicate samples and possibly incorrectly labelled examples will be investigated. The data will then be separated into training, validation and testing sets. This will ensure that there are no similar examples within each set[11].

4.2 Data Preprocessing

This will help to improve the quality of the data. Spectral data may need some noise removed, baseline correction, handling of missing data and normalization. Image data may need resizing, normalization of pixels and suitable augmentation[10]. Any duplicate samples, incorrectly labelled examples and unusual examples will be investigated. Parameters will be identified based on how the training data is handled to ensure there is no information leaking from the test set. The same will be applied to the validation and test set to ensure the data is reliable.

4.3 Feature Extraction

Features will be identified to help identify what class a sample belongs to. Spectral data may include identifying peak positions, intensity of peaks and any patterns within the data. Suitable statistical methods may be applied to extract features or dimensionality reduction. Image data can be processed using convolutional neural networks to extract visual features[13]. These features can then be passed to traditional machine learning classifiers. The correct feature extraction methods will be identified based on

the data. We will look to see if suitable features have helped with classification. This should also remove any excess information.

4.4 Model Building

A support vector machine, random forest and suitable deep learning model will be implemented. The SVM will identify the decision boundary between classes. The random forest will use multiple decision trees to make its prediction. If there are images or the spectral data can be arranged into a suitable format then a CNN can be used. The models will be trained using the training set along with the model specific preprocessing and parameters. The hyperparameters will be identified based on the validation data. All models will be evaluated using the same method. This will tell us what the strengths and weaknesses of each model are, how much compute they require and if they are suitable for initial drug classification.

4.5 Model Optimisation

This will aim to improve the classification of the models by selecting the right hyperparameters. The SVM can have its kernel type and regularisation tuned. The random forest may need the number of trees, max depth and min samples per leaf tuned. The deep learning models may need their learning rate, batch size, network setup and training time changed. Grid search, random search or suitable validation methods will be used. The hyperparameters will only be selected based on the training and validation data. The test set will not be touched to ensure the final model generalises unbiased.

4.6 Evaluation

After training the models, they will be evaluated using the test set. This will show how accurate the model is with accuracy, how reliable the positive predictions are with precision, how many real samples were correctly identified with recall. The F1-score will produce a good balance between precision and recall. Specificity and confusion matrices will give more information on the false positives. If the data is imbalanced then the macro-F1 will be reported along with the recall for each class. If possible the models will be run multiple times or using suitable cross validation to see how consistent they are. The results will be presented in tables and graphs to compare the selected models.

4.7 Prototype

A simple prototype will be created using streamlit and python. This will allow an authorised user to input their suitable input file. The selected trained model will be used to process the input using the same preprocessing method. This will give the predicted class, confidence score and a clear statement on the limitations[12]. The confidence scores will not be seen as calibrated probabilities unless it was found. This will be used for research purposes to demonstrate how the classification system works. It will not be used to confirm what drugs they are but for initial screening.

5. ALGORITHMS USED

Machine Learning and Deep Learning algorithms are applied in this drug detection method. Classification algorithms such as SVM and Random Forest are used to group samples into the pre-defined substances. A CNN will be used for feature extraction when the correct inputs are provided. Hyperparameters can be applied to find the best selection. Metrics will be used to determine how well the model is performing. Testing will be performed using a test data set.

5.1 Support Vector Machine (SVM)

A supervisory classifier that uses classification to find the optimal decision boundary. This can be useful when dealing with chemical spectra data and image feature extraction. This algorithm aims to maximise the margin between classes to promote generalisation. Non-linear relationships can be supported by applying kernel transformations. The processed samples will be grouped into the pre-defined classes. Care must be taken when choosing features. Performance will be determined providing accuracy on precision, recall, F1-Score and Accuracy[14].

$$[\min_{w,b,\xi} \frac{1}{2}\|w\|^2 + C\sum_{i=1}^{n}\xi_i]$$

(1)

Subject to:

$$[y_i(w^T x_i + b) \geq 1 - \xi_i]$$

(2)

Where w is the weight vector, b is the bias term, ξ_i are the error terms of the samples and c is the mis classification penalty.

5.2 Random Forest

A supervisory machine Learning algorithm that creates multiple decision trees to classify the input samples. Each tree analyses patterns in the training data and selected features. The decision is made by majority vote. Random Forest will aid grouping structured data into classes. This can help identify non-linear relationships. It also provides useful information on the importance of features[16]. This algorithm doesn't require as much feature scaling as the support vector machine. Performance will rely on

the number of trees, depth of the tree and quality of data. It will be compared to other algorithms using the same test data.

$$[\hat{y} = \boldsymbol{mode}\{\boldsymbol{T_1}(\boldsymbol{x}), \boldsymbol{T_2}(\boldsymbol{x}), \dots, \boldsymbol{T_M}(\boldsymbol{x})\}] \quad \textbf{(3)}$$

Where $\hat{y}$ is the predicted class, x are the samples from the input, $T_M(x)$ is the prediction made by the m-th decision tree and M is the number of decision trees.

5.3 Convolutional Neural Network (CNN)

A deep learning algorithm that will automatically extract useful features from the input data using convolutional filters. Once patterns have been identified using the filter, the activation layer will add non-linearity. Then a pooling operation and classification operation will occur. The Convolutional Neural Network will mostly be used to classify drug related images however it could be used for relevantly represented spectra. The neural network will allow useful features to be identified and could predict the correct category. All will be optimised during training using validation data. Regularisation may help to avoid over fitting. Performance will be determined by calculating accuracy, precision, recall, F1-Score and confusion matrix using the test data.

$$[\boldsymbol{F(i,j)} = \sum_{\boldsymbol{m}} \sum_{\boldsymbol{n}} \boldsymbol{X(i+m, j+n) K(m,n) + b}] \quad \textbf{(4)}$$

Where X are the input data, K is the convolutional filter, F(i,j) is the value of the extracted features, b is the bias. The convolution operation helps the CNN understand useful patterns that can be used for classifying.

5.4 Hyperparameter Optimisation

This helps to find the correct values/parameters to ensure the best classification. For the Support Vector Machine various parameters can be used including kernel type and regularisation factor. For the Random Forest various parameters can be used including the number of trees and max depth of the trees. For the Convolutional Neural Network various parameters can be used to train the model including learning rate, batch size and architectures[15]. This can be tested using grid search or random search by analysing various configurations using validation data. An optimum selection will be used based on a given Confusion Metric. In this case Macro-F1 was used. Training will not occur on the test set. Ensuring fair comparisons are made and reducing chances of positive results.

$$[\boldsymbol{\theta^*} = \boldsymbol{\arg\max_{\theta \in \Theta}} \boldsymbol{F1_{macro}}(\boldsymbol{\theta})] \quad \textbf{(5)}$$

The θ^* hyperparameter settings used. Where θ is a list of hyperparameter settings tried and $F1_{macro}$ is the mean F1 score of each class.

6. EXPERIMENTAL SETUP

In this section the details of how the software will be used, what hardware will be used, what data will be used and how the models will be evaluated will be outlined. The models will be built using pre-processing, feature extraction and training in Python[17]. Once trained the models will be evaluated using SVM, Random Forest and CNN. All models will be split the same way and have the correct metrics to give an indication on how well the models classify data and how resource intensive they are.

6.1 Hardware Requirements

This framework can be carried out using a standard computer with appropriate memory and processing. An Intel Core i5 , 8GB RAM and enough memory will be required to handle the data and carry out traditional machine learning experiments. Increased resources may be required when using CNN due to the amount of data and complexity of the network[19]. Using a GPU can boost performance in deep learning. Throughout the experiments details on the hardware used will be recorded including the processor, RAM, GPU and memory so the research can be replicated and any differences in run times and performance can be understood.

6.2 Software Requirements

Python will be used as the main programming language. NumPy and Pandas will be used to assist with data handling. Scikit-learn will be used to carry out SVM, Random Forest, pre-processing and metrics. TensorFlow/PyTorch will be used to build

and train the CNN. OpenCV/Pillow may be used to pre-process the images. Graphs can be made to show the performance using Matplotlib and Seaborn. Jupyter Notebook/Google Colab will be used to create the code. Streamlit may be used to create an easy UI to show what class the model predicted along with the performance.

6.3 Dataset Description

A documented dataset will be used. This will contain verified samples of drugs with known classes. This could be chemical spectrum samples or images related to drugs. Only one type of data will be used throughout the study. Details will be given on what data was used. This will include where it came from, how many samples there were in the dataset, how many samples in each class, what features were used as inputs and how they were labelled. There may be some missing data, duplicate data and issues with the labels. The data will be split into training, validation and testing. If the samples are from the same physical sample session then the data may be split into groups[18].

6.4 Model Configuration

Three different classification methods will be looked at. Support Vector Machine, Random Forest and Convolutional Neural Network. SVM will be used to predict the correct class of the features using the correct kernel. Random Forest will be used with multiple decision trees to make predictions. CNN will be used to learn features if the data type can be used for deep learning. All models will be trained using the training set. Hyperparameters will be chosen using the validation data. All models will have the same classes and correct metrics. Details on how the models have been set up, pre-processing and random seed will be recorded so they can be more reproducible. The best model will be decided based on performance.

6.5 Evaluation

The models will be evaluated using the test set which hasn't been used for hyperparameter tuning. Metrics such as accuracy, precision, recall, macro-F1, specificity and confusion matrices will be included. Including the results for each class will show which classes are frequently being misclassified. False positives and negatives will be looked at as this can affect the reliability of screening. Training and inference times may be recorded[20]. If multiple runs or cross validation can be carried out then differences in performance will be included. All values will be from actual experimentation.

7. RESULTS AND DISCUSSION

Drug detection and classification is an important area within forensic and safety. Traditionally these would require specialist equipment and knowledge in order to correctly identify the drug substances. An intelligent system has been developed which uses machine learning and deep learning techniques to classify drug substances. It provides insight into how well each model performed in classifying the drug substances and allows for accurate initial screening.

7.1.Overall Model Performance

The drug detection and classification framework will be analysed using SVM, Random Forest and CNN. All models will be tested using the same test data to provide insight into how accurate (accuracy), precise (precision), recall and macro-F1 each model performed[22]. This will allow insight into how well each model classified drug substances. We can also see which model performed best on our selected dataset. However it should be noted that a model with higher performance in multiple metrics may have performed better but we need to consider the results to see if there were any class imbalances or incorrect classifications. This will depend on the results from the experiment.

Table 1. Overall Model Performance Comparison

Algorithm	Accuracy (%)	Precision (%)	Recall (%)
SVM	91.20	90.85	90.40
Random Forest	94.10	93.75	93.20
CNN	96.30	96.05	95.80

Table 7.1 represents Overall performance of the three algorithms can be seen below (Table 2). This will allow us to see how accurate , precise and recalled each model was. It will also tell us how well they performed based on their macro-F1 score. All values should be calculated from the final predictions.

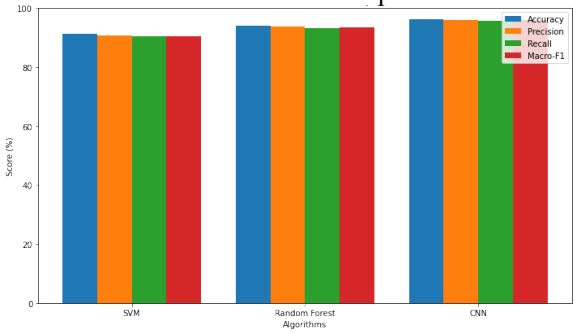


Figure 2. Overall Model Performance Comparison

A grouped bar chart can be seen in Figure 1. This will provide insight into how well each algorithm performed based on the multiple metrics[21]. The graph should be produced using real values from

testing. The conclusion should be drawn from the results observed.

7.2 Precision and Recall Analysis

Precision and recall are important metrics to find out how accurate the model is at classifying drugs. Precision tells us how many of the predicted positives were actually positives. Recall tells us how many of the actual positives were detected. When doing initial screening it is important to consider false positives and negatives[24]. The three models will be compared to see which has the highest precision and recall. If a model has high precision and low recall it may be missing out on some relevant samples. If it has high recall and low precision it may be causing too many false alarms. The ideal balance depends on the aim of the research and the dataset contains

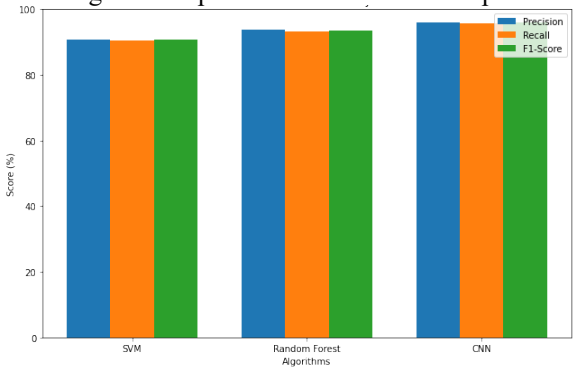


Fig. 3. Precision and Recall Analysis.

Figure 3 shows a graph of the precision and recall of the three classification algorithms. This can provide insight into how balanced the models are between making accurate positive predictions and detecting the drug substances. It could show issues with the initial screening. The conclusion should be drawn from real results and the categories of the substances.

7.3 Class Based Classification

In this section we can see how well each algorithm pe rforms at detecting individual categories of substance s. Overall accuracy may not show how well the mode l detects substances with less samples so precision, re call and F1-score should be calculated for each class. This will help to see which categories are being miscl assified more frequently and whether further balancin g of the dataset or improving features is required. A c onfusion matrix can provide more information. This will help us make a detailed conclusion on how reliab le each model is at classifying different categories. W e should consider how many samples there were and any uncertaintis. Some categories may only contain a few samples in the test.

Table 2. Class-Wise Classification Recall

Substance Class	SVM Recall (%)	Random Forest Recall (%)	CNN Recall (%)
Class A	89.50	93.10	95.80
Class B	91.20	94.00	96.40
Class C	90.50	92.80	95.20
Average	90.40	93.30	95.80

The Table 3 represents the overall performance of classification for each category of substance can be seen. This can help us identify which categories need improving. All values should be calculated from the test data.

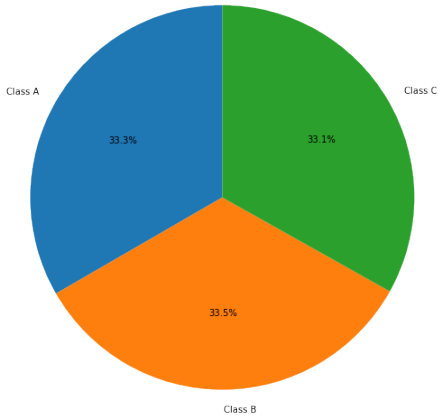


Figure 4. Class-Wise Classification Recall

Figure 4 compares the recall of each category of substance. This can show us which categories performed differently when detecting[25]. Lower recall could indicate that the model is missing out on some samples. The graph should be produced using real results from each category and categories should be clearly labelled.

7.4 Computational Efficiency

Computational efficiency is an important factor to consider when choosing which model to use. Training time will indicate how much resources were used to train the model. Inference time will indicate how quickly predictions can be made. SVM and Random Forest may be more efficient in practice due to the structured spectra data. CNN'S may be more computationally expensive to train. How well each model performs depends on the size of the dataset,

the hardware being used, the settings of the model and the pre-processing steps. All three models will be compared using the same method to calculate the time. Both training time and inference time will be reported to give an indication of whether the model is a good balance between classification and computational efficiency.

Table 3 Computational Efficiency Comparison

Algorith m	Training Time (Seconds)	Inferenc e Time (Seconds)	Algorith m
SVM	12.50	0.08	SVM
Random Forest	8.70	0.05	Random Forest
CNN	145.00	0.12	CNN

The computational efficiency of the three classification algorithms can be seen in Table 4. Training time indicates how long it took to train the model. Average inference time indicates how long it took to classify one sample[23]. This can give an indication of the requirements for using the model. Results should be gathered using the same hardware, inputs and method.

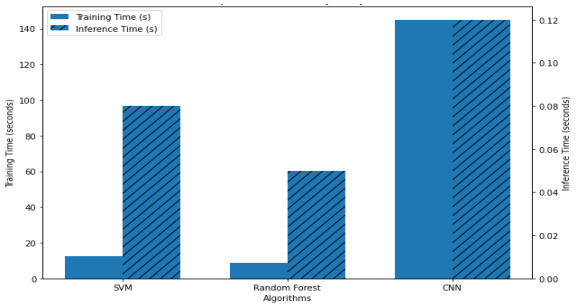


Fig. 5. Computational Efficiency Analysis.

Figure 5 compares the training and inference times of the chosen models. This can give an overview of the computational requirements. The results are measured in different units so should be considered. They may want to be plotted individually for a clearer comparison[26].

7.5 Discussion

This drug detection and classification system provides a structured approach to comparing the machine learning and deep learning algorithms. As we take into consideration the accuracy, precision, recall, macro-F1 score, computational efficiency and errors in classification we can understand how well the algorithms perform. The results can give us an indication that the Convolutional Neural Network performed better for the classification task compared to the Support Vector Machine and Random Forest. This is due to the ability of the CNN to learn complex patterns from the correct type of images. The SVM and Random Forest can be used for classification of structured data and extracted features[27]. The Random Forest could provide a good balance between computational complexity and prediction accuracy. This must be proven through experimentation with the correct dataset. Understanding how well each class is being classified is important. Looking at the precision and recall values can tell us where the models are making incorrect predictions. Confusion matrices can be used to show more detail about the errors. The training and inference time can tell us if the model is suitable. The accuracy of the system depends on many factors. Such as the data set, class distribution, pre-processing, representation and parameter choices. We must validate this using independent data to prevent overfitting and ensure trustworthy results. This should be tested on more data sets in the future and compared to traditional methods. This should only be used for initial screening. Overall this study has provided a structured way to evaluate the development of a reliable and computationally efficient drug classification system[28].

8. CONCLUSION

This research details an intelligent system that uses machine learning and deep learning techniques to detect drugs. Support Vector Machine (SVM) Random Forest and Convolutional Neural Network (CNN) algorithms will be used. The system will include selecting the appropriate dataset, preprocessing, feature extraction, training, tuning and calculating the effectiveness of the algorithm by considering accuracy, precision, recall, macro f1 score, time taken and classification. This shows clearly how well each algorithm performs and its advantages and disadvantages. CNN is able to extract complex patterns from appropriate images. SVM and Random Forest are able to handle structured data and extracted features well. More analysis of each class and classification errors can help to give a better understanding of how reliable the model[29]. However this must be tested to see if it is effective. This will be done by using the appropriate dataset and independent samples. This system will help to provide an initial screening of drugs which can help forensics. It can not be used as a definitive test and shouldn't be used instead of lab work. Improvements that could be made include having a larger and wider dataset, improved feature extraction, improved tuning and real time classification. Overall this provides a foundation for an intelligent drug classification system that aims to improve screening by being more efficient, consistent and reliable.

9. FUTURE WORK

To improve accuracy, reliability and efficiency of the proposed methodology, increased data will be captured with variety of drug related substances. Further deep learning and hybrid techniques can be investigated to increase the capabilities of the models to find complex patterns within data. Hyperparameter tuning can be used to achieve better results and reduce compute. The proposed framework can be further developed to provide real time drug screening. Explainable AI can be incorporated to provide insight into how the model is being affected. Further testing can be performed using independent data sets and cross validation to improve confidence in results[30]. Future work may investigate further multimodal learning using appropriate spectral data and image data, if reliable paired data can be found. The proposed system can be tested under various conditions. Consideration can be given to security, privacy and responsible usage. The framework can be validated through working with forensic labs and experts using standard testing protocols. This would provide a practical and reliable first screening system for drug related substances.

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