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A Machine Learning Binary Classification Model Based on the Chemical Structure and Delivery Parameters of Functional Polymers: Predicting the Cancer Cell Inhibition Effectiveness of Polymer-based Delivery Systems for Ocular Cancers

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Abstract. The treatment of ocular cancer faces unique challenges. The complex physiological structures of the eye, such as the corneal barrier and the blood-eye barrier, restrict the efficiency of drug delivery. Traditional chemotherapy drugs, due to their low solubility and poor stability, not only have poor therapeutic effects but also are prone to cause side effects such as ocular irritation. Polymer-based delivery systems, with their controllable chemical structure, good biocompatibility and targeted delivery capabilities, have become key carriers for optimizing the delivery effect of drugs for ocular cancer. The current commonly used machine learning algorithms are difficult to meet the requirements of the refined assessment of the ocular cancer delivery system. Therefore, this paper proposes the LSTM-Adaboost classification algorithm. Firstly, violin graph analysis and correlation analysis are carried out, and then multiple machine learning algorithms are used for testing. The results show that the core evaluation indicators of this algorithm are generally superior to those of ExtraTrees, decision tree, GBDT, Random Forest, CatBoost, AdaBoost and XGBoost algorithms. Its accuracy rate and recall rate both reach 89.3%, and the precision rate and F1 value are both 89.2%. Compared with the suboptimal ExtraTrees algorithm, all indicators were 87.4%, increasing by 1.9, 1.9, 1.8, and 1.8 percentage points respectively. Compared with the decision tree algorithm, which has an accuracy rate and recall rate of 78%, an precision rate of 80%, and an F1 value of 78.7%, and the GBDT algorithm, which has an accuracy rate and recall rate of 81.1%, an precision rate of 81.7%, and an F1 value of 81.4%, its advantages are more significant. The AUC indicator is 94.9%, which is slightly lower than the 95.1% of the ExtraTrees algorithm, but higher than other algorithms. Overall, it still leads. This algorithm provides a reliable method for the refined evaluation of ocular cancer delivery systems and is of great significance for promoting the optimization of drug delivery technologies for ocular cancer treatment.

Keywords: Eye cancer, polymer-based, Adaboost

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1. Introduction

The treatment of ocular cancer faces unique challenges. The complex physiological structures of the eye, such as the corneal barrier and the blood-eye barrier, limit the efficiency of drug delivery. Traditional chemotherapy drugs are prone to insufficient efficacy and side effects such as ocular irritation due to low solubility and poor stability [1]. Polymer-based delivery systems, with their controllable chemical structure, good biocompatibility and targeted delivery capabilities, have become important carriers for improving the drug delivery effect of ocular cancers [2]. However, the cancer cell inhibition effectiveness of polymer-based delivery systems is synergistically influenced by multiple factors such as the molecular weight of the polymer, the density of functional groups, the particle size of nanoparticles, and the drug encapsulation rate. The traditional method of optimizing through experimental screening has problems of long cycle and high cost, making it difficult to rapidly and efficiently evaluate the effectiveness of a large number of candidate systems. There is an urgent need to establish an efficient prediction method [3].

Machine learning algorithms, with their powerful data mining and complex relationship modeling capabilities, have demonstrated significant advantages in performance prediction tasks in the biomedical field. For the effectiveness evaluation of polymer-based delivery systems, machine learning can construct predictive models by analyzing the potential correlation between multi-dimensional features and inhibitory effectiveness, significantly shortening the evaluation cycle and reducing experimental costs [4]. Although the commonly used binary classification algorithms such as logistic regression and random forest can handle some linear or nonlinear relationships, they have limitations when capturing dynamic dependencies among features and dealing with small samples and imbalanced data. They are difficult to fully explore the complex laws under the collaborative effect of multiple factors, which affects the accuracy and stability of the prediction model. It cannot meet the demand for refined assessment of the ocular cancer delivery system [5].

To address the deficiencies of the existing algorithms, this paper proposes the LSTM-Adaboost classification algorithm. LSTM (Long Short-Term Memory Network) has the ability to capture the dynamic dependency relationship of sequence data, and can effectively explore the correlation between temporal characteristics such as polymer degradation and drug release half-life and inhibitory effectiveness, making up for the defect that traditional algorithms are difficult to handle dynamic relationships. Adaboost (Adaptive Boosting Algorithm) enhances the model's recognition ability for minority class samples and improves the classification performance of the model under imbalanced data by iteratively optimizing the weights of weak classifiers.

2. Data sources

The dataset used in this article contains 527 sample data for polymer-based delivery systems targeting ocular cancers, covering 12 characteristic variables reflecting the chemical structure of functional polymers and key parameters of the delivery system, as well as 1 binary predictive variable representing the effectiveness of cancer cell inhibition. The characteristic variables cover polymer chemical structure-related indicators such as molecular weight, hydrophilic and hydrophobic balance value, density of targeted functional groups, glass transition temperature, degree of branch, and charge density, as well as core parameters of the delivery system such as nanoparticle size, drug encapsulation rate, drug loading capacity, polymer-drug binding strength, in vitro release half-life, and uptake efficiency by cancer cells. The predictor variables were expressed as 0 and 1 respectively, indicating that the delivery system was ineffective and effective in inhibiting ocular cancer cells.

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Output the violin plots of each variable to observe the data distribution of each variable, as shown in Figure 1.

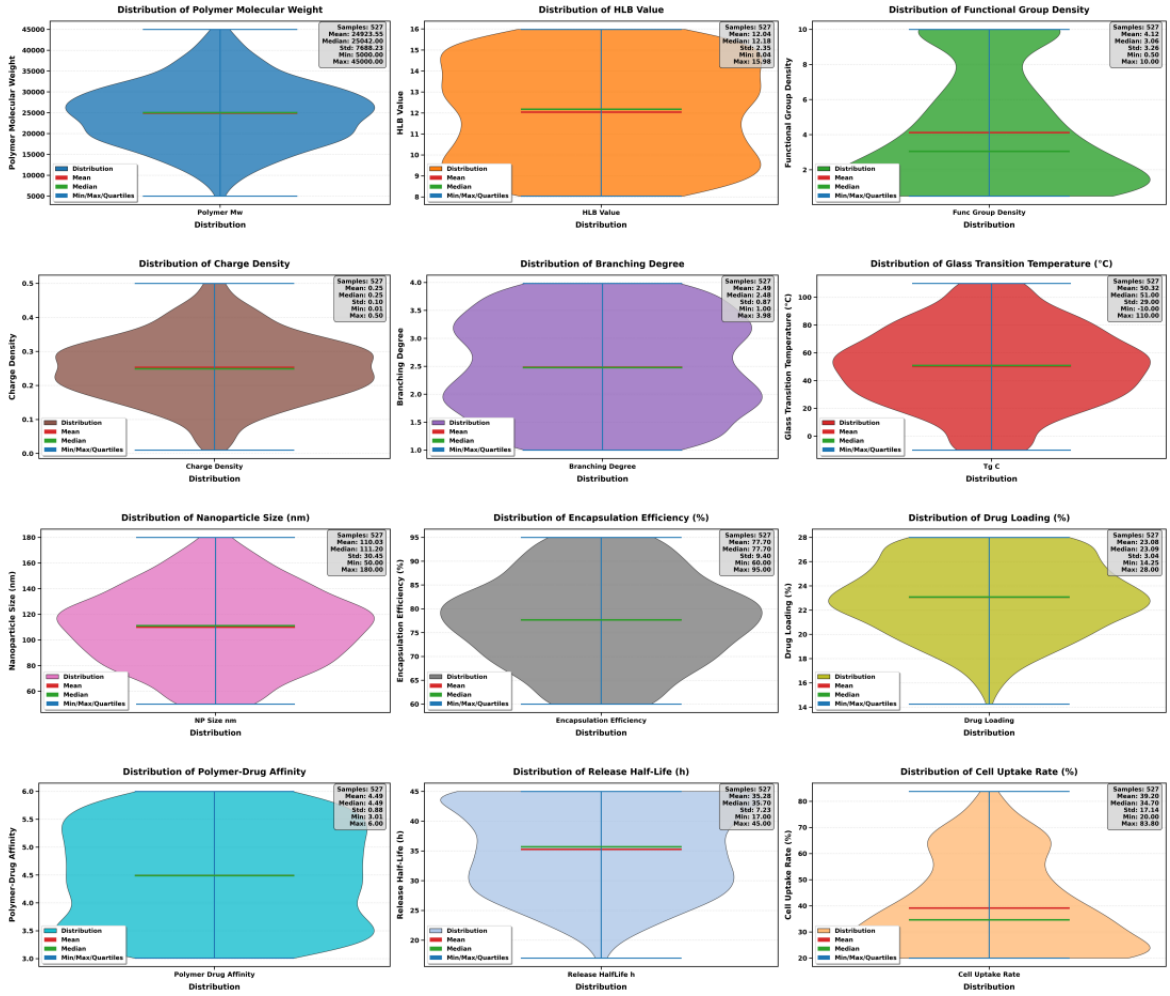


Figure 1. Violin diagrams of each variable

Output the correlation heat maps of each variable, as shown in Figure 2.

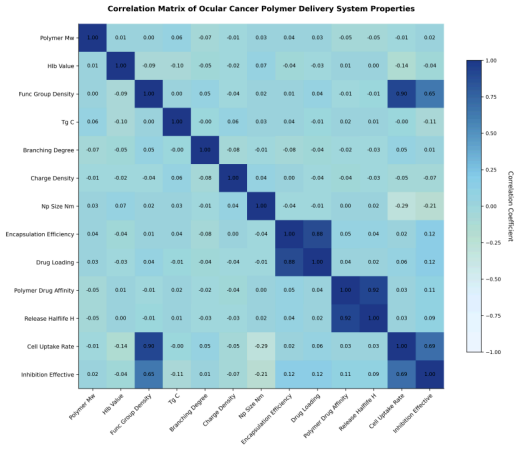


Figure 2. The correlation heat map

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3. Method

3.1. LSTM

LSTM, or Long Short-Term Memory Network, is an important improved algorithm of recurrent neural networks. Its core solution is the problem of vanishing or exploding gradients that often occurs when traditional recurrent neural networks process long sequence data [6]. Internally, through the collaborative effect of four core modules - input gate, forgetting gate, output gate and cell state - it can selectively retain long-term valid information and forgotten redundant information in sequence data, and update key features, thereby precisely capturing the temporal dependency relationships among data. The network structure of LSTM is shown in Figure 3.

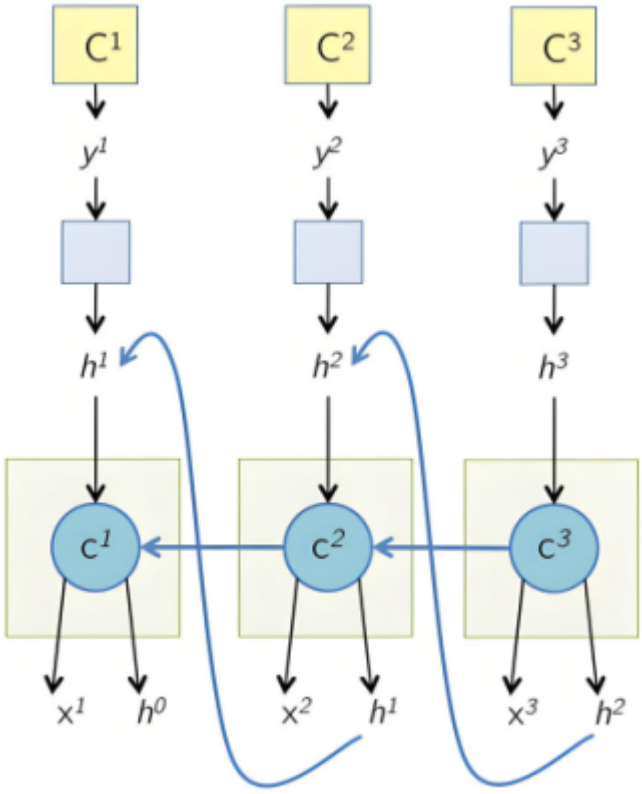


Figure 3. The network structure of LSTM

3.2. Adaboost

The Adaboost algorithm is a classic boosting algorithm in the field of ensemble learning. Its core logic is to iteratively train a series of weak classifiers and combine them weighted to form a stronger classifier with better performance [7]. In each iteration round, the algorithm adjusts the sample weights based on the classification error rate of the weak classifier in the previous round - the weights of wrongly classified samples are increased, while those of correctly classified samples are decreased, enabling the subsequent weak classifier to focus more on difficult-to-classify samples. Finally, all the weak classifiers are weighted and summed according to their classification accuracy to form the final strong classifier. The network structure of Adaboost is shown in Figure 4.

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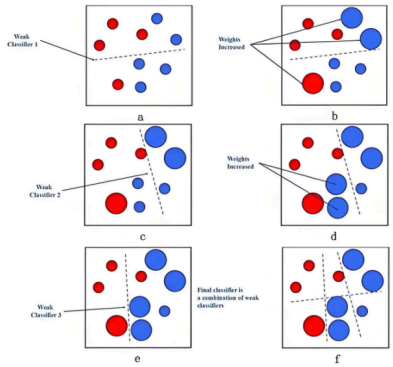


Figure 4. The network structure of Adaboost

3.3. Lstm-adaboost

The LSTM-Adaboost classification algorithm is a hybrid algorithm that combines the feature extraction advantages of LSTM with the integrated optimization capabilities of Adaboost. It is designed for the multi-feature and strong temporal characteristics of the effectiveness prediction of polymer-based delivery systems for ocular cancer [8]. This algorithm first uses LSTM to deeply extract multi-dimensional features such as polymer chemical structure parameters and dynamic parameters of the delivery system, focusing on capturing the temporal dependencies and nonlinear correlations among the features, and converting the high-dimensional original features into more discriminative low-dimensional feature vectors. Subsequently, the feature vector is input into the Adaboost algorithm for integrated classification. By iteratively optimizing the weights of weak classifiers, the recognition ability for difficult-to-distinguish samples is enhanced, and the classification accuracy of the model is further improved [9].

4. Result

The parameter Settings of the project include a ratio of the training set to the dataset of 0.7, setting the flag bit to 1 to open the confusion matrix, the number of weak regressors to 10, and the number of hidden layer nodes to 6. The training adopts the Adam gradient descent algorithm, with a maximum of 500 training sessions, an initial learning rate of 0.001, a segmented learning rate scheduling method, a learning rate descent factor of 0.1, and a learning rate descent period of 40. Each training session will disrupt the dataset [10]. Output the comparison results of the indicators of each model, as shown in Table 1.

Table 1. The results of the comparative experiment

Model	Accuracy	Recall	Precision	F1	AUC
ExtraTrees	0.874	0.874	0.874	0.874	0.951
Decision tree	0.78	0.78	0.8	0.787	0.78
GBDT	0.811	0.811	0.817	0.814	0.882
Random Forest	0.849	0.849	0.861	0.835	0.93
CatBoost	0.836	0.836	0.828	0.826	0.934
AdaBoost	0.818	0.818	0.81	0.813	0.91
XGBoost	0.849	0.849	0.844	0.845	0.936
Our model	0.893	0.893	0.892	0.892	0.949

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The results of this comparative experiment show that the LSTM-Adaboost algorithm proposed in this paper performs overall better than the ExtraTrees, Decision Tree, GBDT, Random Forest, CatBoost, AdaBoost and XGBoost algorithms in terms of core evaluation indicators. The accuracy rate and recall rate of this algorithm both reach 89.3%, and the precision rate and F1 value are both 89.2%. Compared with the suboptimal ExtraTrees algorithm, its accuracy rate, recall rate, precision rate and F1 value are all 87.4% The former increased by 1.9 percentage points, 1.9 percentage points, 1.8 percentage points and 1.8 percentage points respectively.

Output the bar comparison charts of each indicator, as shown in Figure 5.

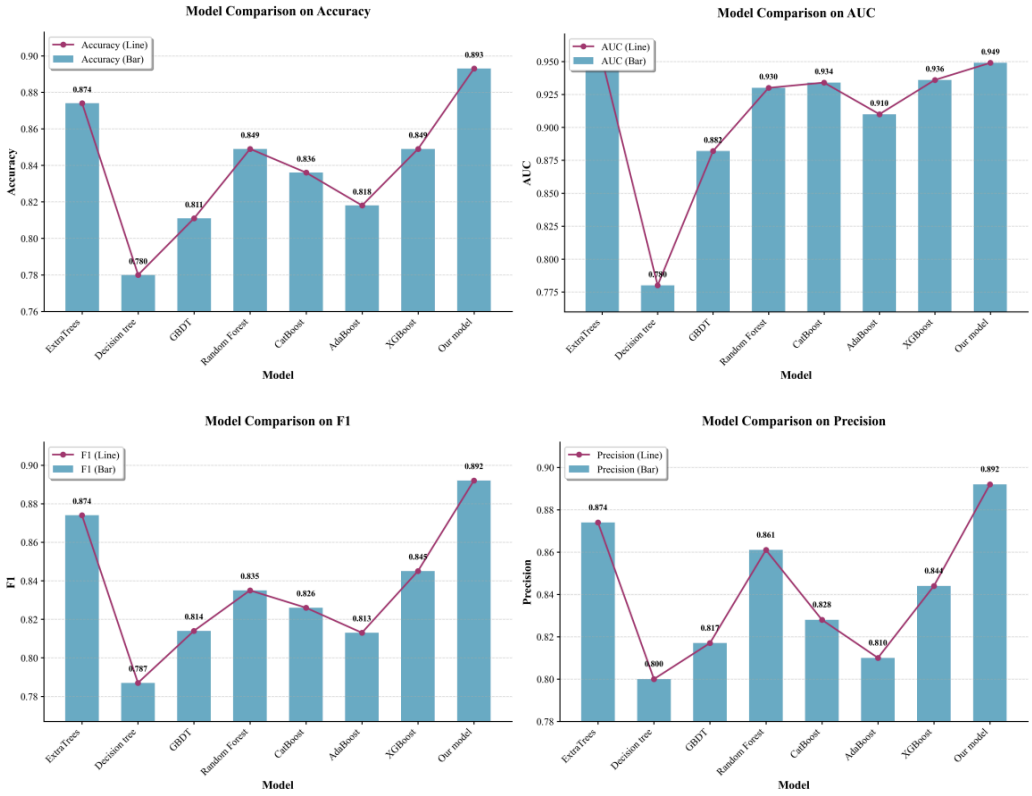


Figure 5. The line graphs comparing the indicators of each model

5. Conclusion

The treatment of ocular cancer faces special challenges. Complex physiological structures such as the corneal barrier and the blood-eye barrier restrict the efficiency of drug delivery. Traditional chemotherapy drugs also have low solubility and poor stability, which not only lead to insufficient efficacy but also easily cause side effects such as ocular irritation. Polymer-based delivery systems, with their controllable chemical structure, good biocompatibility and targeted delivery capabilities, have become important carriers for improving the drug delivery effect of ocular cancers. However, the existing commonly used machine learning algorithms cannot meet the refined evaluation requirements of this delivery system. For this purpose, this paper proposes the LSTM-Adaboost classification algorithm. Firstly, violin graph analysis and correlation analysis are conducted, and then tested through multiple machine learning algorithms. The results show that the core evaluation indicators of this algorithm are generally superior to those of ExtraTrees, decision tree, GBDT, Random Forest, CatBoost, AdaBoost and XGBoost algorithms. Its accuracy rate and recall rate both reach 89.3%, and the precision rate and F1 value are both 89.2%. Compared with the suboptimal

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ExtraTrees algorithm (with all indicators at 87.4%), it has improved by 1.9, 1.9, 1.8, and 1.8 percentage points respectively. Compared with the decision tree (accuracy rate and recall rate 78%, precision rate 80%, F1 value 78.7%) and GBDT (accuracy rate and recall rate 81.1%), Algorithms with an accuracy rate of 81.7% and an F1 value of 81.4% have more significant advantages. Although its AUC index of 94.9% is slightly lower than the 95.1% of the ExtraTrees algorithm, it is still higher than many other algorithms and remains at the leading level overall. This algorithm provides strong support for the precise assessment of polymer-based delivery systems for ocular cancer and helps promote the progress of drug delivery technology in the field of ocular cancer treatment.

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