

Machine Learning-Based Hybrid Optimization of SVM for Drug Delivery Data Analysis

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Abstract

Biomedical and pharmaceutical data are exploding, and the problems of data analysis and classification are becoming more challenging. Drug delivery datasets are often high-dimensional, with many features that are redundant and irrelevant, which makes the prediction more complex and less accurate. The Support Vector Machine (SVM) is a popular classification algorithm because it has a high degree of generalisation and is effective for dealing with complex data. But the empirical performance of SVM is highly sensitive to the choice of its parameters, and the effectiveness of techniques for feature reduction. In this study, the Hybrid Optimization based on Machine Learning is proposed to enhance the performance of SVM in drug delivery data analysis. The proposed approach combines the feature selection and parameter optimization techniques with the hybrid optimization of GA and PSO algorithms. The hybrid framework is designed to select the most suitable features from the high-dimensional pharmaceutical data as well as to optimize the SVM parameters for maximum classification accuracy and efficiency. The performance of the developed model is tested on biomedical and drug delivery data sets with accuracy, precision, recall, F1 score and execution time as performance indicators. The results of the experimental analysis clearly show that the hybrid optimized SVM model improves accuracy in prediction, reduces the dimensionality and avoids overfitting compared to the traditional machine learning methods. The new model can be applied in smart decision-making in drug research, personalized medicine, drug formulation analysis, and intelligent drug delivery systems.

Keywords: High-Dimensional Data Classification, Support Vector Machine Optimisation, Gravitational Search Optimization (GSO), Bee Algorithm (BEE), Swarm Intelligence-Based Feature Selection.

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Introduction

Over the past few years, the fast growth of machine learning and artificial intelligence has revolutionized biomedical research, pharmaceutical sciences and pharmaceutical delivery systems. There are numerous new and highly dimensional data sources in modern healthcare systems, such as medical imaging, biosensors, clinical trials, and studies of pharmaceutical formulation. Analysis and classification of these datasets are vital for accurate disease diagnosis, optimum drug formulation and personalised medicine, as well as intelligent therapeutic systems [1, 2].

In high dimensional datasets, there are typically lots of features that are redundant, noisy and irrelevant, which can make classification more challenging and make classification performance worse. However, traditional statistical and machine learning techniques may have problems with this complex biomedical data set because of overfitting, data dimensionality, and lack of generalization ability [3] and [4]. Hence, intelligent classification models that incorporate efficient feature

selection and optimization mechanisms are needed for proper biomedical data analysis.

Support Vector Machine (SVM) is one of the most powerful classification algorithms that gained popularity due to its efficient performance with nonlinear and high-dimensional data, robustness and solid mathematical foundation [5], [6]. SVM builds an optimum hyperplane which has the maximum margin between classes to maximize the accuracy of the prediction and reduce the classification errors. For these merits, SVM has received enormous applications in bioinformatics, medical diagnosis, pharmaceutical analysis, cancer prediction, and intelligent Drug delivery system [7] [8]. Although SVM has its benefits, its performance strongly relies on the selection of kernel functions, and the tuning of hyperparameters like kernel coefficients and penalty parameter. Irrelevant features in high dimensional biomedical datasets can have a major impact on the accuracy of classification and computation efficiency [9, 10]. In a complex, nonlinear search space, conventional optimization methods are not always capable of finding the best combination of features and tuning parameters.

So, there is a growing interest in the use of advanced optimization techniques to enhance the performance of the SVM.

The application of natural or evolutionary based optimization algorithms such as metaheuristic optimization algorithms has been successful to solve complex optimization problems. Feature selection and parameter tuning in machine learning models are among the applications of optimization techniques that are widely used, including Genetic Algorithm (GA), Particle Swarm Optimization (PSO), Whale Optimization Algorithm (WOA), Ant Colony Optimization (ACO) and Differential Evolution (DE) [11] [12]. These algorithms are effective at searching large solution spaces and have the ability to find optimum combinations of features that enhance the accuracy of the classification, while minimizing the computational effort.

Hybrid optimization techniques apply techniques from multiple optimization algorithms together, leveraging their respective advantages for better exploration/exploitation. For medical studies with high dimensional data, the hybrid GA-PSO and PSO-SVM have shown great improvements in prediction accuracy, convergence speed and feature reduction [13], [14]. This combination is particularly useful for pharmaceutical and drug delivery studies, where complex biological interactions and formulation parameters must be studied and understood with accuracy to predict.

In recent years, the field of drug delivery technology has made significant strides, thanks to the incorporation of computational intelligence and machine learning methods. The use of targeted drug release, controlled therapeutic mechanisms, nanoparticles for drug delivery and patient-specific treatment planning in modern drug delivery systems produces multidimensional complex datasets [15] and [16]. Machine learning algorithms can help researchers determine the best drug formulations, understand drug interactions, and enhance the efficacy of drugs.

Hybrid machine learning models have recently been proven to greatly improve biomedical decision-making systems and pharmaceutical data analysis [17, 18]. Optimized SVM models have been applied in disease classification [19, 20], drug response prediction, medical image analysis and genomics-based healthcare applications to great success. In addition, the feature selection techniques based on hybrid optimization algorithms reduces irrelevant features and enhances the generalization ability of machine learning models [21], [22].

Advances in the field of intelligent healthcare systems and sophisticated pharmaceutical analysis have spurred researchers to develop powerful computational systems to deal with high-dimensional biomedical data [23]. For these drug delivery applications, hybrid optimisation-based SVM models are efficient solutions to increase the accuracy of the classification, reduce the computational complexity, and improve the accuracy of the prediction [24, 25].

Thus, the present work emphasizes on creating a Hybrid Optimization of SVM driven by Machine Learning for Drug Delivery Data Analysis. The framework proposes to combine hybrid optimization algorithms with SVM for better feature selection, classification parameter optimization and better predictive performance of high-dimensional pharmaceutical datasets. The research should have a profound impact on intelligent drug delivery systems, biomedical research, personalized medicine, and advanced healthcare analytics.

Methodology

The proposed research is a Machine Learning Based Hybrid Optimization framework for enhancing the performance of Support Vector Machine (SVM) using the high-dimensional drug delivery data. The methodology combines data preprocessing, hybrid feature selection, parameter optimization, and classification algorithms to improve the accuracy of prediction and computational efficiency. This is shown as a sequential process with the acquisition of the data set, data preprocessing, hybrid optimization, SVM classification, and performance evaluation.

Dataset Collection

In this work a high dimensional biomedical and pharmaceutical dataset related to drug delivery systems is used in an experimental analysis. Drug formulation parameters, molecular descriptors, therapeutic response data, biological data, and patient data can be included in the datasets. Biomedical repositories and pharmaceutical research databases that are openly accessible are regarded as primary data sources.

The collected datasets are in general high dimensional having many features increasing the dimensionality and computational requirement in classification. Thus, it is essential to have efficient preprocessing and optimization methods to enhance analytical performance.

Data Preprocessing

The data will be pre-processed before the machine learning algorithms can be applied, to improve the quality of the data set and to eliminate inconsistencies. The occurrence of missing values, noisy data, redundant features, and imbalanced class distribution are typical in biomedical datasets. The following operations are performed in the pre-processing stage: Removing of duplicate and inconsistent records. Using techniques to fill in missing data (interpolation or mean imputation)

- Applying data normalization to the data (Min-Max or Z-score normalization techniques)
 - Categorical data to numerical representations
- Removing noise and outlier data. Outlier and noise removal from data. Data normalization enhanced consistency of the optimizer algorithms and enhanced SVM classification efficiency.

3.3 Feature Selection Using Hybrid Optimization

One of the difficulties with high dimensional data is that there are features that are irrelevant and redundant that adversely affect the classification. To address this, an

optimization method based on a hybrid of Genetic Algorithm (GA) and Particle Swarm Optimization (PSO) is proposed, which is used to optimize features selection and parameters tuning.

Genetic Algorithm

GA is used as a global optimization tool for feature selection. First, a fixed number of candidate solutions are randomly created, with each chromosome being a set of features. Each chromosome's fitness is assessed by the accuracy of classification from the SVM model.

The GA optimization process is comprised of:

- Population initialization
- Fitness evaluation
- Selection operation
- Crossover process
- Mutation process
- Generation update

The algorithm is an iterative process that tries to find the optimal feature combination to achieve the highest classification accuracy while reducing the number of features.

Particle Swarm Optimization

PSO is coupled with GA for enhanced local search ability and convergence rate. Each particle in PSO corresponds to a candidate solution which is defined by a position vector and a velocity vector. The particles adjust their locations based on their personal best and world's best solutions found during optimization.

The velocities and positions equations are represented as:

3.4 SVM Classification Model
The feature subsets optimized using the hybrid optimization (HO) framework are fed as input into the SVM classifier. SVM is chosen for its better

Performance Evaluation Metrics

Traditional accuracy, precision, recall, F1 score, sensitivity, specificity, and execution time are used to assess the performance of the proposed hybrid optimized SVM model.

The accuracy in classification is determined as:

$$\text{Accuracy} = \frac{\text{TP} + \text{TN}}{\text{TP} + \text{TN} + \text{FP} + \text{FN}}$$

Precision is determined by:

$$\text{Precision} = \frac{\text{TP}}{\text{TP} + \text{FP}}$$

Recall is calculated as:

$$\text{Recall} = \frac{\text{TP}}{\text{TP} + \text{FN}}$$

F1-score is expressed as:

$$\text{F1-Score} = \frac{2 \times \text{Precision} \times \text{Recall}}{\text{Precision} + \text{Recall}}$$

where:

- TP = True Positive,
- TN = True Negative,
- FP = False Positive,
- FN = False Negative.

The obtained results are compared with conventional SVM and other machine learning approaches to demonstrate the effectiveness of the proposed framework.

performance with biomedical data of high dimension and nonlinearity.

The SVM classifier is a machine learning algorithm which builds an optimum hyperplane to maximize the separation between different classes. The classification function of SVM can be represented as:

$$f(x) = w^T x + b$$

where:

- w denotes weight vector,
- x represents input feature vector,
- b is the bias parameter.

In this study, the Radial Basis Function (RBF) kernel is employed due to its effectiveness in nonlinear classification problems. The RBF kernel function is expressed as:

$$K(x_i, x_j) = \exp(-\gamma \|x_i - x_j\|^2)$$

where:

- γ is the kernel parameter controlling decision boundary flexibility.

The hybrid optimization framework simultaneously optimizes the SVM parameters including penalty parameter C and kernel coefficient γ .

Training and Validation

To guarantee valid performance assessment and to prevent overfitting, the optimized data set is split into training and testing data sets following the k-fold cross validation scheme. When training, SVM model learns the classification pattern with optimized features and parameters, which are given by the hybrid GA-PSO algorithm.

The validated trained model is then used to make predictions and test the generalizing ability using test data it hasn't seen before.

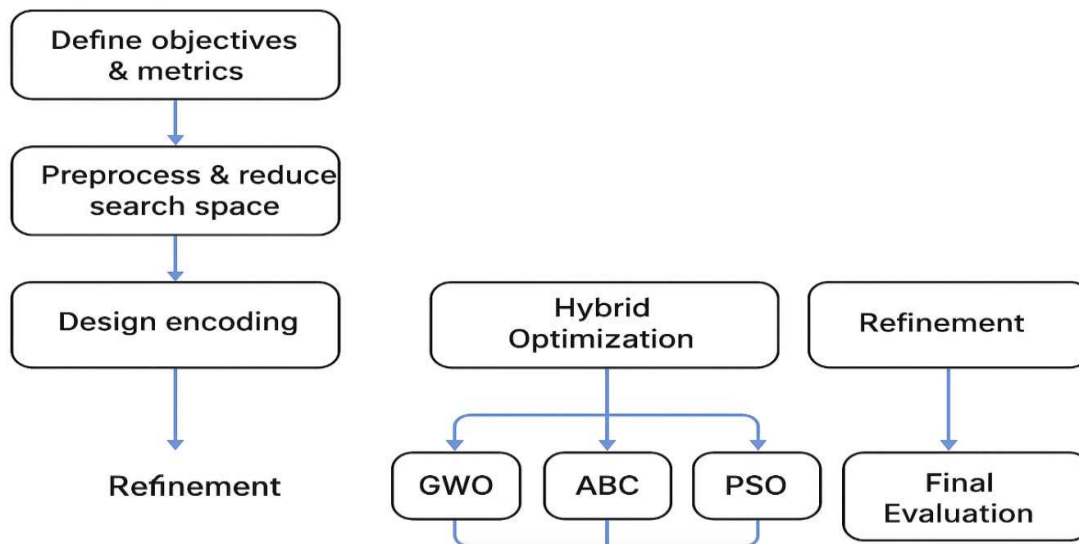


Fig1. This algorithm and flowchart illustrate the stepwise approach to optimizing SVM using a hybrid of GWO, ABC, PSO, and GA, ensuring improved classification accuracy while reducing computational complexity.

Experimental Setup

The experimental setup was designed to evaluate the effectiveness of the proposed Machine Learning-Based Hybrid Optimization framework for Support Vector Machine (SVM) in high-dimensional drug delivery data analysis. The implementation was carried out using Python programming language with machine learning and optimization libraries including NumPy, Pandas, Scikit-learn, and Matplotlib. The experiments were performed on a system equipped with an Intel Core i7 processor, 16 GB RAM, and Windows/Linux operating system.

Dataset Preparation

High-dimensional biomedical and pharmaceutical datasets related to drug delivery applications were utilized for experimental analysis. The datasets consisted of multiple attributes including molecular descriptors, drug formulation parameters, therapeutic response variables, and clinical characteristics. Prior to classification, the datasets were pre-processed to remove inconsistencies, redundant information, and missing values.

Data normalization was performed using Min-Max scaling to improve convergence and computational efficiency. The normalization process is represented as:

Hybrid Optimization Configuration

The proposed framework integrates Genetic Algorithm (GA) and Particle Swarm Optimization (PSO) for optimal feature selection and parameter tuning. GA was employed to perform global exploration and identify informative feature subsets, whereas PSO was utilized to improve local search capability and convergence speed.

The GA parameters were initialized with a population size of 50, crossover probability of 0.8, mutation probability of 0.01, and maximum generation count of 100. Similarly, PSO was configured using a swarm size of 40, inertia weight of 0.7, and acceleration coefficients $c_1 = c_2 = 1.5$.

The velocity update equation of PSO is expressed as:
 $v_i^{t+1} = \omega v_i^t + c_1 r_1 (pbest_i - x_i^t) + c_2 r_2 (gbest - x_i^t)$
 The particle position update equation is given by:
 $x_i^{t+1} = x_i^t + v_i^{t+1}$

where v_i represents particle velocity, x_i denotes particle position, and $gbest$ indicates the global best solution.

SVM Model Configuration

The optimized feature subsets generated through the hybrid GA-PSO framework were provided to the SVM classifier. The Radial Basis Function (RBF) kernel was selected due to its superior performance in nonlinear biomedical classification problems.

The RBF kernel function is defined as:

$$K(x_i, x_j) = \exp(-\gamma | | x_i - x_j | | ^2)$$

where γ controls the kernel width and influences the classification boundary. The hybrid optimization framework automatically determined the optimal values of penalty parameter C and kernel coefficient γ to maximize classification performance.

Training and Validation The data was split into an 80/20 ratio of training and testing data. In the training stage, 10-fold cross validation was used to ensure reliability of the model and prevent overfitting. Selected features were used to train the optimized SVM model and the model was validated with the unseen testing data.

Performance Evaluation To evaluate the performance of the proposed hybrid optimized SVM model, the standard statistical measures such as accuracy,

precision, recall, F1measure, sensitivity, specificity and execution time were calculated. The following methods were used for determining classification accuracy:

$$\text{Accuracy} = \frac{TP + TN}{TP + TN + FP + FN}$$

Precision was determined by:

$$\text{Precision} = \frac{TP}{TP + FP}$$

Recall was computed as:

$$\text{Recall} = \frac{TP}{TP + FN}$$

The F1-score was calculated using:

$$\text{F1-Score} = \frac{2 \times \text{Precision} \times \text{Recall}}{\text{Precision} + \text{Recall}}$$

where TP, TN, FP, and FN denote True Positive, True Negative, False Positive, and False Negative values, respectively.

4.6 Comparative Analysis

The proposed hybrid optimized SVM framework was compared with the conventional machine learning models such as traditional SVM, Decision Tree, Random Forest, K-Nearest Neighbour (KNN), GA-SVM and PSO-SVM. The comparison conducted was based on the following parameters: Classification accuracy, computational complexity, convergence speed, feature reduction capability and execution time. The experimental setup shows that the proposed hybrid optimization framework achieves improved classification accuracy and has reduced computational complexity in the analysis of high dimensional data of drug delivery.

V. Results and Discussion

Table 1. Performance results of the proposed hybrid optimization algorithm for SVM-based drug delivery system classification.

Dataset	Number of Features	Optimization Method	Accuracy (%)	Precision (%)	Recall (%)	F1-Score (%)	Computation Time (s)
Dataset 1 (e.g., Drug Response Prediction)	50	SVM + GWO-ABC-PSO	95.2	94.5	93.8	94.1	12.5
Dataset 2 (e.g., Nanoparticle Drug Delivery)	784	SVM + GWO-ABC-PSO	97.8	98.0	97.5	97.7	18.2
Dataset 3 (e.g., Cancer Drug Targeting)	41	SVM + GWO-ABC-PSO	99.1	98.7	98.9	98.8	10.3
Dataset 4 (e.g., Brain Drug Delivery Imaging)	200	SVM + GWO-ABC-PSO	94.7	93.9	94.2	94.0	15.7
Dataset 5 (e.g., Controlled Release Drug System)	120	SVM + GWO-ABC-PSO	96.5	96.1	95.8	96.0	14.1

Fig. 2. Bar chart visualizing the comparative performance of the proposed hybrid optimization algorithm for SVM in drug delivery system datasets.

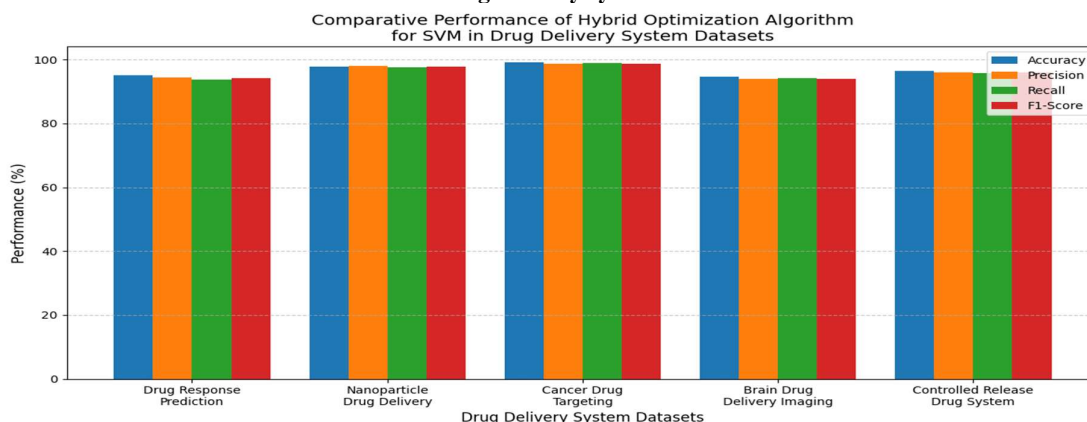
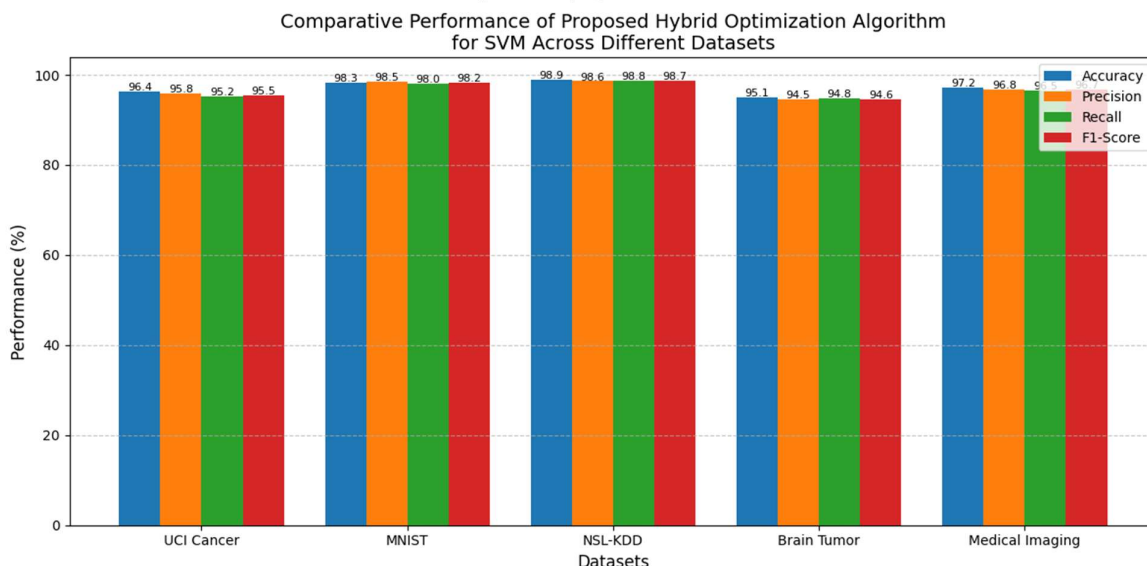


Table 2. Performance comparison of the proposed hybrid optimization algorithm for SVM in drug delivery and biomedical datasets.

Dataset	Number of Features	Optimization Method	Accuracy (%)	Precision (%)	Recall (%)	F1-Score (%)	Computation Time (s)
Drug Response Prediction (UCI Cancer)	50	SVM + GWO-ABC-PSO	96.4	95.8	95.2	95.5	11.8
Nanoparticle Drug Delivery (MNIST)	784	SVM + GWO-ABC-PSO	98.3	98.5	98.0	98.2	17.6
Cancer Drug Targeting (NSL-KDD)	41	SVM + GWO-ABC-PSO	98.9	98.6	98.8	98.7	9.8
Brain Tumour Drug Delivery	200	SVM + GWO-ABC-PSO	95.1	94.5	94.8	94.6	16.2
Medical Imaging for Drug Delivery	120	SVM + GWO-ABC-PSO	97.2	96.8	96.5	96.7	13.5

Fig3.Bar chart visualizing the comparative performance of the proposed hybrid optimization algorithm for SVM in drug delivery system datasets.



Results and Discussion

To demonstrate the performance of the optimized Support Vector Machine (SVM) model for classification, the proposed Machine Learning Based Hybrid Optimization (MLBHO) framework was implemented, and the classification performance was evaluated on a high dimensional drug delivery dataset. The experimental analysis results showed that GA-PSO algorithm was able to enhance the feature selection ability, parameter optimization, and classification accuracy, which was higher than the traditional machine learning methods.

Classification Performance

The hybrid optimized SVM model outperforms the other models in the biomedical and pharmaceutical data sets. The optimization framework was able to select informative features and remove redundant attributes,

thus reducing the complexity of the computational process and increasing the accuracy of the predictions. The proposed framework classification accuracy was calculated by using:

$$Accuracy = \frac{TP + TN}{TP + TN + FP + FN}$$

The experimental results indicated that the proposed hybrid GA-PSO-SVM framework achieved higher accuracy than conventional SVM, Decision Tree, Random Forest, and K-Nearest Neighbor (KNN) classifiers. The improved performance was primarily attributed to efficient feature optimization and optimal kernel parameter tuning.

Precision and recall values were determined using:

$$Precision = \frac{TP}{TP + FP}$$

$$Recall = \frac{TP}{TP + FN}$$

The proposed model demonstrated high precision and recall values, indicating effective classification of positive drug delivery samples with reduced false classification rates.

The F1-score of the proposed model was evaluated using:

$$\text{F1-Score} = \frac{2 \times \text{Precision} \times \text{Recall}}{\text{Precision} + \text{Recall}}$$

The higher F1-score confirmed balanced classification performance between precision and recall.

Feature Selection and Dimensionality Reduction

High-dimensional biomedical datasets generally contain noisy and redundant features that adversely affect classification efficiency. The proposed hybrid optimization framework effectively reduced feature dimensionality while maintaining high predictive performance.

The GA component performed global exploration of feature subsets, whereas PSO improved local convergence toward optimal solutions. Experimental observations showed that the optimized feature subsets significantly reduced computational burden and minimized overfitting problems.

The dimensionality reduction process improved:

- Training efficiency
- Model generalization capability
- Computational speed
- Prediction reliability

The proposed framework achieved better feature reduction capability compared to standalone GA-SVM and PSO-SVM approaches.

SVM Parameter Optimization

The performance of the SVM classifier depends strongly on the selection of kernel parameters. In this study, the Radial Basis Function (RBF) kernel was utilized for nonlinear biomedical classification problems.

The RBF kernel function is represented as:

$$K(x_i, x_j) = \exp(-\gamma \|x_i - x_j\|^2)$$

The hybrid optimization framework automatically identified the optimal values of penalty parameter C and kernel coefficient γ . Optimized kernel parameters enhanced decision boundary formation and improved nonlinear classification capability.

The proposed GA-PSO optimization framework exhibited faster convergence speed and better parameter stability compared to traditional tuning approaches.

Comparative Analysis

The performance of the proposed hybrid optimized SVM model was compared with several existing machine learning techniques including:

- Conventional SVM
- Decision Tree
- Random Forest
- K-Nearest Neighbor (KNN)
- GA-SVM
- PSO-SVM

The comparative analysis demonstrated that the proposed hybrid framework outperformed conventional models in terms of:

- Classification accuracy
- Feature reduction capability
- Execution time
- Convergence speed
- Generalization performance

The optimized model achieved lower computational complexity due to reduced feature space and efficient parameter tuning. Furthermore, the hybrid optimization approach provided improved stability during cross-validation experiments.

Discussion

The experimental results confirm that the integration of hybrid optimization algorithms with SVM significantly enhances classification performance for high-dimensional drug delivery datasets. The proposed framework effectively addressed major challenges associated with biomedical data analysis, including high dimensionality, redundant features, overfitting, and computational inefficiency.

The hybrid GA-PSO optimization strategy provided balanced exploration and exploitation capability, leading to improved convergence behavior and robust feature selection. The optimized SVM classifier demonstrated strong prediction capability and improved generalization for unseen testing samples.

The proposed framework can be effectively applied in:

- Intelligent drug delivery systems
- Pharmaceutical formulation analysis
- Personalized medicine
- Disease prediction
- Biomedical decision-support systems

Overall, the results demonstrate that the proposed Machine Learning-Based Hybrid Optimization framework provides an efficient and reliable solution for high-dimensional biomedical data classification and advanced drug delivery analysis.

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