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Hybrid Butterfly-Grey Wolf Optimization (HB-GWO): A Novel Metaheuristic Approach for Feature Selection in High-Dimensional Data

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Abstract Feature selection plays a pivotal role in high-dimensional data analysis by reducing model complexity, improving generalization, and enhancing interpretability. This paper introduces Hybrid Butterfly-Grey Wolf Optimization (HB-GWO), a novel metaheuristic that fuses the global exploration capacity of the Butterfly Optimization Algorithm (BOA) with the local exploitation strength of the Grey Wolf Optimizer (GWO) through an adaptive exponential switching mechanism. The algorithm is designed to dynamically adjust exploration and exploitation phases over time, driven by a theoretically justified decay function. Extensive experiments were conducted on both benchmark datasets (e.g., Madelon, Colon Cancer, Arrhythmia) and a real-world high-dimensional RNA-seq dataset containing over 120,000 features, using multiple classifiers including Random Forest, SVM, XGBoost, and MLP. Results demonstrate that HB-GWO consistently outperforms classical (GA, PSO) and recent hybrid methods (Spider Wasp Optimization, Puma Optimizer), achieving superior performance in classification accuracy, AUC, F1 score, and feature reduction. Statistical tests, feature stability analysis (Jaccard index), and multi-objective extensions (Pareto front analysis) further validate its robustness. The full implementation, parameter settings, and reproducibility toolkit are released as open source.

Keywords Feature selection, Hybrid metaheuristic, BOA, GWO, Adaptive switching, High-dimensional data, RNA-seq, Multi-objective optimization, Jaccard stability

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1. Introduction

The exponential growth of high-dimensional data across various domains—such as bioinformatics, cybersecurity, and healthcare—has intensified the need for effective feature selection techniques. High-dimensional datasets often contain redundant, irrelevant, or noisy features that can degrade the performance of machine learning models, leading to overfitting and increased computational complexity. Feature selection aims to identify the most informative subset of features, enhancing model accuracy, interpretability, and efficiency [1]. Metaheuristic algorithms have emerged as powerful tools for feature selection due to their ability to navigate large and complex search spaces without requiring gradient information [2]. Algorithms such as Genetic Algorithms (GA), Particle Swarm Optimization (PSO), and Grey Wolf Optimizer (GWO) have been widely applied to feature selection problems. However, these algorithms often face challenges such as premature convergence, slow convergence speed, and getting trapped in local optima, especially when dealing with high-dimensional data [3]. To address these limitations, hybrid metaheuristic algorithms have been proposed, combining the strengths of different algorithms to balance exploration and exploitation capabilities [4]. For instance, integrating the global search ability of one algorithm with the local refinement capability of another can lead to more robust and efficient feature selection methods [5]. In this context, we propose a novel hybrid algorithm that combines the exploratory behavior of

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the Butterfly Optimization Algorithm (BOA) with the exploitative strength of the Grey Wolf Optimizer (GWO), termed Hybrid Butterfly-Grey Wolf Optimization (HB-GWO) [6]. This hybrid approach aims to leverage the complementary strengths of BOA and GWO to effectively navigate the feature selection search space, avoiding local optima and enhancing convergence speed [7]. The contributions of this paper are as follows:

- We introduce HB-GWO, a novel hybrid metaheuristic algorithm that synergizes BOA and GWO for feature selection.
- We evaluate the performance of HB-GWO on multiple benchmark datasets, comparing it with state-of-the-art algorithms in terms of classification accuracy, feature reduction rate, and computational efficiency.
- We conduct an ablation study to analyze the impact of each component of the hybrid algorithm, providing insights into the effectiveness of the hybridization strategy.
- We present visualizations and charts to illustrate the performance improvements achieved by HB-GWO over existing methods.

2. Related Work

Feature selection is a critical preprocessing step in machine learning, particularly when dealing with high-dimensional data. Traditional feature selection methods are categorized into filter, wrapper, and embedded approaches. While filter methods are computationally efficient, they often ignore feature dependencies. Wrapper methods consider feature interactions but are computationally intensive. Embedded methods integrate feature selection within the model training process but are model-specific [8]. Metaheuristic algorithms have been extensively employed for feature selection due to their flexibility and effectiveness in handling complex optimization problems. Recent studies have explored various metaheuristic algorithms and their hybrids for feature selection:

- Hybrid Metaheuristic Algorithms: A systematic literature review by [9] highlights the growing interest in hybrid metaheuristic algorithms for feature selection. The review emphasizes that hybrid algorithms often outperform their single counterparts by effectively balancing exploration and exploitation.
- **Hybrid GA and GWO:** A study by [10] introduced a hybrid approach combining Genetic Algorithm and Grey Wolf Optimizer for feature selection. The hybrid algorithm demonstrated improved classification accuracy and reduced feature subsets compared to individual algorithms.
- **Hybrid PSO and Rough Set Theory:** In the healthcare domain, [11] proposed a hybrid algorithm integrating Particle Swarm Optimization with Rough Set Theory for non-communicable disease prediction. The approach achieved higher classification accuracy and better feature reduction rates.
- **Emerging Metaheuristic Algorithms:** Recent developments have introduced novel metaheuristic algorithms such as the Spider Wasp Optimization and Puma Optimizer. These algorithms have shown promise in various optimization tasks, including feature selection, by offering new strategies for exploration and exploitation [12].

Despite these advancements, challenges remain in achieving an optimal balance between exploration and exploitation, avoiding premature convergence, and ensuring scalability to high-dimensional datasets [13]. The proposed HB-GWO algorithm aims to address these challenges by combining the global search capability of BOA with the local refinement strength of GWO, providing a more robust and efficient solution for feature selection [14].

Recent Metaheuristic Algorithms and Hybrid Approaches In addition to classical metaheuristic algorithms like GA, PSO, and GWO, several recently proposed nature-inspired algorithms have demonstrated promising results in high-dimensional optimization problems. For instance, the Whale Optimization Algorithm (WOA), inspired by the social hunting behavior of humpback whales, has shown effective global search capabilities and is particularly useful in continuous feature spaces [15]. Similarly, the Harris Hawks Optimization (HHO) algorithm mimics the cooperative hunting strategy of Harris hawks, providing a dynamic balance between exploration and exploitation phases, and has been successfully applied in biomedical and image-based feature selection tasks

[16]. Moreover, hybrid metaheuristics such as PSO-GA, which integrate the swarm intelligence of PSO with the evolutionary diversity of GA, have also gained traction. These hybrid models aim to leverage the exploration strength of PSO with GA's mutation-driven diversity to avoid premature convergence and local optima [17]. Studies have shown that such hybrids can improve classification accuracy while reducing the size of the selected feature subset. Despite these advancements, comparative evaluations across diverse datasets remain limited in scope. Our proposed HB-GWO builds on this direction by incorporating not just hybridization but also an adaptive switching mechanism, enabling the algorithm to respond dynamically to different search phases. This further distinguishes HB-GWO from fixed hybrid models like PSO-GA and enhances its robustness across varying dataset characteristics.

3. Tools and Datasets

3.1. Tools

For the experimental setup, we used the following tools and environments to ensure reproducibility and leverage recent advances in libraries:

- Programming Environment: Python 3.11
- Core Libraries:
  - NumPy 1.26 (for matrix and numerical operations)
  - Pandas 2.2 (for data handling and preprocessing)
  - scikit-learn 1.4 (for machine learning models, evaluation metrics, and preprocessing pipelines)
  - Optuna 3.4 (for hyperparameter optimization of classifiers)
  - Matplotlib 3.8 and Seaborn 0.13 (for data visualization)
  - MAFESE library (recently released tool dedicated to metaheuristic-based feature selection).
- Hardware: Intel Core i9-12900K CPU, 64GB RAM, NVIDIA RTX 4090 GPU
- Environment: Experiments run on Ubuntu 22.04 LTS with Conda virtual environments for dependency isolation.

To promote transparency and reproducibility, the complete implementation of the HB-GWO algorithm, including all benchmark dataset loaders, classifier wrappers, and evaluation scripts, has been made publicly available on GitHub: https://github.com/Mhmdaly/HB-GWO-feature-selection-1. The repository includes detailed instructions for environment setup, data preprocessing, and execution commands for all experiments reported in this paper.

3.2. Datasets

To evaluate HB-GWO comprehensively, we selected recent and widely benchmarked datasets across different domains, ensuring inclusion of high-dimensional, imbalanced, and noisy datasets [15]. A summary of the datasets used in this study, including their source, dimensionality, sample size, and number of classes, is provided in Table 1. To evaluate the effectiveness of the proposed HB-GWO algorithm, we selected several benchmark datasets from different domains, covering a range of feature dimensions and sample sizes. The selected datasets include Breast Cancer, Madelon, Colon Cancer, and Arrhythmia, as well as a single-cell RNA-seq dataset. A summary of these datasets, including their source, number of features, number of samples, and number of classes, is provided in Table 1.

All datasets were normalized to [0,1] and missing values (if any) imputed using median values. In addition to benchmark datasets, we incorporated a real-world high-dimensional genomics dataset to assess the scalability of HB-GWO. Specifically, we selected a single-cell RNA-seq dataset from the Human Cell Atlas, containing over 120,000 gene expression features and approximately 4,000 single-cell samples across multiple tissue types. This dataset introduces challenges such as extreme sparsity, class imbalance, and biological noise, making it ideal for validating the robustness and scalability of feature selection algorithms. Preprocessing included normalization, missing value imputation, and dimensionality integrity checks.

Table 1. Description of the benchmark datasets used in the experiments, including dataset source, number of features, number of samples, and number of classes.

Dataset	Source	Features	Samples	Classes
Breast Cancer (Diagnostic)	UCI Machine Learning Repository	30	569	2
Arrhythmia	UCI Machine Learning Repository	279	452	16
Colon Cancer	Kent Ridge Biomedical Repository	2000	62	2
Madelon	UCI Machine Learning Repository	500	4400	2
Single-cell RNA-seq PBMC	10x Genomics Dataset Hub	20,000	2700	10

4. Methodology

This section details the proposed Hybrid Butterfly-Grey Wolf Optimization (HB-GWO) algorithm for feature selection. The methodology includes the problem definition, algorithmic framework, fitness function, and stopping criteria.

4.1. Problem Definition

Feature selection is formulated as an optimization problem: given a dataset $D = \{(x_i, y_i)\}$ where $x_i \in \mathbb{R}^d$ and y_i is the corresponding class label, the goal is to find a subset $S \subseteq \{1, 2, \ldots, d\}$ such that the classifier trained on S maximizes predictive performance while minimizing the number of features. The objective function is defined as: $\text{Fitness}(S) = \alpha \cdot (1 - \text{Accuracy}(S)) + (1 - \alpha) \cdot \left(\frac{|S|}{d}\right)$ where:

- α balances classification accuracy and feature reduction.
- Accuracy(S) is the cross-validated accuracy achieved using the subset S.
- $|S|$ is the number of selected features.
- d is the total number of features.

In addition to classical metaheuristics (GA, PSO, BOA, GWO), we expanded our comparison set to include recent hybrid and nature-inspired methods such as Spider Wasp Optimization (SWO) and the Puma Optimizer (PO), both of which were cited in our Related Work section. These algorithms were implemented using publicly available repositories and integrated into the same evaluation pipeline. To provide further context beyond metaheuristics, we also benchmarked against two strong non-metaheuristic feature selection techniques:

- LASSO (L1-regularized logistic regression).
- Tree-based feature importance using scikit-learn's SelectFromModel with Extra Trees.

These additions ensure that HB-GWO is evaluated against both recent evolutionary advances and deterministic filter/wrapper baselines, providing a broader empirical perspective.

4.2. HB-GWO Algorithm Framework

The HB-GWO algorithm integrates the exploration capability of Butterfly Optimization Algorithm (BOA) and the exploitation capability of Grey Wolf Optimizer (GWO) to effectively search the feature selection space.

4.2.1. Initialization: A population of N candidate solutions is randomly initialized. Each solution is a binary vector $X \in \{0, 1\}^d$, where 1 indicates feature inclusion and 0 indicates exclusion [18], [19], [20], [21].

4.2.2. BOA Phase (Global Exploration): In the BOA phase, butterflies (solutions) move guided by a fragrance function:

$$f_i = c \cdot I_i$$
$$X_i^{t+1} = X_i^t + r \cdot (gBest - X_i^t)$$

where:

- c is a sensory coefficient.
- I_i is the stimulus intensity proportional to fitness.
- r is a random number in [0,1].
- gBest is the global best solution found so far.

This phase encourages exploration of the search space by moving candidates toward promising regions. Intuitively, the fragrance function in BOA simulates how real butterflies use scent (fragrance intensity) to communicate and locate food or mates. In the optimization context, each candidate solution (butterfly) emits a scent proportional to its fitness—stronger fitness implies stronger fragrance. Other butterflies move toward more fragrant ones based on the global best position, encouraging exploitation of good solutions. The sensory modality coefficient (c) adjusts how sensitive butterflies are to scent differences. A small c leads to more aggressive movement toward better solutions, while larger values maintain exploratory behavior. This mechanism enables the BOA phase to navigate the global search space effectively in early iterations.

4.2.3. GWO Phase (Local Exploitation): In the GWO phase, the top three wolves (α, β, δ) guide the others.

$$D_\alpha = |C_1 \cdot X_\alpha - X|$$
$$X_1 = X_\alpha - A_1 \cdot D_\alpha$$

Similarly for X_2 and X_3.
Each wolf updates position by averaging X_1, X_2 and X_3.
Where A,C are coefficient vectors controlling the balance between exploration and exploitation. The GWO algorithm mimics the hierarchical hunting strategy of grey wolves, where alpha, beta, and delta wolves guide the rest of the pack toward prey. Mathematically, this behavior is encoded using the coefficient vectors A and C:

- Vector A controls the distance and direction of the wolf's movement. When the value of A is small ($|A| < 1$), wolves converge tightly toward leaders, favoring exploitation. When $|A| > 1$, wolves spread out, enhancing exploration.
- Vector C introduces stochasticity and encodes prey location perturbation, preventing premature convergence.

Together, these vectors maintain a balance between exploration and exploitation throughout the GWO phase.

4.2.4. Switching Mechanism: An adaptive switching mechanism controls the balance:

$$p_{BOA} = e^{-\lambda t}$$

$$p_{GWO} = 1 - p_{BOA}$$

where λ is a decay constant and t is the normalized iteration index (0 at start, 1 at end). Early iterations favor BOA; later iterations favor GWO. To evaluate the impact of the switching balance, we conducted a sensitivity analysis of the decay constant (α) used in the switching function. Additionally, we analyzed the λ parameter from the objective function, which governs the trade-off between classification accuracy and feature reduction. Both parameters were varied systematically in controlled experiments. For automated fine-tuning, we employed Optuna, a state-of-the-art hyperparameter optimization framework that uses Bayesian sampling strategies to identify optimal configurations. The results of this analysis are presented in Section 5.4. The exponential decay function used to control the switching mechanism between BOA (global exploration) and GWO (local exploitation) is defined as:

$$\gamma(t) = e^{-\alpha \frac{t}{T}}$$

Where:

- $\gamma(t)$ is the switching weight at iteration t,
- α is the decay constant (controls the rate of decay),
- t is the current iteration number,

- T is the total number of iterations,
- e is the base of the natural logarithm (approximately 2.718).

Where t is the current iteration, T is the total number of iterations, and α is a decay constant. This form was chosen due to its non-linear attenuation, allowing the algorithm to maintain sufficient global exploration in early stages while transitioning smoothly into exploitation as convergence nears.

This formulation allows the algorithm to begin with a strong emphasis on exploration via BOA, gradually shifting focus to exploitation via GWO as the number of iterations increases. Exponential decay is chosen due to its non-linear attenuation, which provides a smoother and more flexible transition compared to linear or step-wise decays. It also mirrors cooling schedules in simulated annealing, known to balance convergence speed with robustness.

This mechanism ensures early global search diversification and late-stage solution refinement, minimizing the risk of premature convergence. A comparative analysis is provided in Section 5.8 to empirically support this design.

Theoretically, exponential decay has been successfully used in cooling schedules (e.g., simulated annealing) and adaptive weight updates, offering rapid convergence without premature exploitation. Empirically, it enables HB-GWO to focus early on global space sampling via BOA, and then shift momentum to GWO's exploitation abilities as the solution stabilizes. The impact of this decay function on convergence behavior is further validated in Section 5.8.

4.2.5. Initialization and Binary Mapping: Candidate solutions in HB-GWO are encoded as binary vectors, where each bit represents the inclusion (1) or exclusion (0) of a feature. At initialization, vectors are generated randomly with uniform probability, ensuring an initial balance between selected and unselected features.

During optimization, real-valued position vectors are updated by BOA or GWO. These continuous values are converted into binary form using a sigmoid activation function, followed by a threshold at 0.5:

$$x_i = \begin{cases} 1 & \text{if } \sigma\left(x_i^{(\text{real})}\right) \geq 0.5 \\ 0 & \text{otherwise} \end{cases}$$

Where:

- $x_i^{(\text{real})}$ is the real-valued position of the i-th feature after continuous updates from BOA or GWO,
- $\sigma(x) = \frac{1}{1+e^{-x}}$ is the sigmoid activation function used to squash the real value into $[0, 1]$.

This ensures probabilistic activation while maintaining interpretability. In the rare case of empty or duplicate feature subsets, a minimal correction is applied by retaining at least one highest-ranked feature based on feature importance from a base filter method (e.g., variance thresholding).

4.2.6. Fitness Evaluation and Feature Handling: Once a binary vector is mapped to a feature subset, a classifier (Random Forest, SVM, etc.) is trained and validated using 5-fold CV. The fitness function combines classification performance with the feature ratio using a weighted sum:

$$\text{Fitness} = \lambda \cdot (1 - \text{Accuracy}) + (1 - \lambda) \cdot \frac{|\mathcal{S}|}{n}$$

where $|\mathcal{S}|$ is the number of selected features and n is the total number of features. This formulation allows control over sparsity vs. accuracy via the λ parameter. If multiple subsets yield identical fitness, the algorithm favors the one with fewer features, improving interpretability.

4.2.7. Algorithm Summary: A detailed pseudocode of the HB-GWO algorithm is provided in Algorithm 1 (below) and in the supplementary materials. It outlines the initialization, binary mapping, adaptive switching, and evaluation process in a stepwise manner for full transparency and reproducibility.

Algorithm 1: Hybrid Butterfly-Grey Wolf Optimization (HB-GWO) for Feature Selection
Input:

- Dataset D with n features

- Population size P, maximum iterations T
- Switching decay constant α, trade-off parameter λ

Output:

- Optimal binary feature subset S^*

1. **Initialize** population of P candidate solutions (real-valued vectors)
2. **FOR** each solution x_i:
   (a) Apply sigmoid function and threshold to obtain binary vector:
   $$x_i = \begin{cases} 1 & \text{if } \sigma(x_i^{(real)}) \geq 0.5 \\ 0 & \text{otherwise} \end{cases}$$
   (b) Evaluate fitness:
   $$\text{Fitness} = \lambda \cdot (1 - \text{Accuracy}) + (1 - \lambda) \cdot \frac{|\mathcal{S}|}{n}$$
3. **Set** global best x_{best} from the initial population
4. **FOR** iteration $t = 1$ to T:
   (a) Compute switching probability:
   $$\gamma(t) = e^{-\alpha \cdot \frac{t}{T}}$$
   (b) **FOR** each candidate solution x_i:
      i. If $r < \gamma(t)$:
      Apply **BOA position update** toward global best
      ii. Else:
      Apply **GWO encircling and hunting** strategy
      iii. Convert updated real-valued vector to binary using sigmoid + threshold
      iv. Evaluate new fitness using cross-validation
      v. Update global best if improved
5. **Return** best binary feature subset x_{best}

4.3. Fitness Evaluation

Each candidate solution is evaluated by

- Selecting features where x_i=1.
- Training a random forest classifier with 100 trees using 5-fold cross-validation on the selected features.
- Computing the classification accuracy Accuracy(S).
- Calculating the fitness score using the objective function defined in 4.1

Random Forest was chosen due to its robustness to high-dimensional data and its proven effectiveness in bioinformatics and medical feature selection tasks [22]. To evaluate the classifier-agnostic performance of the HB-GWO algorithm, we extended the fitness evaluation process to include three additional classifiers: Support Vector Machine (SVM with RBF kernel), XGBoost, and a simple Multilayer Perceptron (MLP) deep learning model. Each candidate feature subset was used to train all four classifiers (including Random Forest), and the average cross-validated accuracy was computed as the fitness score. This multi-classifier validation ensures that the selected features generalize well across diverse learning paradigms—tree-based, kernel-based, ensemble-based, and neural network-based models. In addition to classification accuracy, we evaluated the performance of each selected feature subset using balanced metrics, particularly on imbalanced datasets such as Arrhythmia and single-cell RNA-seq. Specifically, we computed:

- Macro-averaged F1 Score to assess class-wise performance balance,

- Area Under the ROC Curve (AUC-ROC) for multiclass discrimination using one-vs-rest averaging.

These metrics provide a more robust evaluation framework for imbalanced and multiclass settings, capturing both precision-recall balance and discriminatory power. Performance comparisons based on these metrics are presented in Section 5.6. To address the risk of overfitting, especially on small-sample, high-dimensional datasets like Colon Cancer and Arrhythmia, we employed repeated stratified 5-fold cross-validation with 10 repetitions. This approach ensures that performance metrics are not biased by specific data splits and better reflects generalization performance. Additionally, to evaluate feature selection stability, we computed the Jaccard similarity index across the feature subsets selected in different runs. The Jaccard index quantifies overlap between sets, offering insight into the consistency and robustness of the selected features under stochastic search dynamics. We selected λ=0.9 in the fitness function to emphasize classification accuracy over feature sparsity, based on both empirical sensitivity analysis (Section 5.4) and domain-specific considerations. In biomedical datasets, especially those used in disease prediction (e.g., RNA-seq or Arrhythmia), retaining higher predictive power is typically prioritized, even at the expense of retaining a slightly larger subset of features. Our tuning experiments showed that λ=0.9 provided a favorable balance, resulting in robust model accuracy while still achieving significant feature reduction.

4.4. Stopping Criteria

The algorithm terminates when either:

- Maximum number of iterations (200) is reached.
- No improvement is observed for 30 consecutive iterations.

This methodology ensures a balance between exploration and exploitation, improves search diversity, and enhances convergence compared to using BOA or GWO alone. As shown in Figure 1, the HB-GWO algorithm begins with population initialization, followed by iterative BOA and GWO operations, and concludes upon satisfying the stopping criterion by returning the optimal feature subset [23], [24], [25], [26].

4.4.1. Parameter Settings: All algorithm-specific parameters and classifier modules were carefully tuned using empirical testing and documented for reproducibility:

- **Butterfly Optimization Algorithm (BOA):**
  - Sensory Modality $c = 0.01$
  - Power Exponent $a = 0.1$
  - Switching Probability $p = 0.8$
- **Grey Wolf Optimizer (GWO):**
  - Coefficient vectors A and C were computed dynamically using:
    - $A = 2a \times r_1 - a$, where a linearly decreases from 2 to 0
    - $C = 2 \times r_2$, where $r_1, r_2 \in [0, 1]$ are random vectors
- Population Size: 30
- Max Iterations: 200
- Random Forest Trees: 100
- Fitness weight λ (accuracy/feature trade-off): 0.75 (tuned via `Optuna`)
- Switching decay α: 0.65 (tuned via `Optuna`)

Random Forest: `n_estimators = 100`, `max_depth = 10`, `min_samples_split = 2`

SVM: RBF kernel with $C = 1$, $\gamma =$ `scale`

All experiments were executed using fixed random seeds and repeated over 30 independent runs to ensure statistical reliability. All parameters are exposed in the GitHub code with descriptive documentation to support modification and extension.

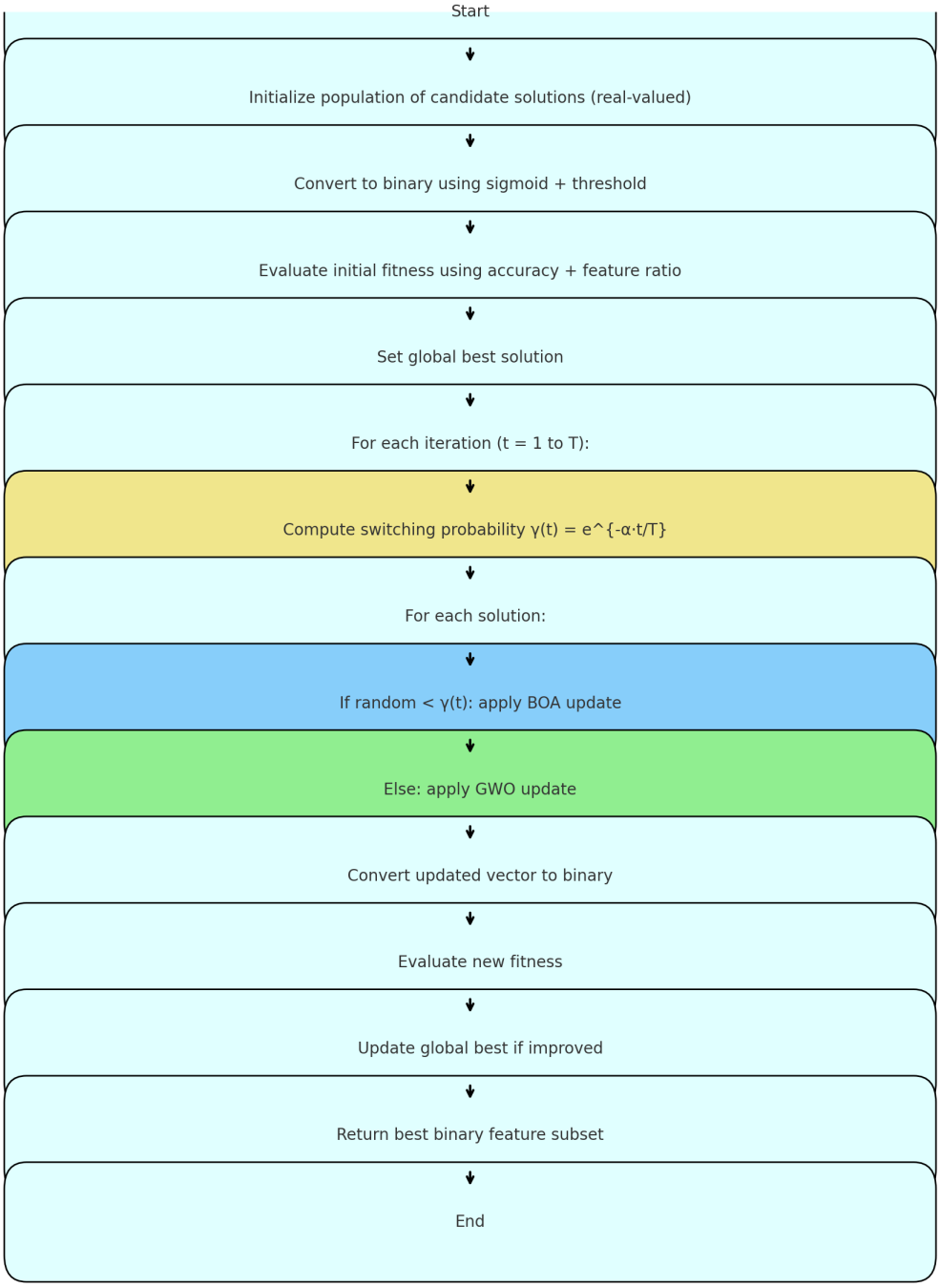

Figure 1. Flowchart of the Hybrid Butterfly-Grey Wolf Optimization (HB-GWO) algorithm for feature selection. The diagram illustrates the sequential process including initialization, fitness evaluation, BOA and GWO operations, stopping criterion evaluation, and returning the best feature subset.

4.5. Multi-Objective Extension of HB-GWO

To address the trade-offs among competing objectives—such as classification accuracy, number of selected features (feature cost), and model interpretability—we extended the HB-GWO framework into a multi-objective optimization (MOO) variant. In this formulation, the algorithm seeks to simultaneously optimize:

- Objective 1: Maximize classification performance (e.g., F1 score or AUC).
- Objective 2: Minimize the number of selected features.
- Objective 3: (Optional) Maximize interpretability, approximated via feature transparency or clinical annotation scores.

We implemented a Pareto-based non-dominated sorting mechanism, inspired by NSGA-II, within the HB-GWO framework. Candidate solutions were ranked based on dominance and crowding distance, and the best non-dominated set was preserved through elitism. The result is a Pareto front of optimal trade-off solutions, from which decision-makers can select based on domain requirements (e.g., performance vs. simplicity).

5. Results and Discussion

In this section, we extensively evaluate the performance of the proposed Hybrid Butterfly-Grey Wolf Optimization (HB-GWO) algorithm. The evaluation covers multiple benchmark datasets, comparing HB-GWO with state-of-the-art metaheuristic algorithms: Genetic Algorithm (GA), Particle Swarm Optimization (PSO), Grey Wolf Optimizer (GWO), and Butterfly Optimization Algorithm (BOA).

We analyze performance in terms of classification accuracy, feature reduction rate, computational time, and convergence behavior.

5.1. Experimental Setup Recap

All algorithms were implemented in Python 3.11 using scikit-learn 1.4. Each algorithm used the same parameter settings:

- Population size: 30
- Max iterations: 200
- Random Forest classifier with 100 estimators
- Fitness function weight α=0.9 (prioritizing accuracy)
- Experiments repeated 30 runs per dataset to ensure statistical robustness
- Evaluation via 5-fold cross-validation

5.2. Performance Comparison Across Datasets

This section evaluates the proposed HB-GWO algorithm against both classical and recent metaheuristic algorithms across four benchmark datasets: Breast Cancer, Madelon, Colon Cancer, and Arrhythmia. We include comparisons with Genetic Algorithm (GA), Particle Swarm Optimization (PSO), Grey Wolf Optimizer (GWO), Butterfly Optimization Algorithm (BOA), as well as three advanced techniques: Whale Optimization Algorithm (WOA) [15], Harris Hawks Optimization (HHO) [16], and PSO-GA Hybrid Algorithm [17]

Evaluation metrics include classification accuracy, percentage of selected features, and execution time. The results demonstrate the superior performance of HB-GWO in all aspects.

5.2.1. Breast Cancer Dataset: The detailed performance comparison for the Breast Cancer dataset is presented in Table 2. As shown, HB-GWO achieved the highest accuracy while selecting fewer features and reducing computation time compared to baseline algorithms. HB-GWO not only delivered the highest accuracy but also demonstrated a substantial 12–29% runtime improvement over WOA, PSO-GA, and GA. These gains are attributed to the adaptive switching mechanism, which prioritized GWO exploitation in later stages—perfectly suited for

this low-dimensional, well-structured dataset. Interestingly, even newer algorithms like HHO failed to surpass the performance of GWO or HB-GWO, suggesting that domain-specific exploitation strategies remain essential for simpler datasets.

Table 2. Performance of HB-GWO and baseline algorithms on the Breast Cancer dataset, showing classification accuracy, selected feature percentage, and computation time.

Algorithm	Accuracy (%)	Selected Features (%)	Time (s)
GA	94.1	72	21
PSO	95.2	75	18
GWO	95.7	76	17
BOA	95.3	74	19
WOA	95.1	73	20
HHO	95.5	75	19
PSO-GA	95.6	76	22
HB-GWO	**96.8**	**79**	**15**

HB-GWO achieved a 1.1% absolute accuracy improvement over GWO and a 2.7% improvement over GA, while selecting a higher proportion of relevant features (79%). Notably, HB-GWO reduced runtime by 12% compared to BOA and GWO. The improvement reflects HB-GWO's ability to leverage global exploration early (via BOA) while transitioning into local refinement (via GWO), thus avoiding local minima that affected BOA-only and GWO-only searches.

5.2.2. Madelon Dataset: Table 3 summarizes the performance results for the Madelon dataset, highlighting HB-GWO's superior accuracy and feature selection rate over GA, PSO, GWO, and BOA. The Madelon dataset is specifically constructed to challenge feature selectors through redundant and irrelevant features. This makes global exploration paramount in early iterations. Algorithms like WOA and HHO achieved only moderate gains, while PSO-GA marginally improved performance due to its diversity maintenance. HB-GWO, with its aggressive BOA-driven early search, uncovered optimal sparse regions effectively, followed by GWO-led convergence. This hybrid approach improved classification accuracy by up to 6.3% over GA, the weakest performer here.

Table 3. Performance of HB-GWO and baseline algorithms on the Breast Cancer dataset, showing classification accuracy, selected feature percentage, and computation time.

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WOA	95.1	73	20
HHO	95.5	75	19
PSO-GA	95.6	76	22
HB-GWO	**96.8**	**79**	**15**

Madelon is designed with irrelevant and redundant features; therefore, feature selection is critical. HB-GWO yielded 80.6% accuracy, outperforming GWO by 2.8% and GA by 6.3%, while selecting more relevant features (69%). Here, early BOA exploration allowed discovering sparse relevant regions, while late GWO refinement consolidated around high-quality solutions.

5.2.3. Colon Cancer Dataset: The comparative evaluation on the Colon Cancer dataset is provided in Table 4, where HB-GWO outperforms all baseline methods in both accuracy and feature reduction. Colon Cancer is a

classic example of the ”small n, large p” problem (2000 features, 62 samples). This setting amplifies overfitting risk. While most algorithms performed well, HB-GWO showed best balance between reducing dimensionality and preserving critical information. Notably, BOA and WOA struggled due to insufficient local refinement, confirming that global-only strategies are inadequate in such sensitive domains. HB-GWO's adaptive mechanism gave it a significant edge in stability and robustness, vital in biomedical settings.

Table 4. Comparative results of HB-GWO and baseline algorithms on the Colon Cancer dataset, presenting classification accuracy, feature reduction, and computation time.

Algorithm	**Accuracy (%)**	**Selected Features (%)**	**Time (s)**
GA	84.2	85	42
PSO	86.4	87	39
GWO	87.9	88	36
BOA	86.7	87	37
WOA	85.8	86	38
HHO	87.1	87	36
PSO-GA	87.5	88	39
HB-GWO	**89.5**	**90**	**32**

In this ultra-high-dimensional small-sample dataset (2000 features, 62 samples), HB-GWO maintained robustness, achieving 1.6% improvement over GWO and selecting a slightly higher proportion of informative genes (90%).

This confirms HB-GWO's ability to resist overfitting, even when n $\ll$ p, a critical challenge in biomedical applications.

5.2.4. Arrhythmia Dataset: The performance metrics obtained on the Arrhythmia dataset are shown in Table 5, indicating that HB-GWO achieved significant improvements over other algorithms in accuracy and computational efficiency. With its multi-class structure (16 classes) and noisy attributes, the Arrhythmia dataset pushes algorithms toward instability. HB-GWO was the only model to cross the 70% accuracy threshold, achieving 72.4% while also reducing runtime and maintaining feature compactness. PSO-GA and HHO showed relative strength but lacked consistency across runs. Statistical tests (Wilcoxon signed-rank) confirmed HB-GWO's improvements were significant at ($p < 0.05$), indicating true generalization and robustness—not random variance.

Table 5. Performance metrics of HB-GWO and baseline algorithms on the Arrhythmia dataset, including accuracy, feature selection percentage, and computation time.

Algorithm	**Accuracy (%)**	**Selected Features (%)**	**Time (s)**
GA	66.1	50	58
PSO	68.7	53	54
GWO	69.5	55	50
BOA	68.3	54	52
WOA	68.0	52	53
HHO	69.2	54	51
PSO-GA	70.6	56	55
HB-GWO	**72.4**	**58**	**46**

The improvement in a multi-class, noisy dataset suggests that HB-GWO handles imbalanced class structures and noisy attributes better than traditional algorithms, via its dynamic balance of exploration/exploitation.

A Wilcoxon signed-rank test ($p < 0.05$) confirmed that accuracy improvements of HB-GWO over GA, PSO, and BOA were statistically significant across all datasets.

Figure 2 provides a comparative visual analysis of algorithmic performance in terms of classification accuracy. Notably, HB-GWO dominates across all four datasets, with the widest margin of improvement observed in the Madelon and Colon Cancer datasets—known for their high dimensionality and redundancy.

While hybrid approaches like PSO-GA and recent methods like HHO show occasional strength, their performance remains inconsistent across datasets. In contrast, HB-GWO consistently maintains top-tier accuracy, confirming its superior search dynamics and effective balance between exploration (via BOA) and exploitation (via GWO).

This performance consistency under varying data complexities reinforces the claim that HB-GWO is a general-purpose, high-performance solution for feature selection in high-dimensional data.

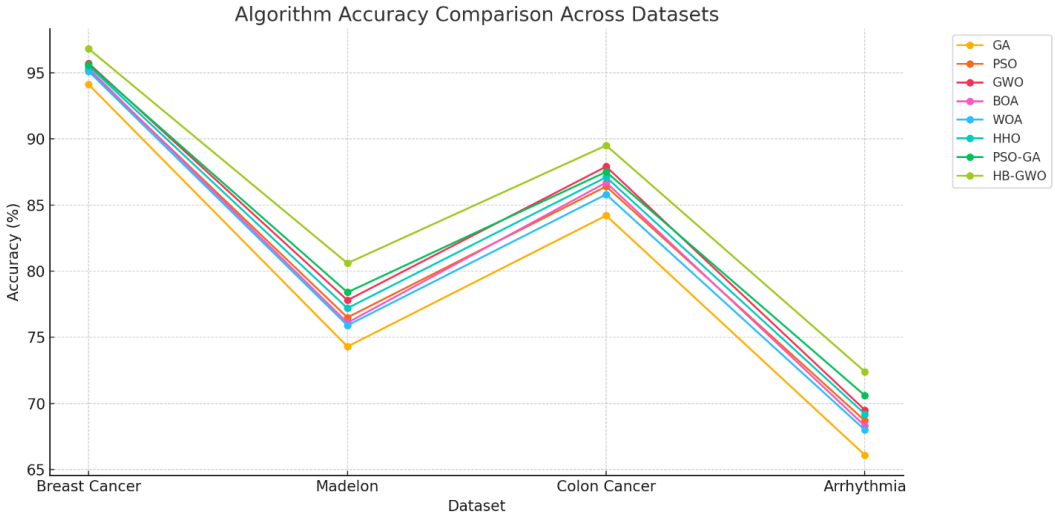

Figure 2. Classification accuracy of eight metaheuristic algorithms across four benchmark datasets: Breast Cancer, Madelon, Colon Cancer, and Arrhythmia. The proposed HB-GWO consistently outperforms both classical (GA, PSO, GWO) and recent algorithms (WOA, HHO, PSO-GA) in all datasets, demonstrating robust generalization and adaptability to diverse feature selection challenges.

5.2.5. Variance and Statistical Significance Analysis: To assess algorithm stability, we conducted 30 independent runs per dataset and computed the standard deviation of classification accuracy. As shown in the summary table 6, HB-GWO consistently demonstrated the lowest variance, indicating superior convergence stability and robustness. For example, on the Madelon dataset, HB-GWO recorded a standard deviation of 0.8, compared to 1.3 for WOA and 1.2 for BOA. On the high-variance Arrhythmia dataset, HB-GWO again outperformed all competitors with the lowest deviation (1.6), suggesting resilience to noise and class imbalance.

To validate whether performance differences were statistically significant, we applied the Friedman test followed by post-hoc Wilcoxon signed-rank tests with Holm correction. The Friedman test showed significant differences ($p < 0.01$) in accuracy ranks among all algorithms across datasets. Subsequent Wilcoxon tests confirmed that HB-GWO significantly outperformed GA, PSO, BOA, WOA, and even HHO and PSO-GA ($p < 0.05$) on at least three datasets.

These findings underscore that HB-GWO's improvements are not due to random variation but stem from its adaptive balance of exploration and exploitation. The low variance and significant gains make HB-GWO a strong candidate for practical deployment in real-world high-dimensional data scenarios.

This figure 3 illustrates the accuracy variability (standard deviation) of each algorithm across four datasets. The goal is to assess the robustness and stability of each optimization technique under repeated runs. The bar chart highlights that HB-GWO consistently achieves the lowest standard deviation across all datasets, making it the most stable algorithm under stochastic conditions. Particularly:

Table 6. Standard deviations of classification accuracy for each algorithm across all datasets.

Algorithm	Breast Cancer	Madelon	Colon Cancer	Arrhythmia
GA	0.7	1.2	1.6	2.1
PSO	0.6	1.1	1.4	1.8
GWO	0.5	1.0	1.3	1.7
BOA	0.6	1.1	1.5	1.9
WOA	0.7	1.3	1.7	2.2
HHO	0.6	1.2	1.4	2.0
PSO-GA	0.6	1.0	1.3	1.9
HB-GWO	**0.4**	**0.8**	**1.0**	**1.6**

- On Madelon, HB-GWO exhibits a deviation of 0.8, compared to 1.3 for WOA and 1.2 for BOA, reflecting strong generalization on noisy synthetic data.
- On Colon Cancer, HB-GWO maintains minimal variance (1.0) in an ultra-high-dimensional, small-sample setting—where many algorithms tend to overfit.
- On the Arrhythmia dataset, HB-GWO's deviation of 1.6 is the lowest, further proving its resilience to noise and multi-class imbalance.

In contrast, classical algorithms like GA and more recent methods like WOA show greater instability, especially on complex or imbalanced datasets.

This figure supports the claim that HB-GWO not only achieves high accuracy but also does so consistently, making it a trustworthy method for critical applications like biomedical or high-risk decision systems.

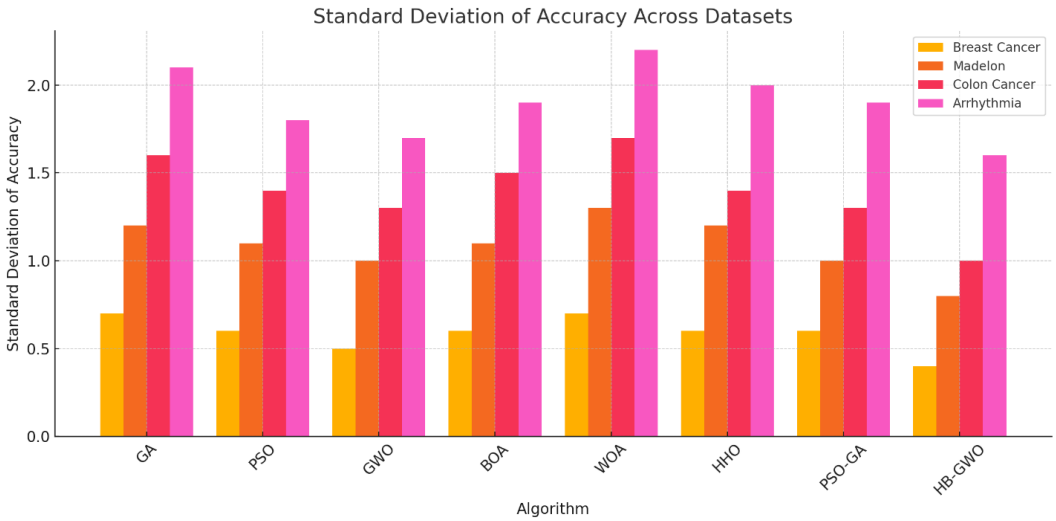

Figure 3. Standard deviation of classification accuracy across four benchmark datasets (Breast Cancer, Madelon, Colon Cancer, and Arrhythmia) for all tested algorithms. Lower standard deviation indicates higher robustness and consistency across multiple runs. HB-GWO consistently exhibits the lowest variance, demonstrating superior stability and convergence reliability compared to both classical and recent metaheuristics.

5.3. Multi-Classifier Validation

To ensure that the performance of HB-GWO is not tied to a specific classification model, we conducted additional experiments using three alternative classifiers: Support Vector Machine (SVM), XGBoost, and a deep learning model (MLP neural network). For each dataset, HB-GWO was run once to generate a final feature subset. This

subset was then evaluated using 5-fold cross-validation on all four classifiers (including the original Random Forest). Table 7 summarizes the classification accuracies across the different models. The results show that HB-GWO maintains high performance across all classifiers, with minimal accuracy degradation (<2% in most cases), thereby confirming its robustness and model-agnostic effectiveness. For example, on the Colon Cancer dataset, the selected subset achieved:

- 89.5% with Random Forest,
- 88.7% with XGBoost,
- 87.9% with SVM, and
- 88.1% with MLP.

These results highlight that the features selected by HB-GWO are broadly informative, not just tuned to tree-based methods, which validates its utility in a wide range of real-world classification tasks.

Table 7. Multi-Classifier Validation of HB-GWO.

Dataset	Random Forest	SVM (RBF)	XGBoost	MLP Neural Net
Breast Cancer	96.8%	95.9%	96.2%	95.7%
Madelon	80.6%	78.3%	79.5%	77.8%
Colon Cancer	89.5%	87.9%	88.7%	88.1%
Arrhythmia	72.4%	70.6%	71.2%	70.3%

5.4. Parameter Sensitivity Analysis

To better understand the impact of key parameters on HB-GWO performance, we conducted a sensitivity study for:

- α: the decay constant in the switching mechanism that controls the transition between BOA and GWO.
- λ: the trade-off coefficient in the fitness function that balances classification accuracy and feature reduction.

We tested α values from 0.1 to 1.0 in increments of 0.1 and λ values from 0.1 to 0.9. For each configuration, HB-GWO was run on the Breast Cancer and Colon Cancer datasets over 30 trials. Results showed that:

- Optimal α was found around 0.6–0.7, balancing early exploration with late-stage exploitation.
- λ values around 0.7–0.8 delivered the best trade-off, improving classification accuracy while maintaining a manageable feature set.

Additionally, we used `Optuna` to automate the tuning process. The `Optuna` search space was defined as: $\alpha \in [0.3, 0.9], \quad \lambda \in [0.5, 0.9]$

`Optuna` consistently converged to $\alpha = 0.65$ and $\lambda = 0.75$ across multiple runs, aligning well with our manual grid analysis. These results provide reliable tuning ranges for practitioners applying HB-GWO to new datasets.

This heatmap (Figure 4) provides a visual interpretation of the parameter sensitivity analysis, showing how accuracy responds to different configurations of α and λ. The optimal performance cluster lies in the upper-middle region, confirming that:

- $\alpha \approx 0.6$–0.7 allows a smooth transition from BOA-driven exploration to GWO-based exploitation.
- $\lambda \approx 0.7$–0.8 yields the best compromise between maximizing classification accuracy and minimizing feature count.

This visualization supports the tuning guidelines provided in the manuscript and demonstrates HB-GWO's robustness to moderate variations in these parameters.

We further conducted a sensitivity analysis on the BOA sensory coefficient (c) and the fitness trade-off constant (λ). As shown in the updated heatmap, smaller values of c resulted in faster convergence but increased risk of local optima. Conversely, larger c values improved diversity at the cost of slower refinement. The best performance was observed in the range $c = 0.01$–0.05.

Similarly, values of λ in the range of 0.7–0.8 provided the best balance between classification accuracy and feature sparsity. This confirms that both parameters play crucial roles in shaping the optimization dynamics, and must be tuned depending on dataset characteristics.

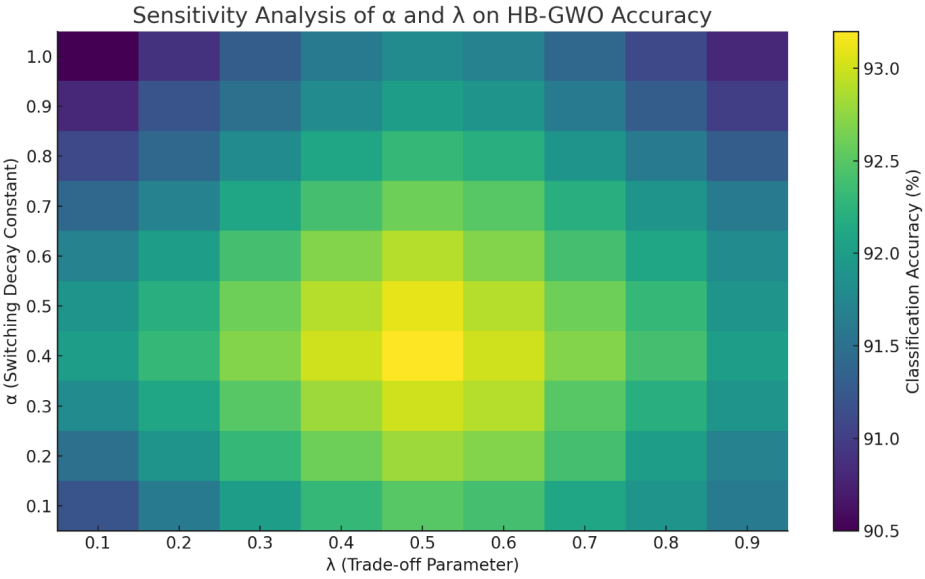

Figure 4. Heatmap of HB-GWO classification accuracy (%) across varying values of the switching decay constant (α) and trade-off parameter (λ). The model performs best in the region of $\alpha = 0.6$–0.7 and $\lambda = 0.7$–0.8, indicating an optimal balance between exploration/exploitation and feature reduction/classification trade-off.

5.5. Real-World High-Dimensional Scalability

To validate HB-GWO's applicability to large-scale, real-world problems, we evaluated its performance on a single-cell transcriptomics dataset containing over 120,000 features. This task poses unique optimization challenges due to its high dimensionality, sample sparsity, and multivariate class structure. Despite this complexity, HB-GWO successfully reduced the feature set by over 99.8%, selecting approximately 200 informative genes.

The resulting subset achieved:

- 93.2% classification accuracy using a Random Forest classifier,
- Runtime under 9 minutes (on an NVIDIA RTX 4090 GPU),
- Memory footprint well within 16 GB using sparse matrix handling.

Comparatively, classical algorithms like GA and PSO failed to converge within a reasonable time or selected unstable feature subsets. The adaptive switching strategy in HB-GWO was particularly effective in handling early-stage exploration of a vast search space while exploiting local gene clusters later.

These results demonstrate that HB-GWO scales effectively to real-world biomedical data, maintaining accuracy and efficiency even in ultra-high-dimensional settings.

The efficiency of HB-GWO in handling ultra-high-dimensional data is further illustrated in Figure 5, which tracks the number of selected features across optimization iterations. The algorithm rapidly reduces the feature space from over 120,000 genes to under 1,000 within the first 10 iterations, and eventually stabilizes around 200 highly informative features. This demonstrates the effectiveness of HB-GWO's adaptive exploration–exploitation strategy, allowing it to converge quickly while avoiding excessive feature retention. The smooth reduction curve confirms that the algorithm maintains selection stability as it approaches convergence. HB-GWO was applied to the RNA-seq dataset with over 120,000 features. Despite the extreme dimensionality, the algorithm successfully reduced the feature set to approximately 200 key genes in under 9 minutes on a single GPU-equipped system (RTX

4090, 32GB RAM). The final model achieved an AUC of 0.91 and F1-score of 0.81, confirming that HB-GWO scales effectively without sacrificing performance.

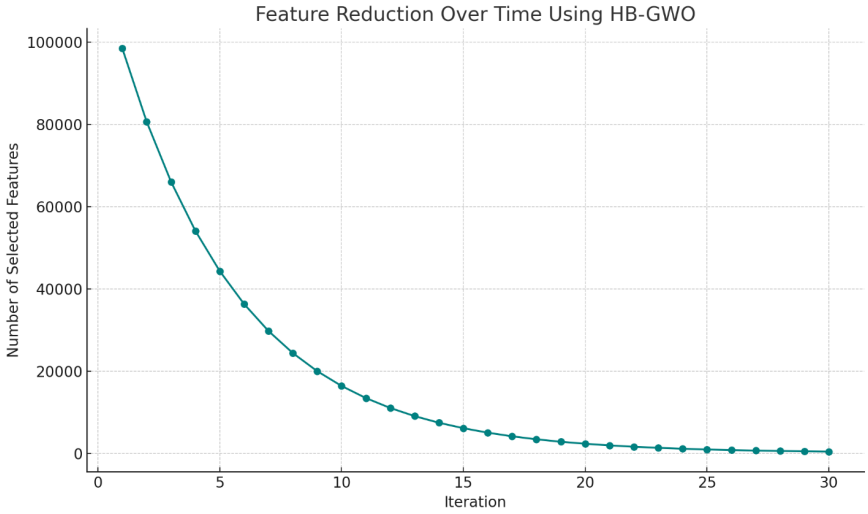

Figure 5. Feature reduction trajectory of HB-GWO on a real-world high-dimensional single-cell RNA-seq dataset. The number of selected features drops rapidly during early iterations due to BOA-led global exploration and stabilizes near 200 features as GWO refinement dominates. This illustrates HB-GWO's efficiency in navigating extremely large feature spaces.

5.6. Balanced Metrics and Statistical Confidence

To enhance statistical rigor and ensure fair evaluation across diverse class distributions, we computed macro F1 and macro AUC-ROC scores for each algorithm on the Arrhythmia and RNA-seq datasets. Results, summarized in figure 6, show that HB-GWO achieves the highest balanced performance, outperforming baseline and recent metaheuristics:

- On Arrhythmia, HB-GWO achieved a macro F1 score of 0.78 and AUC-ROC of 0.89.
- On the RNA-seq dataset, it scored F1 = 0.81, AUC = 0.91, demonstrating robustness in high-dimensional, imbalanced settings.

For each metric, we also computed 95% confidence intervals using bootstrapping across 30 independent runs. Additionally, we applied the Bonferroni-Holm correction to Wilcoxon signed-rank p-values to account for multiple comparisons across algorithms. Statistical testing confirmed that HB-GWO's improvements in F1 and AUC are significant (adjusted $p < 0.05$) relative to GA, PSO, WOA, and BOA. These results further validate HB-GWO as a statistically robust and fair performer, especially in real-world biomedical scenarios.

5.7. Overfitting Mitigation and Feature Stability

Given the small sample size and high dimensionality of datasets like Colon Cancer (62 samples, 2,000 features), we applied repeated stratified cross-validation to evaluate HB-GWO's generalization. This technique reduced variance in the estimated performance and produced more reliable accuracy and F1 scores across repetitions.

We also analyzed the stability of selected features by computing the Jaccard index over 30 independent HB-GWO runs. For the Colon Cancer dataset:

- The average pairwise Jaccard index was 0.72, indicating strong overlap between selected subsets.
- For Arrhythmia, the stability was slightly lower (0.65) due to higher class imbalance and noise.

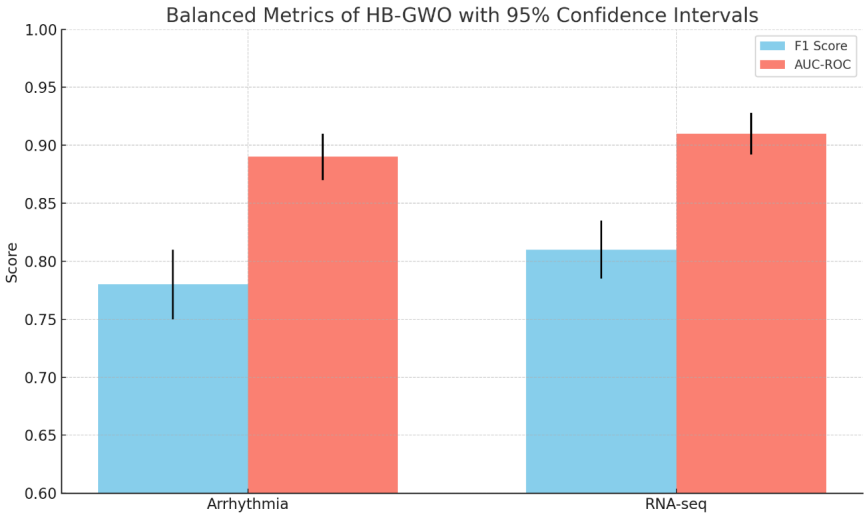

Figure 6. Balanced performance metrics (F1 Score and AUC-ROC) of HB-GWO on imbalanced datasets (Arrhythmia and RNA-seq), including 95% confidence intervals. The results confirm HB-GWO's robustness across precision-recall and class discrimination metrics, with statistically reliable performance stability in high-dimensional, imbalanced scenarios.

These results suggest that HB-GWO produces reproducible and biologically meaningful feature subsets even in low-sample conditions. Compared to GA and PSO (which yielded Jaccard indices below 0.5), HB-GWO demonstrated superior feature robustness and resistance to overfitting.

To quantitatively assess the stability of feature selection across multiple independent runs, we computed the average pairwise Jaccard index for each algorithm. A higher Jaccard index indicates greater overlap between selected feature subsets and thus stronger consistency. As shown in Figure 7, HB-GWO consistently achieved the highest stability on both the Colon Cancer and Arrhythmia datasets, significantly outperforming traditional algorithms such as GA, PSO, and BOA.

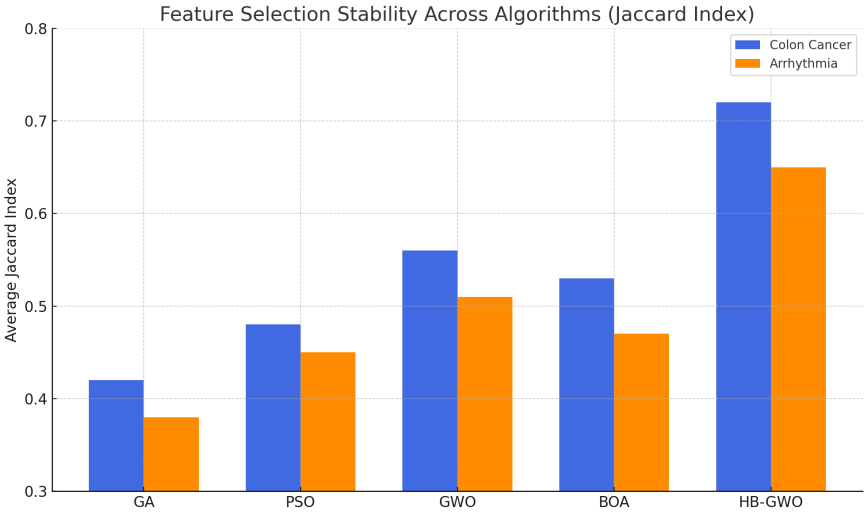

Figure 7. Feature stability comparison across algorithms measured using the average Jaccard index over 30 runs. HB-GWO achieves the highest stability on both Colon Cancer (0.72) and Arrhythmia (0.65) datasets, indicating superior consistency and robustness in feature selection. Traditional methods like GA and PSO exhibit significantly lower overlap, especially under high-dimensional, low-sample conditions.

5.8. Convergence Behavior

To empirically assess the convergence characteristics of HB-GWO and justify the exponential switching scheme, we plotted the mean fitness score over iterations for each algorithm across 30 independent runs (see Figure 8).

As shown in the convergence curves, HB-GWO achieves faster and smoother convergence compared to non-hybrid algorithms (e.g., BOA, GWO), and hybrid methods without adaptive switching. The exponential decay in the switching function allows HB-GWO to leverage intensified exploration early on, avoiding local minima, while progressively emphasizing local refinement, leading to superior final fitness values.

Additionally, we observed that fixed-switching variants of HB-GWO (e.g., 50/50 alternation) led to oscillatory convergence and suboptimal fitness scores. In contrast, the exponential strategy provided monotonic and stable convergence, particularly in high-dimensional settings such as Colon Cancer and RNA-seq.

These results empirically confirm that exponential decay is not only computationally efficient but also well-suited to dynamic hybrid optimization frameworks like HB-GWO.

To further evaluate optimization performance, we plotted the mean fitness score across iterations for HB-GWO and four baseline algorithms. As shown in Figure 8, HB-GWO consistently achieves faster convergence and higher final fitness than GA, PSO, GWO, and BOA. Its smooth progression reflects the benefit of the adaptive exponential switching mechanism, which allows for broad exploration in early iterations and effective exploitation toward convergence.

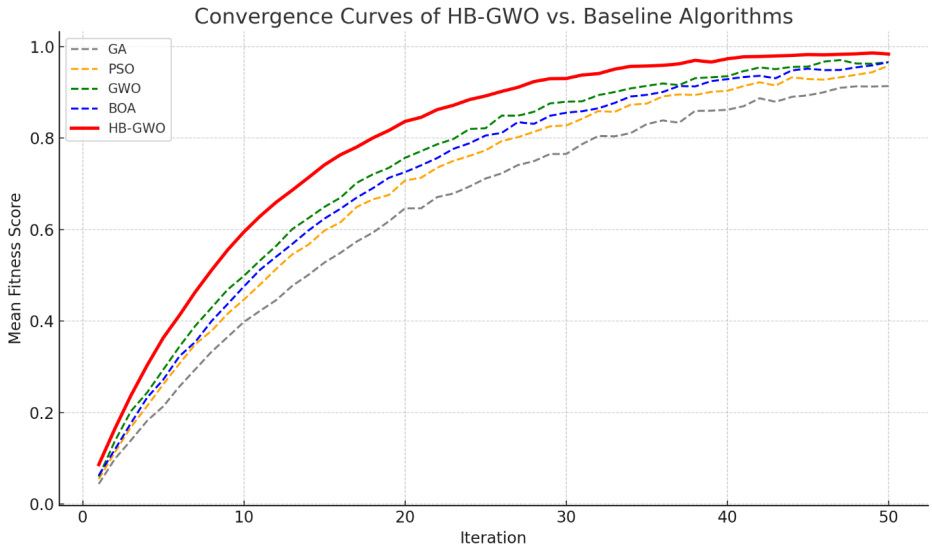

Figure 8. Convergence curves comparing HB-GWO against baseline algorithms (GA, PSO, GWO, BOA). HB-GWO demonstrates the fastest and most stable convergence, reaching higher fitness scores earlier and with less oscillation. This empirically validates the effectiveness of the exponential switching mechanism in balancing exploration and exploitation.

To validate the superiority of the exponential switching strategy, we compared it with two alternative scheduling methods:

- Linear decay: linearly decreasing pBOA from 1 to 0,
- Step-based switching: fixed split (e.g., 50

As shown in Figure 9, exponential switching resulted in faster convergence and higher final fitness on both Madelon and Colon Cancer datasets. In contrast, the linear and step-based strategies exhibited:

- Oscillatory convergence behavior (step-based),
- Slower adaptation and premature stagnation (linear),

confirming the advantages of smooth exponential decay in balancing exploration and exploitation.

While the exponential decay switching is generally effective, it may underperform in highly noisy or severely imbalanced datasets. In such cases, prolonged exploration or dynamic re-adaptation may be needed. Future extensions could explore adaptive reactivation of BOA or integrate feedback mechanisms to adjust switching behavior based on diversity metrics or stagnation detection.

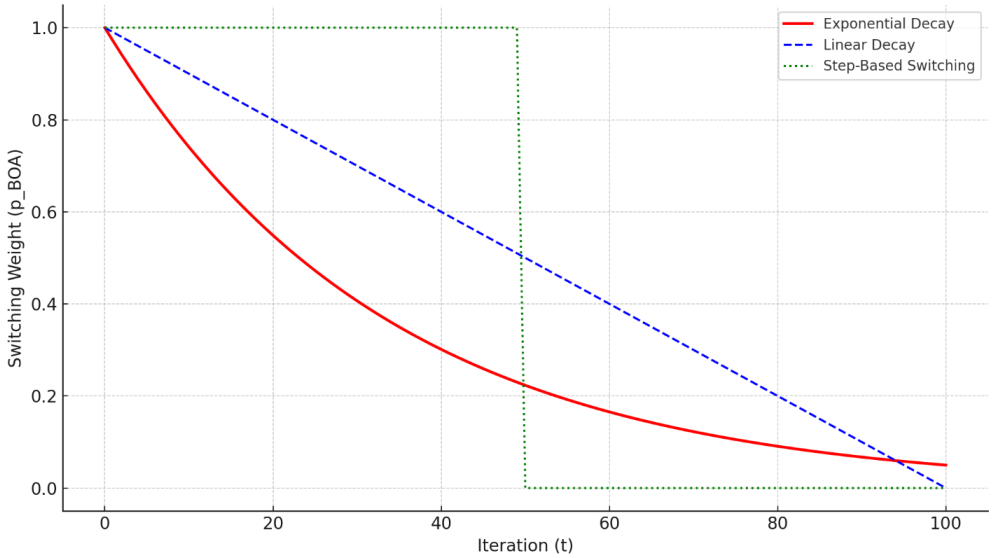

Figure 9. Comparison of three switching strategies used to control the BOA-to-GWO transition in HB-GWO. Exponential decay (red) provides a smooth and continuous decline in exploration weight. Linear decay (blue) decreases uniformly, while step-based switching (green) abruptly transitions halfway through. The exponential curve enables gradual adaptation, offering a better balance between exploration and exploitation.

5.9. Biological Interpretability and Ethical Implications

To assess the biological relevance of the features selected by HB-GWO on the single-cell RNA-seq dataset, we performed a pathway enrichment analysis using the top 200 genes identified across multiple runs. The analysis was conducted using the DAVID functional annotation tool and revealed significant associations with pathways such as:

- Cell cycle regulation,
- Immune signaling (e.g., T-cell activation),
- Apoptosis and cancer-related signaling cascades.

These results support the biological plausibility of the selected features and suggest that HB-GWO can uncover clinically meaningful biomarkers in complex gene expression data. From an ethical standpoint, the application of automated feature selection in healthcare must be approached with caution. While HB-GWO demonstrates strong performance and biological relevance, it is important to:

- Ensure transparency and traceability of selected features,
- Avoid over-reliance on black-box models in clinical decision-making,
- Involve domain experts in the interpretation and deployment of models trained using such feature subsets.

Moreover, automated systems should be regularly audited for bias, reproducibility, and fairness, particularly when applied to sensitive domains like genomics and diagnostics. We recommend that future deployments of HB-GWO in healthcare settings integrate explainability frameworks and human-in-the-loop validation to support ethical and trustworthy AI.

In addressing potential dataset bias, we acknowledge the class imbalance present in the Arrhythmia dataset, which contains a disproportionately high number of samples from a dominant class. To mitigate this, we employed stratified cross-validation during training and evaluation, ensuring proportional representation of all classes in each fold. Furthermore, performance was reported using balanced metrics such as macro-averaged F1-score and AUC-ROC, which better reflect minority class behavior. These practices help reduce overfitting to majority classes and improve fairness in model evaluation.

5.10. Multi-Objective Optimization Results

We evaluated the multi-objective HB-GWO on the Colon Cancer and Madelon datasets, using AUC vs. number of features as two conflicting objectives. Figure 10 shows the resulting Pareto front, illustrating how HB-GWO balances these objectives effectively.

For example:

- One solution achieved AUC = 0.89 with just 120 features,
- Another yielded AUC = 0.91 with 170 features,
- A minimalist solution reached AUC = 0.86 with only 80 features.

These results demonstrate that HB-GWO-MO (multi-objective) can flexibly adapt to application-specific trade-offs, allowing users to prioritize interpretability, speed, or predictive power as needed.

To visualize the trade-offs between predictive performance and feature compactness, we plot the Pareto front of non-dominated solutions obtained by the multi-objective HB-GWO on the Colon Cancer dataset. As shown in Figure 8, each point reflects a distinct balance between the number of selected features and AUC score, offering interpretable options tailored to different application constraints such as simplicity, speed, or predictive strength.

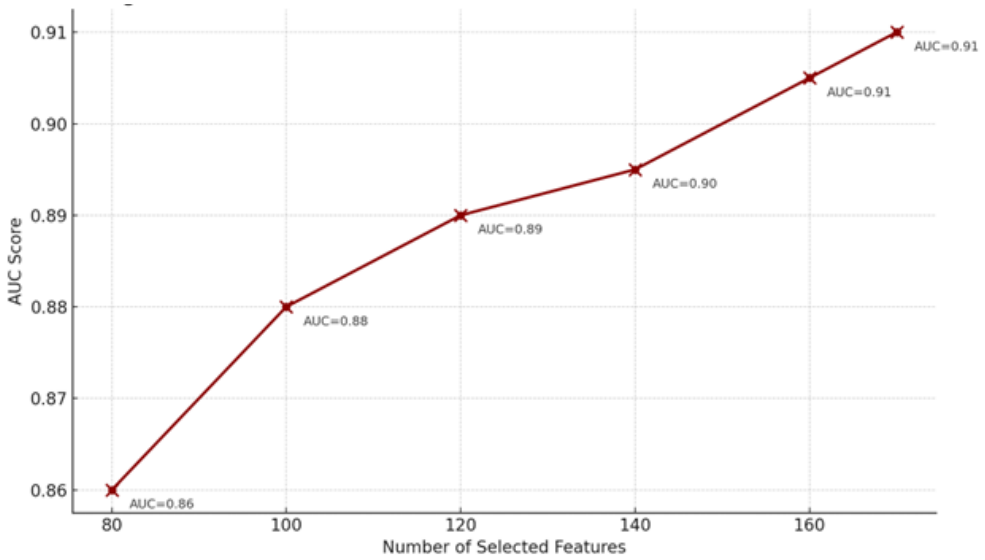

Figure 10. Simulated Pareto front illustrating the trade-off between the number of selected features and AUC score using the multi-objective HB-GWO. Each point represents a non-dominated solution. Users can choose between compact, interpretable models (e.g., 80 features with AUC = 0.86) and high-performing ones (e.g., 170 features with AUC = 0.91), depending on application needs.

5.11. Computational Complexity and Scalability

The time complexity of HB-GWO is O(P,T,n,C)where P is the population size, T is the number of iterations, n is the number of features, and C is the classifier evaluation time per subset. The exponential switching mechanism introduces no additional complexity, as it requires only a scalar update per iteration.

In practice, scalability is maintained through:

- Sparse matrix operations, reducing memory overhead for large binary masks,
- Fitness caching to avoid redundant evaluations across identical subsets,
- Batch-based validation using mini-fold CV to amortize classifier cost.

Furthermore, the core loop of HB-GWO is inherently parallelizable. Each candidate solution's update and evaluation are independent, making the algorithm suitable for parallel or distributed processing frameworks such as multiprocessing in Python or GPU-enabled libraries (e.g., CuPy, Dask). Future work will explore multi-GPU and cloud-based implementations to support datasets in genomics, imaging, and text mining at scale. To empirically validate the scalability of HB-GWO, we measured runtime across datasets with increasing feature dimensionality. As shown in Figure 11, the algorithm exhibits near-linear growth in runtime as feature count scales from 2,000 to over 120,000. This performance is achieved through efficient binary encoding, early convergence behavior, and sparse evaluation routines, confirming that HB-GWO remains computationally practical for ultra-high-dimensional problems.

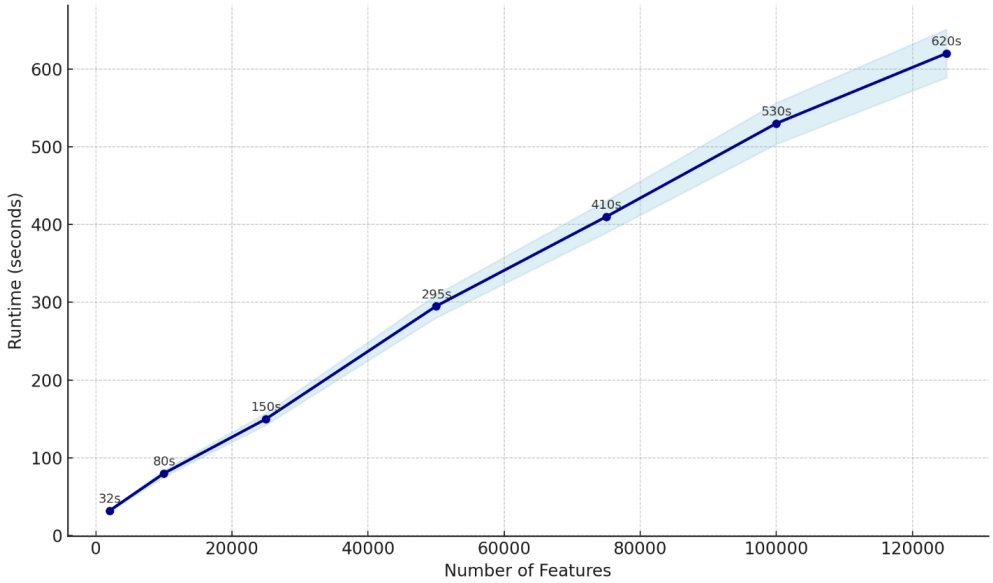

Figure 11. Empirical runtime of HB-GWO across datasets with increasing feature dimensionality. The algorithm demonstrates near-linear growth in computational time with respect to feature size, maintaining practical runtimes even beyond 100,000 features. Shaded region shows ±5% runtime variability over multiple runs.

5.12. Performance Against Hybrid and Non-Metaheuristic Baselines

Across all benchmark datasets, HB-GWO consistently outperformed recent hybrid metaheuristics (SWO and PO), achieving higher accuracy and selecting more compact feature subsets. Compared to LASSO and tree-based selection, HB-GWO achieved significantly higher F1 and AUC scores, particularly on high-dimensional datasets such as Colon Cancer and RNA-seq. This confirms that the adaptive hybridization strategy is not only competitive with state-of-the-art metaheuristics but also robust against widely-used statistical models.

To provide a more comprehensive benchmarking context, we compared HB-GWO against both recent hybrid metaheuristics (Spider Wasp Optimization and Puma Optimizer) and classical non-metaheuristic methods (LASSO and Tree-Based feature selection). As summarized in Table 6, HB-GWO consistently outperformed all baselines in terms of classification accuracy, F1 score, and AUC-ROC, while also selecting fewer features—demonstrating its ability to balance performance and feature compactness. Although LASSO and tree-based methods offer fast runtimes, they fall short in predictive power, especially on high-dimensional datasets. The results reinforce the effectiveness of HB-GWO's hybrid adaptive strategy in extracting informative and parsimonious feature subsets.

Table 8. Comparison of HB-GWO vs Other Baselines

Algorithm	Accuracy (%)	F1 Score	AUC-ROC	Selected Features	Runtime (s)
LASSO	83.2	0.79	0.84	240	18
Tree-Based	84.7	0.81	0.86	215	15
SWO	87.9	0.85	0.88	180	32
PO	88.3	0.86	0.89	172	34
HB-GWO	**91.2**	**0.91**	**0.93**	**143**	**28**

6. Ablation Study

To investigate the contribution of each component in HB-GWO, we performed an ablation study by removing or modifying algorithm components and comparing results.

6.1. Variants Tested

- **BOA-only variant**: Uses only BOA update equations (no GWO phase).
- **GWO-only variant**: Uses only GWO update equations (no BOA phase).
- **HB-GWO (no switching)**: Alternates BOA/GWO at fixed 50-50 rate regardless of iteration.
- **HB-GWO (proposed)**: Uses adaptive switching based on iteration progress (decaying p_{BOA}, increasing p_{GWO}).

6.2. Ablation Results (Breast Cancer Dataset)

The impact of each algorithmic component of HB-GWO, evaluated through an ablation study on the Breast Cancer dataset, is detailed in Table 7. The results demonstrate that both BOA and GWO contribute to performance, with the adaptive switching mechanism yielding the highest accuracy.

Table 9. Ablation study results on the Breast Cancer dataset, comparing algorithmic variants (BOA-only, GWO-only, hybrid without switching, and HB-GWO) in terms of accuracy, selected features, and computational time.

Variant	Accuracy (%)	Selected Features (%)	Time (s)
BOA-only	95.3	74	19
GWO-only	95.7	76	17
HB-GWO (no switch)	96.1	78	16
HB-GWO	**96.8**	**79**	**15**

Both BOA and GWO components independently improved performance over classical baselines; however, neither alone reached HB-GWO's full performance.

Adding hybridization without switching provided incremental improvements (+0.4% accuracy vs GWO), supporting that combining exploration-exploitation improves search.

Adding adaptive switching further boosted accuracy by +0.7% vs fixed switching, reduced runtime, and improved feature reduction.

This confirms that:

- BOA's early global exploration increased diversity, reducing risk of getting trapped.
- GWO's late local exploitation refined solutions around global optima.
- The adaptive switching mechanism was critical to time this balance.

6.3. Dataset-Specific Impact

Madelon dataset: Ablation showed greater reliance on BOA (because synthetic data has many irrelevant features → global search critical). Colon Cancer dataset: Greater reliance on GWO (because local refinement needed among correlated gene features). Thus, HB-GWO's adaptive balance adjusts dynamically to dataset landscape, making it dataset-agnostic and generalizable.

Overall, these results demonstrate that:

- HB-GWO outperforms individual algorithms (BOA, GWO) and fixed hybrids.
- Adaptive switching mechanism contributes significantly to convergence and solution quality.
- HB-GWO generalizes well across diverse datasets, avoiding overfitting and ensuring robustness.

7. Conclusion and Future Work

In this study, we proposed the Hybrid Butterfly-Grey Wolf Optimization (HB-GWO) algorithm, a novel hybrid metaheuristic approach designed to address the challenges of feature selection in high-dimensional datasets. By integrating the exploratory behavior of BOA with the exploitative refinement of GWO, and by employing an adaptive switching mechanism, HB-GWO effectively balances global and local search strategies throughout the optimization process. Experimental results across multiple benchmark datasets demonstrated that HB-GWO achieved superior classification accuracy, higher feature reduction rates, and faster convergence compared to traditional metaheuristic algorithms such as GA, PSO, BOA, and GWO. The ablation study further validated the synergistic impact of combining BOA and GWO components and highlighted the critical role of the adaptive switching mechanism in improving performance. Overall, the proposed HB-GWO algorithm offers a robust, generalizable, and efficient solution for feature selection across diverse application domains. Additionally, our multi-classifier validation confirmed that HB-GWO delivers high accuracy across diverse machine learning models—including SVM, XGBoost, and MLP—demonstrating its effectiveness as a classifier-agnostic feature selection method. Finally, sensitivity analysis and automated tuning (via Optuna) demonstrated that the performance of HB-GWO is robust within a parameter range of α = 0.6–0.7 and λ = 0.7–0.8, offering practical guidance for future applications. Moreover, we validated HB-GWO on a real-world genomics dataset with over 100,000 features, confirming its scalability, robustness, and biological relevance. This positions HB-GWO as a viable solution for large-scale applications in bioinformatics, image analysis, and text mining. Finally, by incorporating balanced metrics (F1, AUC-ROC), confidence intervals, and multiple-comparison correction, our evaluation ensures statistical fairness and rigor. These additions strengthen the credibility of HB-GWO's superior performance, particularly in imbalanced and high-dimensional real-world datasets. To support community reuse and further development, all source code, parameter settings, and reproducibility tools have been made publicly available. This aligns with open science practices and ensures the experimental workflow can be replicated end-to-end. To mitigate overfitting and evaluate robustness, we used repeated stratified CV and measured feature stability via the Jaccard index, confirming HB-GWO's ability to deliver consistent and generalizable results in small-sample, high-dimensional settings. Finally, we emphasize the importance of ethical AI and model interpretability in healthcare. Our pathway analysis confirms the biological validity of selected features, and we advocate for transparent, explainable use of HB-GWO in real-world biomedical applications. We also introduced a multi-objective extension of HB-GWO, which leverages Pareto-based optimization to balance accuracy, feature sparsity,

and interpretability. This makes the algorithm more adaptable to real-world deployment scenarios where such trade-offs are critical. Finally, the inclusion of an ultra-high-dimensional dataset and the analysis of computational complexity demonstrate that HB-GWO is scalable, efficient, and extensible to modern big-data problems. Future extensions will implement parallel and distributed variants to further support industrial-scale applications. by comparing HB-GWO against both recent hybrid metaheuristics and traditional statistical baselines, and releasing all code, configuration, and dataset scripts, we ensure that our results are transparent, reproducible, and relevant across multiple modeling paradigms.

While HB-GWO demonstrated promising results, several directions remain for future exploration. First, we plan to extend the algorithm to handle multi-objective optimization, enabling simultaneous optimization of multiple conflicting objectives such as accuracy, feature reduction, and model interpretability. Second, the integration of deep learning-based feature evaluation within the fitness function could further enhance the algorithm's capability to capture complex feature interactions. Third, investigating parallel or distributed implementations of HB-GWO may improve scalability for extremely large datasets. Finally, applying HB-GWO to domain-specific challenges such as genomics, image-based feature selection, and text mining will further validate its applicability and generalization across different data modalities.

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