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Libreries

Moduls

Functionality

1. DateProcessor
2. Recombination
3. Chromosome
4. NSGAII
5. Fast-NSGAII
6. PlotProcessor

Results

1. DS02
2. DS04
3. DS05
4. DS07
5. DS08
6. DS10

Overall Result

1. Wise initialization
2. Effect of columns number expansion
3. Effect of samples number expansion
4. Effect of fast-non-dominated sorting parallelization
5. Effect of objective evaluation parallelization

### Libraries Used:

- scikit-learn: Utilized for machine learning tasks, including the implementation of K-nearest neighbors and Random Forest classifiers.

- pymoo: A Python library for multi-objective optimization algorithms. It provides tools for handling optimization problems with multiple objectives.

- concurrent.futures: Used for parallel execution of tasks to enhance performance.

- matplotlib: Employed for data visualization, particularly for creating scatter plots and line plots.

- pandas: Used for data manipulation and handling datasets.

- numpy: A fundamental library for numerical operations in Python, used extensively for array manipulations.

- json: Used for handling JSON configuration files.

- docx: A library for creating and modifying Microsoft Word (.docx) files.

### Modular Organization:

1. NSGAConfig: This module handles the loading of configuration parameters from a JSON file. It provides methods to retrieve specific parameters for a given dataset.

2. Recombination: Defines different crossover methods for recombining genetic information between parent chromosomes.

3. Chromosome: Represents an individual solution in the population. It includes methods for dominance checking and crowding distance calculation.

4. DataProcessor: Handles loading and processing of input datasets. It provides methods to obtain the number of features and labels from a dataset.

5. NSGAII: The main class implementing the NSGA-II algorithm. It includes methods for initialization, crossover, mutation, dominance comparison, and environmental selection. The algorithm's main loop, as well as fitness functions and termination criteria, are defined here.

6. Main Execution Loop: The script includes a loop to run the NSGA-II algorithm on multiple datasets. The results, such as Pareto fronts, IGD values, and hypervolume values, are visualized and summarized.

### Overall Functionality:

1. Initialization: The algorithm initializes a population of solutions randomly or based on specific criteria. Three methods have been implemented: random initialization, wise initialization based on feature importance, and wise initialization based on the maximum number of features in the true Pareto front for each dataset, inspired by the plots in the provided paper.

2. Crossover and Mutation: Parent solutions are selected, and crossover is applied with a certain probability. The process of selecting crossover is adaptive, as mentioned in the provided paper. Mutation is also applied with a predefined probability.

3. Fitness Calculation: Fitness functions are applied to evaluate the performance of solutions based on classification error and solution size. Additionally, this process is performed in parallel; after the generation of offspring, all of them are evaluated simultaneously since they are independent.

4. Environmental Selection: The NSGA-II environmental selection mechanism is applied to identify non-dominated solutions and maintain diversity in the population. Additionally, the first part of non-dominated sorting is performed in parallel, as checking chromosome domination against each other can be executed simultaneously.

5. Convergence Criteria: The algorithm monitors changes in hypervolume and IGD values. If no improvement is observed for a certain number of generations, the algorithm terminates.

The `NSGAII` class implements the NSGA-II algorithm, and it includes several methods to handle different aspects of the algorithm. Here are the main functions implemented in the `NSGAII` class:

1. \_\_init\_\_:

- Initializes the NSGA-II algorithm with parameters such as population size, maximum number of generations, crossover and mutation probabilities, and other configuration details.

2. initialize\_population:

Random\_initialize\_population

Wise\_initialize\_population

Wise\_initialize\_population2

- The population is initialized, as mentioned before, using three different methods: random initialization, wise initialization – which involves two distinct approaches. One is based on important features selected using the random forest algorithm, and the other is based on the Pareto front of other algorithms, considered the true Pareto front.

3. create\_offspring:

- Generates offspring through crossover and mutation operations. It selects parent individuals based on their ranks and crowding distances, applies crossover and mutation, and adds the resulting offspring to the next generation.

4. evaluate\_population:

Fitness\_function\_1

Fitness\_function\_2

- Since the problem is multi-objective, there are two fitness functions: the first one calculates the classification error using KNN, while the other measures the size of the feature space.

5. fast\_non\_dominated\_sort:

- Performs fast non-dominated sorting of the population based on dominance relationships, categorizing solutions into different fronts according to their dominance levels. Initially, we calculate the domination relationships for each chromosome, forming a list that indicates which other chromosomes is dominated by it. Subsequently, we create the first front (front\_0) comprising chromosomes that are not dominated by any other. To identify subsequent fronts, we use the domination information from the previous front, ensuring that each new front consists of solutions dominated only by the chromosomes in the preceding front.

6. crowding\_distance\_assignment:

- The calculation involves sorting the solutions in the front based on each objective individually. The boundary solutions (first and last) are assigned a crowding distance of infinity to ensure they are always selected for the next generation. For the interior solutions, the crowding distance is incremented by the difference in the objective values of adjacent solutions along each objective axis. The sum of crowding distances across all objectives is used to measure the overall density of solutions. Solutions with larger crowding distances are preferred because they are in less crowded regions, indicating a more diverse and spread-out set of solutions.

7. environmental\_selection:

- Individuals for the next generation are selected based on non-dominated sorting and crowding distance. This method combines the current population and offspring, performs non-dominated sorting, and selects individuals for the next generation. Additionally, for the last front that is not completely fit in the population, crowding distance is calculated, and a larger distance is preferable.

8. get\_hypervolume:

- Calculates the hypervolume indicator for a set of points in the objective space. Hypervolume is a metric used to evaluate the quality of Pareto fronts.

9. get\_IGD:

- Calculates the inverted generational distance (IGD) metric for a set of points in the objective space. IGD measures the convergence of a Pareto front to the true Pareto front.

10. nsga2:

- The NSGA-II algorithm is executed, involving the initialization of the population, evaluation of the initial population, and iterative creation of offspring. Individuals for the next generation are selected until the maximum number of generations is reached. Additionally, a termination condition is based on a lack of improvement situation, configured differently for each dataset.

11. init\_OSP:

- This method initializes the operator success probabilities (OSP) for each crossover operator used in NSGA-II. It sets equal probabilities for all crossover operators initially, ensuring a fair starting point for exploration.

12. update\_OSP:

- The method adjusts the operator success probabilities based on the historical performance of crossover operators during the evolutionary process. It considers the number of times each operator was rewarded and penalized, updating the probabilities to favor operators that have demonstrated better performance in generating promising offspring.

13. credit\_assignment:

- This method evaluates the dominance relationships between parent and offspring solutions and assigns credits (rewards and penalties) accordingly. It considers non-dominated solutions and penalizes or rewards them based on their ability to dominate or be dominated by other solutions, contributing to the credit assignment mechanism in NSGA-II.

14. dominance\_comparison:

- The dominance\_comparison method identifies non-dominated solutions within a set of chromosomes. It categorizes solutions into non-dominated and dominated sets based on their dominance relationships. This information is crucial for evaluating the Pareto front and guiding the environmental selection process.

15. avoid\_zero\_offspring:

- This method ensures that offspring generated through mutation or crossover are not entirely composed of zero values. It applies uniform mutation until a non-zero offspring is obtained, helping maintain diversity in the population and preventing degenerate solutions with all zero values.

16. roulette wheel selection

- This selection method simulates a roulette wheel, where each crossover operator has a section of the wheel proportional to its probability. The random value determines which section of the wheel is selected, and the corresponding crossover operator is chosen. This mechanism ensures that crossover operators with higher probabilities are more likely to be selected, mimicking a probabilistic selection process.Results:

Dataset: DS02:

Num-features: 56

Num-samples: 27

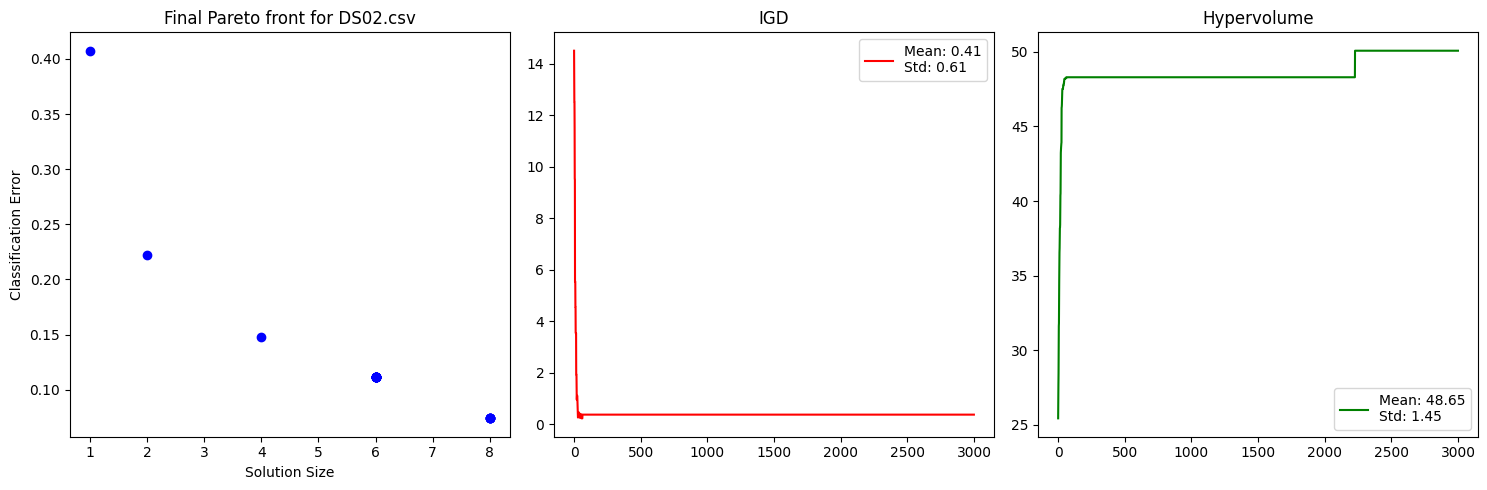
Initialization: random

MAXFE: 300000

Evaluations: 100000, Hypervolume: 48.29629629629629

Evaluations: 200000, Hypervolume: 48.29629629629629

Evaluations: 300000, Hypervolume: 50.07407407407407

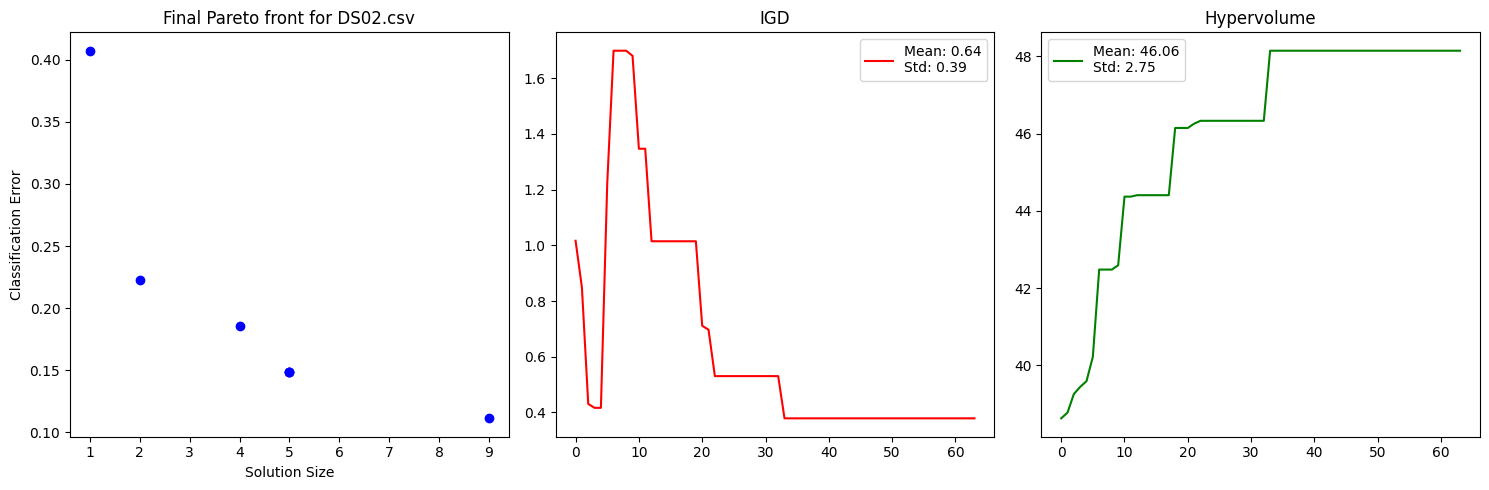
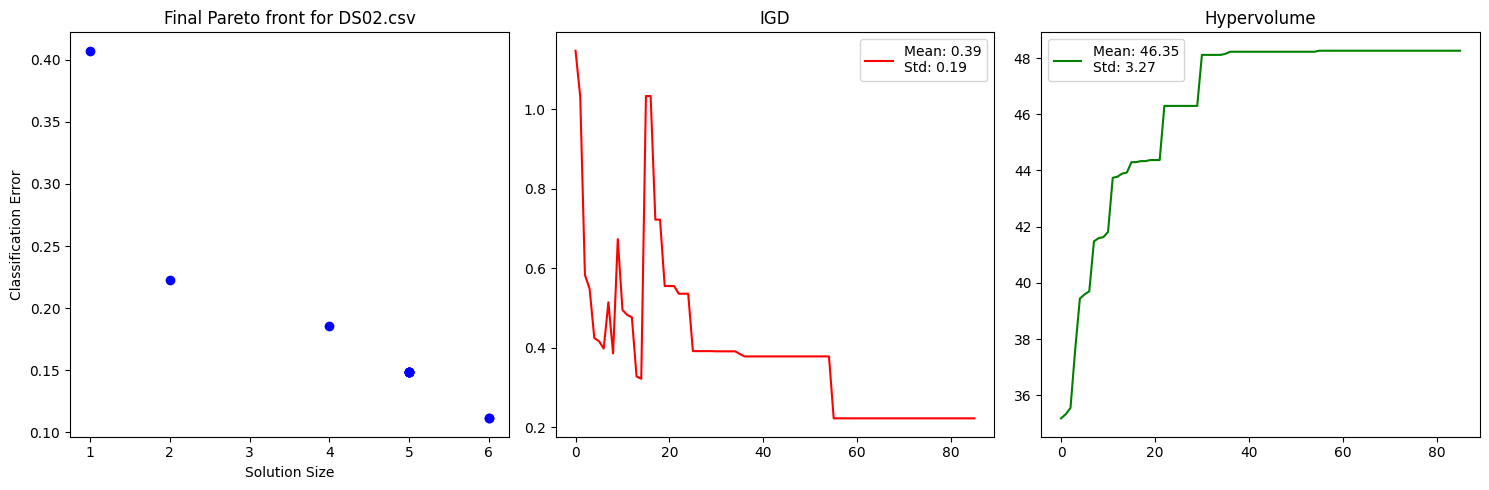
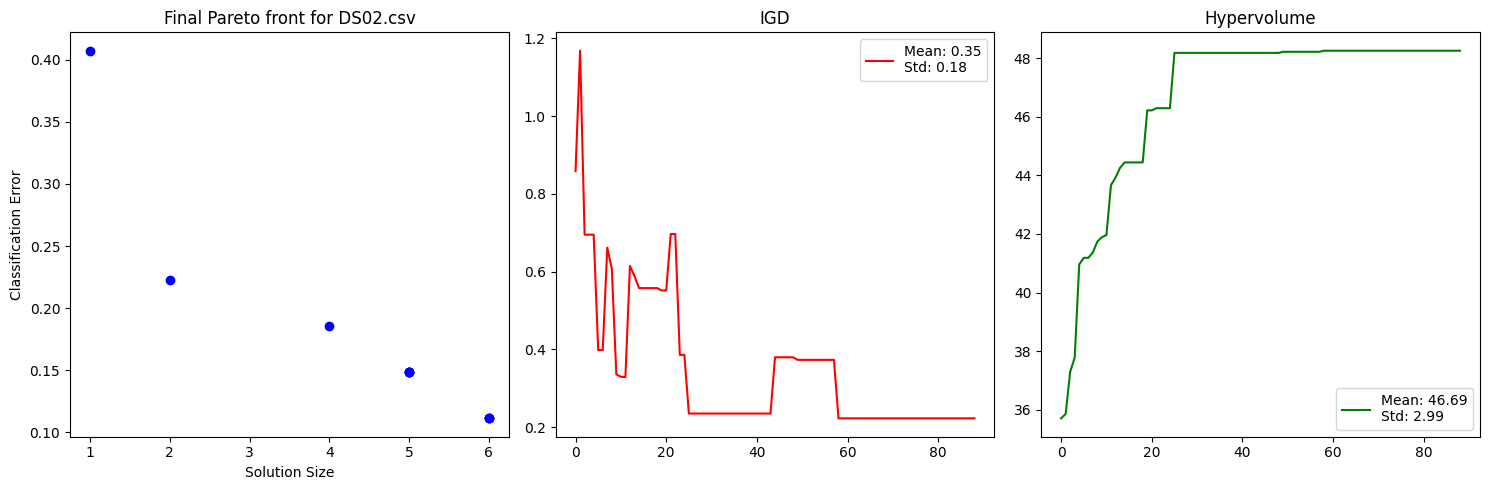
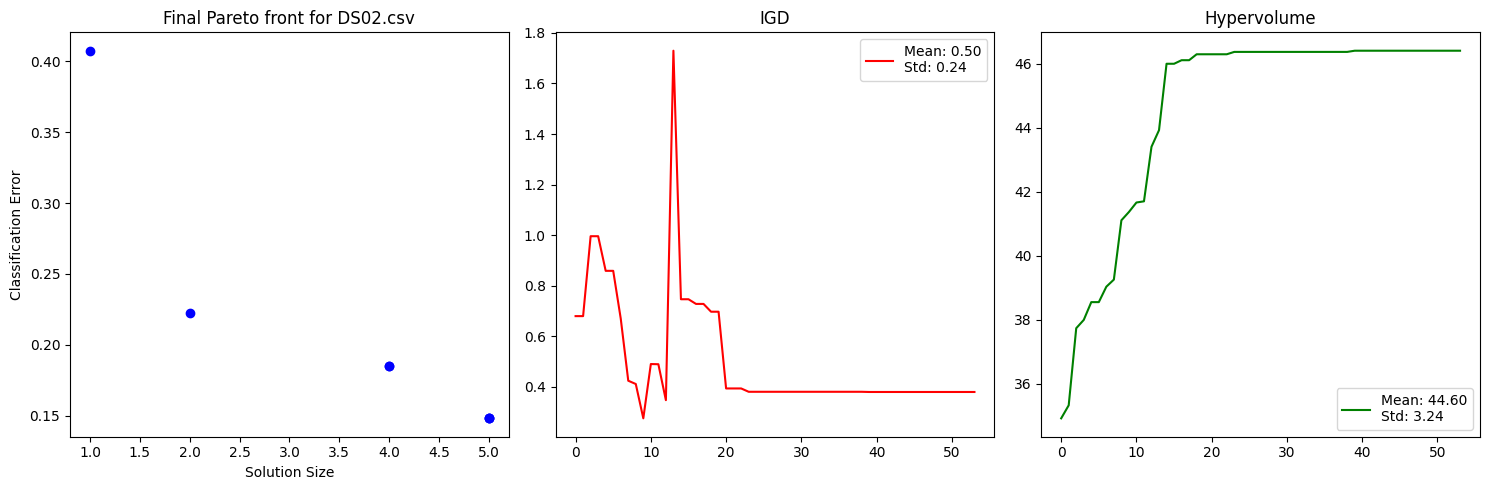
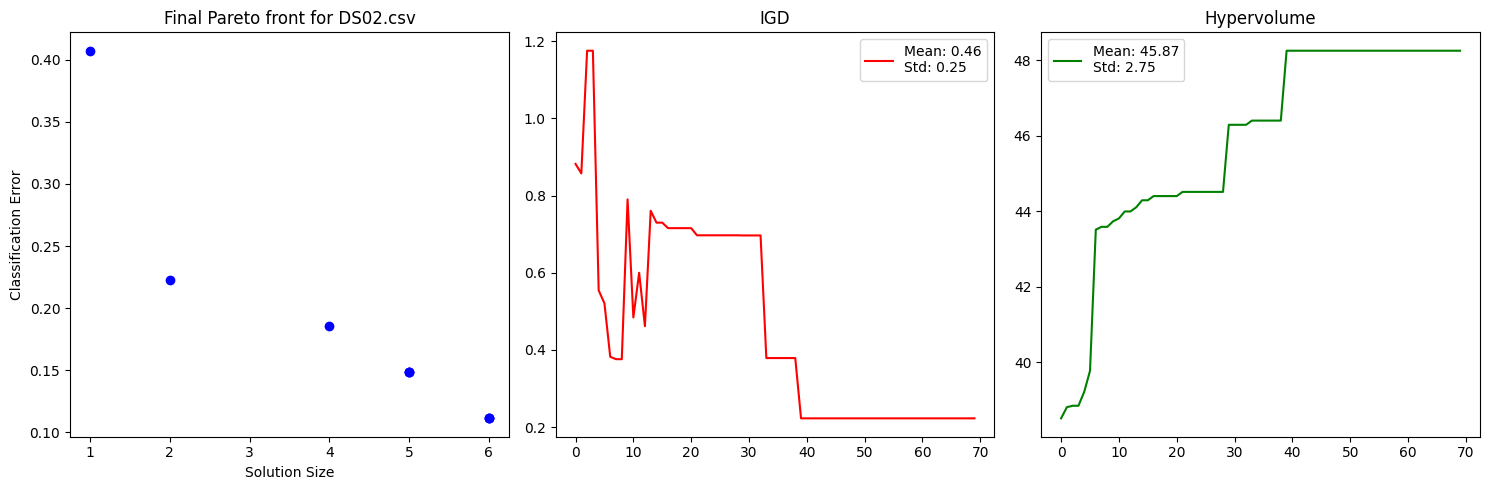


Initialization: random

MAXFE: 10000

Termination condition: hv\_threshold: 0.1, igd\_threshold: 0.005, no\_improvement\_limit: 30

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Dataset | Generation# | HV\_mean | HV\_std | IGD\_mean | IGD\_std | Duration |
| DS02.csv | 70 | 45.8693 | 2.74661 | 0.456694 | 0.254774 | 2 |
| DS02.csv | 54 | 44.5988 | 3.23781 | 0.503211 | 0.244547 | 1 |
| DS02.csv | 89 | 46.6866 | 2.99346 | 0.348842 | 0.179997 | 2 |
| DS02.csv | 86 | 46.3488 | 3.266 | 0.388342 | 0.194258 | 2 |
| DS02.csv | 64 | 46.0642 | 2.74646 | 0.639479 | 0.385097 | 1 |



Dataset: DS04

Num-features: 64

Num-samples: 1000

Initialization: random

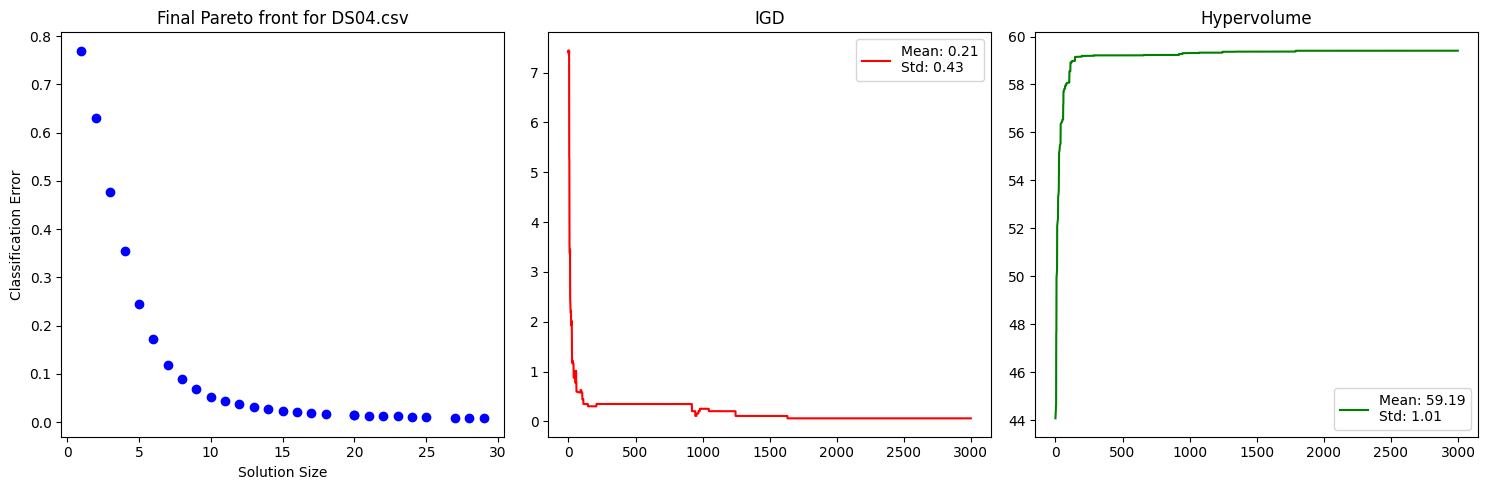
MAXFE: 300000

number of features: 64

Evaluations: 100000, Hypervolume: 59.31214747681813

Evaluations: 200000, Hypervolume: 59.40911570252888

Evaluations: 300000, Hypervolume: 59.40911570252888

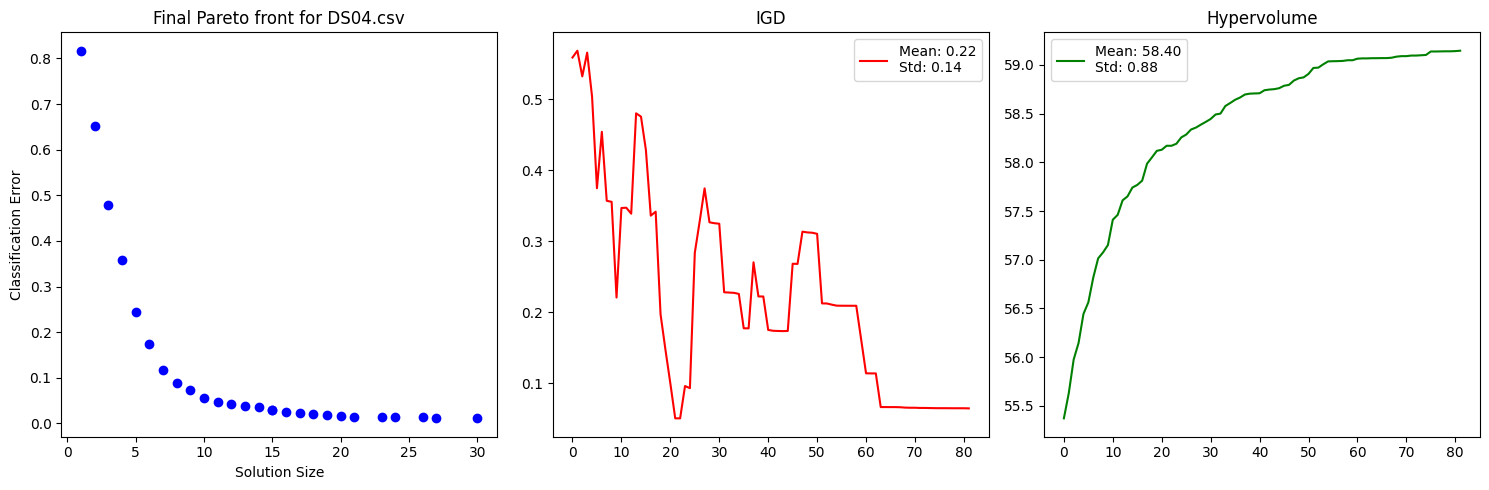
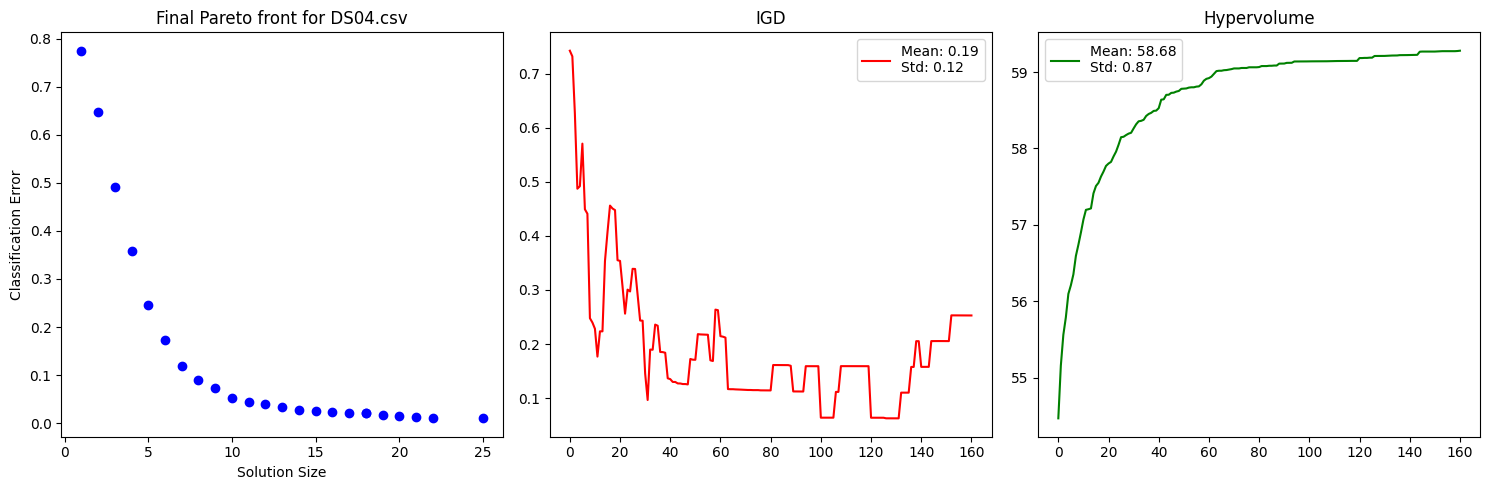
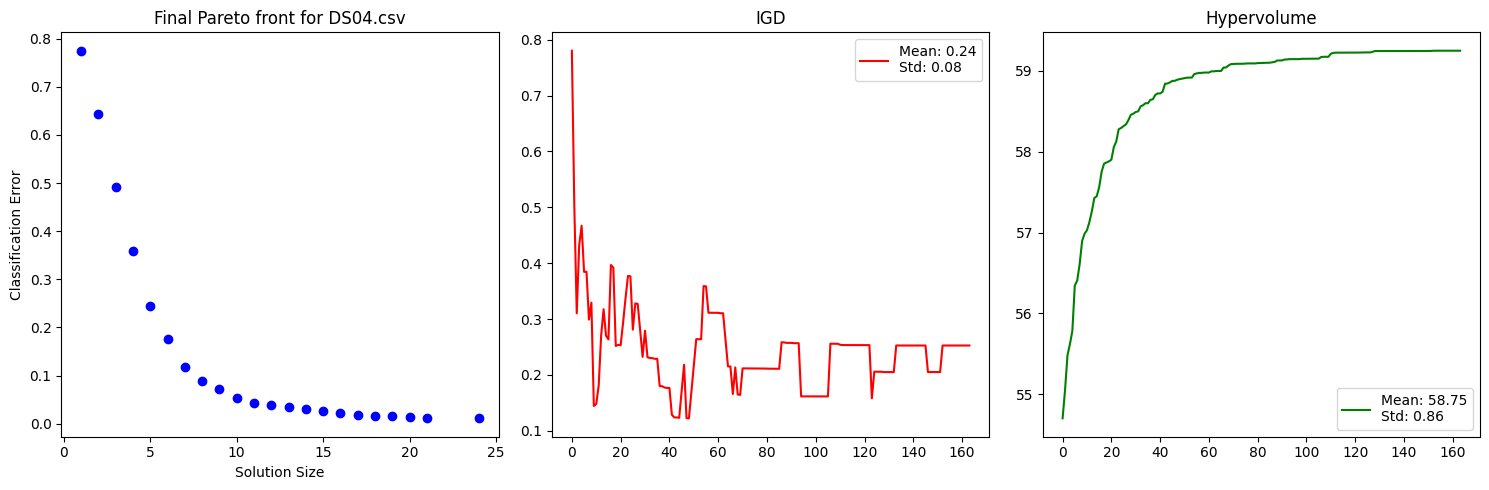
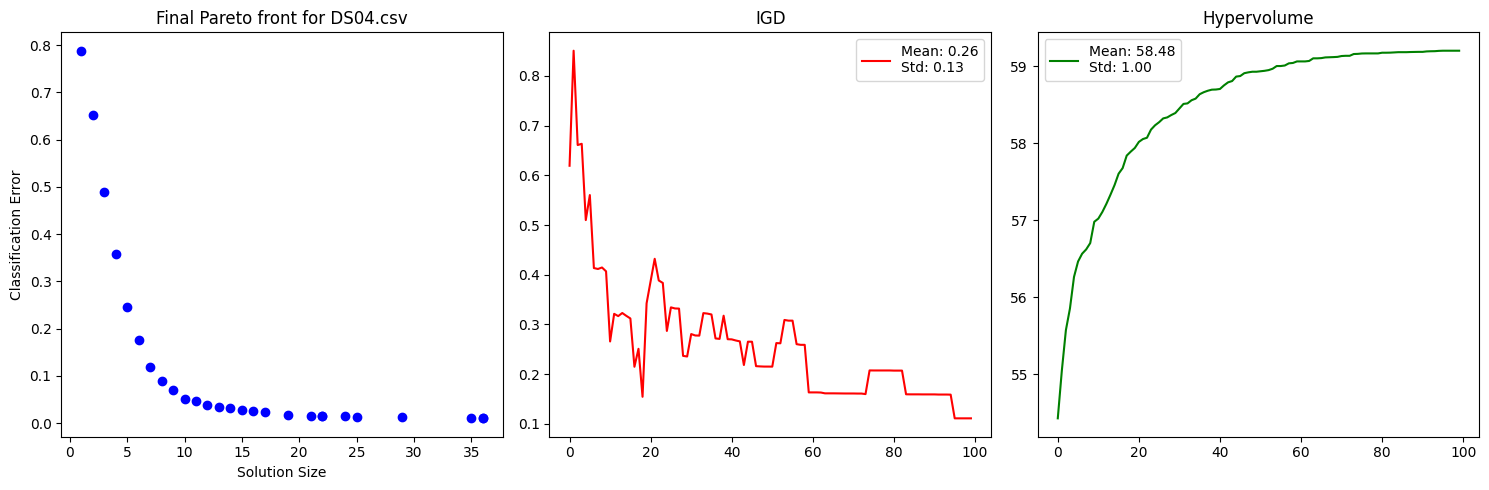
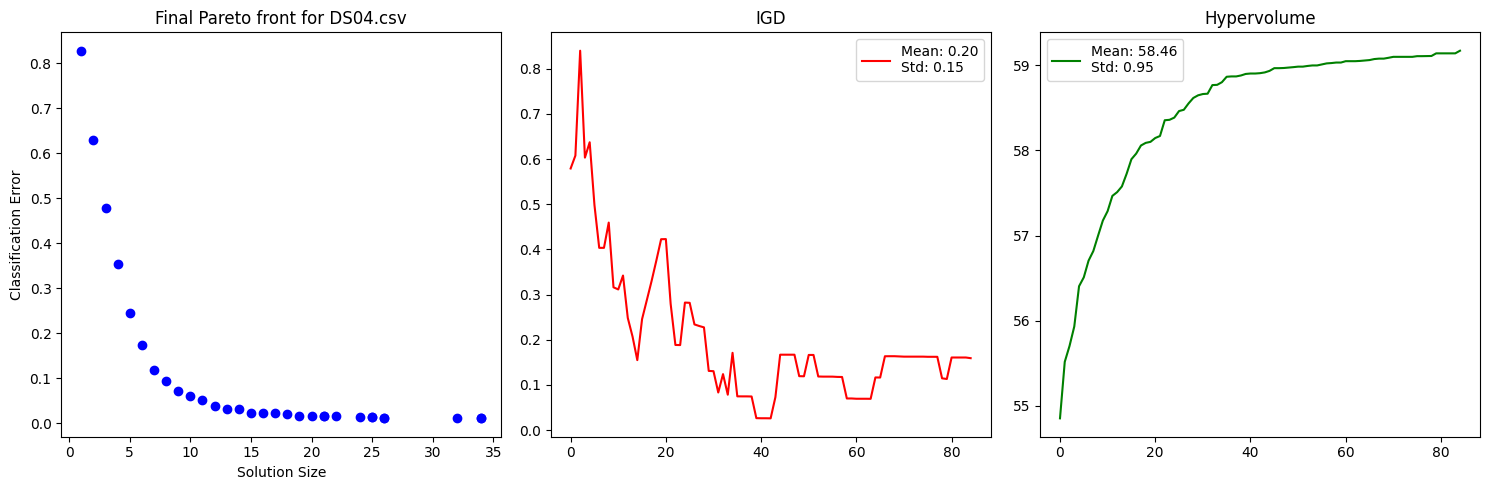


Initialization: random

MAXFE: 20000

Termination condition: hv\_threshold: 1, igd\_threshold: 0.05, no\_improvement\_limit: 30

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Dataset | Generation# | HV\_mean | HV\_std | IGD\_mean | IGD\_std | Duration |
| DS04.csv | 85 | 58.465 | 0.945286 | 0.204455 | 0.153442 | 29 |
| DS04.csv | 100 | 58.4846 | 0.995055 | 0.262293 | 0.12707 | 34 |
| DS04.csv | 164 | 58.7548 | 0.857002 | 0.244203 | 0.0768767 | 56 |
| DS04.csv | 161 | 58.683 | 0.87241 | 0.193206 | 0.118905 | 52 |
| DS04.csv | 82 | 58.3991 | 0.884551 | 0.223908 | 0.140849 | 28 |



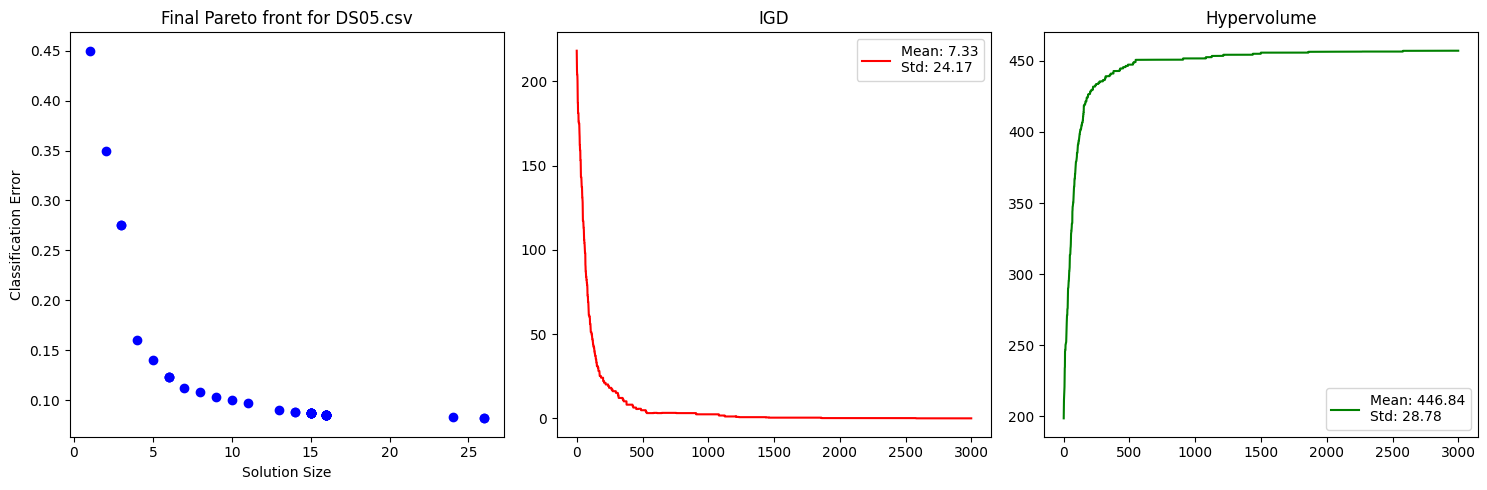
Dataset: DS05

Num-features: 500

Num-samples: 600

Initialization: random

MAXFE: 300000



Initialization: wise\_2 (based on their Pareto front max feature size)

MAXFE: 30000

Termination condition: hv\_threshold: 3, igd\_threshold: 0.1, no\_improvement\_limit: 25

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Dataset | Generation# | HV\_mean | HV\_std | IGD\_mean | IGD\_std | Duration |
| DS05.csv |  |  |  |  |  |  |
| DS05.csv |  |  |  |  |  |  |
| DS05.csv |  |  |  |  |  |  |
| DS05.csv |  |  |  |  |  |  |
| DS05.csv |  |  |  |  |  |  |

Dataset: DS07

Num-features: 561

Num-samples: 900

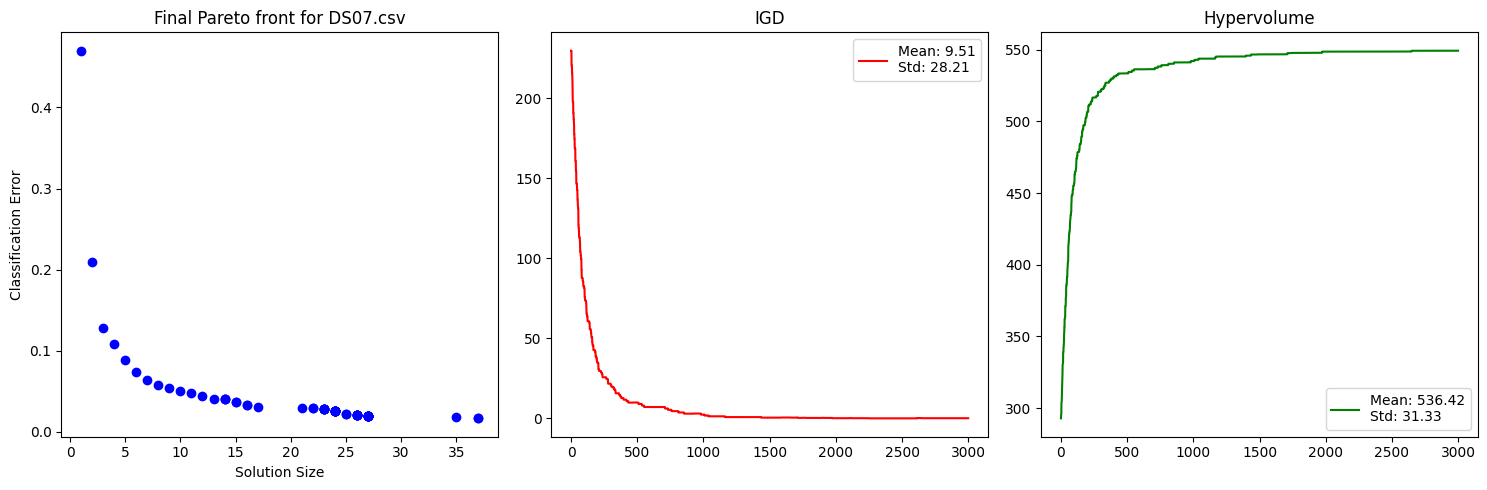
Initialization: random

MAXFE: 300000

Evaluations: 100000, HV: 542.0255555555556, IGD: 2.4288419141085584

Evaluations: 200000, HV: 548.6122222222222, IGD: 0.18200412428615262

Evaluations: 300000, HV: 549.2444444444444, IGD: 0.17772037702437637



Dataset: DS08

Num-features: 561

Num-samples: 1200

Initialization: random

MAXFE: 300000

Dataset: DS10

Num-features: 649

Num-samples:

Initialization: random

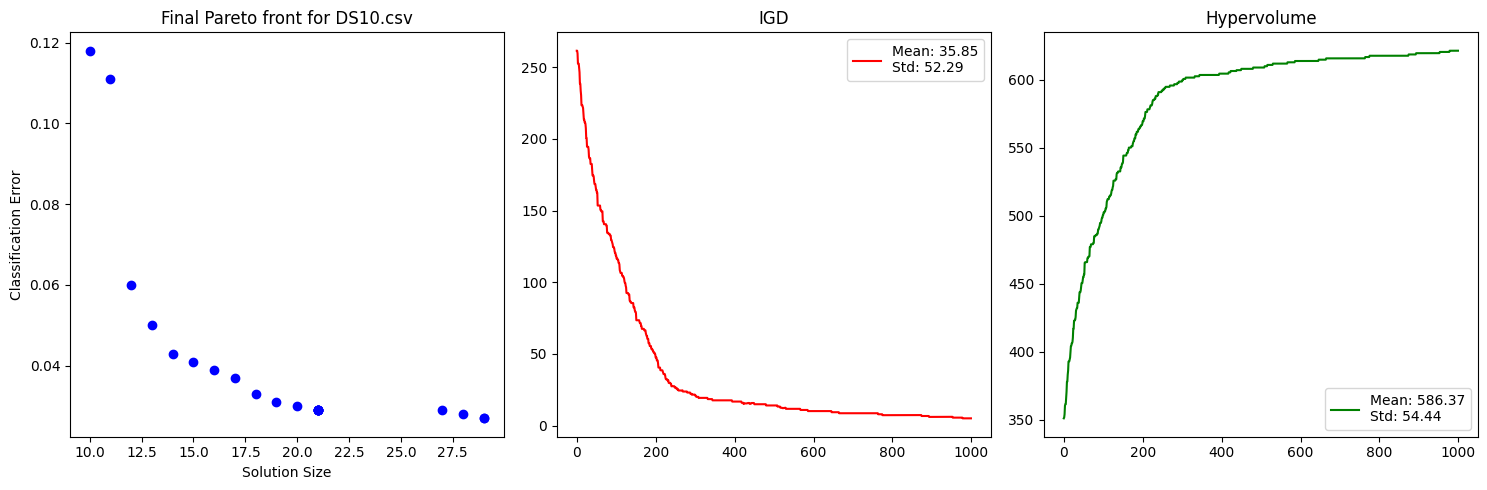
MAXFE: 100000

Evaluations: 25000, HV: 591.9554824285364, IGD: 26.928896199185708

Evaluations: 50000, HV: 609.0753687819556, IGD: 14.073136268640786

Evaluations: 75000, HV: 615.8413743084402, IGD: 8.64583942329659

Evaluations: 100000, HV: 621.4474144803486, IGD: 5.086199016790782



More sample, more runtime

DS05, binary classification, integer numbers