

Ranking-Prediction Based Evolutionary Algorithm for Expensive Many-Objective Optimization Problems

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COIN Report 2025006

ABSTRACT

To deal with challenging expensive many-objective optimization problems, this study proposes a novel ranking-prediction based evolutionary algorithm. Instead of approximating the objectives directly, our algorithm introduces M symmetrical ranking cases in the generalized Pareto dominance to construct a single comprehensive Kriging model. Moreover, we design a novel method referred to as the expected ranking advantage (ERA) for model management to cooperate with ranking-prediction, which is capable of providing sufficient information and avoiding the accumulation of errors compared to traditional surrogate models. In addition, our proposed algorithm achieves a significant improvement in the time complexity of model construction. The outstanding performance and efficiency of the ERA-based algorithm are demonstrated in two benchmark test suites with the comparison of four state-of-the-art algorithms.

KEYWORDS

Many-objective Optimization Problems, Evolutionary Algorithm, Expensive Optimization, Ranking Prediction

1 INTRODUCTION

Expensive multi-objective optimization problems (EMOPs) arise in real-world applications (e.g., engineering design, drug discovery), where each evaluation requires significant resources, such as time, computational power, or physical experiments. Surrogate-assisted evolutionary algorithms (SAEAs) effectively address EMOPs with limited function evaluations (FEs, e.g., a few hundred) [11]. However, traditional SAEAs struggle with expensive many-objective optimization problems (EMaOPs) due to the loss of Pareto-based selection pressure. It becomes essential to assess the quality of candidate solutions reliably for EMaOPs. Consequently, many research efforts have been directed towards developing new methods based on indicators and reference vectors that do not rely on Pareto dominance. For example, in HSMEA [4], the Euclidean distance between the candidate solution and the ideal point is used for selection. The current limitation is that the performance of existing non-Pareto-dominance-based SAEAs depends heavily on the reference vectors and the shape of the problem's Pareto front (PF). Although there are SAEAs dedicated to predicting the dominance relationship of candidate solutions with classification models, these algorithms have not yet been reported to be competitive in providing desirable performance in different kinds of problem [5]. Therefore, it is necessary to develop an efficient algorithm to deal with these challenging but meaningful problems.

Kriging is a widely used surrogate model in SAEAs as it can provide estimated fitness as well as uncertainty information. Despite its poor computational efficiency when dealing with high-dimensional decision variables or large samples, it is highly competitive for EMaOPs. For the decision variables $X = [x_1, x_2, \dots, x_n]$ in the training samples and their responses are $Y = [y_1, y_2, \dots, y_n]$. A Kriging model can learn the latent function $f(X)$. For new input data $z^* \in R$, the approximation is as follows [8]:

$$\bar{f}(z^*) = \psi(z^*) + \mathbf{k}^{*T} \left(K + \delta_n^2 I \right)^{-1} (Y - \psi(X)), \quad (1)$$

$$\sigma^2 [f(z^*)] = k(z^*, z^*) - \mathbf{k}^{*T} \left(K + \delta_n^2 I \right)^{-1} \mathbf{k}^*, \quad (2)$$

where $\psi(X)$ is the mean vector of X , \mathbf{k}^* is the covariance vector between X and z^* , K is the covariance matrix of X , and $k(z^*, z^*)$

is the Gaussian kernel computation of z^* . $\delta_n^2 I$ is the covariance matrix for the noise term, where δ_n^2 is the noise variance, and I is the identity matrix. This term is added to the kernel matrix K to account for the noise in the data. σ^2 represents the predictive variance of the function $\tilde{f}(z^*)$.

Pareto-dominance-based multi-objective evolutionary algorithms (MOEA) usually show poor performance in dealing with many-objective optimization problems (MaOPs) due to the rapid growth of non-dominated solutions with increasing objectives. Zhu et al. [13] proposed the ' $M-1$ ' + 1 framework of generalized Pareto dominance (GPD), abbreviated as $(M-1)$ -GPD. It can guarantee the identity of expanding the dominance area to improve the selection pressure. However, calculating the actual $(M-1)$ -GPD rankings requires precise fitness, which is challenging to achieve with existing regression models. In addition, using traditional binary classification models results in loss of information.

To address the limitations of $(M-1)$ -GPD in SAEAs, we propose a novel ranking-prediction method, termed expected ranking advantage (ERA), which integrates $(M-1)$ -GPD and expected improvement (EI) to assess solution quality while balancing model uncertainty and predicted performance[7]. The proposed algorithm, ERA-MOEA, offers the following key contributions.

- A ranking-prediction method is proposed for the SAEA framework. Unlike traditional methods, our model predicts the average front number in $(M-1)$ -GPD instead of the objectives, thus improving the algorithm's reliability and efficiency.
- A novel criterion is designed to achieve a balance between performance and uncertainty without reference vectors and indicators, which is applicable to a wider variety of Pareto fronts with diverse characteristics.
- Comprehensive experiments are conducted on representative benchmarks, and the performance of our algorithm is validated via comparisons with several state-of-the-art SAEAs.

2 METHODOLOGY

2.1 GENERAL FRAMEWORK

Algorithm 1 presents the pseudocode of ERA-MOEA. ERA-MOEA starts with the Latin Hypercube Sampling (LHS) method for the initial population, and all solutions are evaluated subsequently. We adopt a generalized Pareto dominance method, called AGPO [13], to sort the solutions. Then, our ranking-prediction model is constructed based on the evaluated solutions' average rankings. After producing offspring, promising candidate solutions are pre-selected according to the ranking predicted by the trained model. The details of the ranking-prediction and model management strategy are introduced in the following subsections.

2.2 Ranking-prediction Method

In ERA-MOEA, a novel surrogate model construction is applied to improve the efficiency and reliability of the algorithm. Figure 1 illustrates the construction of the model by a bi-objective example with five candidate solutions. The blue and yellow lines, respectively, represent two cases of dominance of $(M-1)$ -GPD. To begin, training samples are ranked by $(M-1)$ -GPD, which is introduced to provide M symmetrical cases of rankings. These rankings differ from those in generalization of Pareto optimality dominance (GPD)

Algorithm 1 General Framework

Require: N (population size), ϕ (the expanding angle), M (number of the objectives), Q (promising solution)
Ensure: P (current population).
1: $P \leftarrow \text{LHS}(N)$;
2: $FE \leftarrow N$ and $A \leftarrow P$;
3: **while** $FE < FE_{max}$ **do**
4: $(r_1, r_2, \dots, r_M) \leftarrow \text{AGPOSort}(A, \phi)$;
5: $r \leftarrow \text{mean}(r_1, r_2, \dots, r_M)$;
6: $model \leftarrow \text{TrainKriging}(A, r)$;
7: **while** $g < g_{max}$ **do**
8: $O \leftarrow \text{GA}(P)$;
9: $P \leftarrow P \cup O$;
10: $(r_{pred}, RMSE) \leftarrow model(P)$;
11: $ERA \leftarrow \text{ExpectedRankingAdvantage}(r_{pred}, RMSE)$;
12: $P \leftarrow \text{SelectionbyER}(ERA, P, N)$;
13: **end while**
14: $Q \leftarrow \text{ModelManagement}(P, ERA)$;
15: $Q \leftarrow \text{RealEvaluation}(Q)$;
16: $FE \leftarrow FE + 1$
17: $A \leftarrow A \cup Q$;
18: $P \leftarrow \text{EnvironmentalSelection}(A, N)$
19: **end while**
20: **return** P ;

[12]. Specifically, they leave one objective unchanged while increasing the selection pressure for the remaining $(M-1)$ objectives. For Case 1 (yellow line), as shown in Figure 1, solutions A and B belong to the first front, solutions C and D belong to the second front, and solution E is located in the third front. However, for Case 2 (blue line), the rankings of solutions are different from those of Case 1. Therefore, to take full advantage of the information provided during the evolutionary process, we calculate the averaging of the M cases of ranking to decide the final ranking of the training samples. This approach enables a more precise differentiation among various solutions. Furthermore, considering all rankings comprehensively contributes to better diversity. Finally, the Kriging model is trained for ranking-prediction, including the predicted front number and the root mean squared error (RMSE).

2.3 EXPECTED RANKING ADVANTAGE

It is crucial to consider both performance and uncertainty when handling EMaOPs. Performance ensures the overall quality of candidate solutions, while uncertainty reflects the reliability of the current model. To utilize the efficiency of our proposed ranking-prediction in SAEAs, we design a model management strategy that comprehensively considers the performance and uncertainty of solutions.

First, the predicted front number can serve as a metric for assessing performance, since the Kriging model produces continuous output. Furthermore, our model has the ability to synthesize M cases of rankings, thus guaranteeing both diversity and convergence. In addition, our ranking-prediction also provides the RMSE, which can be used as a measure of the uncertainty. Then, inspired by the concept of expected improvement (EI), we propose expected rank advantage (ERA) to integrate these two metrics. Specifically,

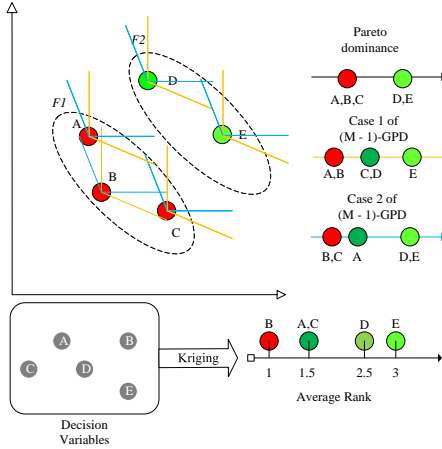


Figure 1: A sketch of the proposed bi-objective ranking-prediction method.

the formulation of ERA is as follows.

$$\begin{aligned} \text{ERA}(x) = & \left(r_{\text{median}} - r_{\text{pred}}(x) \right) \times \Phi \left(\frac{r_{\text{median}} - r_{\text{pred}}(x)}{\text{RMSE}(x)} \right) \\ & + \text{RMSE}(x) \times \phi \left(\frac{r_{\text{median}} - r_{\text{pred}}(x)}{\text{RMSE}(x)} \right), \end{aligned} \quad (3)$$

where r_{median} denotes the median value within the training samples. r_{pred} and RMSE represent the performance and uncertainty, respectively. Φ and ϕ respectively represent the cumulative distribution function (CDF) and the probability density function (PDF) of the standard normal distribution. $r_{\text{median}} - r_{\text{pred}}(x)$ represents the degree of advantage of the prediction ranking relative to the threshold, here taken as the median ranking. When the threshold is set too low, it can lead to a situation where there is no improvement. The criterion becomes excessively stringent, leading to the exclusion of potentially promising solutions. Contrarily, if the threshold is set too high, it may result in a loss of selection pressure. The proposed ERA may fail to identify superior solutions. Therefore, we adopt the median ranking as the threshold to strike a better balance. In summary, ERA represents the expectation of a candidate solution achieving better results relative to the median ranking. As a result, solutions with higher ERA are selected.

During the surrogate-assisted optimization process, all candidate solutions are sorted according to the ERA. The better half of them are selected to regenerate offspring with the genetic algorithm. In this method, ERA directs the candidate solutions towards those predicted to be better than the current median level of the population. Finally, a solution with the best ERA is evaluated using the real function. ERA takes into account both the distribution of the ranking-prediction and the corresponding uncertainty. The evaluation of the new solution helps to refine the current model and enhance the reliability of its subsequent predictions. In addition, it facilitates the convergence of the population.

2.4 COMPLEXITY AND PROPERTY ANALYSIS

In our method, the computational complexity is dominated by the model construction procedure. Suppose that the size of the training

samples is N and the objective number is M . The complexity of traditional SAEAs based on the Kriging model is $O(MN^3)$. But the complexity of our SAEAs is $O(N^3)$. This reduction in complexity implies that our algorithm achieves a significant saving of more than 90% computational resources for model construction.

3 EXPERIMENTAL STUDY

In this section, the proposed algorithm is examined in two benchmark test suites with comparison of four other SAEAs, that is, AB-SAEA [10], KTA2 [9], K-RVEA [2] and REMO [5]. The experiment aims to verify the effectiveness of the proposed ERA-MOEA. Furthermore, all experiments are conducted on a PC equipped with AMD EPYC and 256GB of RAM.

3.1 EXPERIMENTAL SETTINGS

- **Statistical Settings:** We use IGD^+ [6] as the performance indicator. The maximum number of FEs is set to 300 for all problems. All instances run 30 times independently. Moreover, the wilcoxon rank test is adopted at a significance level of 0.05, where "+", "-", and " \approx " indicate that the results of other algorithms are significantly better, significantly worse, and statistically similar to that obtained by ERA-MOEA.
- **Problem Settings:** DTLZ1-7 [3] and MAF1-6 [1] are used in our experiments. For all the problems, the number of objectives M is set to 5, 10, and 15, respectively. The number of decision variables D is the default setting in the benchmarks.
- **Evolutionary Operators:** Simulated binary crossover (SBX) and polynomial mutation (PM) are used for the generation of offspring in all algorithms, where the distribution index is set to 20, the crossover probability is set to 1, and the mutation probability is set to $1/D$.
- **Population Size:** It is set to 100 for all SAEAs.
- **Specific Parameters:** The maximum number of evaluations with surrogate model are respectively set to 2000, 2000, 2000, 3000 and 1000 for AB-MOEA, KTA2, K-RVEA, REMO and ERA-MOEA. In ERA-MOEA, the expanding angle ϕ in ERA-MOEA is set to be equivalent to twice the value of M . For the purpose of a fair comparison, the other parameter settings are the same as those in the original literature.

3.2 RESULTS AND ANALYSIS

The mean results of IGD^+ values achieved by the five algorithms under comparison are summarized in Table 1, where the best results are highlighted. Upon observing these results, it is evident that ERA-MOEA demonstrated superior performance, achieving the best results in 30 of the 39 test instances.

Specifically, ERA-MOEA shows overwhelmingly better performance on most problems, except for showing disadvantages in MAF1 and MAF2. In these two problems, solutions are distributed close to the PF, which is conducive to establishing an accurate regression model. As a result, SAEAs based on objective approximation models perform better in these problems. Whereas REMO and ERA-MOEA distinguish good solutions from poor solutions, their surrogate models are reliable in various problems. ERA-MOEA obtained well-converged solutions in various problems and particularly achieves favorable results in MAF3-6 and DTLZ5-7, which

Table 1: Comparison of IGD⁺ metric on four algorithms and ERA-MOEA, which is statistically better in 29 to 36 problems out of 39 problems.

Problem	M	ABSAEA	KTA2	KRVEA	REMO	ERA-MOEA
DTLZ1	5	2.69e+1 (8.07e+0)	1.88e+1 (7.32e+0)	3.69e+1 (5.89e+0)	1.67e+1 (5.49e+0)	1.28e+1 (5.88e+0)
	10	2.09e+1 (6.70e+0)	1.61e+1 (5.42e+0)	2.77e+1 (8.19e+0)	1.31e+1 (5.33e+0)	1.09e+1 (3.84e+0)
	15	2.75e+1 (1.07e+1)	1.67e+1 (5.62e+0)	2.29e+1 (7.16e+0)	1.66e+1 (6.60e+0)	1.05e+1 (6.01e+0)
DTLZ2	5	3.36e-1 (4.33e-2)	2.77e-1 (4.68e-2)	3.94e-1 (5.18e-2)	3.65e-1 (6.06e-2)	2.56e-1 (6.77e-2)
	10	6.70e-1 (6.01e-2)	6.25e-1 (4.77e-2)	6.43e-1 (7.36e-2)	6.52e-1 (6.42e-2)	5.52e-1 (8.62e-2)
	15	9.01e-1 (5.60e-2)	7.27e-1 (5.41e-2)	8.86e-1 (5.28e-2)	7.39e-1 (7.98e-2)	6.61e-1 (6.04e-2)
DTLZ3	5	3.36e+2 (8.11e+1)	3.09e+2 (7.66e+1)	3.87e+2 (7.74e+1)	2.34e+2 (6.30e+1)	1.73e+2 (6.87e+1)
	10	3.87e+2 (9.12e+1)	3.11e+2 (7.12e+1)	3.66e+2 (8.66e+1)	2.26e+2 (6.51e+1)	3.01e+2 (9.40e+1)
	15	4.24e+2 (9.89e+1)	2.96e+2 (7.43e+1)	4.06e+2 (8.60e+1)	2.11e+2 (5.15e+1)	2.96e+2 (1.04e+2)
DTLZ4	5	5.22e-1 (1.08e-1)	5.14e-1 (8.10e-2)	5.82e-1 (9.44e-2)	3.68e-1 (5.73e-2)	3.47e-1 (1.19e-1)
	10	8.02e-1 (7.54e-2)	6.78e-1 (8.63e-2)	7.67e-1 (5.96e-2)	6.59e-1 (6.69e-2)	5.78e-1 (1.23e-1)
	15	9.48e-1 (5.24e-2)	7.58e-1 (6.61e-2)	9.42e-1 (3.52e-2)	7.69e-1 (6.61e-2)	6.62e-1 (1.00e-1)
DTLZ5	5	1.25e-1 (3.99e-2)	1.26e-1 (2.78e-2)	1.66e-1 (5.89e-2)	2.38e-1 (5.93e-2)	7.77e-2 (3.61e-2)
	10	2.84e-1 (5.72e-2)	2.33e-1 (3.53e-2)	2.11e-1 (5.64e-2)	2.20e-1 (5.89e-2)	1.84e-1 (4.78e-2)
	15	3.39e-1 (4.57e-2)	3.01e-1 (4.36e-2)	2.79e-1 (6.59e-2)	2.35e-1 (6.05e-2)	1.87e-1 (4.82e-2)
DTLZ6	5	5.22e+0 (5.56e-1)	4.95e+0 (1.03e+0)	4.67e+0 (4.84e-1)	7.37e+0 (6.07e-1)	2.83e+0 (6.94e-1)
	10	7.61e+0 (5.72e-1)	7.52e+0 (3.60e-1)	6.08e+0 (5.14e-1)	7.67e+0 (5.49e-1)	4.81e+0 (8.32e-1)
	15	8.21e+0 (3.00e-1)	7.69e+0 (4.49e-1)	8.15e+0 (2.18e-1)	7.66e+0 (5.52e-1)	5.23e+0 (8.55e-1)
DTLZ7	5	1.31e+1 (2.03e+0)	1.39e+0 (5.44e-1)	1.26e+0 (3.62e-1)	7.04e+0 (1.44e+0)	1.43e+0 (4.42e-1)
	10	2.83e+1 (2.20e+0)	5.33e+0 (2.50e+0)	2.80e+1 (2.48e+0)	2.93e+1 (2.79e+0)	2.45e+0 (8.84e-1)
	15	4.49e+1 (2.73e+0)	3.12e+1 (6.90e+0)	4.46e+1 (2.81e+0)	4.58e+1 (4.02e+0)	4.53e+0 (1.49e+0)
MaF1	5	2.05e-1 (4.50e-2)	1.30e-1 (1.55e-2)	1.78e-1 (3.53e-2)	3.49e-1 (7.27e-2)	1.71e-1 (2.84e-2)
	10	6.78e-1 (2.61e-1)	3.32e-1 (3.24e-2)	4.58e-1 (7.47e-2)	5.02e-1 (6.05e-2)	3.57e-1 (2.61e-2)
	15	1.58e-1 (9.81e-3)	1.24e-1 (2.92e-3)	1.67e-1 (6.80e-3)	1.84e-1 (7.95e-3)	1.72e-1 (1.04e-2)
MaF2	5	6.66e-2 (1.77e-3)	6.61e-2 (1.41e-3)	6.57e-2 (1.75e-3)	7.98e-2 (1.76e-3)	6.72e-2 (3.98e-3)
	10	1.58e-1 (9.81e-3)	1.24e-1 (2.92e-3)	1.67e-1 (6.80e-3)	1.84e-1 (7.95e-3)	1.72e-1 (1.04e-2)
	15	2.13e-1 (1.13e-2)	1.46e-1 (6.37e-3)	2.14e-1 (1.19e-2)	2.38e-1 (1.47e-2)	2.21e-1 (1.48e-2)
MaF3	5	7.37e+5 (2.22e+5)	7.80e+5 (3.92e+5)	3.42e+5 (1.20e+5)	1.88e+5 (1.10e+5)	1.31e+4 (1.40e+4)
	10	6.61e+5 (1.84e+5)	8.57e+5 (2.90e+5)	4.32e+5 (1.40e+5)	2.72e+5 (1.80e+5)	1.23e+5 (6.65e+4)
	15	5.80e+5 (2.14e+5)	8.69e+5 (3.80e+5)	4.56e+5 (1.31e+5)	4.15e+5 (2.86e+5)	1.46e+5 (6.91e+4)
MaF4	5	4.80e+3 (1.27e+3)	3.46e+3 (1.12e+3)	4.29e+3 (1.23e+3)	3.15e+3 (7.81e+2)	1.78e+3 (1.07e+3)
	10	1.68e+5 (4.66e+4)	9.41e+4 (3.00e+4)	1.38e+5 (4.20e+4)	8.43e+4 (2.65e+4)	3.67e+4 (1.44e+4)
	15	6.71e+6 (1.34e+6)	4.25e+6 (1.31e+6)	6.45e+6 (1.36e+6)	2.23e+6 (5.70e+5)	1.22e+6 (5.77e+5)
MaF5	5	2.77e+0 (9.70e-1)	2.42e+0 (1.33e+0)	2.91e+0 (9.40e-1)	1.54e+0 (2.08e-1)	1.44e+0 (1.20e-1)
	10	1.24e+1 (1.63e+1)	3.83e+0 (3.17e+0)	1.21e+1 (2.38e+1)	6.90e+0 (6.66e+0)	3.11e+0 (2.19e+0)
	15	1.15e+5 (1.40e+3)	7.00e+0 (1.18e+1)	1.35e+2 (2.44e+2)	5.07e+1 (1.05e+2)	3.79e+0 (2.09e+0)
MaF6	5	1.72e+0 (9.53e-1)	3.35e-1 (2.48e-1)	5.38e+0 (6.21e+0)	6.47e+0 (2.90e+0)	2.83e-1 (4.54e-1)
	10	1.16e+1 (7.89e+0)	7.50e-1 (5.98e-1)	9.43e+0 (3.92e+0)	8.94e+0 (4.30e+0)	2.89e-1 (2.02e-1)
	15	2.50e+1 (5.41e+0)	3.83e+0 (3.72e+0)	1.56e+1 (6.07e+0)	1.02e+1 (3.90e+0)	4.89e-1 (5.57e-1)
+/-/≈		2/36/1	4/29/6	2/33/4	2/35/2	-/-/-

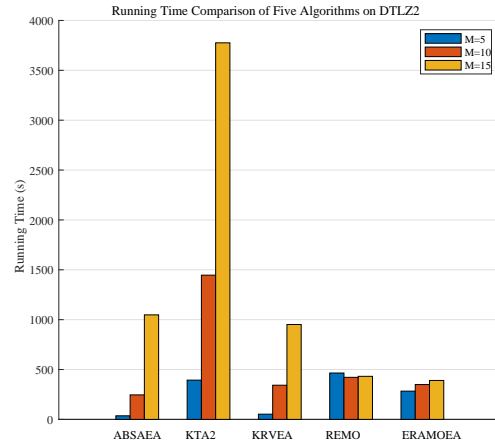


Figure 2: The mean running time comparison on DTLZ2.

ACKNOWLEDGMENTS

This work was supported by the Natural Science Foundation of China under Grant 62206113 and the Natural Science Foundation of Jiangsu Province under Grant BK20221067, BK20230923.

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have irregular PFs. This illustrates that ERA-MOEA is reliable regardless of the shape of the PFs. DTLZ1 and DTLZ3 are multi-modal problems where ERA-MOEA and REMO both perform well, demonstrating the ability to escape local optima. Even without reference vectors, ERA-MOEA maintains good distribution and outperforms reference-vector-based SAEAs on DTLZ2 and DTLZ4.

In addition, ERA-MOEA not only demonstrates performance advantages, but also does not consume excessive time, especially when M is as large as 15. The statistical results on running time are shown in Figure 2. ERA-MOEA exhibits the shortest running time because its time complexity in model construction does not change with the number of objectives. In summary, ERA-MOEA can outperform SAEAs based on objective approximation while maintaining reliability.

4 CONCLUSION

In this work we develop an evolutionary algorithm for expensive many-objective optimization, named as ERA-MOEA, which utilizes ranking-prediction to avoid error accumulation in traditional SAEAs. Unlike reference-vector-based approaches, ERA-MOEA relies on generalized Pareto dominance [13], ensuring reliability of the convergence and diversity of population across diverse problems. However, without the approximation of objectives, it is impossible to assess the diversity of the population with traditional methods. As a result, there is a demand for a new method that can enhance diversity without requiring predicted objectives.