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Riemannian 多様体における永続性ベースの Clustering の多峰性最適化問題への応用

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1 Introduction

In the realm of optimization and data analysis, the process of clustering plays a pivotal role in discerning patterns and uncovering hidden structures within complex datasets. Traditional clustering algorithms partition a collection of objects into groups using shared characteristics. In the pursuit of solving single-objective multi-modal optimization problems, the challenge lies in exploring intricate search spaces efficiently using proper clustering algorithms.

This paper introduces a novel approach that leverages persistence-based clustering in Riemannian manifolds within evolutionary computation (EC) algorithms to address multi-modal optimization problems. The method leverages the concepts of topology and geometry to discern topological features in the EC search space, allowing for a robust and insightful clustering of objects. Moreover, the proposed approach operates seamlessly in Riemannian manifolds, capturing the inherent non-linear structures in the population.

To enhance the effectiveness of our method, we integrate it with the chaotic evolution (CE) algorithm, resulting in a synergistic fusion of topological data analysis and global search capabilities. This integration harnesses the chaotic dynamics of the CE algorithm to navigate complex landscapes efficiently. The iterative optimization strategy em-

bedded within our approach ensures the discovery of previously overlooked peaks, safeguarding against the omission of local optima.

To evaluate the performance of the proposed algorithm, we conduct experiments employing nine multi-modal benchmark functions derived from the annual CEC competition. A comparative analysis is undertaken between the new algorithm, the CE algorithm, and the classical Genetic Algorithm (GA). An array of evaluation metrics drawn from CEC2021⁹⁾ is employed to comprehensively assess the proposal's performance.

Through our research, we aim to not only present a robust solution to the challenges posed by multi-modal optimization but also contribute to the broader landscape of data analysis methodologies. Our focus remains on the innovative application of topological data analysis in Riemannian manifolds, demonstrating its potential to revolutionize the way we approach clustering and multi-modal optimization problems.

The subsequent sections of this paper are delineated as follows: Section 2 provides a mathematical exposition of the clustering algorithm, the CE algorithm, and delineates the proposed Chaotic Evolution with Clustering methodology. Section 3 furnishes an elaborate description of the conducted experiments. Section 4 expounds upon the experimental results. Finally, Section 5 summarizes the salient points of this article, proffers prospective solutions, and charts forthcoming avenues of development.

Evolutionary Multi-modal Optimization Using Persistence-Based Clustering in Riemannian Manifolds

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2 An Overview of Clustering Methods for Multi-Modal Optimization and Chaotic Evolution

The concept of single-objective multi-modal optimization problem implies the presence of multiple local optimal solutions within a search space, necessitating the discovery of the global optimal solution. The integration of clustering methods into single-objective multi-modal optimization algorithms enhances the algorithm's capacity to effectively explore the search space, thereby increasing the likelihood of identifying the local and global optimal solutions.

2.1 Clustering Algorithms

Clustering algorithms, essential in unsupervised learning, categorize data based on inherent similarities, revealing underlying patterns. Methods include Partition-based ⁴⁾, Density-based ²⁾, and Hierarchical ⁷⁾, along with specialized approaches like quantum clustering ⁸⁾ and spectral clustering ⁵⁾. Persistent clustering on Riemannian manifolds ¹⁾ utilizes Riemannian metrics, transforming data into a persistence diagram. These insights enhance traditional clustering, enabling efficient data clustering on manifolds, which is a model of fitness landscape in EC.

Clustering algorithms are vital in single-objective optimization, especially for high-dimensional and multi-modal optimization challenges. Clustering algorithms significantly enhance efficiency, enabling more effective searches for multi-modal problems.

2.2 Persistence-Based Clustering in Riemannian Manifolds

In this section, we present a novel approach for persistent clustering on Riemannian manifolds, leveraging Riemannian metrics, which is introduced to EC algorithms for multi-modal optimization.

Riemannian metrics offer a natural means of quantifying distances between points on a manifold. We utilize both the Riemannian metric and the Euclidean metric to compute the geodesic distance between data points. We create a persistence diagram, which records the inception and cessa-

tion of topological features as the spatial scale undergoes transformation. Subsequently, clusters are derived from the persistence diagram, enabling the discernment of significant and enduring clusters on the Riemannian manifold.

In optimization algorithms, a "neighborhood" typically denotes a set of feasible solutions surrounding the present solution. In such neighborhoods, only one or a few variables have undergone modification relative to the current solution. These neighborhoods delineate a search space, representing a local region surrounding the current solution that is considered a candidate set for potentially superior solutions.

The incorporation of neighborhoods into optimization algorithms generally serves to heighten their efficiency and precision. This is primarily due to their capacity to narrow the scope of the search space, expediting the process of identifying the optimal solution while obviating the necessity of exploring the entire solution space.

When identifying the neighborhoods of points, it becomes imperative to compare their fitness values. As depicted in Figure 1, the neighborhood of point D encompasses both point C and point E. Notably, the fitness value of point C surpasses that of point D, whereas the fitness value of point E falls below that of point D. Consequently, based on their fitness values, points C and D are unambiguously categorized together.

2.3 Chaotic Evolution Algorithm

The CE algorithm ⁶⁾ represents a global optimization algorithm that draws upon the principles of chaotic systems and evolutionary algorithms. It melds the stochastic and non-linear characteristics of chaotic systems (as expressed in equation 1) with the adaptive and global search capabilities inherent in EC algorithms. This amalgamation equips the algorithm to effectively address non-linear, non-convex, and multi-modal optimization problems.

Within the framework of the CE Algorithm, the chaotic system (as defined by equation 1) serves as the exploration mechanism for the search space. The introduction of chaotic sequences ensures that the search process continually executes random

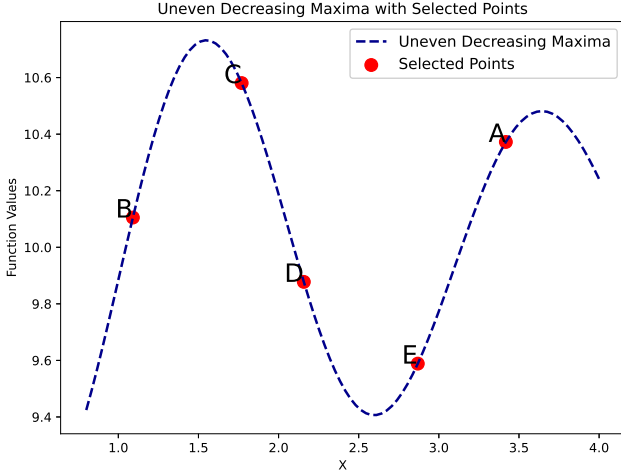


Fig. 1: Neighborhood diagram. There are three points C, D, and E. Points C and D are classified into the same category, while points E and D are classified into different categories.

jumps, thereby preventing entrapment in local optima.

In a chaotic system (equation 1), the chaotic parameter (CP_i) governs the search range of the CE algorithm within the search space. The direction factor, D_i , regulates the exploration and exploitation functions of the CE algorithm.

$$mutant_i = target_i \cdot (D_i \cdot CP_i). \quad (1)$$

3 Multi-modal Optimization with Persistence-Based Clustering in Riemannian Manifolds

The CE with clustering algorithm (CECA) is a clustering algorithm grounded in the principles of chaotic evolution. Our proposed CECA algorithm is shown in Algorithm 1. It amalgamates the erratic traversal of chaotic dynamics with the global search capabilities of the CE algorithm to enhance the clustering effectiveness.

The effectiveness of our method is assessed through the application of established metrics tailored for clustering on Riemannian manifolds. Additionally, we engage in comprehensive parameter tuning to optimize the clustering outcomes, thereby ensuring the method's robustness across diverse multi-modal problems.

Algorithm 1 Chaotic Evolution with Clustering Algorithm (CECA)

Require:

- 1: Fitness function $f(x)$, Search space X , Maximum number of iterations max_iter , Population size N , Neighborhood radius R

Ensure: Best solution x^*

- 2: Initialize population P with N individuals randomly in X
 - 3: Initialize the chaotic system
 - 4: **for** $t = 1$ **to** max_iter **do**
 - 5: Generate a chaotic sequence $r(t)$ using the chaotic map
 - 6: Evaluate fitness of each individual in P
 - 7: Find the best individual x^* in P
 - 8: **for** $i = 1$ **to** N **do**
 - 9: Find neighboring individuals of P_i within radius R
 - 10: Set $F_{max} = F_i$
 - 11: **for** each neighbor $B_{i,j}$ **do**
 - 12: **if** $F_{B_{i,j}} > F_{max}$ **then**
 - 13: Set $F_{max} = F_{B_{i,j}}$
 - 14: **end if**
 - 15: **end for**
 - 16: **if** $F_i = F_{max}$ **then**
 - 17: Record P_i as a vertex
 - 18: **else**
 - 19: **for** each neighbor $B_{i,j}$ **do**
 - 20: **if** $F_{B_{i,j}} > F_i$ and $dist(P_i, B_{i,j}) < dist(P_i, B_{k,j})$ for all $k \neq i$ **then**
 - 21: Classify P_i and $B_{i,j}$ as the same vertex
 - 22: Break the loop
 - 23: **end if**
 - 24: **end for**
 - 25: **end if**
 - 26: **end for**
 - 27: **for** each vertex P_i **do**
 - 28: Using the Gaussian noise
 - 29: Get the optimal value x^* of each peak point from each vertex P_i
 - 30: **end for**
 - 31: **end for**
 - 32: **return** $number(x^*)$ and $fitness(x^*)$
-

To illustrate the application of the CECA algorithm, we selected a one-dimensional benchmark function from the test set of the CEC2021 competition. Figure 2 illustrates a general experimental procedure diagram. The experiment begins with a randomly generated initial population. We then performed ten generations to optimize the population. CECA is used to find the position and number of peaks in each generation. finally, we will accumulate the different peaks found in each generation. In addition, in order to enhance the discovery of the optimal peak of the objective function, we apply Gaussian mutation (as shown in equation 2) to the best individual in each peak of every generation, where μ represents the fluctuation the mean value, σ represents the standard deviation of the fluctuation. The larger σ is, the greater the noise fluctuation is, and the smaller σ is, the smaller the noise fluctuation is.

$$Gaussian(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}} \quad (2)$$

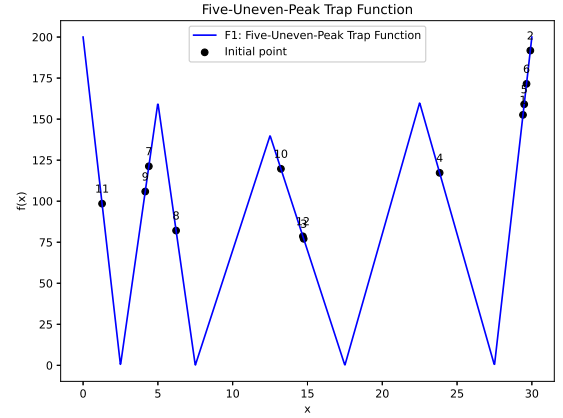
Figure 2 depicts the population distribution subsequent to the application of Gaussian mutation, highlighting the gradual convergence of the population toward the optimal peak during the search process.

CE algorithms have demonstrated their ability to swiftly navigate away from local optima and discover global optima, rendering them proficient in global search tasks. Additionally, the CE algorithm incrementally approaches the optimal solution by emulating the natural process of survival of the fittest and the mechanism of cross-mutation between generations. The CE algorithm is distinguished by its robust global search performance, adaptability, and ease of implementation. Our proposed approach furnishes a potent technique for multi-modal optimization using persistent clustering on Riemannian manifolds.

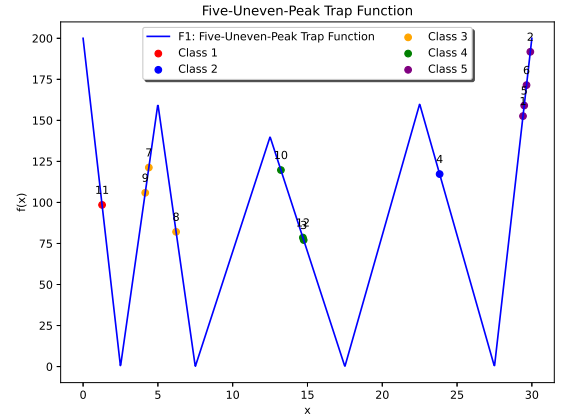
4 Experimental Evaluation

4.1 Experimental Settings

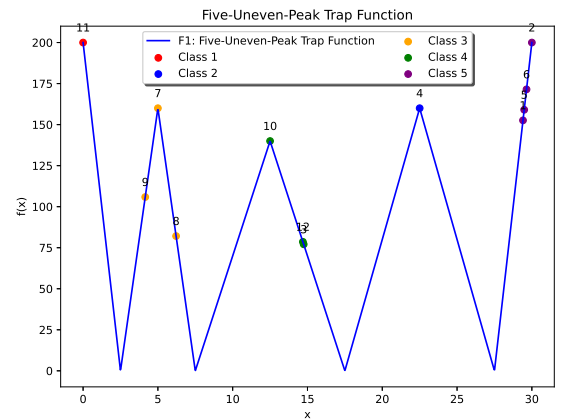
In this study, we conduct a comprehensive performance assessment of our proposed algorithm using the CEC2021 benchmark. The CEC2021



Initial Population



Persistence-Based Clustering



Gaussian mutation

Fig. 2: Comparison of distributions after initial population, application of CECA algorithm and application of Gaussian mutation

Table 1: Test Function

No.	Name	dimension	Form	Range	Peak maximum	Peak number
F1	Five-Uneven-Peak Trap	1D	$f(x) = \begin{cases} 80(2.5 - x), 0 \leq x < 2.5, \\ 64(x - 2.5), 2.5 \leq x < 5.0, \\ 64(7.5 - x), 5.0 \leq x < 7.5, \\ 28(x - 7.5), 7.5 \leq x < 12.5, \\ 28(17.5 - x), 12.5 \leq x < 17.5, \\ 32(x - 17.5), 17.5 \leq x < 22.5, \\ 32(27.5 - x), 22.5 \leq x < 27.5, \\ 80(x - 27.5), 27.5 \leq x < 30 \end{cases}$	$x \in [0, 30]$	200.0	5
F2	Equal Maxima	1D	$f(x) = \sin^6(5\pi x)$	$x \in [0, 1]$	1.0	5
F3	Uneven Decreasing Maxima	1D	$f(x) = \exp(-2\log(2)(\frac{x-0.08}{0.854})^2) \sin^6(5\pi(x^{\frac{3}{4}} - 0.05))$	$x \in [0, 1]$	1.0	5
F4	Himmelblau	2D	$f(x) = 200 - (x^2 + y - 11)^2 - (x + y^2 - 7)^2$	$x, y \in [-6, 6]$	200.0	4
F5	Six-hump-camel-back	2D	$f(x, y) = (4 - 2.1x^2 + \frac{x^4}{3})x^2 + xy + (-4 + 4y^2)y^2$	$x \in [-1.9, 1.9], y \in [-1.1, 1.1]$	1.03163	4
F6	Shubert	2D	$f(\vec{x}) = -\prod_{i=1}^2 \sum_{j=1}^5 j \cos[(j+1)x_i + j]$	$x, y \in [-10, 10]^2$	186.731	18
F7	Vincent	2D	$f(\vec{x}) = \frac{1}{2} \sum_{i=1}^2 \sin(10\log(x_i))$	$x, y \in [0.25, 10]^2$	1.0	36
F8	Shubert	3D	$f(\vec{x}) = -\prod_{i=1}^D \sum_{j=1}^5 j \cos[(j+1)x_i + j]$	$x_i \in [-10, 10]^D$	2709.0935	81
F9	Vincent	3D	$f(\vec{x}) = \frac{1}{D} \sum_{i=1}^D \sin(10\log(x_i))$	$x_i \in [0.25, 10]^D$	1.0	216

benchmark is a well-established and publicly accessible test suite widely recognized in the field of EC. This benchmark encompasses a diverse array of optimization problems, encompassing continuous, constrained, and multi-objective optimization scenarios. Leveraging the standardized evaluation metrics offered by the CEC2021 benchmark, we systematically compared our algorithm with state-of-the-art methodologies. This approach allowed us to objectively gauge the algorithm’s efficacy and efficiency across a spectrum of problem instances.

We employ a set of nine multi-modal functions, which are detailed in Table 1, as the experimental subjects. The table (Table 1) provides a clear summary of the function dimensions and the number of peaks. The experimental environment is Windows 11 system. The algorithm is implemented by anaconda’s spyder and implemented in python3.9 language.

4.2 Evaluation Metrics

The peak ratio(PR) metric offers distinct advantages in the evaluation of single-objective multi-modal optimization problems. It provides a comprehensive performance assessment and demonstrates robustness. By normalizing the objective

function values, the PR metric furnishes a straightforward yet effective means of evaluating and comparing the efficacy of various single-objective multi-modal optimization algorithms. CE, GA and CECA are used to evaluate the performance of searching for global optimal performance and finding multi-modal capabilities.

- **Peak Ratio:** PR ³⁾ is a commonly used performance metric for evaluating multi-modal optimization algorithms, typically for continuous multi-modal optimization problems. In equation (3), NPF_i denotes the number of global optima found at the end of the i-th run, NKP is the number of known global optima, and NR is the number of runs.

$$PR = \frac{\sum_{run=1}^{NR} NPF_i}{NKP * NR}. \quad (3)$$

- **Objective Function Value:** The value of the objective function of the global optimum found by the algorithm, used to measure the optimization performance.

4.3 Experiment Results

CECA exhibited exceptional performance across the benchmark functions $F1$ to $F9$ (Table 1), con-

Table 2: Peak Ratio

No.	Name	F_{CE}	F_{GA}	F_{CECA}
F1	Five-Uneven-Peak Trap	1.00	0.95	1.00
F2	Equal Maxima	1.00	1.00	1.00
F3	Uneven Decreasing Maxima	1.00	1.00	1.00
F4	Himmelblau	0.98	1.00	1.00
F5	Six-hump-camel-back	0.95	0.97	1.00
F6	Shubert_2D	0.91	0.87	0.99
F7	Vincent_2D	0.96	0.83	0.99
F8	Shubert_3D	0.94	0.88	0.98
F9	Vincent_3D	0.96	0.80	0.96

sistently delivering outstanding results. In terms of identifying the maximum fitness values, the CECA algorithm outperformed the other two algorithms across all tested benchmarks. However, it notes that the CECA algorithm necessitated more time to reach the maximum values in certain benchmark tests compared to the other two algorithms, as CECA operates as an iterative optimization algorithm that incrementally refines solutions.

From Table 2, we conducted an in-depth analysis of the PR for the benchmark functions. The CECA algorithm demonstrated exceptional performance across all benchmark functions, including F1, F2, and F3, achieving a PR of 1, signifying proximity to all peak numbers. For the F5 function, the CECA algorithm achieved a PR of 1, while the GA algorithm and CE algorithm achieved PRs of 0.97 and 0.95, respectively. Overall, the CECA algorithm delivered satisfactory PR results in the majority of benchmark functions, either matching or surpassing the performance of the alternative algorithms.

Figure 3 presents the benchmark functions and the number of peaks identified during the CECA process. For most benchmark functions, CECA successfully identified all solutions. In the cases of the Shubert and Vincent benchmarks, CECA located all peaks after 20 generations on the $shubert_{2D}$ function, surpassing the performance of the other two algorithms. As the dimensionality increases, the search space required by the algorithm grows larger, and the number of peaks exceeds those at lower dimensions, increasing the complexity of the search. In multiple experiments,

it may not be guaranteed that all peaks can be identified every time in high dimensions. For 3-dimensional functions, the CECA algorithm consistently located all peaks in most cases, as indicated by Table 2. This data corroborates the superior performance of the CECA algorithm when compared to the other two algorithms.

4.4 Discussions

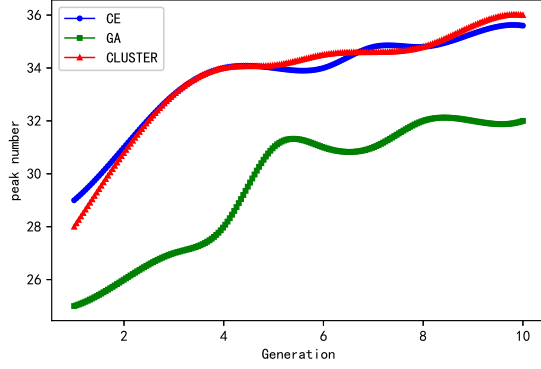
Table 2 illustrates the superior performance of the CECA concerning PR when compared to other benchmarked algorithms. Consistently, the CECA algorithm attains significantly higher PR values than its alternative counterparts. These results substantiate the efficacy of the CECA algorithm in capturing inherent clustering structures within the initial population, ultimately leading to improved PR values. It demonstrates a remarkable ability to accurately identify and emphasize distinctive peak regions.

Table 3 indicates that the CECA algorithm consistently achieves high fitness values throughout the optimization process. The CECA algorithm demonstrates exceptional convergence toward optimal solutions, as evidenced by its superior fitness values. These outcomes underscore the CECA algorithm’s capacity to optimize clustering performance, resulting in the maximization of cluster fitness. Figure 4 presents three illustrations to elucidate CECA’s performance in benchmarking fitness across varying dimensions.

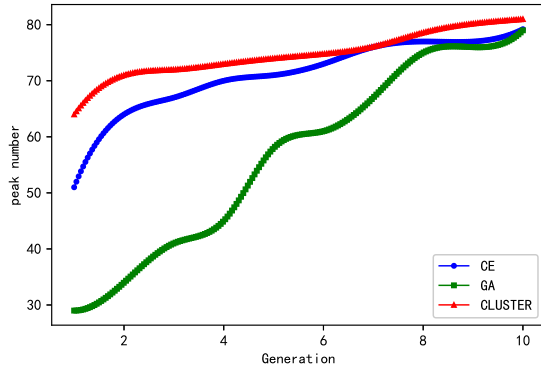
Table 3: Peak Fitness

No.	Name	F_{CE}	F_{GA}	F_{CECA}
F1	Five-Uneven-Peak Trap	199.9971	199.9234	199.9717
F2	Equal Maxima	0.9999	0.9999	0.9999
F3	Uneven Decreasing Maxima	1.000	1.000	1.000
F4	Himmelblau	199.9985	199.9681	199.9996
F5	Six-hump-camel-back	0.975	0.971	1.000
F6	Shubert_2D	186.729	186.601	186.7308
F7	Vincent_2D	0.9999	0.9995	0.9999
F8	Shubert_3D	2709.0359	2673.8931	2709.0902
F9	Vincent_3D	0.9999	0.9962	0.9999

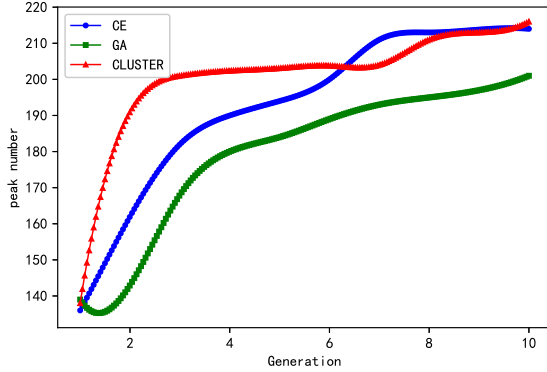
In summary, the CECA algorithm exhibited commendable performance in terms of maximizing fitness values across the majority of the test functions. Notably, it excelled in capturing global optima for test functions $F3$ and $F8$ demonstrat-



Vincent 2D



Shubert 3D



Vincent 3D

Fig. 3: Peak number. Above three figures show the peak number results of the three methods in the three functions.

ing its effectiveness in addressing complex and multi-modal optimization challenges. These out-

comes suggest that the CECA algorithm possesses a strong capacity to optimize fitness values and converge toward optimal solutions for a variety of test functions.

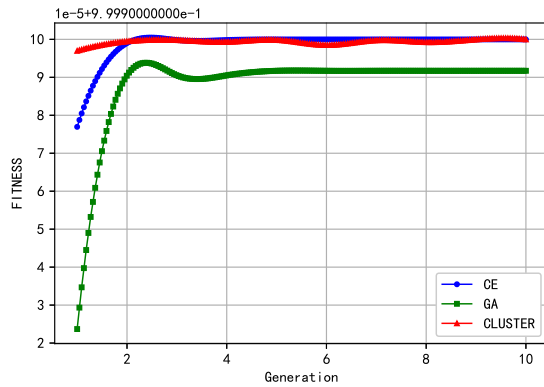
In conclusion, the CECA algorithm displayed promising performance in terms of maximizing fitness values across a broad spectrum of test functions. However, its performance in the context of the peak number metric exhibited variability among different functions, with notable success observed in functions $F7$ and $F8$. These findings underscore both the strengths and potential limitations of the CECA algorithm, underscoring the need for ongoing research to enhance its performance and address the challenges associated with accurately determining the peak number in optimization problems.

5 Conclusion and Future Work

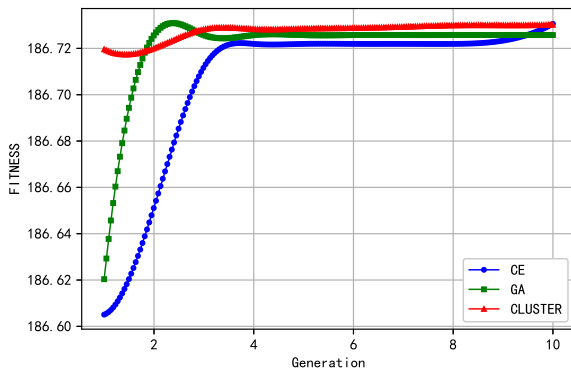
We have introduced a pioneering concept that employs persistence-based clustering in Riemannian manifolds in EC algorithm for multi-modal optimization. The proposal transforms the landscape of evolutionary algorithms to Riemannian manifold for complex multi-modal optimization challenges.

Our framework provides a versatile methodology applicable to various evolutionary algorithms. Applied to the CE algorithm, it led to the development of the CECA.

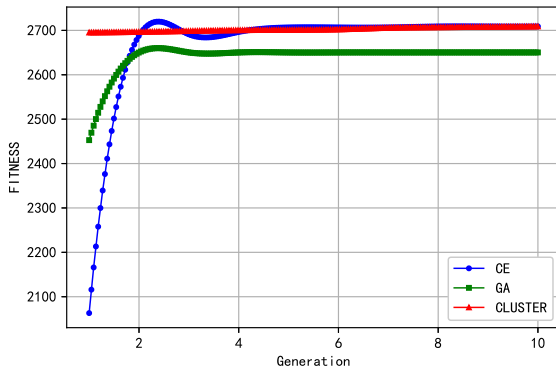
Extensive experiments, including rigorous testing on benchmark functions like the CEC functions, demonstrated proposal's effectiveness. It showcased faster convergence and superior global and local search capabilities compared to traditional methods for multi-modal optimization, highlighting the framework's adaptability and robustness. Furthermore, our research will extend beyond the domain of single-objective multi-modal optimization, venturing into the intricate realm of multi-objective multi-modal optimization tasks.



Vincent 2D



Shubert 2D



Vincent 3D

Fig. 4: Fitness value. Above three figures show the max fitness results of the three methods in the three functions.

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