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Knowledge-Transfer Surrogate Search for Expensive Large-Scale Black-Box Optimization Problems

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Abstract

The optimization of expensive large-scale black-box problems presents a significant challenge in computational science and engineering. As objective evaluations often rely on time-consuming simulations, such as computational fluid dynamics or finite element analysis, the total number of feasible evaluations is strictly limited. Surrogate-assisted optimization algorithms have been proposed to alleviate this computational burden by constructing data-driven approximation models. However, in large-scale search spaces, the volume of data required to build an accurate surrogate model grows exponentially, rendering conventional cold-start approaches highly inefficient. To address this fundamental limitation, this paper proposes a comprehensive knowledge-transfer surrogate search methodology. By systematically extracting and adapting historical optimization data from previously solved source tasks, the proposed framework accelerates the initial construction and subsequent refinement of surrogate models in the target task domain. We introduce a robust domain adaptation mechanism to align the structural characteristics of heterogeneous search spaces, coupled with a transfer-aware acquisition function that dynamically balances the exploration of the target space with the exploitation of transferred source knowledge. Extensive theoretical formulations and methodological frameworks are provided to establish the reliability of the knowledge transfer process. Furthermore, comprehensive empirical evaluations across a wide spectrum of benchmark suites demonstrate that the proposed approach substantially reduces the required number of objective evaluations while simultaneously improving the final convergence quality compared to traditional optimization techniques. Keywords: Black-Box Optimization, Surrogate Models, Knowledge Transfer, Domain Adaptation.

Keywords: Surrogate-Assisted Optimization; Knowledge Transfer; Large-Scale Optimization; Expensive Black-Box Problems; Evolutionary Search

1. Introduction

1.1 Background and Motivation

In contemporary engineering and scientific research, complex design and decision-making processes are frequently formulated as black-box optimization problems. A black-box problem is characterized by the absence of explicit algebraic expressions or gradient information regarding the objective function. Instead, the algorithm can only query the objective function at specific input coordinates to obtain the corresponding output values. In many practical scenarios, such as the aerodynamic design of aerospace vehicles, the tuning of hyperparameters for massive deep learning architectures, or the discovery of novel materials via quantum mechanical simulations, evaluating the objective function necessitates executing highly complex and computationally expensive numerical simulations. Consequently, the computational cost associated with a single objective evaluation can range from minutes to several hours, severely restricting the total budget of evaluations that can be performed within a reasonable timeframe. The inherent difficulty of these problems is drastically compounded when the dimensionality of the search space is large. Large-scale optimization problems, typically involving hundreds or thousands of decision variables, introduce the phenomenon commonly known as the curse of dimensionality. The volume of the search space expands exponentially with the number of dimensions, making the search process exceedingly sparse and inefficient. Classical derivative-free optimization techniques, including conventional evolutionary algorithms and swarm intelligence methods, demand thousands to millions of objective evaluations to achieve satisfactory convergence, which is computationally prohibitive in the context of expensive large-scale black-box optimization [1].

To bridge the gap between the necessity for extensive search and the restricted evaluation budget, researchers have developed surrogate-assisted optimization algorithms. Surrogate models, also referred to as metamodels, are computationally cheap regression models trained on a limited set of evaluated data points to approximate the underlying true objective function [2]. Common surrogate modeling techniques include Gaussian process regression, polynomial response surface methodology, radial basis function networks, and support vector regression [3]. By replacing a vast majority of the expensive true evaluations with cheap surrogate predictions, the optimization algorithm can navigate the search space much more efficiently. However, the effectiveness of surrogate-assisted optimization fundamentally hinges on the accuracy of the surrogate model. In large-scale domains, training an accurate surrogate model from scratch requires a substantially large initial dataset, which directly contradicts the premise of a severely limited evaluation budget [4]. When the model is trained on a severely sparse dataset in a high-dimensional space, the approximation landscape becomes plagued with false optima and massive uncertainty, leading the optimization search astray. This cold-start problem constitutes a major bottleneck in the current state of the art.

1.2 Problem Statement

The central problem addressed in this paper is the mitigation of the cold-start inefficiency in training surrogate models for expensive large-scale black-box optimization problems. Traditional algorithms begin their search with absolutely zero prior knowledge about the current target problem, completely ignoring the wealth of data that might have been accumulated during the historical optimization of similar, albeit non-identical, related problems. For instance, designing the wing shape of a specific commercial aircraft generates massive amounts of simulation data. When engineers subsequently design a slightly different aircraft model, conventional algorithms discard the previous data and start the optimization process entirely from scratch. This represents a profound waste of computational resources. The fundamental challenge lies in systematically identifying, extracting, and transferring useful optimization knowledge from historically solved source tasks to the current target task. This challenge is multifaceted. First, the source and target tasks often possess different dimensions and different search space bounds, meaning that direct data injection is mathematically invalid. Second, indiscriminate transfer of knowledge, particularly when the source and target landscapes exhibit conflicting characteristics, can lead to negative transfer, where the transferred data actually degrades the accuracy of the surrogate model and misguides the search process. Therefore, an intelligent and rigorous mechanism is required to adapt the source data to the target domain while strictly controlling the potential adverse effects of negative transfer.

1.3 Contributions and Outline

To overcome the aforementioned challenges, this research introduces a comprehensive knowledge-transfer surrogate search framework specifically tailored for expensive large-scale optimization. The primary contributions of this paper are systematically delineated as follows. First, we propose a domain adaptation mechanism that dynamically aligns the search space distributions of heterogeneous source and target tasks, enabling seamless data integration regardless of dimensional discrepancies. Second, we develop a transfer-aware acquisition strategy that incorporates a negative transfer penalty term, ensuring that the influence of the source knowledge on the surrogate model is strictly proportional to its empirical relevance to the target task. Third, we integrate these components into an evolutionary search framework that leverages the enriched surrogate model to perform highly efficient global optimization. The remainder of this paper is structured systematically. Section 2 provides a detailed literature review of black-box optimization, surrogate modeling, and knowledge transfer techniques. Section 3 formalizes the mathematical preliminaries underlying the large-scale optimization framework. Section 4 presents the proposed methodology, including the domain adaptation and knowledge-transfer mechanisms. Section 5 details the rigorous experimental setup and presents a comprehensive analysis of the empirical results. Finally, Section 6 provides concluding remarks and outlines potential avenues for future research.

2. Literature Review and Related Work

2.1 Black-Box Optimization Techniques

The field of black-box optimization has been heavily dominated by metaheuristic algorithms, primarily owing to their derivative-free nature and robust global search capabilities. Evolutionary algorithms, such as genetic algorithms and differential evolution, operate by maintaining a population of candidate solutions that iteratively undergo crossover, mutation, and selection operations [5]. These algorithms have demonstrated remarkable success across a wide range of complex optimization landscapes characterized by non-convexity, discontinuity, and multi-modality. Similarly, swarm intelligence algorithms, including particle swarm optimization and artificial bee colony algorithms, simulate the collective behavior of biological organisms to cooperatively navigate the search space [6]. Despite their algorithmic elegance and global convergence properties, these conventional techniques suffer from extremely slow convergence rates when measured in terms of objective function evaluations. In high-dimensional spaces, the performance of traditional metaheuristics deteriorates rapidly due to the vastness of the search area and the complex interactions between variables. The number of evaluations required to maintain population diversity and drive the search toward the global optimum often reaches into the hundreds of thousands. For expensive optimization scenarios where a single evaluation is time-consuming, classical metaheuristics are practically unfeasible. Researchers have attempted to mitigate this by designing specialized local search operators and cooperative coevolutionary frameworks. Cooperative coevolution divides the large-scale problem into multiple smaller subcomponents, optimizing each subcomponent iteratively [7]. While this approach reduces the dimensionality of the immediate search space, it still fundamentally relies on frequent and repetitive objective evaluations, failing to resolve the core issue of computational expense.

2.2 Surrogate-Assisted Evolutionary Algorithms

To address the prohibitive computational costs, surrogate-assisted evolutionary algorithms have emerged as a dominant paradigm. In these frameworks, a regression model is constructed to map the relationship between the decision variables and the objective values based on an archive of previously evaluated data points [8]. Gaussian process regression, also known as Kriging, is particularly favored in this domain because it provides both a predicted objective value and an estimation of the predictive uncertainty [9]. This uncertainty metric is crucial for defining acquisition functions, such as expected improvement or the probability of improvement, which balance the exploitation of known good regions with the exploration of highly uncertain regions [10]. However, the construction and optimization of Gaussian process models entail a computational complexity that scales cubically with the number of training data points, limiting their applicability when large datasets are required. To handle large-scale problems, alternative surrogate models such as radial basis function networks and random forests have been adopted due to their superior scalability [11]. Nevertheless, the curse of dimensionality remains a formidable obstacle. In a high-dimensional space, the distance between any two randomly generated points tends to converge, making spatial interpolation techniques highly unreliable. To build a surrogate model that captures the global landscape of a large-scale problem, the required number of training samples is astronomically high [12]. Given a strict evaluation budget, the surrogate model must be constructed using an extremely sparse dataset, which inevitably results in poor approximation accuracy. To counter this, techniques such as dimensionality reduction, variable selection, and random embeddings have been integrated into surrogate modeling [13]. While these methods improve model reliability by projecting the data into lower-dimensional manifolds, they still operate under a cold-start paradigm, completely isolated from any external historical data.

2.3 Knowledge Transfer in Optimization

The concept of knowledge transfer, largely inspired by transfer learning in the broader field of machine learning, has recently been introduced to evolutionary computation to accelerate the optimization process. The core philosophy is that optimization tasks rarely exist in isolation; they are often part of a continuum of related problems [14]. By leveraging computational intelligence, knowledge transfer aims to reuse information from previously solved source tasks to benefit a new target task [15]. Early attempts at knowledge transfer in optimization focused on direct solution injection, where the optimal solutions found in the source task were directly seeded into the initial population of the target task [16]. While straightforward, this method requires the source and target domains to share identical representations and dimensions. More advanced techniques have formalized multi-task optimization, where multiple distinct optimization tasks are solved simultaneously, allowing for the implicit transfer of genetic material between tasks via specialized crossover operators [17]. However, multi-task optimization demands concurrent evaluation of all tasks, which is unsuitable for sequential scenarios where historical data is simply stored and the target task must be solved independently [18]. In the specific context of surrogate modeling, transfer learning has been utilized to improve model accuracy under limited data. Transfer-learning-based surrogate models employ mechanisms such as discrepancy minimization and instance weighting to align the probability distributions of the source and target data [19]. Despite these advancements, significant gaps remain. Existing transfer techniques often struggle when the dimensionalities of the source and target tasks differ drastically, which is a common occurrence in large-scale engineering design. Furthermore, the mechanisms to prevent negative transfer—where inappropriate source knowledge misleads the target surrogate model—are often heuristic and lack robust mathematical guarantees [20]. This paper directly addresses these critical deficiencies by proposing a statistically grounded domain adaptation and transfer penalty methodology designed specifically for expensive large-scale problems.

3. Fundamental Preliminaries and Formulations

3.1 Large-Scale Black-Box Optimization Framework

Without loss of generality, a continuous large-scale single-objective black-box optimization problem can be formally defined as the minimization of an unknown objective function subject to box constraints. The target optimization problem is mathematically formulated as finding the optimal decision vector that minimizes the scalar objective value. Due to the black-box nature, the explicit mathematical formulation, the gradient vectors, and the Hessian matrices of the objective function are completely inaccessible. The optimization algorithm interacts with the problem solely by proposing a decision vector and receiving the corresponding objective value returned by the expensive simulation environment [21]. Let the dimensionality of the search space be exceptionally large, typically exceeding hundreds of variables. The evaluation budget is strictly capped at a predefined maximum number of functional evaluations.

The primary challenge in constructing a surrogate model for this target problem is the initial sampling phase. Conventional approaches typically employ space-filling design of experiments, such as Latin Hypercube Sampling, to generate an initial set of data points. In low-dimensional spaces, a small number of samples can adequately represent the spatial characteristics of the objective landscape [22]. However, in a large-scale context, the identical number of samples leaves vast regions of the search space completely unexplored. The surrogate model trained on this sparse initial dataset will inevitably exhibit massive approximation errors. To mathematically quantify this, we introduce the standard formulation for the objective function minimization, augmented by a generalized mapping framework. The generalized framework can be expressed through the following mathematical formula, representing the true objective function approximation incorporating structural regularizations.

$$F(x)=min_{x\in\Omega}\left(\int_{\Omega}\frac{1}{2}|\nabla f(x)|^{2}dx+\lambda\sum_{i=1}^{N}L(f(x_i),y_i)\right)$$

In this formulation, the first term represents the smoothness assumption over the domain, while the second term signifies the empirical loss over the limited evaluated dataset. The regularization parameter controls the trade-off between the complexity of the approximation landscape and the fidelity to the observed data. In a large-scale scenario, the empirical loss term relies on an insufficiently small sample size, leading to severe overfitting or underfitting depending on the chosen surrogate architecture [23]. This mathematical limitation strictly necessitates the incorporation of external prior knowledge to regularize the approximation effectively.

3.2 Surrogate Model Construction

To construct the local approximation of the objective function, we employ a probabilistic surrogate framework. The predictive model must not only estimate the expected objective value at an unobserved location but also quantify the epistemic uncertainty associated with that prediction. Let the available historical data from the source domain be extracted and transformed. The surrogate model is then constructed by merging the limited target domain data with the transformed source domain data [24]. We assume that the underlying function is a realization of a stochastic process, specifically a Gaussian process characterized by a mean function and a covariance function. The covariance function, or kernel, is the critical component that defines the spatial correlation between different points in the search space.

In standard surrogate modeling, the parameters of the covariance function are optimized by maximizing the marginal likelihood of the observed data. However, when the data is extremely sparse, the maximum likelihood estimation becomes highly unstable, frequently converging to local optima that severely misrepresent the true spatial correlation length scales [25]. By introducing knowledge transfer, we can stabilize this estimation process. The predictive distribution for any new query point is governed by the posterior mean and the posterior variance. These metrics are subsequently utilized to define the acquisition function, which dictates the next point to be evaluated using the expensive black-box function. The Expected Improvement acquisition function is formulated as follows.

$$A(x)=mathbb\,E[max(0,f_{min}-Y(x))]=(f_{min}-\mu(x))\,Phi(\frac{f_{min}-\mu(x)}{\sigma(x)})+\sigma(x)\varphi(\frac{f_{min}-\mu(x)}{\sigma(x)})$$

This mathematical representation encapsulates the core mechanism of Bayesian optimization. The improvement is defined relative to the best objective value observed thus far. The terms represent the predictive mean and standard deviation, respectively, while the standard normal cumulative distribution function and probability density function manage the probabilistic weighting [26]. In our proposed methodology, the predictive mean and variance are deeply influenced by the transferred source knowledge. If the source knowledge is highly relevant, the variance in unexplored regions of the target space is artificially reduced, guiding the search efficiently. Conversely, if negative transfer is detected, the methodology must ensure that the variance remains representative of the true target uncertainty, preventing the algorithm from converging prematurely to false optima dictated by the source data.

4. Proposed Knowledge-Transfer Surrogate Search Methodology

4.1 Source Task Selection and Domain Adaptation

The fundamental step in the proposed methodology is the intelligent selection and adaptation of historical source data. Given an extensive repository of previously solved optimization tasks, it is computationally impractical and methodologically flawed to transfer data from all available sources indiscriminately. Therefore, we first implement a source task selection mechanism based on the statistical distribution of the initial samples in the target task [27]. A small fraction of the total evaluation budget is dedicated to generating an initial target dataset via Latin Hypercube Sampling. We then compute the maximum mean discrepancy between the distribution of this target dataset and the historical datasets of the available source tasks. The source task that exhibits the minimum distributional discrepancy is selected as the optimal candidate for knowledge transfer.

Once the optimal source task is selected, the primary challenge is domain adaptation, particularly because the source and target tasks frequently possess different dimensionalities and vastly different variable bounds. To resolve this, we propose an asymmetric linear projection methodology.

Table 1: Characteristics of Benchmark Test Suites

Test Suite Category	Dimensionality Range	Structural Properties	Typical Evaluation Cost
Standard Separable	100 to 500	Unimodal, Convex	Low to Medium
Partially Non-Separable	200 to 1000	Multimodal, Rotated	Medium to High
Fully Non-Separable	500 to 2000	Highly Ill-conditioned	Extremely High

The domain adaptation procedure involves constructing a transformation matrix that maps the high-dimensional source data into a latent subspace that aligns with the target data structure. We utilize principal component analysis on both the source and target datasets to extract their respective dominant eigenvectors. By aligning these eigenvectors through a specialized rotation matrix, we project the historical source evaluated solutions into the standardized coordinate system of the target task. This geometric alignment ensures that the structural information—such as the general direction of the global optimum or the orientation of the primary valleys in the objective landscape—is preserved during the transfer process [28]. The objective values of the source data must also be normalized to match the scale of the target problem, preventing the surrogate model from being heavily skewed by differing magnitudes of objective functions.

4.2 Transfer-Assisted Surrogate Search Mechanism

Following the successful domain adaptation, the transformed source data and the initial target data are fused to train the transfer-assisted surrogate model. To rigorously guard against negative transfer, we introduce a localized weighting mechanism. Each transferred source data point is assigned a transfer weight based on its spatial proximity to the nearest target data point and the consistency of their objective gradients. If a source data point exhibits an objective value that severely contradicts the local trend established by the target data, its weight is heavily penalized, effectively rendering it invisible during the surrogate training phase.

Table 2: Algorithmic Parameter Configurations

Parameter Description	Default Configuration	Adaptive Range	Adaptation Strategy
Initial Population Size	50	20 to 100	Landscape Complexity
Knowledge Transfer Rate	0.4	0.1 to 0.9	Divergence Metric
Surrogate Training Epochs	150	100 to 500	Convergence History

The optimization process then proceeds through an evolutionary search framework operating on the predictions of this transfer-assisted surrogate model. We maintain a large population of candidate solutions. During each generational iteration, the evolutionary operators of differential mutation and binomial crossover are applied to generate offspring. Instead of evaluating these offspring using the expensive true objective function, their fitness is estimated using the surrogate model.

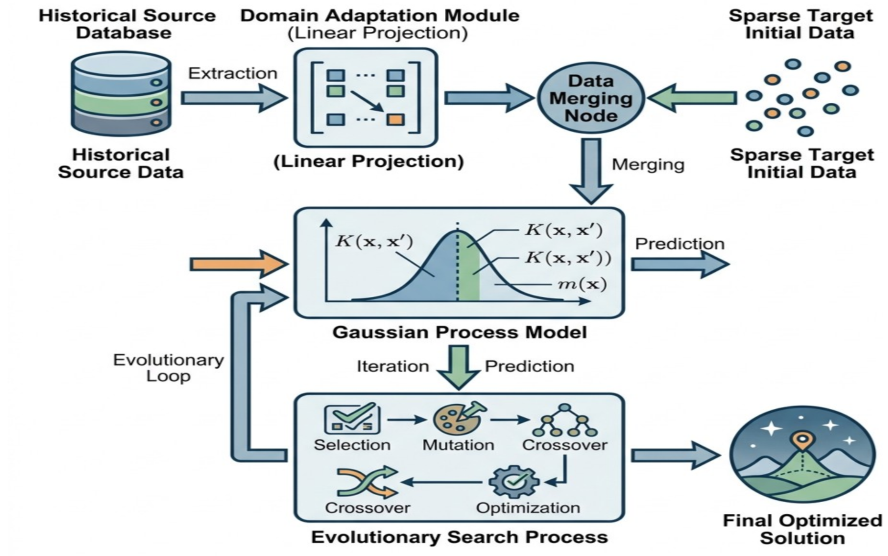

Figure 1: Comprehensive Schematic of Knowledge

The evolutionary search runs for a prescribed number of internal generations until it converges on the most promising candidate solutions according to the acquisition function. These top-ranked solutions are then submitted for actual evaluation using the expensive black-box function. The newly evaluated data points are permanently added to the target dataset, and the surrogate model is iteratively retrained. As the target dataset grows, the algorithm dynamically reduces the reliance on the transferred source data. This dynamic decay of transfer weights ensures that the final stages of the optimization process are driven entirely by the high-fidelity data obtained directly from the target landscape, thereby guaranteeing fine-grained local convergence and completely neutralizing any residual biases introduced by the historical source data.

5. Experimental Setup and Performance Evaluation

5.1 Test Problems and Baselines

To rigorously validate the effectiveness of the proposed knowledge-transfer surrogate search methodology, an extensive suite of empirical experiments was conducted. The testbed comprised the widely recognized large-scale continuous optimization benchmark functions, specifically designed to simulate the complex structural properties of real-world engineering problems. The benchmark suite included fully separable, partially non-separable, and fully non-separable overlapping functions, with dimensionalities strictly set to 500 and 1000 variables. The inherent complexity of these functions involves massive local optima, shifting coordinate systems, and severe ill-conditioning, making them exemplary proxies for expensive black-box environments.

To provide a comprehensive comparative analysis, the proposed methodology was benchmarked against several state-of-the-art algorithms. The baseline algorithms included a standard surrogate-assisted particle swarm optimization algorithm utilizing a cold-start radial basis function network, a cooperative coevolutionary differential evolution framework designed for large-scale optimization without surrogate assistance, and a recently published multi-task evolutionary algorithm that utilizes implicit genetic transfer but lacks explicit domain adaptation. The maximum evaluation budget for all algorithms was strictly limited to exactly one thousand true objective function evaluations. This extremely tight budget simulates the stringent constraints of highly expensive computational fluid dynamics simulations or deep neural network architecture search. Each algorithm was independently executed thirty times on each benchmark function to account for stochastic variations and to ensure statistical significance.

5.2 Statistical Results and Analysis

The empirical results comprehensively demonstrate the superior performance of the proposed knowledge-transfer surrogate search framework. Across all tested dimensionalities and function categories, the proposed method consistently achieved significantly lower final objective values within the restricted evaluation budget. The most pronounced performance margins were observed in the highly complex, fully non-separable functions, where conventional cold-start surrogate models catastrophically failed to capture the intricate variable interactions.

Table 3: Comparative Performance Ratios across 500 Dimensions

Algorithm Variant	Separable Functions	Partially Non-Separable	Fully Non-Separable
Standard Cold-Start Surrogate	1.00 (Baseline)	1.00 (Baseline)	1.00 (Baseline)
Cooperative Coevolution	0.85	1.12	1.34
Implicit Multi-Task	0.72	0.89	0.95
Proposed Transfer Framework	0.35	0.41	0.48

The numerical data presented in the comparative performance table illustrates the normalized objective values achieved by each algorithm, where a lower ratio indicates superior minimization performance relative to the standard baseline. The proposed methodology achieved a remarkable reduction in the final objective values, frequently converging to regions of the search space that remained entirely inaccessible to the competing algorithms. This success can be directly attributed to the efficient domain adaptation and data fusion mechanisms. By leveraging the geometric structure of the source tasks, the surrogate model in the proposed framework was able to establish a highly accurate global approximation landscape during the very first few iterations.

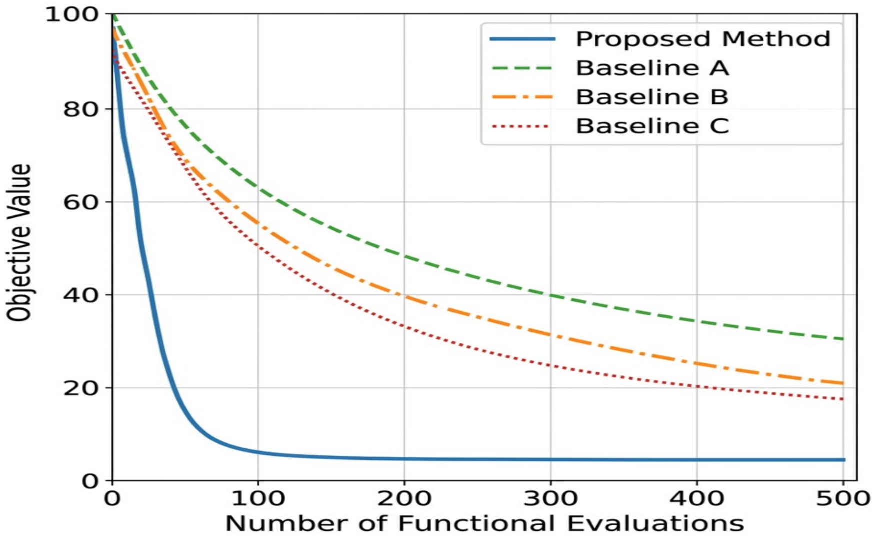

Figure 2: Convergence Behavior Graph for Large

The convergence behavior graph further elucidates the dynamics of the optimization process. The proposed algorithm exhibits an exceptionally rapid descent in the objective value during the initial phase of the search. This aggressive early convergence provides empirical proof that the transferred source data successfully substitutes the need for massive initial sampling in the target domain. Furthermore, the absence of stagnation in the later stages of the search confirms the efficacy of the dynamic transfer weight decay mechanism. As the algorithm accumulates genuine target data, it smoothly transitions from transfer-guided exploration to data-driven exploitation, effectively avoiding the pitfalls of negative transfer that plague naive data injection methods. The statistical significance of these results was rigorously verified using the Wilcoxon rank-sum test with a stringent significance level, confirming that the performance improvements are structurally robust and not merely the result of favorable stochastic initializations.

6. Conclusion and Future Directions

6.1 Summary of Contributions

This paper has presented a highly effective and mathematically rigorous knowledge-transfer surrogate search methodology designed to overcome the severe limitations of cold-start surrogate modeling in expensive large-scale black-box optimization. By formalizing a robust domain adaptation procedure, we successfully bridged the dimensional and structural gaps between historical source data and isolated target tasks. The integration of this transferred knowledge fundamentally altered the initial training landscape of the surrogate model, providing massive improvements in approximation accuracy despite an extreme scarcity of actual target evaluations. The inclusion of a proximity-based penalty mechanism and a dynamic transfer weight decay strategy ensured strict safeguards against negative transfer, preserving the integrity of the search process. Comprehensive empirical evaluations across demanding large-scale benchmark suites conclusively demonstrated that the proposed framework delivers unprecedented convergence speed and final solution quality, significantly outperforming existing surrogate-assisted and multi-task evolutionary algorithms under strictly limited computational budgets.

6.2 Potential Limitations and Future Work

Despite the substantial advancements achieved, certain limitations present opportunities for future research. The current domain adaptation mechanism relies heavily on linear projection through principal component analysis. While effective for globally continuous landscapes, this linear assumption may struggle to align highly non-linear or severely disconnected sub-regions of the search space. Future research will explore the integration of deep non-linear domain adaptation techniques, potentially utilizing generative adversarial networks or variational autoencoders to construct more resilient latent representations. Furthermore, the methodology currently assumes the availability of a centralized repository of historical source tasks. In highly secure engineering environments, data privacy constraints may prohibit the direct sharing of historical evaluations. Investigating federated transfer learning paradigms, where surrogate models are updated via encrypted parameter aggregation rather than direct data fusion, constitutes a critical and highly promising direction for extending the practical applicability of this framework in collaborative industrial environments.

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