Efficient Black-box Optimization via Deep Surrogate Models and Transfer Learning

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Abstract. Black-box optimization (BBO) deals with optimizing functions that are expensive to evaluate, lack closed-form expressions, or are defined implicitly through complex simulators. Evolutionary algorithms, particularly the Covariance Matrix Adaptation Evolution Strategy (CMA-ES), have become a standard tool in this field due to their robustness and gradient-free nature. Despite their flexibility, evolutionary methods are often sample-inefficient. To address this, surrogate-assisted optimization introduces predictive models that approximate the objective function to guide the search. Recent advances in deep learning, particularly transformers and transfer learning, offer new avenues to improve surrogate modeling. This starting research explores how modern deep architectures, enhanced by prior knowledge from related tasks, can improve efficiency and generalization in black-box optimization when combined with state-of-the-art evolutionary algorithms.

1 Motivation and Research Questions

Black-box optimization plays a central role in many scientific and engineering applications, ranging from hyperparameter tuning [7] and reinforcement learning [23] to industrial design [3] and biological systems [24]. Unlike standard optimization methods that rely on gradient information or convexity assumptions, BBO methods are applicable in situations with non-smooth, multimodal, or noisy objectives.

Among BBO techniques, CMA-ES [1, 8] stands out for its self-adaptive search distribution and strong empirical performance across benchmark functions and real-world problems [10]. However, such methods often require a large number of objective function evaluations.

That is why surrogate models are introduced to approximate the objective function and guide the optimizer toward promising areas of the search space. Historically, the first surrogate models used in evolutionary optimization were low-order polynomials [9, 14, 27], which offered a simple yet effective way to capture local structure. These were later followed by more flexible models, including Gaussian Processes (GPs) [22] and random forests [13], which are widely used in Bayesian optimization due to their ability to model uncertainty.

Recent research suggests that deep neural networks (DNNs), including autoencoders [26], CNNs [16], and especially transformers [19, 25], could outperform classical surrogate models in high-dimensional and structured domains. Furthermore, transfer learning [20, 30] has shown promise in leveraging prior knowledge to accelerate convergence in related optimization tasks.

While transfer learning has become a well-established concept in many areas of machine learning, its application to surrogate modeling for black-box optimization remains relatively rare. To date, only a few recent works have directly addressed this intersection. For instance, Hu et al. [12] proposed a method for transferring the parameters of Gaussian Process (GP) surrogate models when the training data distributions of a source and target task are sufficiently similar, as measured by the Wasserstein distance. Their framework dynamically decides whether to apply transfer or to re-estimate the surrogate via maximum likelihood, and they suggest its use in surrogate-assisted evolutionary optimization, where earlier generations can act as knowledge sources.

In contrast, Chen et al. [5] consider a more elaborate transfer mechanism in GP modeling, one that incorporates the distance of the predicted optimum to the target data and the prediction error of the source model. However, their method requires user selection of the source and is not specifically aimed at evolutionary optimization.

Since GPs are a central model in both surrogate-assisted and Bayesian optimization, these studies represent an emerging bridge between the two areas. Indeed, there has been growing interest in knowledge transfer within Bayesian optimization itself, as seen in works such as [17, 18, 28].

Building on this state of the art, my research investigates the following questions:

- How can modern deep architectures, such as transformers and ConvNets, enhance the expressiveness and generalization of surrogate models in BBO?
- In what ways can transfer learning be leveraged to reuse knowledge across optimization tasks and reduce sample complexity?
- How can these models be integrated with adaptive evolutionary strategies such as CMA-ES in a principled, data-efficient manner?

2 Research Approach and Methodology

The proposed research explores the intersection of evolutionary optimization, deep learning, and transfer learning. The core idea is to augment evolutionary search—especially CMA-ES—with deep surrogate models that are either pretrained on similar tasks or dynamically adapted using transfer learning techniques. This allows the optimizer to benefit from prior experience, improving convergence in domains where each function evaluation is costly.

Inspired by previous work on Gaussian surrogates [2] and landscape-aware methods [21], I investigate how to embed prior structure using neural representations. Drawing from recent developments such as TransOpt [4] and deep active learning [25], I explore architectures that incorporate attention mechanisms, uncertainty estimation, and meta-learning.

Furthermore, I examine the use of pretrained networks on structured domains (e.g., COCO-inspired parameter spaces) to initialize surrogate models, a direction influenced by neural architecture search [6] and meta-optimization [29]. Active sampling strategies and uncertainty-aware loss functions are explored to ensure that each additional evaluation adds maximal information.

The experimental evaluation will be conducted across a range of BBO tasks, including synthetic functions from the BBOB benchmark suite [11], constrained optimization [15], and discrete domains. Evaluation metrics include data efficiency, final performance, and model calibration.

3 Planned Contributions and Future Work

The main objectives of my doctoral research are:

- Systematically evaluate the role of deep surrogate models in black-box optimization, comparing architectures such as GPs, MLPs, CNNs, and transformers.
- Develop a framework for transfer learning in surrogate-assisted BBO, enabling cross-task generalization with minimal adaptation.
- Integrate this framework with CMA-ES and similar evolutionary strategies, leveraging active sampling, representation learning, and model uncertainty.
- Validate the framework across diverse benchmarks, including structured image-like tasks and real-world optimization domains.

Ultimately, the goal is to establish a general-purpose optimization approach that combines the flexibility of evolution strategies with the power of deep learning and transfer-based inductive bias.

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