West University of Timişoara
Doctoral School of Exact Sciences and Natural Sciences
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Analysis of population dynamics for difference-based evolutionary algorithms

Analiza dinamicii populaţiei pentru algoritmii evolutivi bazaţi pe diferenţe

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1 Introduction

Evolutionary algorithms (EAs), inspired by natural evolutionary processes, are powerful optimization techniques. Among them, Differential Evolution (DE) has proven effective for continuous optimization problems across various domains (Qing 2009; Chen et al. 2017) since its introduction by Storn and Price (Storn and Price 1997). Despite extensive research on DE's strategies and properties (Peng et al. 2017; Tian and Gao 2018; Mousavirad and Rahnamayan 2020; Tanabe and Fukunaga 2013; Tanabe and Fukunaga 2014; Stanovov et al. 2018; Dasgupta et al. 2009; Rudolph 1999), a critical aspect, Bound Constraint Handling Methods (BCHMs), has been largely overlooked. BCHMs are essential for managing solutions that violate search space boundaries, a common occurrence in DE due to the randomness in mutation and crossover (Arabas et al. 2010; Kononova et al. 2022). How these violations are handled significantly impacts search dynamics, diversity, and convergence. This thesis addresses this gap by systematically investigating the role and impact of BCHMs in DE, treating them not just as implementation details but as active algorithmic components.

The main objectives of the thesis are:

- Develop a theoretical framework analyzing how BCHMs influence DE properties such as search direction, bound violation probability, and population variance.
- To design and evaluate adaptive BCHM strategies that dynamically select appropriate methods to enhance DE performance.
- Establish a geometric monitoring framework for characterizing DE population dynamics and BCHM effects, using axis-aligned and PCA-based measures.
- To assess BCHM impact in a real-world context: neural network hyperparameter optimization.

This research aims to elevate the status of BCHMs to recognized components requiring careful design and adaptation. The research is guided by four main groups of questions:

- RQ_A: How do BCHMs influence DE's theoretical properties and empirical behavior (search direction, violation probability, population distribution)? The question is addressed in Chapter 3 where it is further divided in four more specific questions: **(RQ_A1):** How does the choice of BCHM theoretically influence the probability of generating infeasible solutions? **(RQ_A2):** To what extent do different BCHMs preserve or alter the search direction intended by the DE mutation operator?; **(RQ_A3):** How accurately do the theoretical models for bound violation probability predict the empirically observed probabilities?; **(RQ_A4):** How does the actual population distribution deviate from the original uniformly initialized population?

- RQ_B: Can adaptive BCHM strategies improve DE performance, and how should they be designed (selection pool composition, selection mechanisms)? Chapter 4 addresses the main question by decomposing it into three more focused research inquiries: **(RQ_B1):** Which BCHMs should be included in the adaptive pool to ensure complementary strengths while avoiding redundancy? **(RQ_B2):** How can the selection process be designed to effectively choose appropriate methods during different optimization phases? **(RQ_B3):** What measures should guide the adaptation process to ensure both short-term effectiveness and long-term optimization success?

- RQ_C: How can DE population spatial and geometric dynamics be characterized, and how do BCHMs affect them? Chapter 5 provides a detailed examination of this question by addressing four more specific aspects of the problem: **(RQ_C1):** How can we effectively characterize the spatial distribution of DE populations during the optimization process? **(RQ_C2):** How do different BCHMs influence the geometric characteristics of the population?; **(RQ_C3):** hat correlations exist between population-related measures and algorithm performance?; **(RQ_C4):** What insights on the population dynamics can be extracted by the proposed analysis, and how can they be used to guide the selection of appropriate BCHMs for specific optimization scenarios.

- RQ_D: What is the impact of BCHMs on DE's effectiveness in a real-world problem, e.g. hyperparameter optimization? Chapter 6 tackles this question by structuring the investigation around five more granular research questions: **(RQ_D1):** How do different BCHMs influence the final solution quality (measured by validation loss, accuracy, regret) achieved by DEHB during the optimization of neural network hyperparameters on real-world classification datasets? **(RQ_D2):** What is the relationship between the employed correction strategy and the frequency of boundary violations necessitating repair, as quantified by the Probability of Repair (PORS)? **(RQ_D3):** Is there an observable trade-off between performance effectiveness (solution quality) and repair frequency (PORS) associated with different correction strategies within the DEHB framework? **(RQ_D4):** Do correction strategies incorporating population-derived information demonstrate discernible performance advantages over simpler, non-adaptive strategies for hyper-parameter optimization utilizing DEHB? **(RQ_D5):** How consistent is the relative performance ranking of the evaluated correction strategies across the diverse set of classification datasets under investigation?

2 Main Results

This section summarizes the main results included in this thesis.

2.1 Particularities of Bound Constraints and Correction Methods (Chapter 3)

Chapter 3 is based on the published papers (Mitran 2021; Mitran 2023; Kononova et al. 2024) and provides a systematic analysis of BCHMs, moving beyond treating them as mere implementation details. It established that the choice of BCHM significantly impacts key DE behaviors. The results can be grouped in two categories:

- **Theoretical Influence (RQ_A1, RQ_A2):** Mathematical models were developed to analyze how different BCHMs affect the probability of subsequent bound violations (e.g., for Saturation and Exponentially Confined strategies), the preservation of the intended search direction (showing that the Saturation and Mirroring strategies can preserve the search direction better than Toroidal under certain conditions), and population variance (suggesting different impacts on diversity).
- **Empirical Validation (RQ_A3, RQ_A4):** Experiments largely validated the theoretical findings, especially regarding search direction preservation (measured by cosine similarity, confirming Saturation's high preservation and Toroidal's disruption). The accuracy of the bound violation probability model for Exponentially Confined strategies was confirmed under specific conditions (e.g. the reference position is R=0.5, and no selection pressure) but showed limitations otherwise. Population distribution analysis using the Kullback-Leibler divergence, quantified the deviations from uniformity, showing that while the uniformity assumption holds in the early evolution stage, it becomes less accurate later, especially with disruptive BCHMs.

Overall, this chapter demonstrated that BCHMs are active components with distinct theoretical properties and empirically verifiable impacts on DE dynamics.

2.2 Adaptive Strategies for Bound Constraints (Chapter 4)

Chapter 4, based on papers (Mitran et al. 2023; Mitran 2024b), addressed the need for adaptive BCHM strategies, given that no single method is universally optimal.

- **Selection Pool Design (RQ_B1):** A method for constructing diverse pools was developed by characterizing BCHMs based on multiple behavioral aspects (bound violation patterns, diversity impact, convergence behavior) and using hierarchical clustering to identify complementary methods. This ensures that the pool covers different search dynamics.

- **Selection Strategies (RQ_B2):** Building upon existing work, adaptive selection mechanisms were designed. A linear combination approach with an inertia coefficient and a more robust method based on modeling success probabilities with the Beta distribution were proposed and evaluated. The Beta distribution approach showed better performance on some functions from the BBOB testsuite. Phase-dependent effectiveness patterns, as depicted from figures 1, 2 suggested potential benefits for explicitly phase-aware adaptation.

- **Guiding Adaptation (RQ_B3):** While success rates offer short-term guidance, the analysis suggested that long-term success might require incorporating measures like population diversity and convergence progress, potentially informed by phase detection using error-variance divergence analysis illustrated in figure 3.

This chapter established the rationale for adaptive BCHMs and provided methodologies for designing effective pools and robust, potentially phase-aware, selection mechanisms.

2.3 Monitoring Population Dynamics (Chapter 5)

Chapter 5, based on paper (Mitran 2024a) introduced a novel framework for monitoring DE population dynamics, focusing on geometric characteristics and the influence of BCHMs.

- **Geometric Monitoring Framework (RQ_C1):** A multi-faceted framework was developed, combining traditional statistical measures with axis-aligned Population Bounding Box (PBB) measures (extension, shape, eccentricity) and novel PCA-based geometric measures (PCA-shape, PCA-eccentricity, PCA-density, PCA-variance structure) to provide a comprehensive view of the population's spatial distribution, illustrated in figures 4 and 5.

- **Value of PCA Measures:** PCA-based measures proved essential for revealing the population's intrinsic structure (shape, orientation, density) independent of axis alignment, capturing details missed by PBB or statistical measures alone. They helped distinguish intrinsic elongation from axis-aligned stretching and true coalescence from mere contraction.

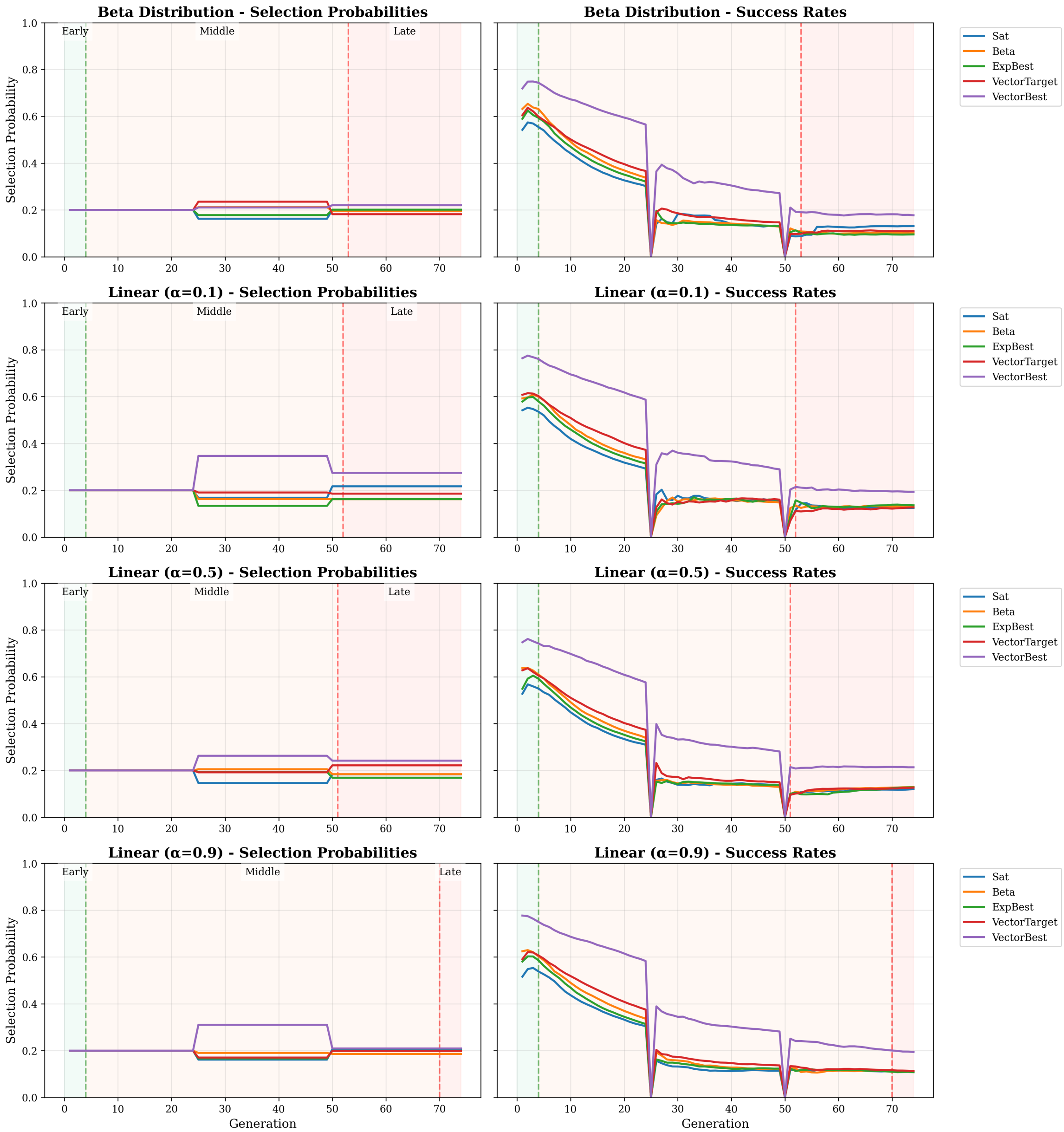

Figure 1: Selection probabilities and success rates on function f_4 of BBOB. The vertical lines split the optimization process into early, middle, and late phases.

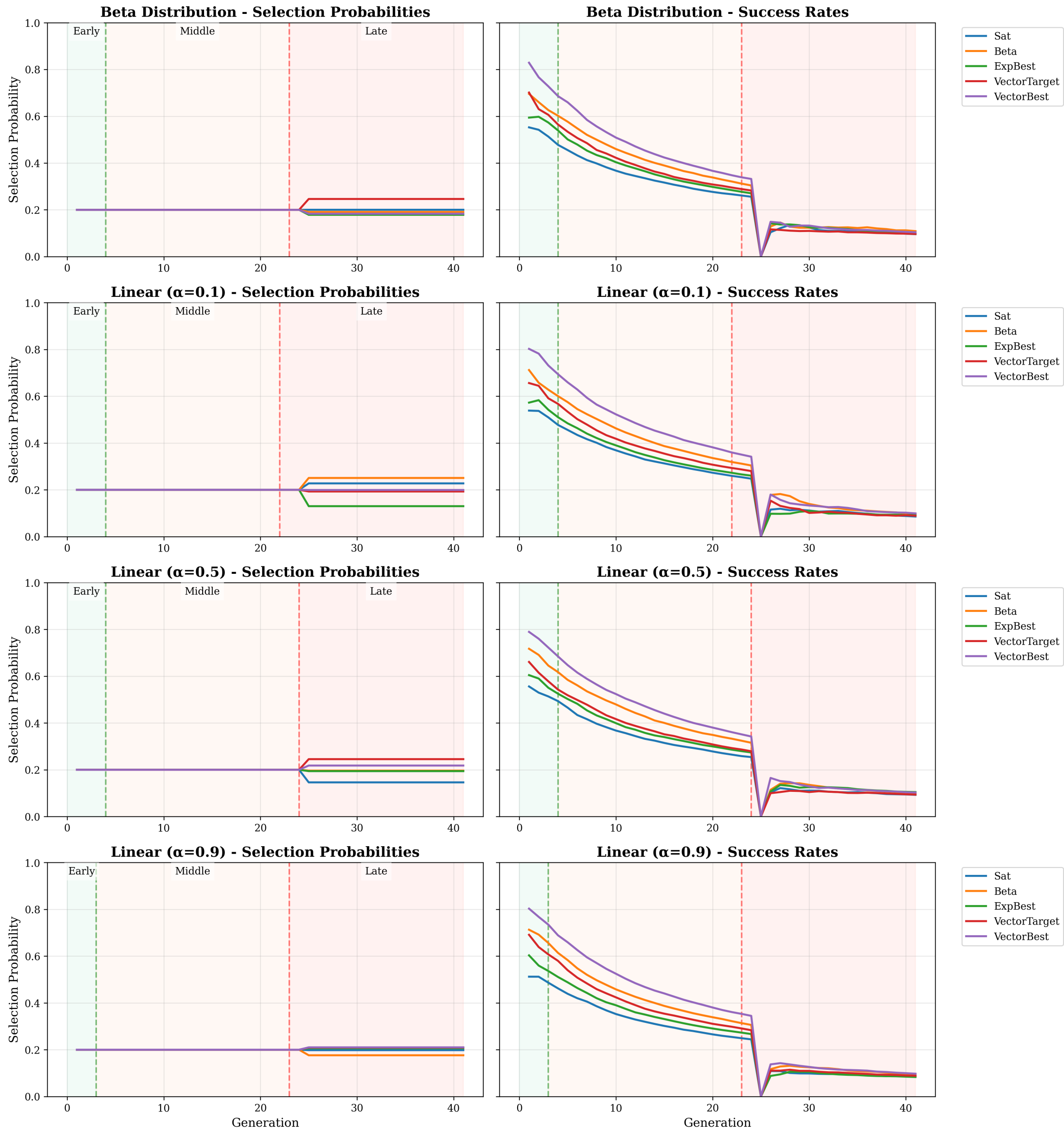

Figure 2: Selection probabilities and success rates on $f_{19}$of BBOB. The vertical lines split the optimization process into early, middle, and late phases.

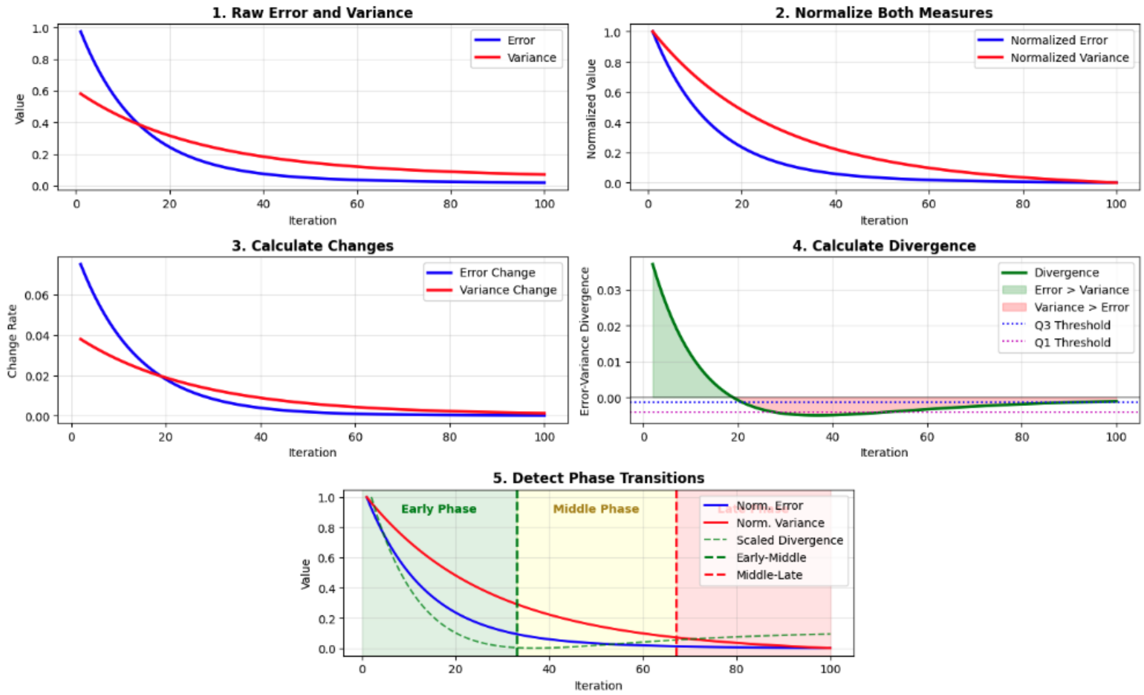

Figure 3: Overview of the error-variance-based phase detection methodology. Panel 1: Raw error and variance. Panel 2: Measures min-max scaled to $[0, 1]$. Panel 3: Generation-wise changes in scaled measures. Panel 4: Divergence measure d_t and its statistical thresholds (Q_1, Q_3). Panel 5: Identified Early, Middle, and Late evolutionary phases. Phase transitions are determined by the divergence curve crossing these thresholds.

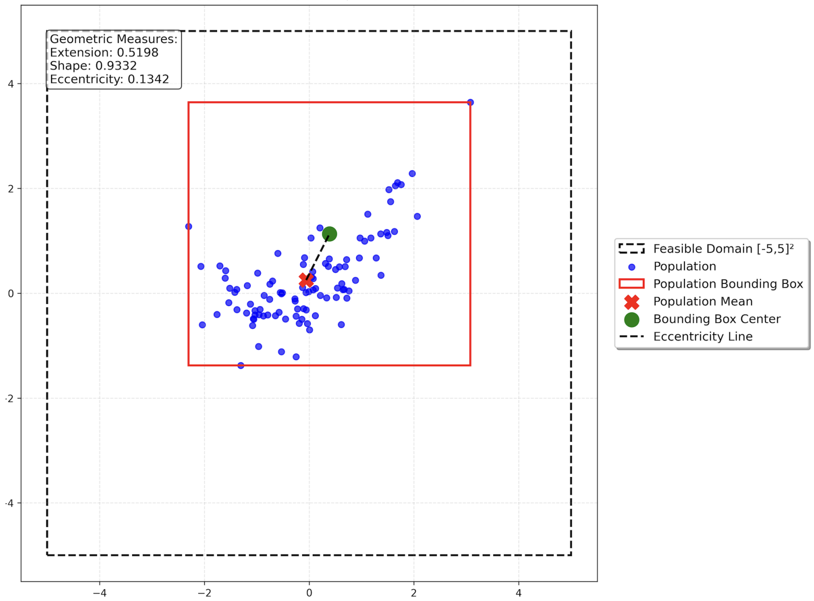

Figure 4: Visualization of PBB (red box), for a population (blue points) distributed inside the feasible domain $[-5,5]^2$, with population mean (red X), PBB center (green circle) and eccentricity line (dashed black). The eccentricity (0.13) reflects the asymmetric distribution within the PBB, and the high shape value (0.933) indicates that the PBB is almost a perfect square.

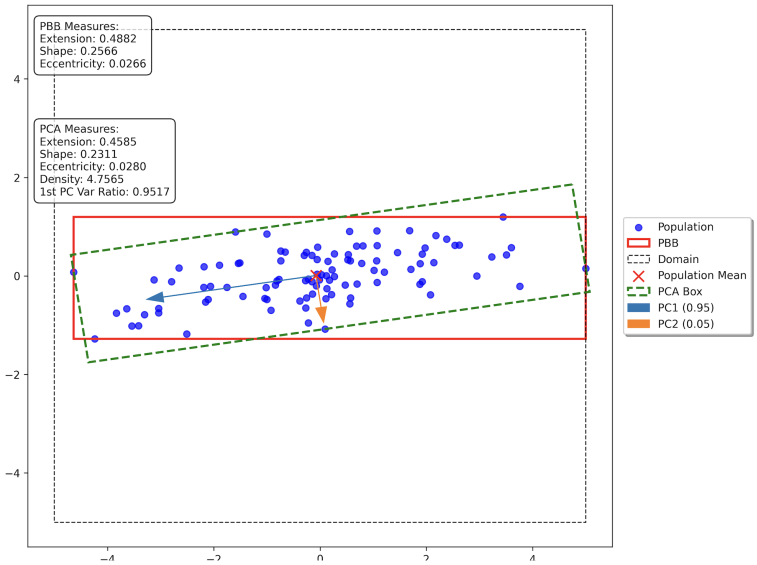

Figure 5: Visualization of an elongated population distribution with both axis-aligned and variance-aligned geometric characterizations. The PBB (red solid rectangle) provides axis-aligned boundary representation, while the PCA Box (green dashed polygon) aligns with the principal directions of variation. Principal components are displayed as arrows originating from the population mean (red X), with PC1 (blue) explaining 95.1% of total variance and PC2 (orange) explaining the remaining 4.83%. The comparison illustrates how PCA-based geometric measures better capture the intrinsic shape of anisotropic distributions.

- **BCHM Influence on Geometry (RQ_C2):** Experiments showed that the BCHMs actively shape population geometry. Vector-based methods induced distinct dynamics compared to component-wise methods. Discrepancies between PBB and PCA measures highlighted BCHM-specific impacts on orientation and internal structure.

- **Correlations and Insights (RQ_C3, RQ_C4):** Strong correlations were confirmed between error and fundamental convergence indicators (contraction, densification, diversity loss). Relationships involving shape, symmetry, internal distribution (KL divergence), and control parameters were more complex and context-dependent. PCA measures provided deeper insights, for example, showing variance concentration in fewer effective dimensions during convergence. The framework offers diagnostic potential for practitioners.

This chapter established the utility of geometric monitoring, particularly with PCA, for a nuanced understanding of DE dynamics and BCHM effects.

2.4 Impact of Correction Strategies on Constrained Optimization Real-World Problems (Chapter 6)

Chapter 6 investigated the impact of BCHMs in a practical application: hyperparameter optimization (HPO) for neural networks using the DEHB (Awad et al. 2021) algorithm.

- **HPO Performance (RQ_D1):** BCHM choice significantly affected DEHB performance. Strategies using the best-so-far solution (`expCB`, `vectB`, `midB`) and the `mir` strategy generally outperformed simpler methods like `sat` and `midT` in terms of validation loss and accuracy. `sat` consistently performed poorly.

- **Repair Frequency (PORS) (RQ_D2, RQ_D3):** There was an inverse relationship between performance and the probability of repair (PORS). The method with the lowest PORS (`midT`) performed poorly, while several top performers had higher PORS values. This suggests that minimizing repairs is not the primary goal; effective exploration might involve transient violations handled well by the BCHM.

- **Value of Population Information (RQ_D4):** Incorporating best-so-far information (e.g., `expCB`, `vectB`, `midB`) consistently led to better results than those using target vector information (`expCT`, `vectT`, `midT`) or non-adaptive strategies, highlighting the benefit of guiding correction towards promising regions.

- **Consistency Across Datasets (RQ_D5):** While general trends held (e.g., 'Best'-based methods are robust, while `sat` behaves rather poorly), the exact ranking of top methods varied across datasets, indicating some problem dependency. However, `expCB` and `vectB` consistently ranked well, suggesting they are reasonable default choices.

This case study confirmed the practical significance of BCHM selection in HPO and validated the effectiveness of information-guided correction strategies.

3 Conclusions and Future Work

This thesis demonstrated that Bound Constraint Handling Methods (BCHMs) are critical components of Differential Evolution (DE), significantly influencing theoretical properties, empirical behavior, population geometry, and real-world performance. Key contributions include a systematic analysis of BCHM properties, a novel geometric monitoring framework using PBB and PCA measures, the design and evaluation of adaptive BCHM strategies, and validation of BCHM impact in Hyperparameter Optimization.

The research challenges the practice of arbitrary BCHM selection and provides tools (geometric monitoring, adaptive frameworks) for a more informed design. The PCA-based geometric measures offer deeper insights into population structure and dynamics than previously available. The HPO study highlighted the practical consequences and the benefit of information-guided corrections, while also cautioning against simply minimizing boundary violations.

Limitations include reliance on simplifying assumptions in the theoretical models and the usage of only some specific algorithms/benchmarks in the empirical studies.

Future work could involve:

- Refine theoretical models for non-uniform distributions and when the selection pressure is taken into account.
- Broader empirical studies across more DE variants, problems (constrained, multi-objective, large-scale), and other metaheuristic algorithms.
- Developing advanced adaptive mechanisms (self-adaptation, phase-awareness, geometry-informed feedback).
- Using geometric measures for online algorithm control (adapting diversity, mutation, population size).
- Investigating BCHMs in other real-world applications.

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