

# The Evolving Landscape of Optimization: Current Trends and Future Directions

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## 1. Introduction

Optimization methodologies constitute the cornerstone of modern scientific discovery, engineering innovation, and decision-making processes across diverse domains. As computational capabilities expand and problem complexity intensifies, the field of optimization continues to evolve at an unprecedented pace. This review synthesizes recent advancements and paradigm shifts in optimization research, examining how novel algorithms, interdisciplinary approaches, and emerging technologies are reshaping solution strategies for increasingly complex challenges. The accelerated development is evidenced by the fact that over 300 new metaheuristic methodologies have emerged within the last decade, reflecting the field's vigorous expansion (Selvarajan, 2024). Contemporary optimization transcends traditional boundaries, integrating insights from artificial intelligence, quantum computing, materials science, and statistical theory to address problems ranging from sustainable energy systems to precision medicine. This review systematically examines current trends, theoretical breakthroughs, and practical applications that define the state of optimization science in 2025, providing researchers with a comprehensive reference for navigating this rapidly advancing domain.

## 2. Nature-Inspired and metaheuristic Optimization

The proliferation of bio-inspired optimization algorithms continues to dominate the landscape of heuristic approaches, drawing inspiration from increasingly diverse biological systems and natural phenomena.

Recent years have witnessed a paradigm shift toward algorithms modeled on specialized behaviors and niche evolutionary adaptations. The 2024 introduction of Painting Training Based Optimization (PTBO) exemplifies this trend, translating human creative processes into an optimization framework that demonstrates competitive performance on the CEC 2011 test suite, outperforming established algorithms like Grey Wolf Optimizer (GWO) and Harris Hawks Optimization (HHO) across all 22 constrained optimization problems (Amin & Dehghani, 2025).

PTBO's position update for artist  $i$  follows:

$$\begin{aligned} X_i^{(t+1)} &= X_i^{(t)} + \alpha \underbrace{(X_{best} - X_i^{(t)})}_{\text{master imitation}} \\ &+ \beta u(-1,1) \odot \underbrace{(X_{rand}^{(t)} - X_i^{(t)})}_{\text{creative exploration}} \end{aligned}$$

Where  $\alpha = \alpha_0 e^{-t/T}$ ,  $\beta \sim \text{Cauchy}(0,1)$  and  $\odot$  denotes element-wise multiplication.

This human-inspired approach represents a significant departure from traditional evolutionary and swarm-based methods, highlighting the field's expanding conceptual horizons.

Metaheuristic strategies have evolved toward specialized hybridization to overcome limitations of standalone approaches. The Fossa Optimization Algorithm combines predatory search patterns with social hierarchy dynamics to enhance convergence properties,

$$\begin{aligned} V_i^{(t)} &= \omega V_i^{(t-1)} + c_1 r_1 (X_\alpha - X_i^{(t)}) \\ &+ c_2 r_2 (X_\beta - X_i^{(t)}) + c_3 r_3 (X_\delta - X_i^{(t)}) \end{aligned}$$

$$X_i^{(t+1)} = X_i^{(t)} + V_i^{(t)} + \sigma N(0,1) \cdot e^{-\|X_\alpha - X_i^{(t)}\|}$$

Where  $X_\alpha, X_\beta, X_\delta$  represents dominant solutions.

while the Spider-Tailed Horned Viper Optimization integrates specialized predation mechanisms with evolutionary operators (Amin & Dehghani, 2025). These hybridizations reflect a growing recognition that complex optimization landscapes require balanced exploration-exploitation strategies. As noted by researchers, "The observed trend indicates an increasing acknowledgement of the effectiveness of bio-inspired methodologies in tackling intricate engineering problems, providing solutions that exhibit rapid convergence rates and unmatched fitness scores" (Selvarajan, 2024).

**Table1: Classification of Contemporary Metaheuristic Approaches**

Category	Representative Algorithms	Key Innovations	Application Domains
Swarm Intelligence	Draco Lizard Optimizer, Wombat Optimization	Niche foraging behaviors, collective tunneling	Supply chain optimization, energy systems
Evolutionary Methods	Genetic Algorithms, Differential Evolution	Adaptive mutation operators, parallel island models	Aerospace design, computational biology
Human-Inspired	PTBO, Sculptor Optimization	Creative process modeling, apprenticeship learning	Engineering design, creative industries
Physics-Based	Simulated Annealing, Gravitational Search	Quantum-inspired tunneling, relativistic effects	Molecular dynamics, materials science

Theoretical understanding of population dynamics and convergence behavior in metaheuristics has deepened substantially. Recent analyses employ Markov chain modeling and computational statistics to quantify exploration-exploitation trade-offs, providing mathematical justification for parameter adaptation strategies (Selvarajan, 2024).

For a population  $P = \{X_1, X_2, \dots, X_N\}$  at iteration  $t$ , the state transition is governed by:

$$P^{(t+1)} = G(P^{(t)}) \quad \mathcal{M}(X_i^{(t)})$$

Where  $G$  represents genetic operators (crossover/mutation), and  $\mathcal{M}$  denotes migration patterns. The *exploration-exploitation trade-off* is quantified by:

$$\Phi(t) = \frac{1}{N} \sum_{i=1}^N \|X_i^{(t)} - \bar{X}^{(t)}\|_2 \cdot e^{-\lambda t}$$

With

$\lambda$  controlling the decay rate of exploration diversity.

This theoretical grounding addresses long-standing criticisms regarding the empirical nature of many metaheuristics. However, the No Free Lunch theorem continues to underscore the importance of domain-specific algorithm selection, as no single optimizer demonstrates universal superiority across all problem classes (Amin & Dehghani, 2025).

### 3. Quality-Diversity and multimodal Optimization

Quality-Diversity (QD) optimization represents a paradigm shift in evolutionary computation by aiming to generate not only the best solutions but also a diverse set of high-performing alternatives. This is particularly beneficial in domains such as robotics, product design, procedural content generation, and synthetic biology, where multiple distinct yet competitive solutions are more desirable than a single global optimum.

#### 3.1 MAP-Elites Algorithm

A foundational method in QD optimization is the MAP-Elites (Multi-dimensional Archive of Phenotypic Elites) algorithm. It partitions the behavior space into a grid (niches), each representing a different type of solution behavior or characteristic, and seeks the best-performing individual (elite) in each niche.

#### Algorithmic Flow:

1. Initialization: Randomly generate a population of candidate solutions.
2. Evaluation: For each candidate  $x$ , evaluate both the objective function  $f(x)$  and its behavioral descriptor  $\phi(x)$ .
3. Archive Update: Place the candidate in the corresponding cell  $c$  of a discretized

behavior space  $B$  only if it outperforms the current elite  $x_c^*$  in that cell:

$$x_c^* = \arg \max_{x \in \text{cell } c} f(x), \quad \text{where } c = \phi(x)$$

4. Variation: Apply genetic operators (e.g., mutation, crossover) to elites and repeat the process.

The final output is not a single solution but a map of diverse, high quality solutions, offering a toolbox for flexible deployment in uncertain or changing environments.

### 3.2 Multimodal Optimization and MMDE

In contrast, Multimodal Optimization algorithm aims to locate multiple optima (both global and local) in the fitness landscape, making them highly suitable for problems with multiple valid answers. One of the prominent approaches is the Multimodal Differential Evolution (MMDE) algorithm.

MMDE extends the classical Differential Evolution (DE) by integrating diversity-preserving mechanisms such as fitness sharing, crowding, or speciation.

The mutation step in standard DE is:

$$v_i^{(t)} = x_{r1}^{(t)} + F \cdot (x_{r2}^{(t)} - x_{r3}^{(t)})$$

where  $x_{r1}, x_{r2}, x_{r3}$  are randomly selected individuals and  $F$  is a scaling factor.

To promote diversity and discourage convergence to a single optimum, fitness sharing modifies the fitness value of each individual  $x_i$  as:

$$f(x_i) = \frac{f(x_i)}{\sum_{j=1}^N sh(d_{ij})}$$

with the sharing function defined as:

$$sh(d_{ij}) = \begin{cases} 1 - \left(\frac{d_{ij}}{\sigma_{share}}\right)^\alpha & \text{if } d_{ij} < \sigma_{share} \\ 0 & \text{otherwise} \end{cases}$$

where:

- $d_{ij}$  is the Euclidean distance between individuals  $x_i$  and  $x_j$ ,
  - $\sigma_{share}$  is the niche radius,
  - $\alpha$  is the sharing exponent controlling decay.
- These mechanisms allow the population to maintain niching behavior, thus converging to multiple optima simultaneously.

### 3.3 Applications and Integration

Both QD and multimodal optimization are highly applicable in:

- Robotics: Generating diverse locomotion patterns.
- Antenna design: Finding multiple configurations with similar radiation properties.
- Drug design: Identifying chemically diverse compounds with comparable efficacy.

Furthermore, hybrid approaches are emerging that combine QD methods like MAP-Elites with multimodal techniques (e.g., clustering-enhanced DE) to exploit both diversity and performance in high-dimensional or deceptive search spaces.

As observed by Chauhan et al. (2025), these strategies provide robust search capabilities in complex real-world optimization problems, offering both innovation and flexibility across disciplines.

### 4. AI-Driven Optimization Paradigms

The fusion of artificial intelligence with optimization has catalyzed transformative methodologies that redefine problem solving capabilities. Data-centric optimization represents a fundamental shift from algorithm-centric approaches, emphasizing the critical role of data quality in determining optimization outcomes. Research indicates that specialized AI applications require customized datasets, with limitations in large language models becoming particularly evident when processing complex scientific data structures such as chemical compounds, knowledge graphs, and time-series

information (CAS., 2024). This recognition has spurred the development of compound AI systems that integrate multiple data sources and employ "mixture of experts" approaches, substantially reducing hallucination incidents and improving solution fidelity in domains like drug repurposing and computer-aided design (CAS., 2024).

Learning-based optimization frameworks have emerged as particularly promising approaches. Optimization-augmented neural networks incorporate combinatorial layers

that enable end-to-end training of contextual multi-stage decision policies (LION19., 2025).

$$y = \arg \min_{z \in \mathcal{C}} \|z - Wh\|_{2^2} + \lambda \mathcal{R}(z)$$

Where  $\mathcal{C}$  is a feasible set (e.g., routing constraints),  $h$  is hidden state, and  $\mathcal{R}(\cdot)$  is a regularizer. Differentiable optimization is achieved via implicit differentiation:

$$\frac{\partial y}{\partial W} = -(A_{zz}^2 \mathcal{L})^{-1} \frac{\partial}{\partial W} (A_z \mathcal{L})$$

with  $\mathcal{L}$  the Lagrangian.

These frameworks demonstrate exceptional performance in dynamic environments, evidenced by their winning solutions in the 2022 EUROMeetsNeurIPS vehicle routing challenge. The paradigm encompasses two principal methodologies:

1. Learning by Experience: Agents explore decision spaces through reinforcement mechanisms, developing optimization policies that maximize long-term rewards in uncertain environments.

2. Learning by Imitation: Neural architectures distill heuristics from expert demonstrations, approximating complex optimization logic through differentiable programming.

The integration of surrogate modeling with Bayesian optimization has yielded significant efficiency improvements for problems involving computationally expensive evaluations.

Surrogate model using  $k$ :

$$f(X) \sim \text{GP}(m(X), k(X, X'))$$

Expected improvement (EI) acquisition:

$$\begin{aligned} EI(X) &= E [\max(f(X) - f(X^+), 0)] \\ &= \sigma(X) [y(X) \Phi(y(X)) \\ &\quad + \phi(y(X))] \end{aligned}$$

where  $y(X) = \frac{m(X) - f(X^+)}{\sigma(X)}$ , and  $\Phi$ ,  $\phi$  are CDF/PDF of  $\mathcal{N}(0,1)$ .

Current research focuses on sustainability-aware implementations that minimize energy consumption during optimization processes. As Antonio Candelieri notes, "By replacing the expensive objectives with a surrogate model, computational resources can be saved that would otherwise be allocated to running heavy physics simulators" (LION19., 2025). Multi-fidelity approaches further enhance this efficiency by strategically allocating

computational resources across varying model accuracy levels.

## 5. Mathematical Foundations and Innovations

The mathematical underpinnings of optimization theory continue to advance through developments in variational analysis and nonsmooth optimization. Recent work extends proximal point methods to nonmonotone settings, enabling more effective handling of nonconvex objectives prevalent in engineering applications and machine learning (Grad et al. 2025; Rigó et al., 2025).

For nonsmooth  $f = g + h$ :

$$X^{k+1} = \text{prox}_{\lambda_k h}(X^k - \lambda_k \text{Ag}(X^k))$$

where  $\text{prox}_{\lambda h}(z) = \arg \min_u \{h(u) + \frac{1}{2\lambda} \|u - z\|^2\}$ .

Convergence is guaranteed when  $\lambda_k > L_g$  (Lipschitz constant).

The forthcoming special issue "Optimization and Variational Analysis in 2025" in the Journal of Optimization Theory and Applications highlights emerging research in splitting algorithms for composite optimization, which decompose complex problems into tractable subproblems while preserving convergence guarantees (Rigó et al., 2025). These theoretical advances facilitate solutions to previously intractable problems in mathematical finance and large-scale network optimization.

Nonconvex optimization has seen particularly significant theoretical breakthroughs, especially in understanding the geometric properties of loss landscapes in overparameterized systems. Research into high-dimensional solution spaces reveals that carefully designed optimization trajectories can avoid spurious local minima, explaining the surprising efficacy of gradient-based methods in deep learning architectures (Rigó et al., 2025). This understanding has informed the development of escape heuristics that actively navigate saddle points in nonconvex landscapes, substantially improving convergence rates in training generative adversarial networks and transformer architectures.



Copositive optimization approaches their 75th anniversary with renewed theoretical and practical relevance. Modern research focuses on reformulating difficult combinatorial and polynomial optimization problems through copositive relaxations, yielding tighter convex approximations than traditional semi definite programming approaches (Rigó et al., 2025).

$$\min_{X \in \mathcal{COP}^n} (C, X) \quad \text{s.t.} \quad (A_i, X) = b_i$$

where  $\mathcal{COP}^n = \{M : v^T M v \geq 0 \quad \forall v \geq 0\}$ . The forthcoming anniversary special issue aims to consolidate historical developments while highlighting computational breakthroughs that have transformed copositive methods from theoretical curiosities into practical tools for quadratic assignment problems and maximum clique optimization.

## 6. Interdisciplinary Applications and Domain-Specific Advances

### 6.1. Sustainable Systems and Climate Optimization

Optimization methodologies play increasingly critical roles in addressing climate challenges and advancing sustainability initiatives. Metal-organic frameworks (MOFs) and covalent organic frameworks (COFs) exemplify materials science innovations optimized for environmental applications, with BASF pioneering commercial-scale production of MOFs for carbon capture due to their exceptional surface area and tunable properties (CAS., 2024).

MOF-based Carbon Capture:

Aldsoption maximization:

$$\max_{\phi} Q_{\text{CO}_2}(\phi) = \int_0^p \Gamma(\phi, p) dp$$

$$\Gamma(\phi, p) = K_L(\phi)p \frac{1 - \left(\frac{\theta}{\theta_{\max}}\right)^n}{1 + K_H(\phi)p}$$

where  $\phi$  are MOF topology parameters.

Optimization-driven designs of MOF-based coatings for air conditioning systems demonstrate 40% energy reduction in humidity extraction, highlighting the significant impact of computational optimization on energy efficiency (CAS., 2024).

Waste management optimization represents another frontier, with hydrothermal carbonization technologies converting wet biomass into hydrochar for energy generation and soil conditioning. Advanced algorithms optimize conversion efficiency while minimizing hazardous byproducts, particularly in processing electronic waste and recovering strategic materials like lithium and cobalt (CAS., 2024). These approaches align with circular economy principles by transforming waste streams into valuable resources through optimized conversion processes.

**Table 2: Optimization Applications in Sustainability Domains**

Application Domain	Optimization Methods	Key Metrics	Impact Potential
Renewable Energy Integration	Stochastic programming, Multi-objective optimization	Energy yield, Grid stability, Storage efficiency	30-50% reduction in renewable intermittency issues
Solid-State Batteries	Topology optimization, Bayesian materials design	Energy density, Charge cycles, Safety performance	50% size reduction in EV batteries by 2028
Plastic Recycling	Enzymatic process optimization, Flow control	Monomer regeneration rate, Purity thresholds	70% PET recycling efficiency through bacterial processing
Smart Grids	Decentralized optimization, Real-time pricing	Load balancing, Transmission loss, Resilience	40% demand-response efficiency improvement

### 6.2. Healthcare and Precision Medicine Optimization

The healthcare sector demonstrates particularly sophisticated applications of optimization

technologies. CRISPR-based therapeutic development employs optimization algorithms at multiple stages, from guide RNA design to delivery vector optimization.

$$\min_g [-\text{on-target efficiency (g)}, \quad \text{off-target score (g)}, \quad \text{GC content dev (g)}]^T$$

subject to  $g \in \{A, U, G, C\}^L$  and  $\|g\| = 20$ .

Cutting-edge approaches now optimize base editing and epigenetic modulation parameters, enabling more precise genetic interventions

with reduced off-target effects (CAS., 2024). Optimization has also enhanced CAR-T cell therapies through knockout of inhibitory genes and introduction of controllable safety switches, creating personalized immunotherapies with improved efficacy profiles.

Molecular editing technologies represent another breakthrough, with optimization algorithms enabling precise atom-level modifications to existing molecular scaffolds. This approach substantially reduces synthetic steps compared to traditional *de novo* synthesis, decreasing toxic solvent use and energy requirements while expanding accessible chemical space for drug discovery (CAS., 2024). Combined with AI-based synthetic pathway optimization, these techniques promise to accelerate pharmaceutical innovation by enabling more efficient exploration of molecular frameworks.

### 6.3 Intelligent Transportation and Logistics

Autonomous systems optimization increasingly integrates combinatorial optimization with deep learning for real-time decision-making. The 2025 LION conference highlights methods that embed optimization layers within neural networks, enabling end-to-end learning of routing policies that adapt to dynamic environmental conditions (LION19., 2025). These approaches demonstrate particular

efficacy in multi-agent transportation systems, where they optimize fleet coordination while balancing competing objectives like fuel efficiency, service equity, and response times. Supply chain optimization has embraced novel metaheuristics like the Wombat Optimization Algorithm (WOA), which models burrow network dynamics to solve complex logistics problems with disrupted flows and stochastic demands (Amin & Dehghani, 2025). These approaches demonstrate superior performance in resilient supply chain design, incorporating real-world constraints like transportation fragility, inventory uncertainty, and sustainability requirements that challenge traditional mathematical programming techniques.

## 7. Emerging Computational Platforms

Quantum optimization approaches transition from theoretical constructs to practical tools, with 2025 designated as the International Year of Quantum Science and Technology. Cleveland Clinic and IBM have installed the first quantum computer dedicated to healthcare research, tackling molecular simulation problems that exceed classical computational capabilities (CAS., 2024). Current research focuses on quantum algorithms for protein folding prediction and materials discovery, potentially reducing computation times for complex molecular dynamics from years to hours. Early applications in agriculture demonstrate quantum optimization of fertilizer formulations and field monitoring strategies, suggesting near-term practical impact beyond theoretical domains (CAS., 2024).

High-performance optimization computing leverages advances in hardware architecture to solve previously intractable problems.

For combinatorial problems:

$$|y, \beta\rangle = e^{-i\beta_p H_B} e^{-iy_p H_C} \dots \cdot e^{-i\beta_1 H_B} e^{-iy_1 H_C} |+\rangle^n$$

$$\min_{y, \beta} \langle y, \beta | H_C | y, \beta \rangle$$

where  $H_C$  is the cost Hamiltonian, and  $H_B = \sum_i \sigma_i^x$  drives transitions.

Heterogeneous computing platforms integrate GPUs, TPUs, and specialized AI accelerators to parallelize population-based metaheuristics and decomposition algorithms. The SIAM Journal on Optimization highlights implementations achieving three orders of magnitude speedup for stochastic gradient descent in large-scale neural network training through innovative parallelization strategies (SIAM., 2025). These hardware-aware optimization approaches co-design algorithms and computing architectures, maximizing resource utilization while minimizing energy consumption, a critical consideration given AI's growing environmental footprint.

## 8. Emerging Methodologies and Future Directions

Human-inspired optimization continues to diversify beyond traditional nature-inspired paradigms. Recent methodologies include Sales Training Based Optimization (modeling knowledge transfer in commercial training), Sculptor Optimization (emulating artistic refinement processes), and Dollmaker Optimization (inspired by iterative design refinement) (Amin & Dehghani, 2025). These approaches demonstrate competitive performance on engineering design problems, suggesting that human creative and pedagogical processes offer rich metaphors for optimization strategy development. Their effectiveness appears particularly pronounced in supply chain management applications, where they outperform established bio-inspired algorithms on real-world implementation challenges (Amin & Dehghani, 2025).

Multi-agent optimization frameworks address complex coordination challenges in sharing economy platforms and virtual power plants. Modern approaches incorporate partial rationality and bounded rationality into agent models, recognizing that human participants rarely exhibit perfect optimization behavior (LION19., 2025).

Agent  $i$ 's response:

$$u_i^{(t)} = \arg \min_{u_i} [J(u_i, u_{-i}^{(t-1)}) + \rho D_{KL}(u_i || u_i^{(t-1)})]$$

where  $D_{KL}$  quantifies deviation from previous strategy, and  $\rho$  is rationality parameter.

The LION19 conference highlights applications in Tesla Virtual Power Plant and similar systems, where optimization algorithms balance energy distribution while accommodating participant behaviors that deviate from purely rational economic models (LION19., 2025). These approaches employ nonlinear control theory and probabilistic fairness guarantees to ensure system stability despite unpredictable human factors.

The algorithm selection problem remains a fundamental challenge, prompting research into meta-optimization frameworks that dynamically match solvers to problem

characteristics. Current approaches employ deep reinforcement learning to construct adaptive portfolios that switch optimization strategies based on landscape analysis and runtime performance metrics (LION19., 2025). These systems demonstrate promising results on the BBOB (Black-Box Optimization Benchmark) testbed, suggesting potential for autonomous optimization systems that continuously refine their approach based on problem characteristics and accumulated experience.

## 9. Conclusion and Research Challenges

The optimization landscape continues to evolve toward greater interdisciplinary integration and specialization. Bio-inspired algorithms maintain their relevance through continuous hybridization and theoretical refinement, while AI-driven approaches transform optimization from standalone algorithms into embedded components of learning systems. The convergence of statistical learning and optimization theory opens new avenues for understanding generalization in overparameterized models, promising tighter integration between learning theory and optimization practice (OPT., 2025). Several critical challenges demand research attention. Algorithm selection methodologies require further development to guide practitioners through the expanding optimizer landscape. Sustainability considerations must become central to optimization research, addressing both the environmental impact of optimization computations and their application to climate challenges. Ethical optimization frameworks need development to ensure equitable outcomes in socially impactful applications like healthcare resource allocation and algorithmic decision-making.

The rapid proliferation of optimization techniques necessitates renewed emphasis on reproducibility and benchmarking standards. Community efforts like the CEC test suites and LION competitions provide valuable evaluation platforms, but require expansion to cover emerging problem classes like multi-objective reinforcement learning and large-scale nonconvex optimization (Amin &

Dehghani, 2025; OPT., 2025). As optimization permeates increasingly consequential domains, maintaining scientific rigor while encouraging methodological innovation represents the field's central challenge moving forward.

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