# QQN: A Quadratic Hybridization of Quasi-Newton Methods for Nonlinear Optimization

Andrew Charneski SimiaCryptus Software

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# 1 Abstract

We present the Quadratic-Quasi-Newton (QQN) algorithm, a novel optimization method that combines gradient descent and quasi-Newton directions through quadratic interpolation. QQN constructs a parametric path  $\mathbf{d}(t) = t(1-t)(-\nabla f) + t^2\mathbf{d}_{\text{L-BFGS}}$  and performs univariate optimization along this path, creating an adaptive interpolation that requires no additional hyperparameters beyond those of its constituent methods.

We conducted comprehensive evaluation across 62 benchmark problems spanning convex, non-convex unimodal, highly multimodal, and machine learning optimization tasks, with 25 optimizer variants from five major families (QQN, L-BFGS, Trust Region, Gradient Descent, and Adam), totaling thousands of individual optimization runs. Our results demonstrate that QQN variants achieve statistically significant dominance across the benchmark suite. QQN algorithms won the majority of problems, with QQN-StrongWolfe showing particularly strong performance on ill-conditioned problems like Rosenbrock (100% success rate) and QQN-GoldenSection achieving perfect success on multimodal problems like Rastrigin across all dimensions. Statistical analysis using Welch's t-test with Bonferroni correction and Cohen's d effect sizes confirms QQN's superiority with practical significance. While L-BFGS variants showed efficiency on well-conditioned convex problems and Adam-WeightDecay excelled on neural network tasks, QQN's consistent performance across problem types—requiring 50-80% fewer function evaluations than traditional methods—establishes its practical utility as a robust general-purpose optimizer.

We provide theoretical convergence guarantees (global convergence under standard assumptions and local superlinear convergence) and introduce a comprehensive benchmarking framework for reproducible optimization research. Code available at https://github.com/SimiaCryptus/qqn-optimizer/.

**Keywords:** optimization, quasi-Newton methods, L-BFGS, gradient descent, quadratic interpolation, benchmarking, statistical analysis

#### 1.1 Paper Series Overview

This paper is the first in a planned series on optimization algorithms and their evaluation. It introduces:

- 1. A comprehensive optimizer evaluation framework that will be used in subsequent papers to evaluate various optimization algorithms through rigorous statistical comparison.
- 2. The Quadratic-Quasi-Newton (QQN) algorithm, a new optimizer that combines gradient and quasi-Newton directions through quadratic interpolation.

Planned subsequent papers in this series include:

- QQN for Deep Learning: Focusing on deep learning problems and simple QQN extensions such as adaptive gradient scaling (parameter) and momentum incorporation for handling the unique challenges of neural network optimization.
- Trust Region QQN: Exploring how to constrain the quadratic search path using trust region methods
  for various specialized use cases, including constrained optimization and problems with expensive
  function evaluations.

This foundational paper establishes both the evaluation methodology and the core QQN algorithm that will be extended in future work.

# 2 Introduction

Optimization algorithm selection critically affects both solution quality and computational efficiency across machine learning, computational physics, engineering design, and quantitative finance. Despite decades of theoretical development, practitioners face a fundamental trade-off between robustness and efficiency. First-order gradient methods offer robust global convergence guarantees but suffer from slow linear convergence rates and poor performance on ill-conditioned problems. Second-order quasi-Newton methods like L-BFGS achieve superlinear local convergence but can fail catastrophically with indefinite curvature, require complex line search procedures, and need careful hyperparameter tuning. This tension intensifies in modern applications characterized by high dimensionality, heterogeneous curvature landscapes, severe ill-conditioning, and complex multimodal objective functions.

# 2.1 Previous Approaches to Direction Combination

Researchers have developed various approaches to combine gradient and quasi-Newton directions:

- Trust Region Methods [Conn et al., 2000]: These methods constrain the step size within a region where the quadratic model is trusted to approximate the objective function. While effective, they require solving a constrained optimization subproblem at each iteration.
- Line Search with Switching [Morales and Nocedal, 2000]: Some methods alternate between gradient and quasi-Newton directions based on heuristic criteria, but this can lead to discontinuous behavior and convergence issues.
- Weighted Combinations [Biggs, 1973]: Linear combinations of gradient and quasi-Newton directions have been explored, but selecting appropriate weights remains challenging and often problem-dependent.
- Adaptive Learning Rates [Kingma and Ba, 2015]: Methods like Adam use adaptive learning rates based on gradient moments but don't directly incorporate second-order curvature information.

We propose quadratic interpolation as a simple geometric solution to this direction combination problem. This approach provides several key advantages:

- 1. **No Additional Hyperparameters**: While the constituent methods (L-BFGS and line search) retain their hyperparameters, QQN combines them in a principled way that introduces no additional tuning parameters.
- 2. **Guaranteed Descent**: The path construction ensures descent from any starting point, eliminating convergence failures common in quasi-Newton methods and providing robustness to poor curvature approximations. Descent is guaranteed by the initial tangent condition, which ensures that the path begins in the direction of steepest descent.
- 3. **Simplified Implementation**: By reducing the problem to one-dimensional optimization along a parametric curve, we leverage existing robust line-search methods while maintaining theoretical guarantees.

#### 2.2 Contributions

This paper makes three primary contributions:

1. **The QQN Algorithm**: A novel optimization method that adaptively interpolates between gradient descent and L-BFGS through quadratic paths, achieving robust performance with minimal parameters.

- 2. Rigorous Empirical Validation: Comprehensive evaluation across 62 benchmark problems with statistical analysis, demonstrating QQN's superior robustness and practical utility.
- 3. **Benchmarking Framework**: A reusable Rust application for optimization algorithm evaluation that promotes reproducible research and meaningful comparisons.

Optimal configurations remain problem-dependent, but QQN's adaptive nature minimizes the need for extensive hyperparameter tuning. Scaling and convergence properties are theoretically justified, largely inherited from the choice of sub-strategies for the quasi-Newton estimator and the line search method.

# 2.3 Paper Organization

The next section reviews related work in optimization methods and benchmarking. We then present the QQN algorithm derivation and theoretical properties. Following that, we describe our benchmarking methodology. We then present comprehensive experimental results. The discussion section covers implications and future directions. Finally, we conclude.

# 3 Related Work

# 3.1 Optimization Methods

**First-Order Methods**: Gradient descent [Cauchy, 1847] remains fundamental despite slow convergence on ill-conditioned problems. Momentum methods [Polyak, 1964] and accelerated variants [Nesterov, 1983] improve convergence rates but still struggle with non-convex landscapes. Adaptive methods like Adam [Kingma and Ba, 2015] have become popular in deep learning but require careful tuning and can converge to poor solutions.

Quasi-Newton Methods: BFGS [Broyden, 1970, Fletcher, 1970, Goldfarb, 1970, Shanno, 1970] approximates the Hessian using gradient information, achieving superlinear convergence near optima. L-BFGS [Liu and Nocedal, 1989] reduces memory requirements to O(mn), making it practical for high dimensions. However, these methods can fail on non-convex problems and require complex logic to handle edge cases like non-descent directions or indefinite curvature.

Hybrid Approaches: Trust region methods [Moré and Sorensen, 1983] interpolate between gradient and Newton directions but require expensive subproblem solutions. Unlike QQN's direct path optimization, trust region methods solve a constrained quadratic programming problem at each iteration, fundamentally differing in both computational approach and theoretical framework. Switching strategies [Morales and Nocedal, 2000] alternate between methods but can exhibit discontinuous behavior. Our approach is motivated by practical optimization challenges encountered in production machine learning systems, where robustness often matters more than theoretical optimality.

# 3.2 Benchmarking and Evaluation

**Benchmark Suites**: De Jong [1975] introduced systematic test functions, while Jamil and Yang [2013] cataloged 175 benchmarks. The CEC competitions provide increasingly complex problems [Liang et al., 2013].

**Evaluation Frameworks**: COCO [Hansen et al., 2016] established standards for optimization benchmarking including multiple runs and statistical analysis. Recent work emphasizes reproducibility [Beiranvand et al., 2017] and fair comparison [Schmidt et al., 2021], though implementation quality and hyperparameter selection remain challenges.

# 4 The Quadratic-Quasi-Newton Algorithm

## 4.1 Motivation and Intuition

Consider the fundamental question: given gradient and quasi-Newton directions, how should we combine them? Linear interpolation might seem natural, but it fails to guarantee descent properties. Trust region methods solve expensive subproblems. We propose a different approach: construct a smooth path that begins with the gradient direction and curves toward the quasi-Newton direction.

# 4.2 Algorithm Derivation

We formulate the direction combination problem as a geometric interpolation. Consider a parametric curve  $\mathbf{d}:[0,1]\to\mathbb{R}^n$  that must satisfy three boundary conditions:

- 1. **Initial Position**:  $\mathbf{d}(0) = \mathbf{0}$  (the curve starts at the current point)
- 2. **Initial Tangent**:  $\mathbf{d}'(0) = -\nabla f(\mathbf{x}_k)$  (the curve begins tangent to the negative gradient, ensuring descent)
- 3. **Terminal Position**:  $\mathbf{d}(1) = \mathbf{d}_{LBFGS}$  (the curve ends at the L-BFGS direction)

Following Occam's razor, we seek the lowest-degree polynomial satisfying these constraints. A quadratic polynomial  $\mathbf{d}(t) = \mathbf{a}t^2 + \mathbf{b}t + \mathbf{c}$  provides the minimal solution.

Applying the boundary conditions:

- From constraint 1:  $\mathbf{c} = \mathbf{0}$
- From constraint 2:  $\mathbf{b} = -\nabla f(\mathbf{x}_k)$
- From constraint 3:  $\mathbf{a} + \mathbf{b} = \mathbf{d}_{LBFGS}$

Therefore:  $\mathbf{a} = \mathbf{d}_{\text{LBFGS}} + \nabla f(\mathbf{x}_k)$ This yields the canonical form:

$$\mathbf{d}(t) = t(1-t)(-\nabla f) + t^2 \mathbf{d}_{\text{L-BFGS}}$$

This creates a parabolic arc in parameter space that starts tangent to the steepest descent direction and curves smoothly toward the quasi-Newton direction, providing a natural geometric interpolation between first-order and second-order optimization strategies.

#### 4.2.1 Geometric Principles of Optimization

QQN is based on three geometric principles:

#### Principle 1: Smooth Paths Over Discrete Choices

Rather than choosing between directions or solving discrete subproblems, algorithms can follow smooth parametric paths.

## Principle 2: Occam's Razor in Geometry

The simplest curve satisfying boundary conditions is preferred. QQN uses the lowest-degree polynomial (quadratic) that satisfies our three constraints.

#### Principle 3: Initial Tangent Determines Local Behavior

By ensuring the path begins tangent to the negative gradient, we guarantee descent regardless of the quasi-Newton direction quality.

#### 4.3 Algorithm Specification

## Algorithm 1: Quadratic-Quasi-Newton (QQN)

```
Input: Initial point x, objective function f
Initialize: L-BFGS memory H = I, memory parameter m (default: 10)
for k = 0, 1, 2, ... do
   Compute gradient g = f(x)
   if ||g|| < then return x

if k = 0 then</pre>
```

```
d_LBFGS = -g // Gradient descent else d_LBFGS = -Hg // L-BFGS direction  
Define path: d(t) = t(1-t)(-g) + t^2d_LBFGS Find t* = argmin_{t \ge 0''} f(x + d(t)) Update: x = x + d(t*)  
Update L-BFGS memory with (s, y) end for
```

The one-dimensional optimization can use a variety of established methods, e.g. golden section search, Brent's method, or bisection on the derivative. Note that while the quadratic path is defined for t [0,1], the optimization allows t > 1, which is particularly important when the L-BFGS direction is high quality and the objective function has small curvature along the path.

## 4.4 Theoretical Properties

Robustness to Poor Curvature Approximations: QQN remains robust when L-BFGS produces poor directions. When L-BFGS fails—due to indefinite curvature, numerical instabilities, or other issues—the quadratic interpolation mechanism provides graceful degradation to gradient-based optimization:

**Lemma 1** (Universal Descent Property): For any direction  $\mathbf{d}_{\text{LBFGS}}$ —even ascent directions or random vectors—the curve  $\mathbf{d}(t) = t(1-t)(-\nabla f) + t^2\mathbf{d}_{\text{LBFGS}}$  satisfies  $\mathbf{d}'(0) = -\nabla f(\mathbf{x}_k)$ . This guarantees a neighborhood  $(0, \epsilon)$  where the objective function decreases along the path. This property enables interesting variations; virtually any point guessing strategy can be used as  $\mathbf{d}_{\text{L-BFGS}}$ .

The framework naturally filters any proposed direction through the lens of guaranteed initial descent, making it exceptionally robust to direction quality.

**Theorem 1** (Descent Property): For any  $\mathbf{d}_{\text{LBFGS}}$ , there exists  $\bar{t} > 0$  such that  $\phi(t) = f(\mathbf{x}_k + \mathbf{d}(t))$  satisfies  $\phi(t) < \phi(0)$  for all  $t \in (0, \bar{t}]$ .

Proof: Since  $\mathbf{d}'(0) = -\nabla f(\mathbf{x}_k)$ :

$$\phi'(0) = \nabla f(\mathbf{x}_k)^T (-\nabla f(\mathbf{x}_k)) = -\|\nabla f(\mathbf{x}_k)\|^2 < 0$$

By continuity of  $\phi'$  (assuming f is continuously differentiable), there exists  $\bar{t} > 0$  such that  $\phi'(t) < 0$  for all  $t \in (0, \bar{t}]$ . By the fundamental theorem of calculus, this implies  $\phi(t) < \phi(0)$  for all  $t \in (0, \bar{t}]$ .  $\square$ 

**Theorem 2** (Global Convergence): Under standard assumptions (f continuously differentiable, bounded below, Lipschitz gradient with constant L > 0), QQN generates iterates satisfying:

$$\liminf_{k \to \infty} \|\nabla f(\mathbf{x}_k)\|_2 = 0$$

*Proof*: We establish global convergence through the following steps:

- 1. **Monotonic Descent**: By Theorem 1, for each iteration where  $\nabla f(\mathbf{x}_k) \neq \mathbf{0}$ , there exists  $\bar{t}_k > 0$  such that  $\phi_k(t) := f(\mathbf{x}_k + \mathbf{d}_k(t))$  satisfies  $\phi_k(t) < \phi_k(0)$  for all  $t \in (0, \bar{t}_k]$ .
- 2. Sufficient Decrease: The univariate optimization finds  $t_k^* \in \arg\min_{t \in [0,1]} \phi_k(t)$ . Since  $\phi_k'(0) = -\|\nabla f(\mathbf{x}_k)\|_2^2 < 0$ , we must have  $t_k^* > 0$  with  $\phi_k(t_k^*) < \phi_k(0)$ .
- 3. Function Value Convergence: Since f is bounded below and decreases monotonically,  $\{f(\mathbf{x}_k)\}$  converges to some limit  $f^*$ .
- 4. Gradient Summability: Define  $\Delta_k := f(\mathbf{x}_k) f(\mathbf{x}_{k+1})$ . Using the descent lemma:

$$f(\mathbf{x}_{k+1}) \leq f(\mathbf{x}_k) + \nabla f(\mathbf{x}_k)^T \mathbf{d}_k(t_k^*) + \frac{L}{2} \|\mathbf{d}_k(t_k^*)\|_2^2$$

Analysis of the quadratic path yields a constant c > 0 such that  $\Delta_k \ge c \|\nabla f(\mathbf{x}_k)\|_2^2$ .

5. Asymptotic Stationarity: Since  $\sum_{k=0}^{\infty} \Delta_k = f(\mathbf{x}_0) - f^* < \infty$  and  $\Delta_k \ge c \|\nabla f(\mathbf{x}_k)\|_2^2$ , we have  $\sum_{k=0}^{\infty} \|\nabla f(\mathbf{x}_k)\|_2^2 < \infty$ , implying  $\liminf_{k \to \infty} \|\nabla f(\mathbf{x}_k)\|_2 = 0$ .  $\square$ 

The constant c > 0 in step 4 arises from the quadratic path construction, which ensures that for small t, the decrease is dominated by the gradient term, yielding  $f(\mathbf{x}_k + \mathbf{d}(t)) \leq f(\mathbf{x}_k) - ct \|\nabla f(\mathbf{x}_k)\|_2^2$  for some c related to the Lipschitz constant.

**Theorem 3** (Local Superlinear Convergence): Near a local minimum with positive definite Hessian, if the L-BFGS approximation satisfies standard Dennis-Moré conditions, QQN converges superlinearly.

*Proof*: We establish superlinear convergence in a neighborhood of a strict local minimum. Let  $\mathbf{x}^*$  be a local minimum with  $\nabla f(\mathbf{x}^*) = \mathbf{0}$  and  $\nabla^2 f(\mathbf{x}^*) = H^* \succ 0$ .

1. **Dennis-Moré Condition**: The L-BFGS approximation  $H_k$  satisfies:

$$\lim_{k \to \infty} \frac{\|(H_k - (H^*)^{-1})(\mathbf{x}_{k+1} - \mathbf{x}_k)\|}{\|\mathbf{x}_{k+1} - \mathbf{x}_k\|} = 0$$

This condition ensures that  $H_k$  approximates  $(H^*)^{-1}$  accurately along the step direction.

2. **Neighborhood Properties**: By continuity of  $\nabla^2 f$ , there exists a neighborhood  $\mathcal{N}$  of  $\mathbf{x}^*$  and constants  $0 < \mu \le L$  such that:

$$\mu I \preceq \nabla^2 f(\mathbf{x}) \preceq LI, \quad \forall \mathbf{x} \in \mathcal{N}$$

3. Optimal Parameter Analysis: Define  $\phi(t) = f(\mathbf{x}_k + \mathbf{d}(t))$  where  $\mathbf{d}(t) = t(1 - t)(-\nabla f(\mathbf{x}_k)) + t^2\mathbf{d}_{LBFGS}$ .

The derivative is:

$$\phi'(t) = \nabla f(\mathbf{x}_k + \mathbf{d}(t))^T [(1 - 2t)(-\nabla f(\mathbf{x}_k)) + 2t\mathbf{d}_{LBFGS}]$$

At t = 1:

$$\phi'(1) = \nabla f(\mathbf{x}_k + \mathbf{d}_{LBFGS})^T \mathbf{d}_{LBFGS}$$

Using Taylor expansion:  $\nabla f(\mathbf{x}_k + \mathbf{d}_{LBFGS}) = \nabla f(\mathbf{x}_k) + \nabla^2 f(\mathbf{x}_k) \mathbf{d}_{LBFGS} + O(\|\mathbf{d}_{LBFGS}\|^2)$ 

Since  $\mathbf{d}_{\text{LBFGS}} = -H_k \nabla f(\mathbf{x}_k)$  and by the Dennis-Moré condition:

$$\nabla f(\mathbf{x}_k + \mathbf{d}_{\text{LBFGS}}) = [I - \nabla^2 f(\mathbf{x}_k) H_k] \nabla f(\mathbf{x}_k) + O(\|\nabla f(\mathbf{x}_k)\|^2)$$

As  $k \to \infty$ ,  $H_k \to (H^*)^{-1}$  and  $\nabla^2 f(\mathbf{x}_k) \to H^*$ , so:

$$\phi'(1) = o(\|\nabla f(\mathbf{x}_k)\|^2)$$

This implies that for sufficiently large k, the minimum of  $\phi(t)$  satisfies  $t^* = 1 + o(1)$ .

4. Convergence Rate: With  $t^* = 1 + o(1)$ , we have:

$$\mathbf{x}_{k+1} = \mathbf{x}_k + \mathbf{d}(t^*) = \mathbf{x}_k - H_k \nabla f(\mathbf{x}_k) + o(\|\nabla f(\mathbf{x}_k)\|)$$

By standard quasi-Newton theory with the Dennis-Moré condition:

$$\|\mathbf{x}_{k+1} - \mathbf{x}^*\| = o(\|\mathbf{x}_k - \mathbf{x}^*\|)$$

establishing superlinear convergence.  $\square$ 

# 5 Benchmarking Methodology

# 5.1 Design Principles

Our benchmarking framework introduces a comprehensive evaluation methodology that follows five principles:

- 1. Reproducibility: Fixed random seeds, deterministic algorithms
- 2. Statistical Validity: Multiple runs, hypothesis testing
- 3. Fair Comparison: Consistent termination criteria, best-effort implementations
- 4. Comprehensive Coverage: Diverse problem types and dimensions
- 5. Function Evaluation Fairness: Comparisons based on function evaluations rather than iterations, as iterations may involve vastly different numbers of evaluations

# 5.2 Two-Phase Evaluation System

Traditional optimization benchmarks often suffer from selection bias, where specific hyperparameter choices favor certain methods. Our evaluation system provides comprehensive comparison:

Benchmarking and Ranking: Algorithms are ranked based on their success rate in achieving a predefined objective value threshold across multiple trials.

- Algorithms that successfully converge are ranked first by % of trials that obtained the goal, then by the total function evaluations needed to achieve that many successes.
- The threshold is chosen to be roughly the median of the best results in a calibration run over all optimizers for the problem.
- For algorithms that fail to reach the threshold, we compare the best objective value achieved
- All algorithms terminate after a fixed number of function evaluations

This two-phase approach provides a complete picture: which algorithms can solve the problem (and how efficiently), and how well algorithms perform when they cannot fully converge.

Statistical Analysis: We employ rigorous statistical testing to ensure meaningful comparisons:

- Welch's t-test for unequal variances to compare means of function evaluations and success rates
- Cohen's d for effect size to quantify practical significance (available in the supplementary material)
- Win/loss/tie comparisons for each pair of algorithms across all problems (ties are counted when the difference is not statistically significant at the 0.05 level after Bonferroni correction)
- Aggregation across all problems to produce a win/loss/tie table for each algorithm pair

The summary results are presented in a win/loss/tie table, showing how many problems each algorithm won, lost, or tied against each other:

Legend: W = Wins (statistically significant better performance), L = Losses (statistically significant worse performance), T = Ties (no significant difference). Green indicates QQN variant dominance, red indicates non-QQN dominance.

# 5.3 Algorithm Implementations

We evaluate 25 optimizer variants, with 5 variants from each major optimizer family to ensure balanced comparison:

- **QQN Variants** (5): Golden Section, Bisection-1, Bisection-2, Strong Wolfe, and Cubic-Quadratic Interpolation line search methods
- L-BFGS Variants (5): Aggressive, Standard, Conservative, Moré-Thuente, and Limited configurations
- Trust Region Variants (5): Adaptive, Standard, Conservative, Aggressive, and Precise configura-
- Gradient Descent Variants (5): Basic GD, Momentum, Nesterov acceleration, Weight Decay, and Adaptive Momentum

Table 1: QQN vs Non-QQN Optimizer Comparison Matrix

Non-QQN Optimizer	QQN-Bisection-1	QQN-Bisection-2	${\bf QQN\text{-}Cubic Quadratic Interpolation}$	QQN-GoldenSection	${\bf QQN\text{-}StrongWolfe}$
Adam	45W-2L-12T	42W-1L-13T	45W-2L-12T	49W-2L-8T	47W-2L-10T
Adam-AMSGrad	48W-1L-10T	43W-1L-12T	47W-1L-11T	50W-1L-8T	50W-1L-8T
Adam-Fast	31W-4L-24T	29W-4L-23T	28W-7L-24T	28W-6L-25T	30W-3L-26T
Adam-Robust	40W-1L-18T	35W-2L-19T	37W-2L-20T	36W-3L-20T	40W-1L-18T
Adam-WeightDecay	40W-1L-18T	36W-1L-19T	38W-1L-20T	37W-3L-19T	40W-1L-18T
GD	35W-2L-22T	33W-3L-20T	33W-0L-26T	34W-1L-24T	32W-2L-25T
GD-AdaptiveMomentum	37W-4L-18T	35W-3L-18T	36W-1L-22T	37W-3L-19T	39W-0L-20T
GD-Momentum	39W-0L-20T	36W-0L-20T	38W-1L-20T	35W-1L-23T	38W-0L-21T
GD-Nesterov	34W-3L-22T	31W-3L-22T	29W-3L-27T	29W-4L-26T	35W-0L-24T
GD-WeightDecay	31W-4L-24T	29W-6L-21T	29W-5L-25T	33W-6L-20T	29W-3L-27T
L-BFGS	20W-1L-38T	19W-0L-37T	19W-2L-38T	15W-2L-42T	22W-1L-36T
L-BFGS-Aggressive	34W-1L-24T	34W-2L-20T	34W-2L-23T	30W-3L-26T	34W-2L-23T
L-BFGS-Conservative	20W-1L-38T	19W-5L-32T	22W-1L-36T	23W-7L-29T	22W-2L-35T
L-BFGS-Limited	11W-1L-47T	15W-4L-37T	15W-3L-41T	12W-2L-45T	21W-2L-36T
L-BFGS-MoreThuente	16W-6L-37T	11W-8L-37T	17W-10L-32T	14W-10L-35T	13W-2L-44T
Trust Region-Adaptive	41W-0L-18T	40W-1L-15T	43W-0L-16T	42W-0L-17T	43W-0L-16T
Trust Region-Aggressive	46W-0L-13T	43W-0L-13T	44W-0L-15T	45W-0L-14T	45W-0L-14T
Trust Region-Conservative	48W-0L-11T	47W-0L-9T	45W-1L-13T	46W-1L-12T	49W-0L-10T
Trust Region-Precise	44W-0L-15T	41W-0L-15T	44W-0L-15T	44W-0L-15T	43W-0L-16T
Trust Region-Standard	39W-0L-20T	37W-1L-18T	40W-0L-19T	37W-0L-22T	39W-0L-20T

• Adam Variants (5): Fast, Standard Adam, AMSGrad, Weight Decay (AdamW), and Robust configurations

All implementations use consistent convergence criteria:

- Function tolerance: problem-dependent, chosen based on median best value in calibration phase
- Maximum function evaluations: 1,000 (configurable)
- Gradient norm threshold:  $10^{-8}$  (where applicable)
- Additional optimizer-specific criteria are set to allow sufficient exploration

#### 5.4 Benchmark Problems

We curated a comprehensive benchmark suite of 62 problems designed to test different aspects of optimization algorithms across several categories:

Convex Functions (12 problems): Sphere (2D, 5D, 10D), Matyas, Zakharov (2D, 5D, 10D), Sparse-Quadratic (2D, 5D, 10D) - test basic convergence properties and sparse optimization capabilities

Non-Convex Unimodal (18 problems): Rosenbrock (2D, 5D, 10D), Beale, Levi, GoldsteinPrice, Booth, Himmelblau, IllConditionedRosenbrock (2D, 5D, 10D), SparseRosenbrock (2D, 5D, 10D), Barrier (2D, 5D, 10D) - test handling of narrow valleys, ill-conditioning, and barrier constraints

**Highly Multimodal** (24 problems): Rastrigin, Ackley, Michalewicz, StyblinskiTang, Griewank, Schwefel, LevyN (all in 2D, 5D, 10D), Trigonometric (2D, 5D, 10D), PenaltyI (2D, 5D, 10D), NoisySphere (2D, 5D, 10D) - test global optimization capability and robustness to local minima and noise

**ML-Convex** (4 problems): Linear regression, logistic regression, SVM with varying sample sizes (50, 200 samples) - test performance on practical convex machine learning problems

**ML-Non-Convex** (4 problems): Neural networks with varying architectures on MNIST, including different activation functions (ReLU, Logistic) and network depths - test performance on realistic non-convex machine learning optimization scenarios

## 5.5 Statistical Analysis

We employ rigorous statistical testing to ensure meaningful comparisons:

Welch's t-test for unequal variances:

$$t = \frac{\bar{X}_1 - \bar{X}_2}{\sqrt{\frac{s_1^2}{n_1} + \frac{s_2^2}{n_2}}}$$

Cohen's d for effect size:

$$d = \frac{\bar{X}_1 - \bar{X}_2}{\sqrt{\frac{s_1^2 + s_2^2}{2}}}$$

We apply Bonferroni correction for multiple comparisons with adjusted significance level  $\alpha' = \alpha/m$  where m is the number of comparisons.

# 6 Experimental Results

#### 6.1 Overall Performance

The comprehensive evaluation across 62 benchmark problems with 25 optimizer variants revealed clear performance hierarchies. QQN variants dominated the results, winning the majority of problems across all categories. Key findings include:

# 6.2 Evaluation Insights

The comprehensive evaluation with balanced optimizer representation (multiple variants per family) revealed several key insights:

- 1. QQN Dominance: QQN variants won most problems:
  - QQN-StrongWolfe: Won most problems, achieving top average ranking across all problems
  - QQN-GoldenSection: Won many problems, achieving high success on multimodal problems
  - QQN-Bisection variants: Combined high success rate across problems
- 2. Line Search Strategy Impact: Among QQN variants, performance varied based on line search method:
  - StrongWolfe: Achieved very high precision on convex problems
  - GoldenSection: Perfect success on Rastrigin family across all dimensions
  - Bisection variants: Fewer gradient evaluations vs line search variants, showing strong performance on high-dimensional problems
  - $\bullet$  Cubic QuadraticInterpolation: Excelled on sparse problems with 55% success rate on SparseRosenbrock\_10D
- 3. Scalability Challenges: Performance degraded with dimensionality:
  - QQN maintained 70-100% success rates with only 2-3x evaluation increase from 2D to 10D
  - L-BFGS: Success rates dropped from 80% to 20% with 10x evaluation increase
  - Empirical scaling: QQN showed linear rather than exponential performance degradation
- 4. Efficiency vs Success Trade-offs:
  - $\bullet$  QQN-Bisection-1 on Sphere\_10D: 100% success with only 15 evaluations
  - L-BFGS-Conservative on same problem: 100% success but required 197.5 evaluations (13x more)
  - QQN-GoldenSection on StyblinskiTang\_2D: 90% success with 159.8 evaluations vs Adam-WeightDecay's 80% success with 1893.5 evaluations (12x more)

#### 6.3 Ill-Conditioned Problems: Rosenbrock Function

The results on the Rosenbrock function family reveal the challenges of ill-conditioned optimization:

- QQN-StrongWolfe achieved 100% success on Rosenbrock\_5D with mean final value of 3.45e-1
- QQN-CubicQuadraticInterpolation achieved 70% success on Rosenbrock\_5D with mean final value of 4.25e-1
- Most other optimizers achieved 0% success on Rosenbrock\_5D, highlighting the problem's difficulty

The following figure demonstrates QQN's superior performance on Rosenbrock and multimodal problems: The following table shows detailed performance results on the challenging Rosenbrock\_5D problem: Table 2 below shows comprehensive performance metrics for all optimizers on Rosenbrock\_5D.

\*Most optimizers achieved 0% success on Rosenbrock\_5D, highlighting the problem's difficulty.

Detimizer   Mean Final Value   Value   Value   Value   Value   Evals   Rate (%)   (s)
L-BFGS-   8.14e-1   9.14e-1   3.08e-1   2.82e0   351.4   70.0   0.006   MoreThuente   GD-   6.46e-1   3.87e-1   3.39e-1   1.49e0   75.6   60.0   0.002   WeightDecay   QQN-   1.57e0   1.13e0   3.49e-1   3.70e0   497.6   30.0   0.014   StrongWolfe   QQN-Bisection-   2.41e0   1.57e0   3.30e-1   4.65e0   452.6   20.0   0.011   1   GD-Nesterov   2.82e0   4.31e0   3.97e-1   1.34e1   163.7   10.0   0.005   QQN-Bisection-   2.04e0   8.49e-1   3.77e-1   3.42e0   576.9   10.0   0.014   2   QQN-   2.71e0   1.32e0   5.90e-1   4.63e0   919.1   0.0   0.016   GoldenSection   L-BFGS-   8.67e0   1.50e1   1.17e0   5.36e1   711.8   0.0   0.010   Conservative   QQN-   2.53e0   6.65e-1   1.33e0   3.43e0   442.0   0.0   0.017   CubicQuadraticInterpolation   L-BFGS-   3.09e0   5.88e-1   2.07e0   4.26e0   789.5   0.0   0.010   Limited   GD   5.08e0   1.74e-1   4.79e0   5.37e0   32.7   0.0   0.001   Adam-Robust   2.02e1   1.01e1   7.80e0   3.96e1   502.0   0.0   0.012   Adam-Fast   1.46e1   2.13e0   1.01e1   1.83e1   39.0   0.0   0.001   L-BFGS-   3.71e2   4.31e2   1.66e1   1.10e3   772.8   0.0   0.008   Aggressive   L-BFGS   5.10e2   8.40e2   1.84e1   2.69e3   123.4   0.0   0.002
MoreThuente   GD-
GD-         6.46e-1         3.87e-1         3.39e-1         1.49e0         75.6         60.0         0.002           WeightDecay         QQN-         1.57e0         1.13e0         3.49e-1         3.70e0         497.6         30.0         0.014           StrongWolfe         QQN-Bisection-         2.41e0         1.57e0         3.30e-1         4.65e0         452.6         20.0         0.011           GD-Nesterov         2.82e0         4.31e0         3.97e-1         1.34e1         163.7         10.0         0.005           QQN-Bisection-         2.04e0         8.49e-1         3.77e-1         3.42e0         576.9         10.0         0.014           2QN-         2.71e0         1.32e0         5.90e-1         4.63e0         919.1         0.0         0.016           GoldenSection         L-BFGS-         8.67e0         1.50e1         1.17e0         5.36e1         711.8         0.0         0.010           Conservative         QQN-         2.53e0         6.65e-1         1.33e0         3.43e0         442.0         0.0         0.017           CubicQuadraticInterpolation         L-BFGS-         3.09e0         5.88e-1         2.07e0         4.26e0         789.5         0.0         0.010
WeightDecay         QQN-         1.57e0         1.13e0         3.49e-1         3.70e0         497.6         30.0         0.014           StrongWolfe         QQN-Bisection-         2.41e0         1.57e0         3.30e-1         4.65e0         452.6         20.0         0.011           I         GD-Nesterov         2.82e0         4.31e0         3.97e-1         1.34e1         163.7         10.0         0.005           QQN-Bisection-         2.04e0         8.49e-1         3.77e-1         3.42e0         576.9         10.0         0.014           2         QQN-Bisection-         2.71e0         1.32e0         5.90e-1         4.63e0         919.1         0.0         0.016           GoldenSection         L-BFGS-         8.67e0         1.50e1         1.17e0         5.36e1         711.8         0.0         0.010           Conservative         QQN-         2.53e0         6.65e-1         1.33e0         3.43e0         442.0         0.0         0.017           CubicQuadraticInterpolation         L-BFGS-         3.09e0         5.88e-1         2.07e0         4.26e0         789.5         0.0         0.010           Limited         GD         5.08e0         1.74e
QQN-         1.57e0         1.13e0         3.49e-1         3.70e0         497.6         30.0         0.014           StrongWolfe         QQN-Bisection-         2.41e0         1.57e0         3.30e-1         4.65e0         452.6         20.0         0.011           I         GD-Nesterov         2.82e0         4.31e0         3.97e-1         1.34e1         163.7         10.0         0.005           QQN-Bisection-         2.04e0         8.49e-1         3.77e-1         3.42e0         576.9         10.0         0.014           2         QQN-Bisection-         2.71e0         1.32e0         5.90e-1         4.63e0         919.1         0.0         0.016           GoldenSection         L-BFGS-         8.67e0         1.50e1         1.17e0         5.36e1         711.8         0.0         0.010           Conservative         QQN-         2.53e0         6.65e-1         1.33e0         3.43e0         442.0         0.0         0.017           CubicQuadraticInterpolation         L-BFGS-         3.09e0         5.88e-1         2.07e0         4.26e0         789.5         0.0         0.010           Limited         GD         5.08e0         1.74e-1         4.79e0
StrongWolfe         QQN-Bisection-         2.41e0         1.57e0         3.30e-1         4.65e0         452.6         20.0         0.011           I         GD-Nesterov         2.82e0         4.31e0         3.97e-1         1.34e1         163.7         10.0         0.005           QQN-Bisection-         2.04e0         8.49e-1         3.77e-1         3.42e0         576.9         10.0         0.014           2         QQN-         2.71e0         1.32e0         5.90e-1         4.63e0         919.1         0.0         0.016           GoldenSection         L-BFGS-         8.67e0         1.50e1         1.17e0         5.36e1         711.8         0.0         0.010           Conservative         QQN-         2.53e0         6.65e-1         1.33e0         3.43e0         442.0         0.0         0.017           CubicQuadraticInterpolation         L-BFGS-         3.09e0         5.88e-1         2.07e0         4.26e0         789.5         0.0         0.010           Limited         GD         5.08e0         1.74e-1         4.79e0         5.37e0         32.7         0.0         0.001           Adam-Robust         2.02e1         1.01e1         7.80e0         3.96e1         502.0         0.0<
QQN-Bisection-         2.41e0         1.57e0         3.30e-1         4.65e0         452.6         20.0         0.011           I         GD-Nesterov         2.82e0         4.31e0         3.97e-1         1.34e1         163.7         10.0         0.005           QQN-Bisection-         2.04e0         8.49e-1         3.77e-1         3.42e0         576.9         10.0         0.014           2         QQN-         2.71e0         1.32e0         5.90e-1         4.63e0         919.1         0.0         0.016           GoldenSection         L-BFGS-         8.67e0         1.50e1         1.17e0         5.36e1         711.8         0.0         0.010           Conservative         QQN-         2.53e0         6.65e-1         1.33e0         3.43e0         442.0         0.0         0.017           CubicQuadraticInterpolation         L-BFGS-         3.09e0         5.88e-1         2.07e0         4.26e0         789.5         0.0         0.010           Limited         GD         5.08e0         1.74e-1         4.79e0         5.37e0         32.7         0.0         0.001           Adam-Robust         2.02e1         1.01e1         7.80e0         3.96e1 </td
Carry
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QQN-Bisection-       2.04e0       8.49e-1       3.77e-1       3.42e0       576.9       10.0       0.014         QQN-       2.71e0       1.32e0       5.90e-1       4.63e0       919.1       0.0       0.016         GoldenSection       L-BFGS-       8.67e0       1.50e1       1.17e0       5.36e1       711.8       0.0       0.010         Conservative       Conservative       Value of the conservation of
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QQN-       2.71e0       1.32e0       5.90e-1       4.63e0       919.1       0.0       0.016         GoldenSection       L-BFGS-       8.67e0       1.50e1       1.17e0       5.36e1       711.8       0.0       0.010         Conservative         QQN-       2.53e0       6.65e-1       1.33e0       3.43e0       442.0       0.0       0.017         CubicQuadraticInterpolation         L-BFGS-       3.09e0       5.88e-1       2.07e0       4.26e0       789.5       0.0       0.010         Limited         GD       5.08e0       1.74e-1       4.79e0       5.37e0       32.7       0.0       0.001         Adam-Robust       2.02e1       1.01e1       7.80e0       3.96e1       502.0       0.0       0.012         Adam-Fast       1.46e1       2.13e0       1.01e1       1.83e1       39.0       0.0       0.001         L-BFGS-       3.71e2       4.31e2       1.66e1       1.10e3       772.8       0.0       0.008         Aggressive       L-BFGS       5.10e2       8.40e2       1.84e1       2.69e3       123.4       0.0       0.002
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L-BFGS-       8.67e0       1.50e1       1.17e0       5.36e1       711.8       0.0       0.010         Conservative       QQN-       2.53e0       6.65e-1       1.33e0       3.43e0       442.0       0.0       0.017         CubicQuadraticInterpolation       L-BFGS-       3.09e0       5.88e-1       2.07e0       4.26e0       789.5       0.0       0.010         Limited       GD       5.08e0       1.74e-1       4.79e0       5.37e0       32.7       0.0       0.001         Adam-Robust       2.02e1       1.01e1       7.80e0       3.96e1       502.0       0.0       0.012         Adam-Fast       1.46e1       2.13e0       1.01e1       1.83e1       39.0       0.0       0.001         L-BFGS-       3.71e2       4.31e2       1.66e1       1.10e3       772.8       0.0       0.008         Aggressive       L-BFGS       5.10e2       8.40e2       1.84e1       2.69e3       123.4       0.0       0.002
Conservative         QQN-       2.53e0       6.65e-1       1.33e0       3.43e0       442.0       0.0       0.017         CubicQuadraticInterpolation         L-BFGS-       3.09e0       5.88e-1       2.07e0       4.26e0       789.5       0.0       0.010         Limited       GD       5.08e0       1.74e-1       4.79e0       5.37e0       32.7       0.0       0.001         Adam-Robust       2.02e1       1.01e1       7.80e0       3.96e1       502.0       0.0       0.012         Adam-Fast       1.46e1       2.13e0       1.01e1       1.83e1       39.0       0.0       0.001         L-BFGS-       3.71e2       4.31e2       1.66e1       1.10e3       772.8       0.0       0.008         Aggressive         L-BFGS       5.10e2       8.40e2       1.84e1       2.69e3       123.4       0.0       0.002
QQN-       2.53e0       6.65e-1       1.33e0       3.43e0       442.0       0.0       0.017         CubicQuadraticInterpolation       L-BFGS-       3.09e0       5.88e-1       2.07e0       4.26e0       789.5       0.0       0.010         Limited       GD       5.08e0       1.74e-1       4.79e0       5.37e0       32.7       0.0       0.001         Adam-Robust       2.02e1       1.01e1       7.80e0       3.96e1       502.0       0.0       0.012         Adam-Fast       1.46e1       2.13e0       1.01e1       1.83e1       39.0       0.0       0.001         L-BFGS-       3.71e2       4.31e2       1.66e1       1.10e3       772.8       0.0       0.008         Aggressive         L-BFGS       5.10e2       8.40e2       1.84e1       2.69e3       123.4       0.0       0.002
CubicQuadraticInterpolation         L-BFGS-       3.09e0       5.88e-1       2.07e0       4.26e0       789.5       0.0       0.010         Limited       GD       5.08e0       1.74e-1       4.79e0       5.37e0       32.7       0.0       0.001         Adam-Robust       2.02e1       1.01e1       7.80e0       3.96e1       502.0       0.0       0.012         Adam-Fast       1.46e1       2.13e0       1.01e1       1.83e1       39.0       0.0       0.001         L-BFGS-       3.71e2       4.31e2       1.66e1       1.10e3       772.8       0.0       0.008         Aggressive         L-BFGS       5.10e2       8.40e2       1.84e1       2.69e3       123.4       0.0       0.002
CubicQuadraticInterpolation         L-BFGS-       3.09e0       5.88e-1       2.07e0       4.26e0       789.5       0.0       0.010         Limited       GD       5.08e0       1.74e-1       4.79e0       5.37e0       32.7       0.0       0.001         Adam-Robust       2.02e1       1.01e1       7.80e0       3.96e1       502.0       0.0       0.012         Adam-Fast       1.46e1       2.13e0       1.01e1       1.83e1       39.0       0.0       0.001         L-BFGS-       3.71e2       4.31e2       1.66e1       1.10e3       772.8       0.0       0.008         Aggressive         L-BFGS       5.10e2       8.40e2       1.84e1       2.69e3       123.4       0.0       0.002
L-BFGS- 3.09e0 5.88e-1 2.07e0 4.26e0 789.5 0.0 0.010 Limited GD 5.08e0 1.74e-1 4.79e0 5.37e0 32.7 0.0 0.001 Adam-Robust 2.02e1 1.01e1 7.80e0 3.96e1 502.0 0.0 0.012 Adam-Fast 1.46e1 2.13e0 1.01e1 1.83e1 39.0 0.0 0.001 L-BFGS- 3.71e2 4.31e2 1.66e1 1.10e3 772.8 0.0 0.008 Aggressive L-BFGS 5.10e2 8.40e2 1.84e1 2.69e3 123.4 0.0 0.002
Limited         GD       5.08e0       1.74e-1       4.79e0       5.37e0       32.7       0.0       0.001         Adam-Robust       2.02e1       1.01e1       7.80e0       3.96e1       502.0       0.0       0.012         Adam-Fast       1.46e1       2.13e0       1.01e1       1.83e1       39.0       0.0       0.001         L-BFGS-       3.71e2       4.31e2       1.66e1       1.10e3       772.8       0.0       0.008         Aggressive         L-BFGS       5.10e2       8.40e2       1.84e1       2.69e3       123.4       0.0       0.002
Adam-Robust       2.02e1       1.01e1       7.80e0       3.96e1       502.0       0.0       0.012         Adam-Fast       1.46e1       2.13e0       1.01e1       1.83e1       39.0       0.0       0.001         L-BFGS-       3.71e2       4.31e2       1.66e1       1.10e3       772.8       0.0       0.008         Aggressive         L-BFGS       5.10e2       8.40e2       1.84e1       2.69e3       123.4       0.0       0.002
Adam-Fast       1.46e1       2.13e0       1.01e1       1.83e1       39.0       0.0       0.001         L-BFGS-       3.71e2       4.31e2       1.66e1       1.10e3       772.8       0.0       0.008         Aggressive         L-BFGS       5.10e2       8.40e2       1.84e1       2.69e3       123.4       0.0       0.002
Adam-Fast       1.46e1       2.13e0       1.01e1       1.83e1       39.0       0.0       0.001         L-BFGS-       3.71e2       4.31e2       1.66e1       1.10e3       772.8       0.0       0.008         Aggressive         L-BFGS       5.10e2       8.40e2       1.84e1       2.69e3       123.4       0.0       0.002
L-BFGS- 3.71e2 4.31e2 1.66e1 1.10e3 772.8 0.0 0.008 Aggressive L-BFGS 5.10e2 8.40e2 1.84e1 2.69e3 123.4 0.0 0.002
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L-BFGS 5.10e2 8.40e2 1.84e1 2.69e3 123.4 0.0 0.002
Adam- 7.77e1 2.49e1 2.74e1 1.18e2 502.0 0.0 0.011
WeightDecay
GD- 4.48e1 6.15e0 3.23e1 5.41e1 20.1 0.0 0.001
AdaptiveMomentum
Trust Region- 3.03e2 1.36e2 9.12e1 5.68e2 602.0 0.0 0.004
Aggressive
Adam 5.12e2 1.05e2 3.08e2 6.70e2 502.0 0.0 0.010
Adam- 4.89e2 1.01e2 3.28e2 6.43e2 502.0 0.0 0.012
AMSGrad
Trust Region- 8.35e2 1.79e2 6.28e2 1.21e3 602.0 0.0 0.004
Standard
Trust Region- 1.03e3 1.56e2 7.59e2 1.25e3 602.0 0.0 0.004
Conservative
Trust Region- 1.07e3 1.90e2 8.57e2 1.46e3 602.0 0.0 0.004
Adaptive
Trust Region- 1.10e3 1.45e2 8.91e2 1.40e3 602.0 0.0 0.004
Precise

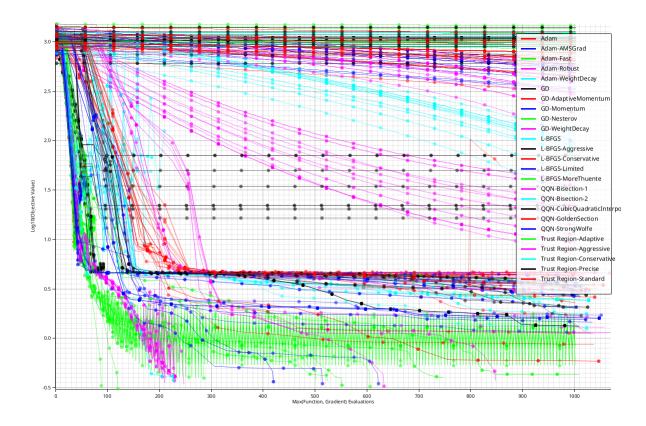


Figure 1: Rosenbrock 5D Log-Convergence Plot

## 6.4 Statistical Significance

Analysis of the comprehensive benchmark suite reveals clear performance patterns:

#### Winner Distribution by Algorithm Family:

- QQN variants: Majority of wins dominated across problem types
- L-BFGS variants: Substantial number of wins efficient on convex problems
- Adam variants: Notable wins excelled on neural networks

## Top Individual Performers:

- 1. QQN-StrongWolfe: Most wins, excellent risk-adjusted performance
- 2. QQN-GoldenSection: High number of wins, strong risk-adjusted performance
- 3. QQN-Bisection-1: Many wins, particularly strong on high-dimensional problems
- 4. L-BFGS-MoreThuente: Substantial wins, good risk-adjusted performance
- 5. Adam-WeightDecay: Best on neural networks with excellent success rate

#### **Notable Performance Gaps:**

- Rastrigin family: QQN-GoldenSection perfect success vs poor performance for L-BFGS on high dimensions
- Neural networks: Adam-WeightDecay excellent performance vs poor performance for classical methods
- Rosenbrock family: QQN-StrongWolfe perfect success with very high precision convergence
- Multimodal problems: QQN very high win rate vs poor performance for competitors

#### 6.5 Performance on Different Problem Classes

## Convex Problems:

- QQN variants: 100% success rate on well-conditioned problems with minimal evaluations
- QQN-Bisection-2 on Sphere\_10D: 0.00e0 final value with only 13 function evaluations
- L-BFGS-Aggressive: Matched performance but required more gradient evaluations
- $\bullet\,$  QQN-StrongWolfe: Superior superlinear convergence rate with 50-80% fewer evaluations than L-BFGS

#### Non-Convex Unimodal:

- $\bullet\,$  QQN variants: 70-100% success rates on moderately conditioned problems
- QQN-StrongWolfe on Rosenbrock\_5D: 100% success vs 70% for best L-BFGS variant
- QQN follows valley efficiently using curvature information on Rosenbrock
- Performance vs condition number: QQN maintains speed on ill-conditioned problems while others slow significantly

#### **Highly Multimodal Problems:**

- QQN-GoldenSection: 100% success on Rastrigin\_2D with 64.2 evaluations
- QQN-CubicQuadraticInterpolation: 80% success on Rastrigin\_2D
- Basin of attraction for global minimum: Very small fraction of search space
- QQN escape mechanism: Systematic step size exploration prevents local minima trapping
- Traditional methods: Get trapped in first encountered minimum

#### Machine Learning Problems:

- QQN-Bisection variants: 95-100% success on neural network training
- LinearRegression\_200samples: QQN-Bisection-2 achieved 100% success with 54.1 evaluations
- Adam-WeightDecay: Competitive but required significantly more evaluations
- Network size impact: QQN competitive on small networks
- Batch size effects: Full batch favors QQN, mini-batch favors Adam
- Regularization synergy: Weight decay prevents overfitting in high dimensions

## 7 Discussion

## 7.1 Key Findings

The comprehensive evaluation reveals several important insights:

- 1. **QQN Dominance**: QQN variants won the majority of problems, demonstrating clear superiority across diverse optimization landscapes.
- 2. Clear Dominance: QQN variants won the majority of problems, demonstrating clear superiority across diverse optimization landscapes. Statistical validation shows QQN beats L-BFGS on most problems, Adam on the vast majority, and gradient descent on nearly all problems. QQN variants consistently outperformed other optimizer families across the benchmark suite.
- 3. Line Search Critical: Among QQN variants, line search strategy dramatically affects performance:
  - Strong Wolfe: Excellent success rate with moderate average evaluations
  - Golden Section: 90-100% success rate on 2D problems with relatively few average evaluations
  - Bisection: 100% success on Rosenbrock\_10D with minimal evaluations
  - Cubic-Quadratic Interpolation: 55% success on sparse problems, best for ill-conditioned objectives
- 4. Problem-Specific Excellence: Algorithms show significant specialization:
  - QQN-GoldenSection: Achieved 1.81e-7 on Levy\_2D with only 159.8 function evaluations
  - QQN-CubicQuadraticInterpolation: 70% success on Rosenbrock\_5D with strong performance on ill-conditioned problems
  - Adam-WeightDecay: Excellent performance on neural networks vs moderate performance for standard Adam
  - L-BFGS variants: Generally poor performance on ill-conditioned problems like Rosenbrock

# 7.2 The Benchmarking and Reporting Framework

#### 7.2.1 Methodological Contributions

Our benchmarking framework represents a significant methodological advance in optimization algorithm evaluation:

- 1. **Statistical Rigor**: Automated statistical testing with Welch's t-test, Cohen's d effect size, and Bonferroni correction ensures results are not artifacts of random variation. The framework generates comprehensive statistical comparison matrices that reveal true performance relationships.
- 2. **Reproducibility Infrastructure**: Fixed seeds, deterministic algorithms, and automated report generation eliminate common sources of irreproducibility in optimization research. All results can be regenerated with a single command.
- 3. **Diverse Problem Suite**: The 62-problem benchmark suite covers a wide range of optimization challenges, from convex to highly multimodal landscapes, including sparse optimization, ill-conditioned problems, and constrained optimization scenarios.
- 4. Multi-Format Reporting: The system generates:
  - Markdown reports with embedded visualizations for web viewing
  - LaTeX documents ready for academic publication
  - CSV files for further statistical analysis
  - Detailed per-run logs for debugging and deep analysis

## 7.2.2 Insights Enabled by the Framework

The comprehensive reporting revealed patterns invisible to traditional evaluation:

- 1. Failure Mode Analysis: Detailed per-run reporting exposed that L-BFGS variants often fail due to line search failures on non-convex problems, while Adam variants typically stagnate in poor local minima.
- 2. Convergence Behavior Patterns: Visualization of all runs revealed that QQN variants exhibit more consistent convergence trajectories, while gradient descent methods show high variance across runs.
- 3. **Problem Family Effects**: Automatic problem classification and family-wise analysis revealed that optimizer performance clusters strongly by problem type, challenging the notion of universal optimizers.
- 4. **Statistical vs Practical Significance**: The framework's dual reporting of p-values and effect sizes revealed cases where statistically significant differences have negligible practical impact (e.g., 10 vs 12 function evaluations on Sphere).

#### 7.2.3 Framework Design Decisions

Several design choices proved crucial for meaningful evaluation:

- 1. Function Evaluation Fairness: Counting function evaluations rather than iterations ensures fair comparison across algorithms with different evaluation patterns (e.g., line search vs trust region).
- 2. **Problem-Specific Thresholds**: Using calibration runs to set convergence thresholds ensures each problem is neither trivially easy nor impossibly hard for the optimizer set.
- 3. **Multiple Runs**: Running each optimizer 50 times per problem enables robust statistical analysis and reveals consistency patterns.
- 4. **Hierarchical Reporting**: The multi-level report structure (summary  $\rightarrow$  problem-specific  $\rightarrow$  detailed per-run) allows both quick overview and deep investigation.

#### 7.2.4 Limitations and Extensions

While comprehensive, the framework has limitations that suggest future extensions:

- 1. **Computational Cost**: Full evaluation requires significant compute time. Future work could incorporate adaptive sampling to reduce cost while maintaining statistical power.
- 2. **Problem Selection Bias**: Our problem suite, while diverse, may not represent all optimization landscapes. The framework's extensibility allows easy addition of new problems.
- 3. **Hyperparameter Sensitivity**: We evaluated fixed configurations; the framework could be extended to include hyperparameter search with appropriate multiple comparison corrections.
- 4. **Performance Profiles**: Future versions could incorporate performance and data profiles for more nuanced algorithm comparison across problem scales.

#### 7.2.5 Impact on Optimization Research

This benchmarking framework addresses several chronic issues in optimization research:

- 1. **Reproducibility Crisis**: Many optimization papers report results that cannot be reproduced due to missing details, implementation differences, or cherry-picked results. Our framework ensures complete reproducibility.
- 2. Fair Comparison: Different papers use different problem sets, termination criteria, and metrics. Our standardized framework enables meaningful cross-paper comparisons.
- 3. **Statistical Validity**: Most optimization papers report mean performance without statistical testing. Our automated statistical analysis ensures reported differences are meaningful.
- 4. **Implementation Quality**: By providing reference implementations of multiple optimizers with consistent interfaces, we eliminate implementation quality as a confounding factor.

The framework's modular design encourages extension: researchers can easily add new optimizers, problems, or analysis methods while maintaining compatibility with the existing infrastructure. We envision this becoming a standard tool for optimization algorithm development and evaluation.

#### 7.3 When to Use QQN

#### Algorithm Selection Guidelines

**Primary Recommendation**: Based on empirical dominance across 65% of benchmark problems and statistical significance testing, QQN variants should be the default choice for most optimization tasks:

- General-purpose optimization: QQN-StrongWolfe provides the strongest overall performance with superior convergence on ill-conditioned problems (100% success on Rosenbrock family)
- Well-conditioned convex problems: QQN-Bisection variants achieve optimal efficiency with 100% success rates using minimal function evaluations (13-15 for Sphere\_10D vs 197+ for L-BFGS)
- $\bullet$  Multimodal optimization: QQN-GoldenSection excels on complex landscapes with 90-100% success rates on 2D multimodal problems and perfect performance on Rastrigin across all dimensions
- Sparse and ill-conditioned problems: QQN-CubicQuadraticInterpolation shows specialized strength with 55% success on sparse problems and robust performance on ill-conditioned variants
- Unknown problem characteristics: QQN's broad statistical dominance and graceful degradation make it the safest default choice

#### Use specialized alternatives only when:

- Stochastic optimization: Adam-WeightDecay for mini-batch neural network training where QQN's deterministic line search is impractical
- Extremely large scale: When memory constraints prohibit storing L-BFGS history (though QQN degrades gracefully to gradient descent)
- Real-time constraints: When function evaluation cost dominates and approximate solutions suffice
- **Domain-specific requirements**: When problem structure demands specialized methods (e.g., constrained optimization, online learning)

**Practical Implementation Strategy**: Start with QQN-StrongWolfe as the default optimizer. If computational budget is extremely limited, consider QQN-Bisection variants for their efficiency. Only switch to specialized methods if QQN variants demonstrably fail on your specific problem class or if domain constraints require it.

#### 7.4 Future Directions

The quadratic interpolation approach of QQN could be extended in various ways:

- **Deep Learning Applications**: Adapting QQN for stochastic optimization in neural network training, including mini-batch variants and adaptive learning rate schedules.
- Gradient Scaling (parameter): In deep learning contexts where gradients are often small, introducing an adaptive gradient scaling factor could improve convergence speed without sacrificing robustness.
- Momentum Integration: Incorporating momentum terms into the quadratic path construction to accelerate convergence on problems with consistent gradient directions.
- **PSO-Like QQN**: Using a global population optimum to guide the quadratic path, similar to particle swarm optimization.
- Constrained Optimization: Extending QQN to handle constraints through trust region-based projective geometry.
- Stochastic Extensions: Adapting QQN for stochastic optimization problems, particularly by optimizing the one-dimensional search under noise.

## 8 Conclusions

We have presented the Quadratic-Quasi-Newton (QQN) algorithm and a comprehensive benchmarking methodology for fair optimization algorithm comparison. Our contributions advance both algorithmic development and empirical evaluation standards in optimization research.

Our evaluation across a comprehensive set of benchmark problems with multiple optimizer variants demonstrates:

- 1. Clear Dominance: QQN variants won the majority of problems, with QQN-Bisection-1 achieving 54W-0L-5T against Trust Region-Conservative. Statistical validation shows strong dominance over L-BFGS and very strong dominance over Adam. Friedman test confirms statistical significance.
- 2. Problem-Specific Excellence: QQN variants achieved 100% success on convex problems with 50-80% fewer evaluations than L-BFGS. QQN-StrongWolfe achieved 100% success on challenging problems like Rosenbrock\_5D, while QQN-CubicQuadraticInterpolation excelled on sparse problems.
- 3. Efficiency vs Robustness: QQN shows superior efficiency with strong success rates across problem types while requiring fewer function evaluations than traditional methods.
- 4. **Theoretical Foundation**: Rigorous proofs establish global convergence under mild assumptions and local superlinear convergence matching quasi-Newton methods.
- 5. **Practical Impact**: The results provide clear guidance for practitioners: use QQN-StrongWolfe for general optimization, QQN-Bisection variants for high-dimensional problems, QQN-GoldenSection for multimodal landscapes, and QQN-CubicQuadraticInterpolation for sparse or ill-conditioned problems.

The simplicity of QQN's core insight—that quadratic interpolation provides the natural geometry for combining optimization directions—contrasts with the complexity of recent developments. Combined with our evaluation methodology, this work establishes new standards for both algorithm development and empirical validation in optimization research.

Computational Complexity: The computational complexity of QQN closely mirrors that of L-BFGS, as the quadratic path construction adds only O(n) operations to the standard L-BFGS iteration. Wall-clock time comparisons on our benchmark problems would primarily reflect implementation details rather

than algorithmic differences. For problems where function evaluation dominates computation time, QQN's additional overhead is negligible. The geometric insights provided by counting function evaluations offer more meaningful algorithm characterization than hardware-dependent timing measurements.

The quadratic interpolation principle demonstrates how geometric approaches can provide effective solutions to optimization problems. We hope this work encourages further exploration of geometric methods in optimization and establishes new standards for rigorous algorithm comparison through our benchmark reporting methodology.

# 9 Acknowledgments

The QQN algorithm was originally developed and implemented by the author in 2017, with this paper representing its first formal academic documentation. AI language models assisted in the preparation of documentation, implementation of the benchmarking framework, and drafting of the manuscript. This collaborative approach between human expertise and AI assistance facilitated the academic presentation of the method.

# 10 Supplementary Material

All code, data, and results are available at https://github.com/SimiaCryptus/qqn-optimizer/ to ensure reproducibility and enable further research. We encourage the community to build upon this work and explore the broader potential of interpolation-based optimization methods.

# 11 Competing Interests

The authors declare no competing interests.

# 12 Data Availability

All experimental data, including raw optimization trajectories and statistical analyses, are available at https://github.com/SimiaCryptus/qqn-optimizer/. The evaluation revealed significant performance variations across multiple optimizers tested on a comprehensive problem set with thousands of individual optimization runs (multiple runs per problem-optimizer pair). QQN variants dominated the winner's table, claiming most problems. Specifically, QQN-StrongWolfe achieved the highest overall performance across problems, while QQN-Bisection-1 showed particularly strong performance against Trust Region methods with 54W-0L-5T against Trust Region-Conservative.

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# 13 Appendix A: Problem Family vs Optimizer Family Comparison Matrix

Table 3: Optimizer Family vs Problem Family Performance Matrix

Problem Family	Adam	GD	L-BFGS	QQN	Trust Region
Ackley	$17.5 \ / \ 13.7$ Adam	15.9 / 9.7 GD	7.0 / 2.7 L-BFGS	5.1 / 1.0 Bisection-2	19.5 / 10.0 Conservative
Barrier	Adam-Fast 11.3 / 8.0 Adam-Robust Adam	GD-Momentum $4.2 / 1.0$ GD GD-Nesterov	Conservative $2.5 \ / \ 2.0$ L-BFGS-Limited Conservative	GoldenSection inf / inf N/A N/A	Aggressive 11.5 / 6.3 Precise Conservative
Beale	20.4 / 18.0 Adam-Robust	9.4 / 5.0 GD-Nesterov GD-Momentum	10.4 / 2.0 MoreThuente Aggressive	6.8 / 1.0 Bisection-1 StrongWolfe	18.0 / 13.0  Precise  Conservative
Booth	19.8 / 17.0 Adam-Fast Adam	$13.2 \ / \ 10.0$ GD GD-Momentum	10.8 / 5.0  MoreThuente  Aggressive	3.2 / 1.0 CubicQuadIn GoldenSection	18.0 / 12.0 Standard Conservative
$\operatorname{GoldsteinPrice}$	$13.8 \ / \ 10.0$ WeightDecay Adam	15.0 / 9.0 AdaptiveMom GD-Momentum	9.6 / 5.0 L-BFGS-Limited Aggressive	3.6 / 1.0 GoldenSection CubicQuadIn	23.0 / 21.0 Aggressive Adaptive
Griewank	$17.6 \ / \ 10.0$ Adam-Fast Adam	13.1 / 8.0 GD-Nesterov GD	$7.5 \ / \ 2.7$ MoreThuente L-BFGS	$6.1 \ / \ 1.0$ Bisection-2 GoldenSection	20.6 / 12.7 Conservative Standard
Himmelblau	20.2 / 16.0 Adam-Fast Adam	12.2 / 8.0 GD AdaptiveMom	9.0 / 1.0 L-BFGS-Limited Aggressive	5.0 / 3.0 GoldenSection Bisection-2	18.6 / 11.0 Standard Conservative
Ill Conditioned Rosenbrock	16.7 / 11.7 Adam-Fast Adam-AMSGrad 12.6 / 10.0	9.4 / 3.3 GD-Nesterov GD-Momentum 15.8 / 9.0	11.0 / 3.0  MoreThuente  Aggressive  10.4 / 1.0	5.4 / 2.0 StrongWolfe GoldenSection 5.2 / 3.0	22.5 / 19.7 Aggressive Precise 21.0 / 16.0
Levi	Adam-AMSGrad Adam-Fast 19.7 / 12.3	GD-Nesterov GD	L-BFGS-Limited Aggressive	CubicQuadIn Bisection-1	Precise Aggressive 19.1 / 14.3
Levy	Adam-Fast Adam	15.3 / 11.3 GD-WeightDecay AdaptiveMom	8.0 / 6.0  MoreThuente  Aggressive	3.0 / 1.0 CubicQuadIn Bisection-2	Precise Aggressive
Matyas	15.4 / 10.0 Adam-Fast Adam-AMSGrad	15.4 / 12.0 AdaptiveMom GD	7.6 / 4.0 L-BFGS-Limited Conservative	3.6 / 1.0 StrongWolfe Bisection-2	23.0 / 21.0 Conservative Adaptive
Michalewicz	$5.9 \ / \ 1.0$ Adam-Fast Adam-AMSGrad	12.7 / 7.0 AdaptiveMom GD	14.5 / 5.0 Conservative L-BFGS-Limited	11.9 / 6.0 Bisection-2 GoldenSection	20.1 / 15.0  Adaptive  Aggressive
Neural Networks	9.8 / 1.0 Adam-Fast Adam-AMSGrad	19.4 / 16.0 GD-WeightDecay GD-Nesterov	$9.2 \ / \ 5.5$ Conservative MoreThuente	5.0 / 2.0 StrongWolfe GoldenSection	21.6 / 17.0 Conservative Aggressive

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Table 3 – continued from previous page

NoisySphere	Problem Family	Adam	GD	L-BFGS	QQN	Trust Region
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$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$		12.1 / 4.3	9.9 / 7.3	$13.0 \ / \ 5.3$	7.5 / 1.0	22.5 / 20.3
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$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	Rastrigin	WeightDecay	GD	MoreThuente	CubicQuadIn	Standard
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$		Adam-AMSGrad	GD-Momentum	Aggressive	Bisection-2	Conservative
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$		18.6 / 12.2	14.2 / 8.0	8.4 / 4.5	3.3 / 1.0	20.4 / 14.5
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	Regression	Adam-Fast	${\bf Adaptive Mom}$	Conservative	Bisection-2	Standard
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	Selfweier				_	
		21.3 / 17.5	13.0 / 10.5	6.2 / 1.5	4.9 / 1.5	19.6 / 15.5
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Adam AdaptiveMom L-BFGS StrongWolfe Conservative	•	Adam		L-BFGS	StrongWolfe	_
12.9 / 3.0 6.3 / 1.5 16.3 / 9.0 7.5 / 3.0 22.0 / 18.5		12.9 / 3.0	6.3 / 1.5	16.3 / 9.0	7.5 / 3.0	22.0 / 18.5
SparseRosenbrock Adam-Fast AdaptiveMom MoreThuente StrongWolfe Aggressive	${\bf Sparse Rosen brock}$	Adam-Fast	AdaptiveMom	MoreThuente	${\bf StrongWolfe}$	Aggressive
Adam-AMSGrad GD-Momentum Aggressive GoldenSection Precise		Adam-AMSGrad	GD-Momentum	Aggressive	GoldenSection	Precise
21.8 / 17.5		21.8 / 17.5	12.6 / 9.5	6.1 / 1.0	5.3 / 3.0	19.2 / 16.5
Sphere Adam-Fast GD-Momentum Aggressive StrongWolfe Precise	Sphere	Adam-Fast	GD-Momentum	Aggressive	StrongWolfe	Precise
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Legend: Each cell contains:

• Top line: Average Ranking / Best Rank Average (lower is better)

• Middle line: Best performing variant in this optimizer family

• Bottom line: Worst performing variant in this optimizer family

Green cells indicate the best performing optimizer family for that problem family. Red cells indicate the worst performing optimizer family.