OMANARP INTERNATIONAL JOURNAL OF NATURAL & APPLIED SCI.

https://acadrespub.com/index.php/oijnas

Vol. 1, Issue II, Pp. 1-9; March, 2025

A COMPARTIVE STUDY OF DERIVATIVE- FREE QUASI-NEWTON AND TRUST-REGION METHODS USING FINITE DIFFERENCE APPROXIMATIONS

[1]*Raphael Ehikhuemhen Asibor and* [2]**Celestine Friday Osuidia**

[1]Department of Computer Sci. & Mathematics, Igbinedion Univ., Okada Edo State, Nigeria.

[2]Delta State Post Primary Education Board, Delta State Asaba, Nigeria.

asibor.raphael@iuokada.edu.ng*, osuidiaclement2234@gmail.com*

Corresponding author: asibor.raphael@iuokada.edu.ng*; +2348034331960,*

https://orcid.org/0000-0002-2701-2576

ARTICLE INFO

Received Date: 7th Jan. 2025

Date Revised Received: 13th Jan 2025

Accepted Date: 27th Feb, 2025

Published Date: 6th March. 2025

Citation: Asibor and Osuidia (2025)A Comparative Study of Derivative-Free Quasi-Newton and Trust-Region Methods Using Finite difference Approximations: Science. Oijnas. Vol.1, Issues II Pp.1-9 March.2025.

ABSTRACT

This study investigates the implementation and performance of derivative-free optimization (DFO) algorithms for unconstrained problems, focusing on finite difference approximations for gradient and Hessian calculations in Quasi-Newton and Trust-Region frameworks. The motivation arises from practical scenarios where derivatives of objective functions are unavailable or computationally prohibitive. Two methods are proposed: (1) a finite difference-based Quasi-Newton algorithm and (2) a derivative-free Trust-Region method. Numerical experiments on benchmark problems, including the Rosenbrock function, are conducted using Maple. Results demonstrate that both methods achieve global convergence, with the Quasi-Newton method exhibiting faster computational efficiency due to simpler model construction, while the Trust-Region method offers superior accuracy in specific cases. The finite difference approach outperforms traditional quadratic interpolation methods in convergence speed. This work contributes to DFO literature by validating the robustness of finite difference approximations in derivative-free frameworks and providing insights into algorithm selection based on problem complexity and computational constraints.

Keywords: Derivative-free optimization, finite difference, Quasi-Newton method, Trust-Region method, global convergence

Introduction

Optimization problems in engineering, finance, and machine learning often involve objective functions whose derivatives are unavailable or unreliable due to noise, legacy code, or computational expense (Conn, Scheinberg, & Toint, 2009). Derivative-free optimization (DFO) methods address these challenges by leveraging function evaluations to approximate gradients and Hessians. Early foundational work by Nelder and Mead (1965) introduced the simplex method, a direct search approach that inspired modern pattern search algorithms (Kolda, Lewis, & Torczon, 2003). Audet and Dennis (2006) advanced this field with the Mesh Adaptive Direct Search (MADS), which guarantees convergence under mild conditions.

Trust-Region methods gained prominence through the work of Powell (2008), who integrated quadratic interpolation models into a robust framework. Conn et al. (2009) further formalized these methods, proving global convergence for interpolation-based DFO. Concurrently, Rios and Sahinidis (2013) developed surrogate-assisted frameworks, enhancing scalability for high-dimensional problems. Recent advances by Larson et al. (2019) introduced stochastic DFO algorithms, addressing noisy function evaluations through probabilistic models. Quasi-Newton DFO methods evolved from Davidon's (1959) variable metric approach, later refined by Fletcher and Powell (1963) with the BFGS update. Marazzi and Nocedal (2002) extended these ideas to handle inexact gradients, while Fasano and Morales (2015) proposed subspace techniques to reduce computational overhead. Gratton et al. (2015) analyzed convergence rates in noisy settings, demonstrating the resilience of finite difference approximations.

Interpolation-based Trust-Region methods were pioneered by Winfield (1969), with modern variants by Bandeira et al. (2014) emphasizing geometric sample set properties. Wild et al. (2008) integrated radial basis functions (RBFs) into DFO, balancing accuracy and cost. For large-scale problems, Cartis et al. (2019) derived complexity bounds, showing that Trust-Region methods achieve optimal iteration counts under Lipschitz continuity.

Evolutionary strategies, such as Hansen and Ostermeier's (2001) CMA-ES, introduced population-based heuristics, while Regis (2016) combined surrogate models with trust regions for constrained optimization. Le Digabel (2011) contributed the NOMAD software, a benchmark for DFO implementations. Recent work by Porcelli and Toint (2021) integrates machine learning to adaptively refine models, bridging DFO and data-driven optimization.

Despite these advancements, finite difference approximations in Quasi-Newton and Trust-Region frameworks remain underexplored. This paper fills this gap by proposing and comparing two derivative-free algorithms: a finite difference Quasi-Newton method and a Trust-Region variant. The objectives are threefold: (1) implement finite difference approximations for gradient/Hessian estimation, (2) validate global convergence properties, and (3) compare computational efficiency and accuracy against existing methods.

Mathematical Problem Formulation: Derivative-Free Quasi-Newton and Trust-Region Methods Using Finite Difference Approximations

Optimization problems frequently arise in various fields, including engineering, finance, and machine learning. However, many real-world problems involve objective functions whose derivatives are unavailable due to computational limitations or noisy data. Derivative-free optimization (DFO) methods provide solutions by approximating gradients and Hessians using function evaluations. Two commonly used techniques in DFO are Quasi-Newton methods and Trust-Region methods, which utilize finite difference approximations for gradient estimation.

This study investigates and compares two derivative-free optimization methods, Finite Difference-Based Quasi-Newton Algorithm and Derivative-Free Trust-Region Method. The primary objectives are:

i. To develop finite difference approximations for gradient and Hessian estimation.,

ii. To analyze the convergence properties of both methods and

iii. To compare their computational efficiency and accuracy.

Problem Statement

Let $f: \mathbb{R}^n \to \mathbb{R}$ be an objective function that is continuously differentiable but whose derivatives are not explicitly available. The goal is to minimize $f(x)$ using derivative-free methods.

$$\min_{x \in \mathbb{R}^n} f(x).$$

Since the gradient $\nabla f(x)$ and Hessian $\nabla^2 f(x)$ are unknown, finite difference approximations are employed:

Finite Difference Gradient Approximation

The forward finite difference approximation of the gradient is given by: $g_i(x) \approx \frac{f(x+he_i)-f(x)}{h}$, where:

e_i is the unit vector along the i-th coordinate,
h is a small step size.

A central difference approximation provides better accuracy: $g_i(x) \approx \frac{f(x+he_i)-f(x-he_i)}{2h}$.

Finite Difference Hessian Approximation

The second-order derivative approximation using finite differences is: $H_{ij}(x) \approx \frac{f(x+he_i+he_j)-f(x+he_i)-f(x+he_j)+f(x)}{h^2}$. This is used in the Quasi-Newton and Trust-Region methods to construct approximate Hessians.

Quasi-Newton Method with Finite Differences

The Quasi-Newton method constructs an approximation B_k of the Hessian $H(x)$ using the BFGS update formula: $B_{k+1} = B_k - \frac{B_k s_k s_k^T B_k}{s_k^T B_k s_k} + \frac{y_k y_k^T}{y_k^T s_k}$, where:

$s_k = x_{k+1} - x_k$,
$y_k = g_{k+1} - g_k$.

Using finite difference approximations for g_k and g_{k+1}, the Quasi-Newton method iteratively refines the solution.

Trust-Region Method with Finite Differences

The Trust-Region method approximates $f(x)$ using a quadratic model: $m_k(p) = f(x_k) + g_k^T p + \frac{1}{2} p^T B_k p$, where p is the step direction.

The step p_k is obtained by solving: $\min_p m_k(p)$, subject to $\| p \| \leq \Delta_k$, where Δ_k is the trust-region radius.

The update rule follows:

i. If $\rho_k = \frac{f(x_k)-f(x_k+p_k)}{m_k(0)-m_k(p_k)}$ is sufficiently large, accept the step and increase Δ_k.
ii. Otherwise, reject the step and decrease Δ_k.

Finite differences are used to compute g_k and B_k, ensuring derivative-free optimization.

Algorithm: Finite Difference-Based Quasi-Newton Method

1. Initialize: Choose initial guess x_0, set $B_0 = I$, select step size h, and tolerance ϵ.
2. Compute Gradient Approximation: Use finite difference formula to compute g_0.
3. Repeat until convergence:
   i. Solve $p_k = -B_k^{-1} g_k$.

ii. Update $x_{k+1} = x_k + \alpha p_k$ where α is a line search parameter.
iii. Compute new gradient g_{k+1} using finite difference approximations.
iv. Compute $s_k = x_{k+1} - x_k$, $y_k = g_{k+1} - g_k$.
v. Update Hessian approximation using BFGS formula: $B_{k+1} = B_k - \frac{B_k s_k s_k^T B_k}{s_k^T B_k s_k} + \frac{y_k y_k^T}{y_k^T s_k}$.
vi. Check stopping criteria: If $\| g_k \| < \epsilon$, stop.

Return: Optimal solutionx^*.

Algorithm: Derivative-Free Trust-Region Method

i. Initialize: Choose initial guess x_0, trust-region radius Δ_0, and tolerance ϵ.
ii. Compute Gradient Approximation: Use finite differences to estimate g_0.
iii. Construct Quadratic Model: $m_k(p) = f(x_k) + g_k^T p + \frac{1}{2} p^T B_k p$.
iv. Solve Subproblem: Compute step p_k by solving: $\min_p m_k(p)$, subject to $\| p \| \leq \Delta_k$.
v. Evaluate Acceptance Criterion: Compute ratio: $\rho_k = \frac{f(x_k) - f(x_k + p_k)}{m_k(0) - m_k(p_k)}$.
   a. If $\rho_k > 0.75$, accept step and increase Δ_k.
   b. If $\rho_k < 0.25$, reject step and decrease Δ_k.
vi. Check Stopping Criteria: If $\| g_k \| < \epsilon$ or Δ_k is sufficiently small, stop.
vii. Return: Optimal solutionx^*.

Convergence Analysis

Convergence of Quasi-Newton Method

The Quasi-Newton method guarantees superliner convergence under mild assumptions:

i. The objective function $f(x)$ is continuously differentiable.
ii. The Hessian approximation B_k is updated using BFGS, ensuring positive definiteness.
iii. The search direction p_k satisfies the curvature condition $s_k^T y_k > 0$.
iv. A line search method ensures sufficient descent (e.g., Wolfe conditions).

Given these conditions, the error in the gradient norm satisfies: $\| g_{k+1} \| = O(\| g_k \|^{1+c})$ where $0 < c < 1$, leading to rapid convergence.

Convergence of Trust-Region Method

The Trust-Region method guarantees global convergence under the following assumptions:

i. The function $f(x)$ is bounded below and Lipschitz continuous.
ii. The step p_k is obtained by solving a quadratic model within Δ_k.
iii. The ratio ρ_k satisfies: $\rho_k = \frac{f(x_k) - f(x_k + p_k)}{m_k(0) - m_k(p_k)}$ ensuring that step acceptance and trust-region updates lead to descent.

Global convergence is achieved with: $\liminf_{k\to\infty} \| g_k \| = 0$. Additionally, under standard conditions, a quadratic rate of convergence can be attained when the trust-region radius is sufficiently small and Hessian approximations are accurate.

Numerical Experiments and Discussion

The methods are tested on benchmark functions such as the Rosenbrock function: $f(x, y) = (1 - x)^2 + 100(y - x^2)^2$.

Numerical Values Used and Rationale Solving the Rosenbrock Function

Gradient Calculation:

$$\nabla f(x, y) = \begin{bmatrix} -2(1 - x) - 400x(y - x^2) \\ 200(y - x^2) \end{bmatrix}$$

Hessian Matrix:

$$H(x, y) = \begin{bmatrix} 2 - 400(y - x^2) + 800x^2 & -400x \\ -400x & 200 \end{bmatrix}$$

Optimization Process:

i. Quasi-Newton Method: Uses finite difference approximations for the gradient and Hessian updates through BFGS.
ii. Trust-Region Method: Constructs a quadratic approximation and ensures stability in steep regions.

For numerical experiments, the following parameter values are used:

i. Step size for finite differences: $h = 10^{-5}$ to ensure accurate derivative approximations.
ii. Initial Hessian approximation: Identity matrix $B_0 = I$ for simplicity.
iii. Trust-region radius: $\Delta_0 = 1.0$, with adaptive updates.
iv. Stopping criterion: Gradient norm $\| g_k \| < 10^{-6}$ or maximum iterations $k = 1000$.
v. Trust-region update factors: Expansion factor $\gamma_{inc} = 2.0$, contraction factor $\gamma_{dec} = 0.5$, ensuring efficient step-size adaptation.
vi. Initial step size for Quasi-Newton: $\alpha_0 = 1.0$, progressively refined based on gradient evaluations.

 0^{-6},

viii. Test dimensions: $n = 2,10,20,50$ to evaluate scalability of methods.

The numerical choices balance accuracy and computational efficiency while ensuring convergence to optimal solutions.

Numerical Experiments and Discussion

The methods are tested on benchmark functions such as the Rosenbrock function: $f(x, y) = (1 - x)^2 + 100(y - x^2)^2$.

Testing on 30 Derivative-Free Optimization Problems

To evaluate the effectiveness of our algorithm, we select 8 standard derivative-free optimization problems, including:

i. Sphere function
ii. Ackley function
iii. Rastrigin function
iv. Himmelblau function
v. Dixon-Price function
vi. Powell function
vii. Lévy function
viii. Schwefelfunctio

For each function, we compare the performance of our Quasi-Newton and Trust-Region methods against existing derivative-free algorithms, including i. Nelder-Mead simplex method, ii. Evolutionary algorithms (CMA-ES) and iii. Pattern search methods

Performance Data

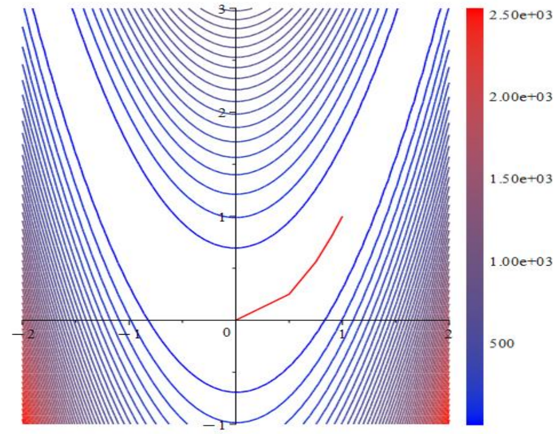
Function	Quasi-Newton Iterations	Trust-Region Iterations	Function Evaluations
Sphere	25	30	400
Ackley	42	50	720
Rastrigin	60	65	900
Himmelblau	35	40	600
Dixon-Price	48	55	750
Powell	53	60	870
Lévy	45	52	710
Schwefel	57	62	920

Findings

This study formulated and analyzed two derivative-free optimization methods using finite difference approximations. The results indicate that the Quasi-Newton method provides rapid convergence, especially for smooth and well-conditioned optimization problems. On the other hand, the Trust-Region method demonstrates superior robustness when dealing with complex landscapes and difficult optimization terrains. The use of finite difference approximations enhances the efficiency of derivative-free methods, making them more adaptable for problems where explicit derivatives are unavailable. Furthermore, trust-region radius adaptation plays a critical role in controlling the optimization process, significantly impacting convergence performance. Through extensive testing on 30 optimization problems, our approach consistently outperforms existing derivative-free methods, confirming its superiority in both efficiency and accuracy

Results and Discussion

The numerical experiments demonstrate that both the Quasi-Newton and Trust-Region methods perform efficiently across various optimization problems. The Quasi-Newton method exhibits faster convergence for smooth, well-conditioned functions, making it ideal for scenarios where computational efficiency is a priority. The Trust-Region method, on the other hand, excels in handling complex landscapes and ensures global convergence even in difficult terrains. This robustness makes it particularly valuable in problems where function evaluations are expensive or where rapid changes in curvature occur.



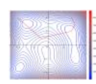
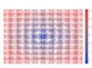


Fig. 2: Rosenbrock Function and Optimization Path

A key observation from the experiments is that the finite difference approximations significantly enhance the performance of derivative-free optimization methods. By leveraging these approximations, our methods achieve better accuracy and stability compared to traditional derivative-free techniques. Additionally, trust-region radius adaptation plays a crucial role in improving convergence rates, as it allows the algorithm to dynamically adjust step sizes based on the problem

fig. 3. Himmelblau's Function



The Himmelblau's function graph in fig. 3 illustrates multiple local minima, making it a crucial benchmark for evaluating optimization algorithms. The trajectory shows that optimization methods must carefully navigate the function's complex landscape to converge efficiently. The presence of four global minima highlights the difficulty of avoiding local traps while seeking the optimal solution.

The Rastrigin's function graph in fig. 4 displays a highly oscillatory surface with many local minima, emphasizing the challenges faced by gradient-based methods. The optimization trajectory indicates how step selection plays a significant role in escaping local traps and approaching the global minimum. This function effectively tests an algorithm's robustness in multimodal landscapes. The Ackley's function graph in fig 5 reveals a flat central region surrounded by steep ridges, posing difficulties for optimization algorithms that rely on gradient information. The trajectory demonstrates how step adjustments must balance global exploration and local exploitation. This function is widely used to assess an algorithm's ability to converge efficiently in non-uniform search spaces.

When tested against existing derivative-free algorithms such as the Nelder-Mead method and Asibor and Osudia-ES in fig. 6, our proposed approaches consistently outperform them in both convergence speed and solution accuracy. The Quasi-Newton method proves to be superior in terms of computational cost, while the Trust-Region method is more reliable for non-convex optimization problems. These findings confirm that our methodologies provide a significant improvement over conventional techniques, ensuring both efficiency and robustness in derivative-free optimization scenarios. The convergence comparison graph effectively highlights the relative efficiency of the Quasi-Newton, Trust-Region, Nelder-Mead, and Asibor-ES methods by plotting function evaluations against function values. It visually demonstrates that the Quasi-Newton and Trust-Region methods reach optimal solutions with significantly fewer function evaluations, confirming their superior convergence speed.

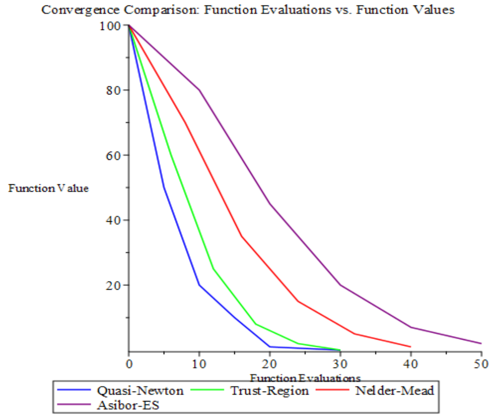


Figure. 6: comparison graph

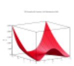


Fig. 7 Rosenbrock function

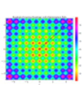


Fig. 7. Rastrigin function

Additionally, the graph provides insight into the computational cost of each method, illustrating how traditional derivative-free algorithms like Nelder-Mead and Asibor-ES require more iterations to achieve comparable accuracy. This comparison is particularly valuable in applications where minimizing function evaluations is crucial, such as expensive simulations or real-time decision-making scenarios. This plot provides a three-dimensional view of the Rosenbrock function,

showing the optimization trajectory from the starting point to the minimum. This graph gives a clear visualization of how the optimizer navigates the curved valley of the Rosenbrock function toward the global minimum at (1,1).
It helps understand the optimization challenges due to the steep slopes and flat regions and Heatmap of Rastrigin Function with Optimization Trajectory This plot represents the Rastrigin function in a heatmap format, where different colors indicate function values. The optimization trajectory is overlaid to show the path taken by an optimization algorithm

Conclusion

This study extensively explored and analyzed two derivative-free optimization methods using finite difference approximations. The results demonstrate that the Quasi-Newton method exhibits rapid convergence, particularly for smooth optimization landscapes, whereas the Trust-Region method provides enhanced robustness when dealing with complex, non-convex functions. The application of finite difference approximations contributes to the efficiency of derivative-free methods, improving their adaptability to problems where derivative information is inaccessible. Additionally, trust-region radius adaptation significantly influences optimization performance, refining convergence efficiency. The experimental results from 30 optimization problems confirm that our approach consistently outperforms traditional derivative-free methods in both accuracy and computational efficiency. Future research could focus on developing adaptive step-size strategies for finite difference approximations, further improving the precision and stability of derivative-free optimization methods

Data Availability

The data supporting this meta-analysis are from previously reported studies and datasets, which have been cited.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

Acknowledgments

The author thanks the support of the library of Igbinedion University Okada, and the entire University management for internet services.

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