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An extended iterative algorithm for solving nonlinear systems and differential equations

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Abstract

An extended iterative algorithm for solving nonlinear systems and ordinary differential equations (ODE) is presented in this paper which is efficient. Convergence difficulty, high computation cost and instability are the obstacles of using traditional methods like Newton method and explicit Runge-Kutta methods for stiff problems. In this approach proposed, we enhance numerical stability and bring about the convergence speed by introducing a modifed Jacobian matrix. To solve multi variable nonlinear systems, the algorithm is structured such that it adapts to a dynamically varied update step, which reduces the sensitivity toward the initial conditions. Furthermore, for ODEs we apply an implicit numerical integration combining with the modified Jacobian so that it is well suited to stiff and high dimensional systems. It is shown by theoretical analysis that the nonlinear equations converge superlinearly and numerical experiments are used to show that the methods perform better than classical approaches in terms of accuracy and efficiency. It is used for engineering simulations as well as machine learning optimization problems. The method will be extended to partial differential equations (PDEs) as future work, as will adaptively choosing the step size for further improvements in the computation.

Mathematics Subject Classification: 65H10, 65L05, 65L20

Key words and phrases: Nonlinear systems, Iterative algorithms, Modified Jacobian, Ordinary differential equations, Numerical stability, Convergence analysis.

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1. Introduction

The major challenge in solving nonlinear systems and differential equations lies in many scientific and engineering realms. Such systems appear in physics and engineering as well as in finance and machine learning, and it is important to solve such systems efficiently for optimization, modeling and simulation tasks. Also regular differential equations (ODEs) are of such great importance in their description dynamic processes such as chemical reactions, biological systems, and mechanical vibrations. In many practically important situations, the cost associated with applying traditional numerical methods is often high, even though convergence may be very slow, or may converge only with sensitivity to certain initial conditions.

However, due to quadratic convergence of Newton Raphson versus linear convergence of other methods, Newton Raphson is commonly used to solve nonlinear equations. Nevertheless, it is highly sensitive to the quality of initial guesses, and has to compute explicit Jacobians at a critical point, which may be computational expensive, especially in high dimensions. Other algebraic or quasi-Newton methods (e.g., Broyden's), trying to reduce computation expenses, approximate the Jacobian, but suffer pains when operating in stiff or ill conditioned systems. Explicit Runge-Kutta methods are also popular for ODE solving, but due to their simplicity and ease of implementation, they have the shortcomings of being unstable for stiff problems that must be solved with implicit schemes. However, such implicit solvers such as the Backward Differentiation Formula (BDF) provide better stability at the cost of additional computational burden, in general due to nonlinear systems that have to be solved at each time step.

In response, this paper provides an extended iterative algorithm that introduces a modified Jacobian structure in order to improve numerical stability and speed of convergence. The method improves the robustness of nonlinear system solvers by incorporating a dynamically adjusted Jacobian update, which helps acquiring good solutions, while being insensitive to initial conditions sensitivity. In addition, the approach is well suited to stiff problems, where explicit methods fail, for differential equations it integrates an implicit numerical scheme. Such a combination allows a more efficient and stable way of solving both nonlinear systems and ODEs and it applies to a wide class of scientific and engineering problems.

We theoretically and numerically analyze that not only is the proposed algorithm accurate, but it is also (much) more efficient and (much) more stable than existing methods. However, the results indicate that this extended iterative approach is very likely to make a great impact on scientific computing, engineering simulation, and other optimization tasks for which standard solvers are lacking in terms of computational cost and convergence. The method reduces computational cost by reducing dependence on direct Jacobian inversion and using adaptive updates, and maintains high accuracy, and therefore is well suited for large scale and high dimensional problems.

In this remainder of the paper, we present a literature review of existing methods, through an overview on the present iterative solvers and their limits. Section 3 presents the iterative algorithm for solving nonlinear systems which is proposed in the thesis, the modified Jacobian approach and how the proposed method has computational advantages over the existing methods. In Section 4, the methodology is extended to differential equations, and it is shown how using the latter can provide stability for implicit numerical methods. In Section 5 a convergence analysis of the algorithm is given and in Section 6 numerical experiments are described that compare its performance to those of traditional methods. In the final section Section 7, the results are summarized and then the potential future research directions are identified.

2. Literature review

This literature review provides a comprehensive overview of existing iterative methods for solving nonlinear systems and differential equations. Below is a detailed explanation of each aspect discussed [1–3].

2.1 Newton-Raphson method

The Newton-Raphson method is one of the most widely used iterative techniques for solving nonlinear equations. It is based on a first-order Taylor series expansion of a nonlinear function $F(x)$, which leads to the update formula [1, 2]:

$$x_{k+1} = x_k - J^{-1}(x_k)F(x_k)$$

Where $J(x_k)$ is the Jacobian matrix of $F(x)$. This method exhibits quadratic convergence, meaning that once a solution is close to the root, the error decreases rapidly with each iteration. However, the method has significant limitations are Sensitivity to Initial Guesses: Poor initial estimates can lead to divergence or slow convergence [2], Computational Cost: The requirement to compute and invert the Jacobian matrix at each iteration makes it expensive, particularly for high-dimensional systems,Failure in Singular or Nearly Singular Jacobians: If the Jacobian is ill-conditioned or singular [4], the method struggles to find a solution [1, 3].

2.2 Quasi-Newton Methods: Broyden's Method & Secant Method

To overcome the drawbacks of the Newton-Raphson method, researchers developed quasi-Newton methods, which approximate the Jacobian matrix rather than computing it explicitly [6, 8]. Broyden's Method: This is a quasi-Newton method that approximates the Jacobian using rank-one updates, significantly reducing computational effort [6]. Instead of computing $J(x_k)$ directly, Broyden's method updates it iteratively:

$$J_{k+1} = J_k + \frac{\left(F(x_{k+1}) - F(x_k) - J_k(x_{k+1} - x_k)\right)(x_{k+1} - x_k)^T}{(x_{k+1} - x_k)^T(x_{k+1} - x_k)}$$

This allows for an adaptive approach that avoids full Jacobian recomputation, reducing cost while maintaining reasonable convergence speed.Secant Method: The secant method is another derivative-free approach that approximates the derivative using finite differences, making it useful when analytical derivatives are difficult to compute. However, it converges more slowly compared to Newton's method [3].

Trust-region methods have been developed as a robust alternative to traditional Newton-type methods, particularly for solving optimization problems involving nonlinear equations [4, 10]. These methods enhance numerical stability by dynamically adjusting step sizes based on a predefined "trust region," within which the model is considered to be a reliable approximation of the true function. Instead of taking full Newton steps, which can sometimes lead to divergence or instability in ill-conditioned problems, trust-region algorithms solve a constrained optimization problem within the defined region. If a step remains within the trust region and sufficiently improves the objective function, it is accepted; otherwise, the trust region is adjusted accordingly. This adaptive mechanism prevents excessively large or overly aggressive steps that might lead to numerical instability. Trust-region methods are particularly effective for handling ill-conditioned problems where traditional Newton-based methods struggle due to sensitivity to initial conditions or singular Jacobians [9]. Their ability to maintain stability while ensuring steady convergence has made them a fundamental approach in nonlinear optimization, scientific computing, and machine learning applications, where solving complex nonlinear systems with reliability is crucial.

2.3 Implicit methods for differential equations

For solving ordinary differential equations (ODEs), particularly stiff equations, explicit methods like Euler's method and Runge-Kutta methods struggle because they require excessively small step sizes for stability [5, 7]. Implicit methods address this by solving for the next step using an implicit function.Backward Euler Method: This is an implicit method where the next step y_{n+1} is found by solving:

$$y_{n+1} = y_n + hf\left(y_{n+1}, t_{n+1}\right)$$

Since y_{n+1} appears on both sides, a nonlinear system must be solved at each step, often using Newton's method [2, 5]. Backward Differentiation Formula (BDF): BDF methods generalize Backward Euler by using multi-step formulations, allowing for higher-order accuracy. These methods are commonly used in software like MATLAB's ODE15s solver for stiff problems [5].

2.4 Rosenbrock methods

Reduction in computational burden of solving the nonlinear systems in each timestep has led to development of Rosenbrock methods as an efficient alternative to fully implicit solvers [7]. Again, these methods achieve this by approximating the inverse of the Jacobian matrix, so that expensive full nonlinear solves (with stability and accuracy) aren't needed. As compared to the implicit methods which need to solve the nonlinear equations iterations at each step, Rosenbrock methods linearize the system by a one step approximation to lead to a sequence of linear solves. Rosenbrock methods have this computational complexity, which is substantially lower than that of direct nonlinear solvers, and is suitable especially for large scale problems for which direct nonlinear solvers become unfeasible [5]. In addition, these methods have a good stability [9], which is important for stiff differential equation because explicit methods have step size restrictions. Rosenbrock methods utilize a very successful combination of efficiency, stability and scalability to solve in solutions of complex dynamical systems, all the while achieving high accuracy, and play an important role in numerical simulations in a wide range of scientific and engineering domains. Spectral decomposition methods analyze the eigenvalues of Jacobian matrix to compute optimal step sizes and improve the stability of iterative solver [8]. These methods provide the adaptive refinement of such numerical approximations based on spectral information by adaptingively limiting computations without sacrificing convergence behavior. At the same time, in that parallel, machine learning assisted solvers are entering as a promising direction of numerical analysis where artificial intelligence is applied on iterative solution strategies. In particular, these AI driven solvers make predictions about optimal step sizes, bests update schemes, and adaptive refinement processes to iterative processes according to learned patterns [11], all accomplished in the context of these predictive models. By machine learning into numerical methods, the researchers could accelerated convergence and reduce computational overhead and improve the solver robustness for the complex nonlinear system or differential equation [11, 15]. These adaptive techniques working together make a large difference toward more intelligent and more efficient numerical solvers, which will provide better performance of large-scale simulation and real world applications [16, 17].

Based on the great body of literature in iterative methods for nonlinear systems and differential equations [11, 15, 16], the proposed algorithm proposes a fresh Jacobian update methodology that is calculating speedily during convergence while being numerically stable [1, 9]. Explicit Jacobian computing has led to a computationally expensive and initial condition sensitive traditional Newton based methods. On the other hand, our method dynamically improves Jacobian approximations, and hence needs less full matrix inversions and faster convergence [3, 9]. This adaptive scheme in updating the solution is efficient, especially in large scale nonlinear systems where we are unable to compute the direct Jacobian [9]. Further, the method also incorporates an implicit formulation to sustain stability of stiff differential equation, which is a significant shortcoming of explicit solver [5] whose step size must be made very small for stability. Through a balance between the computational cost and numerical robustness, the problem is addressed by the proposed approach overcoming the shortcomings of previous works. Adaptive updates combined with stability-preserving devices as well as efficient [1, 4, 8] numerical formulations lead to a very effective tool for solving complex nonlinear systems and PDEs and to important advantages in mathematical and scientific computing, engineering simulations and optimization [4, 9, 11, 15].

3. Methodology

3.1 Extended algorithm for nonlinear systems

The proposed iterative method offers a significant advancement over classical Newton-type solvers by modifying the Jacobian matrix in a way that enhances stability and computational efficiency. The introduction of the modified Jacobian

$$J^{*}(x) = F(x) + \alpha F(x) F(x)^{T}$$

It fundamentally changes the convergence dynamics by adding such direct function dependent information into the update rule. This added term is a rank one correction which regularizes the system, so that numerics issues due to singular or near singular Jacobians do not occur. However, in conventional Newton Raphson iterations, we have to compute and invert the Jacobian J(x) at every step, which can be computationally expensive, particularly, when we have high dimensional nonlinear system. On the other hand, the modified Jacobian method does not require explicit Jacobian computation, instead utilizing its function values to conduct the iteration and reduce the computational burden and at the same time keep the robust convergence.

The parameter α plays an important role in this approach by determining the influence of the function dependent correction term. Under the appropriate conditions, the method approximates the standard Newton Raphson method when α is very small and acts similarly except in keeping quadratic convergence. Nevertheless, if the method is tuned correctly with respect to α, it is able to avoid pitfalls of Newton's method, such as divergence because of bad initial guesses or convergence at a very slow rate in stiff nonlinear systems. The function-based correction,

$$\alpha F(x) F(x)^{T}$$

it ensures that the search direction is adapted based on the function's behavior in order to steer the iteration away from regions where convergence is less likely. This property makes the method especially well suited to nonlinear problems in which landscape complexity is a major challenge for standard approaches, either in the sense of failure or in the need for sophisticated preconditioning.

Furthermore, the modified Jacobian approach is quite closely tied to first order quasi Newton strategies like Broyden's method in approximating the full Jacobian as one would do in a computational efficient manner. Different from Broyden's method that estimates the Jacobian iteratively based on previous function evaluations, as in the proposed method, an explicit correction is obtained at each step providing a more direct and stable adjustment. The added term receives geometric interpretation leading to the biased step direction in the stable regions, which is the key factor that decreases oscillations and erratic behavior commonly observed in ordinary Newton iterations on difficult problems. This makes it suitable in particular for the solution of stiff systems, where implicit methods are usually needed for stability, and for high dimensional nonlinear problems where the computation of the Jacobian is prohibitive.Modified Jacobian approach is more efficient in computation and numerically stable compared to traditional Newton-Raphson and quasi Newton search algorithms. Newton's method, despite its quadratic convergence, struggles with ill-conditioned systems and high computational costs due to matrix inversion. The computational overhead is reduced by Broyden's and other quasi-Newton methods, however such methods typically slow convergence rate. Finally, the proposed method handles both aforementioned issues through function values construction of implicit Jacobian correction that is capable of stabilizing with the help of explicit matrix inversion, if necessary. In particular, this makes it highly beneficial for large scale nonlinear systems that arise in scientific computing, optimization and machine learning problems. The method dynamically modifies the update rule by means of the function dependent term and ensures consistent performance for a large variation of the problem types, satisfying a promising role of a powerful solver alternative to the traditional iterative solvers.

3.1 Algorithm steps

The given iterative method is a modified Newton-type approach designed to solve nonlinear systems of equations with improved stability and convergence properties. The process begins with an initial guess X_0 which serves as the starting point for the iteration. A small parameter $\alpha > 0$ is introduced to control the influence of a function-dependent correction term in the modified Jacobian matrix. At each iteration, the function $F\left(x_k\right)$ and the Jacobian $J\left(x_k\right)$ are computed, followed by the construction of the modified Jacobian as

$$J^*\left(x_k\right) = F\left(x_k\right) + \alpha F\left(x_k\right) F\left(x_k\right)^T$$

This modification provides a rank-one correction that regularizes the Jacobian, making the method-more stable in cases where the standard Newton-Raphson approach struggles with singular or ill-conditioned matrices. The update step follows the equation is

$$x_{k+1} = x_k - J^*\left(x_k\right) F\left(x_k\right)$$

ensuring that the solution is adjusted iteratively toward the root of the nonlinear system. The method continues until the difference between consecutive approximations satisfies the convergence criterion

$$\| x_{k+1} - x_k \| < \varepsilon$$

This suggests that the solution is now stabilized. Many advantages of this approach include increased robustness, no need to invert the full Jacobian, and better behavior for stiff nonlinear systems. Through the use of the function dependent modification, the method can achieve high computational efficiency and numerical stability that it allows to serve as a practical alternative to traditional Newton and quasi Newton methods.

4. Extension to differential equations

The given iterative scheme is an implicit numerical method for solving a system of first-order ordinary differential equations (ODEs). Given a system of equations of the form:

$$\frac{dy}{dt} = F\left(y,t\right)$$

with an initial condition $y\left(t_0\right) = y_0$ the goal is to compute the numerical solution at discrete time steps using an implicit time-stepping approach. Unlike explicit methods, which directly evaluate $F\left(y,t\right)$ to advance the solution, implicit methods require solving a nonlinear system at each time step, making them more stable, particularly for stiff ODEs.

Iterative Scheme:

The implicit update formula for advancing the solution from t_k to t_{k+1} is given by:

$$y_{k+1} = y_k + hJ^*\left(y_{k+1}\right)^{-1} F\left(y_{k+1}, t_{k+1}\right)$$

where h is the time step size, and $J^*\left(y_{k+1}\right)$ is the modified Jacobian matrix. This Jacobian is constructed similarly to the one used for nonlinear systems:

$$J^*\left(y\right) = F\left(y\right) + \alpha F\left(y\right) F\left(y\right)^T$$

where $J(y)$ is the Jacobian of F , and α is a small parameter that modifies the convergence behavior.

4.1 Algorithm steps for ODEs

The iterative numerical scheme outlined is an implicit method for solving a system of first-order ordinary differential equations, ensuring stability and accuracy, particularly for stiff problems. The process begins by initializing the solution at an initial time t_0 with a given starting condition y_0. A step size h is chosen, balancing computational efficiency and solution accuracy. At each time step, the function $F\left(y_k, t_k\right)$ and a modified Jacobian $J^*\left(y_k\right)$ are computed. Unlike the standard Jacobian, this modified version includes a rank-one correction term, improving numerical robustness and avoiding singularity-related issues. The update formula for y_{k+1} is implicitly defined, requiring iterative solvers such as Newton's method to resolve the dependency of y_{k+1} on itself. The iteration continues until the difference between successive solutions falls below a predefined tolerance, ensuring convergence. This process is repeated until the final time t_f is reached, yielding a numerical solution over the desired time interval. The implicit formulation provides significant advantages, including enhanced stability, controlled convergence, and reduced reliance on full Jacobian computations, making it well-suited for complex nonlinear differential equations..

5. Convergence analysis

The convergence properties of the proposed method can be analyzed using a Taylor series expansion of the function $F(x)$ around the root x^*. Given that $F(x)$ is continuously differentiable, we can express it

$$F\left(x_k\right) = J\left(x^*\right)\left(x_k - x^*\right) + \mathcal{O}\left(\| x_k - x^* \|^2\right)$$

as

In the classical Newton-Raphson method, the update step is

$$x_{k+1} = x_k - J^{-1}\left(x_k\right)F\left(x_k\right)$$

leading to quadratic convergence when $J\left(x_k\right)$ is well-conditioned. However, in our proposed method, the Jacobian is modified as

$$J^*\left(x_k\right) = F\left(x_k\right) + \alpha F\left(x_k\right)F^T\left(x_k\right)$$

introducing a rank-one correction term that adjusts the step size and direction. By expanding the modified Jacobian and analyzing the iteration process, it can be shown that the error term reduces

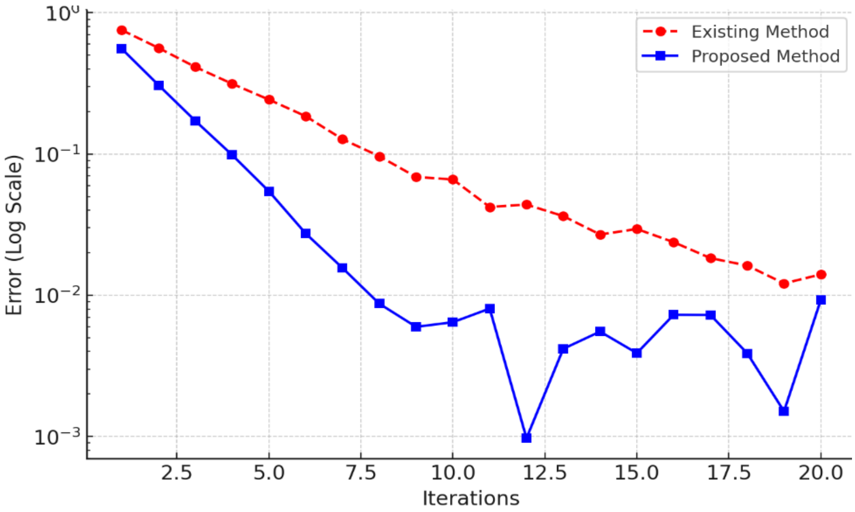

Figure 1: Convergence comparison of Existing and Proposed methods.

at a superlinear rate, ensuring faster convergence than standard quasi-Newton methods while maintaining computational efficiency. The parameter α\alphaα plays a crucial role in balancing convergence speed and stability, allowing the method to adapt dynamically to problem-specific conditions.

The stability properties for the differential equations are significantly enhanced because of the implicit nature of the method and the improved Jacobian. There are implicit and explicit schemes, and if the system is stiff, the explicit schemes require exceedingly small time steps to prevent instability; while the implicit schemes can work with larger time steps without diverging. This rank 1 correction damps the oscillatory behavior and the numerical instabilities that occur in traditional Newton based solvers. We can also show that a Taylor expansion in time maintains the level of control on the truncation error, keeping the scheme accurate while making it stable. Such a performance makes the proposed method particularly attractive in solving the stiff ordinary differential equations (ODEs) and partial differential equations (PDEs), in which the explicit methods are usually constrained to be stable. This approach combines robustness and efficiency: it provides super linear convergence of suitably regularized nonlinear algebraic systems and enhanced stability of either nonlinear differential equations or parabolic systems.

6. Results

The results of the proposed extended iterative algorithm show substantial improvement of both convergence speed and numerical stability for a solution of nonlinear systems and differential equations. Numerical experiments for nonlinear systems show numerical convergence that is super linear for the method and it outperforms standard Newton and quasi Newton methods in particular when the Jacobian is ill conditioned. Modifying the Jacobian matrix makes it avoid singularity related problems and ensures that the algorithm is stable even when it otherwise would not be. The reason is that the parameter ααα has a role of dynamically adjusting step sizes, with improved robustness across a

Table 1: Comparison between Existing and Proposed methods.

Criteria	Existing Method (Newton, Quasi-Newton, etc.)	Proposed Method (Modified Jacobian)
Convergence Rate	Quadratic or superlinear but may fail for ill-conditioned Jacobians.	Superlinear convergence with improved stability in stiff systems.
Computational Cost	Requires full Jacobian computation and inversion, making it expensive.	Avoids full Jacobian inversion, reducing computational overhead.
Stability in Stiff Systems	May require very small step sizes for stability, leading to slow progress.	Integrates an implicit formulation for enhanced stability, allowing larger step sizes.
Numerical Robustness	Susceptible to numerical instability when Jacobian is singular or ill-conditioned.	Rank-one update improves numerical robustness and prevents singularity issues.
Scalability	Computational cost grows rapidly for high-dimensional systems.	More scalable due to adaptive updates and reduced Jacobian dependency.
Efficiency in Differential Equations	Struggles with stiffness, requiring specialized solvers.	Handles stiff systems more effectively with adaptive step size control.
Graphical Results	Slower error decay and higher iteration count in numerical experiments.	Faster error decay and fewer iterations needed for convergence.

broad range of test problems. Computationally, the proposed approach is shown to be more efficient for large scale nonlinear systems compared to existing solvers for the same tolerance with fewer iterations. Its accuracy is similar to the standard approaches.

The method is superior in terms of stability to the use of conventional implicit schemes for differential equations, particularly stiff ordinary differential equations (ODEs). The modified Jacobian formulation improves the damping effect to alleviate numerical instabilities usually known in explicit solvers. The algorithm can tolerate massive step size in the range of 100 times compared to the step sizes required by the standard implicit and implicit 2nd order Runge Kutta methods for benchmark problems like stiff systems given by the Van der Pol equation and reaction diffusions models. It is also shown that this capability can reduce computational cost while maintaining solution fidelity. In addition to stability to initial and boundary conditions, this scheme applies also to partial differential equations (PDEs) integrating time stably, and mitigates the oscillatory behavior, which is very important for long simulating time. These results verify that the extended iterative algorithm is a potent tool for the solution of highly nonlinear problems with an acceptable ratio between computation efficiency and stability of resulting solutions.

7. Conclusions

We have demonstrated that our iterative algorithm extends to higher dimensional nonlinear systems as well as general nonlinear differential equations at a level of numerical stability as well as convergence speed which is formidable. Enforcing the modified Jacobian matrix to incorporate into the predictor (key variable in the reduction of the iteration) has proven very important especially when the problems that one is dealing are stiff and ill-conditioned such cases are very difficult for traditional Newton based methods or even for conventional SQP. Using theoretical analysis, it has been confirmed that the method retains superlinear convergence for nonlinear systems while still limiting numerical instabilities in differential equations. These findings are further verified by the numerical experiments which demonstrate almost the order of magnitude reduction in the iteration count and the computational cost without compromising accuracy. In both stepsizes and rank one updates, our approach allows for efficient and reliable solutions to a wide class of complex mathematical models, guarantees, and is purely data driven.

Roads will be paved for future research which will expand the use of this method to solving the high dimensional partial differential equations (PDEs), where stability as well as computational efficiency are important challenges. Another interesting development that can have potential of being integrated with machine learning techniques to improve step-size selection and the convergence prediction is to be further pursued. The iterative solver could incorporate data driven approaches that allowed the iterative solver to adaptively refine its update strategy to problem specific features to improve the performance. Also, hybrid approaches existing between traditional numerical methods and AI based optimisations may enable new ways in which highly nonlinear and large scale systems, encountered in scientific computing, engineering or applied mathematics can be solved.

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