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NUMERICAL OPTIMIZATION OF NONLINEAR FUNCTION

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Abstract

A combination of measurements and modeling is often used when dealing with engineering problems. When taking measurements, engineers design and set up laboratory equipment to produce data which are collected and analyzed. When modeling, engineers work to understand the theories and principles underlying the physical phenomena, and write or use computer programs to perform virtual experiments as an aid to ensure that results from the physical experiments are reasonable. Mathematical models for engineering applications, such as in the areas of finite elasticity and inverse kinematics, are often expressed in terms of systems of nonlinear equations which are difficult to solve. There is a problem with uniqueness and existence because a nonlinear system can have multiple solutions or no solution at all. When engineers are conducting numerical research, they either write their own programs or use available computer packages to solve nonlinear systems. Numerical analysis is at the core of both methods, and is directed towards developing and improving the mathematical algorithms required to perform the associated calculations.

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Introduction

Motivation for Research – Challenges in Solving Nonlinear Equations

The mathematical methods for solving engineering problems can be divided into two main categories: (1) linear and (2) nonlinear systems. The term "systems of equations" might refer to ordinary differential equations (ODEs), partial differential equations (PDEs), integral equations, and/or algebraic equations. In this thesis, the mathematics of nonlinear algebraic equations arising in engineering applications were investigated. To give a definition for nonlinear algebraic equations, the definition of linear operator must first be reviewed.

Numerical Methods

Numerical methods, and in particular iterative methods, are used to determine the solution to nonlinear systems arising in engineering applications since there is usually no analytical solution available. Issues with current numerical techniques include the rate of convergence and the uniqueness of the solution. Throughout the centuries, mathematicians and scientists have been using the well-known Newton's method (NR), an iterative technique to determine the solution to nonlinear equations. There exist other numerical schemes to determine the roots of nonlinear systems, such as modified versions of the Newton's method (MNR) and Newton-Homotopy continuation methods, but the NR method is by far the popular choice among academics and industries due to its rapid rate of convergence. The algorithm, however, depends on the initial guess, and neither stability nor convergence is guaranteed.

The iterative methods that were investigated in this research included the Newton's method (NR), J.H. He's modified Newton-Raphson method (HMNR) [4], a Newton-Homotopy continuation method by Wu [5] (to be referred to as "Homotopy" in this thesis), and the new method proposed here – a modified Newton's method combined with the Vector Epsilon Algorithm (MNR-VEA). The engineering application considered in this thesis is the inverse kinematics of robot arms. A review of the literature showed that NR is the method normally used for inverse kinematic calculations (e.g., [6, 7]), and, occasionally, Homotopy is also used (e.g., [8]). This has provided the rationale for the choice of iterative methods considered in this thesis.

Iterative Methods

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In this section, the techniques for solving nonlinear equations, the Vector Epsilon Algorithm (VEA) and some inverse kinematics applications are discussed. Notation for system of nonlinear equations in here is $\mathbf{F}(\boldsymbol{x}) = 0$. Numerous numerical methods are based on the Newton's method, and some of them will be reviewed in upcoming sections. The book by Kelley [11], S*olving nonlinear equations with Newton's method*, is an introductory textbook for academics who are working on numerical analysis. Some of the algorithms are written in pseudocode and MATLAB® [12] code for users to experiment with a Newton iteration.

Inverse Kinematics Problems

Kinematics describes the motion of bodies within a system without consideration of the forces causing the motion. Hence, kinematics is the study of motion based on geometry and changes in geometry. The motion of each body is modelled through mathematical formulas for calculating position, velocity, and acceleration. The area of kinematics can be divided into forward and inverse problems. When positions are the primary consideration for a mechanism, forward kinematics is a straightforward process: given a set of joint angles and link parameters defining a configuration, the aim is to find the position of an end-effector. The inverse problem is the reverse of the forward kinematic process: given the end-effector position, find the joint angles and link parameters to achieve that position [36]. In this thesis, the focus will be on inverse kinematics which, as will be shown, is highly nonlinear and therefore is the more challenging problem.

In the literature, there are several techniques used to perform inverse kinematics. A problem of particular interest is the inverse kinematics of robot manipulators, and different iterative methods have been used to solve the corresponding nonlinear equations. Cai et al. [37] and Lenarcic [38] solved nonlinear kinematic equations using iterative algorithm based on the conjugate gradient method. This method [39] solves systems of linear equations in the form of $Ax = b$ where A is a symmetric and positive-definite matrix. It is equivalent to finding the minimum of quadratic form

$$\mathbf{F}(\boldsymbol{x}) = \frac{1}{2}\boldsymbol{x}^{\mathrm{T}}\mathbf{A}\boldsymbol{x} - \boldsymbol{x}^{\mathrm{T}}\boldsymbol{b}, \qquad (2.22)$$

$$\mathbf{F}'(\boldsymbol{x}) = \mathbf{A}\boldsymbol{x} - \boldsymbol{b}. \qquad (2.23)$$

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The minimum of F(x) is a solution to Axb . Caccavale and Wroblewski [40] compared the effectiveness and robustness of Newton-Raphson and Jacobian transpose methods, where they used the transpose instead of the inverse of a Jacobian [41], for determining the roots of nonlinear kinematic equations. Tagawa and Haneda [42] developed a computer program to implement a fast interval bisection (FIB) algorithm based on interval analysis. It reduced the number of operations and storage space of variables. Cai and Zhang [43] programmed a solver based on the gradient descent method in neural networks, and Martin el al. [44] used the gradient descent method to solve the inverse kinematics of multi-link robots by means of neuro- controllers. Chu and Wu [45] showed that a modified secant method has a better performance, assessed via several numerical examples, than the Newton’s method. Ren et al. [46] used the cyclic coordinates descent (CCD) algorithm to perform inverse kinematics for virtual human approximate solution of the equation

$$\mathbf{F}'(x_n)s_n = -\mathbf{F}(x_n)$$

Applications with Vector Epsilon Algorithm

The Vector Epsilon Algorithm (VEA) is an efficient method in accelerating the convergence ofvector sequences [26]. Later on, Gekeler [27] showed that the VEA was able to accelerate

convergence when solving non-singular systems of linear and non-linear equations. As for usingthe VEA to accelerate convergence when solving singular systems, Brezinski [28] and Sidi [29] showed success in systems of linear equations, and Brezinski [30] for systems of non-linear equations. Brezinski and Redivo-Zaglia [31] released a MATLAB toolbox named EPSfun that included codes for Scalar Epsilon Algorithm (SEA) and VEA. Waldvogel [32] used the VEA forexploration of data to lessen the computation time with their own MATLAB code. The algorithm has been applied to engineering applications, such as in fluid dynamics applications, with Hafez and Cheng [33] and Hafez et al. [34] using the SEA to reduce solving time in transonic flow calculations; Cheung [35] used the VEA to reduce solving time in viscous and inviscid hypersonic flow calculations. The algorithm has also been applied to kinematic problems, which is the focus of this thesis.

NR is commonly used when an iterative method is needed to solve certain problems. The reasonfor its popularity is due to its fast convergence. Wu’s version of Homotopy is similar to NR in some ways, in that it provides better performance since it is independent of initial

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guesses and always converges. HMNR is an altered form of NR, and it operates like NR except there is a parameter which controls the iterative process. The proposed method in this thesis, MNR-VEA, combines a modified version of Newton's method with a type of convergence accelerator, the Vector Epsilon Algorithm. Numerical analysis was performed for the investigation of the above iterative techniques. One of the primary issues that will form the basis for comparison is the need for finding *all* the roots of a system of nonlinear equations. For example, for the application of a robot manipulator, this would correspond to finding *all* the configurations that would achieve a specified position of the end effector. The "best" configuration could then be chosen based on some optimization criterion. As will be seen, this is a particular challenge for any iterative method, and depends on the technique's ability to find the closest root to a giveninitial guess.

The Issue of Closest Root

Numerical methods are used to solve equations involving trigonometry functions, such as load flow analysis [51, 52] and inverse kinematics [53, 54]. There is a need to find the closest solution from the given initial guess of nonlinear equations. For Chemical Engineering applications, finding the closest solution is essential in the synthesis, design and control of chemical processes [55, 56] and useful roots can be selected [57]. For Electrical Engineering applications, finding the closest solution is crucial to computer-aided design of integrated circuitssince they are the operating points [58-61].

In order to find solutions within a certain domain systematically, a common approach is to forma grid of points which are used as a series of initial guesses. For each initial guess, the goal is to use the iterative method to find the root closest to that initial guess. If the iterative method does not give the closest root relative to the initial guess, the process is no longer systematic, and it cannot be concluded that all the roots have been found. For example, the classical numerical method NR is dictated by the initial guess used in the iterative process. This method fails when a singularity occurs and is highly unstable near a singularity. It could result in a root distant from the initial guess that may even be outside the defined domain. Due to this, in the literature there are numerous versions of MNR which try to eliminate unfavourable qualities from the original recipe.

To illustrate the meaning of closest root, consider Figure 2.1 and Figure 2.2. Both figures are

$$f(x, y) \,\square\, 0 \qquad (2.31)$$

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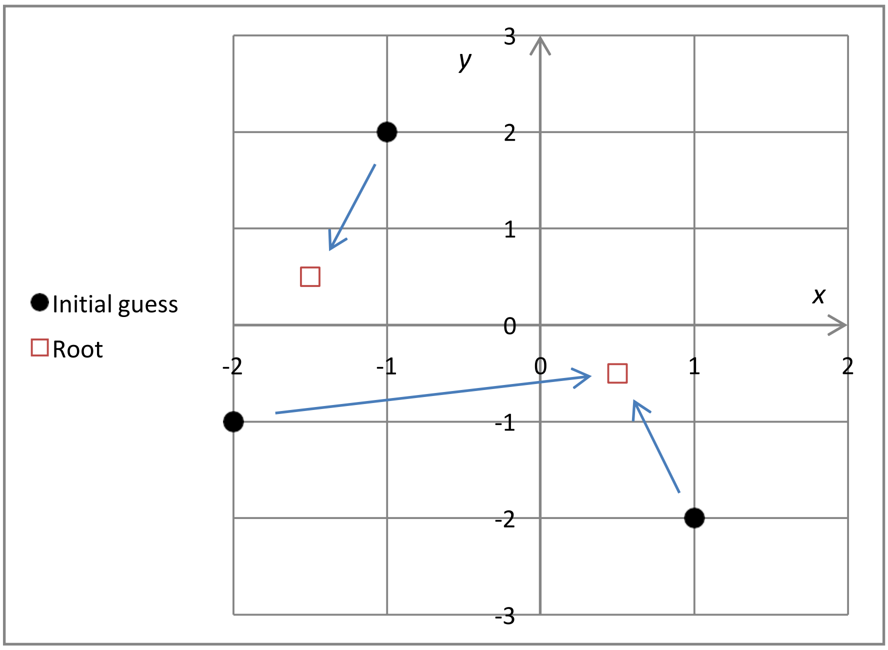
$g(x, y)$ □ 0

of two nonlinear equations in two unknowns. A two degree of freedom (2-DOF) system is considered for this illustration, since it is easier to visualize the numerical approach for two variables as compared to the difficulty in drawing a function of three or more variables. Figure 2.1 demonstrates that, depending on the iterative method, an initial guess may not give the closest root, and in fact the root finding process may become random. Figure 2.2 demonstrates a case where all initial guesses are able to converge to the closest root. Here, by definition, the closest root occurs when the Euclidean distance between the initial guess and the solution is the smallest. In the sections to follow, each iterative method to be considered in this thesis is presented and, later in the thesis, each method was evaluated in terms of its ability to find the closest root for an initial guess.



A case where initial guesses do not all converge to the closest root.

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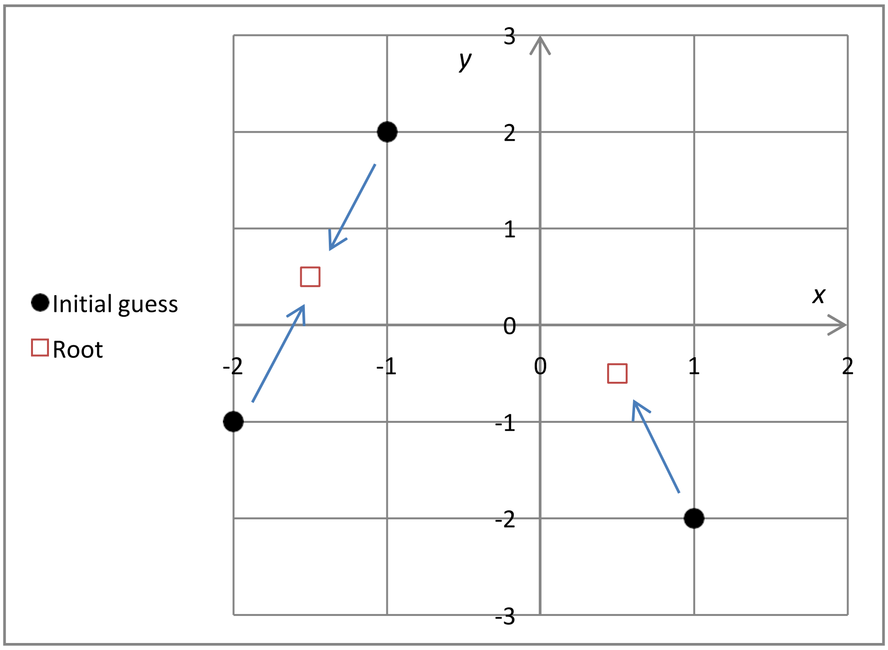

A case where all initial guesses converge to the closest root.

Conclusion

In this study various numerical methods and test cases were evaluated to solve systems of non- linear equations.

For the 1 DOF test case, MNR-VEA (with □ of 0.0001) and Homotopy did not fail to converge. Also, success with Homotopy in the root-finding process was independent of the value of □t; though, Homotopy did require many more iterations to find a solution (5 to 20 times more iterations than MNR-VEA). NR, HMNR and some cases of MNR-VEA (with □ values of 0.1,

0.01 and 0.001) failed to converge on closest root specifically when the initial guesses were inthe region close to the critical point of 1.5708.

For the 2 DOF test case, MNR-VEA had a better performance in converging to the closest root, and was more consistent in obtaining valid solutions. Homotopy was consistent in arriving at theclosest root, and more frequently arrived at the closest root as □*t* decreased;

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though, the number of required iterations was large. HMNR gave the worst performance out of the four methods (andeven resulted in complex numbers), and the choice of *r* was crucial in HMNR.

For the 2/1 DOF test case, MNR-VEA has a best performance in achieving x^* and x^{**}. MNR- VEA. These results, combined with the 1 DOF analysis, indicated that MNR-VEA is the best choice when dealing with 1 DOF problems.

For the 3 DOF test case, Homotopy was consistent in arriving at the closest root, and more frequently arrived at the closest root as □*t* decreased. With Homotopy though, as well as NR, average □ and maximum □ were large, indicating solutions outside the domain. MNR-VEA with □ = 0.1 had its best performance in obtaining valid results converging to the closest root, with low average □. Though, solutions with □ = 0 were minimal. HMNR was not able to solve the 3 DOF test case due to division by zero.

Computation time and percentage of giving closest root were measured to evaluate the performance of each numerical method. MNR-VEA is recommended for 1 and 2 DOF, and Homotopy (□*t* = 0.02, 0.01) is recommended for 3 DOF.

Overall, the results of this analysis indicate different results for MNR-VEA and Homotopy. Specifically, MNR-VEA worked best with 1 and 2 DOF test cases (as well as the 2/1 DOF test case) whereas Homotopy worked moderately well with 1 and 2 DOF test cases and best with the 3 DOF test case. If the goal of the optimization is a mixture of both accuracy and minimal number of iterations, and the initial guess is approximately near the closest root, MNR-VEA maybe more desirable to use for 1 and 2 DOF scenarios. Further, it is important to note thatHomotopy has two parameters to be chosen: the auxiliary function, $g(x)$, and time increment, □*t*. For Homotopy, there are rules to follow in picking $g(x)$ and □*t*, and, even so, it does not guarantee convergence. As such, MNR-VEA may be more desirable to use since the choice of picking parameter *r* and relaxation parameter □ is more intuitive (i.e., □ < 1).

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