Finding the Steady States of Nonlinear Systems using the Canonical S-system Form

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Short Abstract — **Models of biological systems are typically multivariate and highly nonlinear. As such, determining every potential steady state of a given biological system is a useful but difficult goal. Similarly, other problems in engineering and applied mathematics require a search for steady states, or roots, of multiple equations. Our work shows that an algorithm based on S-system methodology and interval Newton methods can efficiently find roots of nonlinear systems and guarantee that every root will be found.**

Keywords — **Root Finding, Zeros, Multivariate Systems, Ordinary Differential Equations, Interval Newton Methods, Reliable Computing**

I. Introduction

Models of biological systems are typically multivariate and highly nonlinear. Most nonlinear systems of equations can be recast to a canonical S-system form [1], a form that provides an excellent systematic basis for general nonlinear algorithms [2]. Previous work suggested that an S-system methodology produced an efficient nonlinear root finding algorithm [3]. The method was promising, but did not guarantee that all roots, or steady states of the biological model, would be found in every case, a useful but difficult goal. Our work improves the algorithm by utilizing interval Newton methods in order to guarantee that every root will be found.

Common multivariate root-finding methods employ Newton's method, in which linearization is used to approximate a nearby root and subsequent iterations converge on the solution. However, such algorithms may converge on any nearby root, making it difficult to craft a strategy that will find every root. On the other hand, so-called interval Newton methods borrow concepts from interval analysis, or reliable computing, in order to bound all possible solutions for a given iteration. Consequently, algorithms based on interval Newton methods can guarantee that every root will eventually be found [4]. We show that the regular structure of the recast S-system form provides computational advantages when using interval Newton methods.

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II. Methods and Results

Using INTLAB [5], an interval analysis package for MATLAB, we implemented two nonlinear root finders based on the Krawczyk method and the Gauss-Seidel method. We tested the solvers using random polynomial systems of one or two variables, increasing in order, with exactly two known positive roots. In the first test, we directed the solvers to use the original functions and the automatic differentiation tools in INTLAB. In the second test, we provided the solvers with the recast system and a fast method of determining the Jacobian of the recast system. The roots were found in every case. The number of iterations and time required to find the roots were compared.

III. Conclusion

As the order of the system increased, the number of iterations required in each test differed by less than a factor of three. However, the methods grew significantly faster when using the recast system. Currently, the S-system form appears to provide two performance advantages when using interval Newton methods to find the steady state of a system. First, recasting performs some work up front, eliminating the need to perform arbitrary function evaluation and automatic differentiation. Second, recasting creates convex nonlinear equations, which lead to fast, tight bounds on the entries in the interval Jacobian matrix.

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