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# Finding all real solutions of nonlinear systems of equations with discontinuities by a modified affine arithmetic

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ABSTRACT

Chemical engineering is a rich area when comes to nonlinear systems of equations, possibly with multiple solutions, (unbounded) discontinuities, or functions which become undefined in terms of real values. In this work, a new approach is proposed for finding all real solutions of such systems within prescribed bounds. A modified affine arithmetic is used in an interval Newton method plus generalized bisection. A special constraint propagation is used to automatically remove regions where the functions are undefined for real numbers. Results for test problems have shown that the proposed implementation requires less computation effort than similar methods available in the literature for small continuous systems. Further, the method is able to find all real solutions of nonlinear systems of equations even when there are unbounded discontinuities or when functions become undefined within the given variable bounds.



## 1. Introduction

Solving systems of nonlinear equations is a fundamental task in many mathematical, engineering, and science applications. Chemical engineering, in particular, is a rich area when comes to nonlinear systems of equations. Usually, the complex physical phenomena present in chemical processes can only be properly described by systems of nonlinear equations. Even though the variables involved are usually limited to a valid physical domain, the model functions can be discontinuous (unbounded or not) or can become undefined.

When solving these equations, we are usually interested in finding at least one solution and a fundamental problem arises when no solution is found. Was no solution found because of convergence failure or does the model actually have no possible solution? In this regard, *structural* analysis can be very helpful in identifying structurally singular models and in aiding the user to fix the defective model (Soares & Secchi, 2012). But, unfortunately, structurally non-singular models can still pose convergence problems for numerical methods. Further, if there are multiple solutions, have all possible solutions been enumerated? In some cases, finding all solutions is mandatory, in other cases, *trivial* or unphysical solutions need to be avoided.

A large body of methods have been proposed in the literature for solving systems of nonlinear equations. According to Maranas and Floudas (1995), these methods may roughly be classified into three classes: (i) Newton and *quasi*-Newton type methods; (ii) homotopy continuation type methods; and (iii) interval-Newton methods. In the work of Rahimian, Jalali, Seader, and White (2011) a list with 7 different categories of methods is suggested. In the present work, no attempt to systematically review all methods is made. Some recent advances and papers found to be relevant in different categories follow below.

Newton-like methods are very common, mainly because they can be very computationally efficient and achieve super-linear convergence in the neighborhood of the solution. However, there is no guarantee for convergence and the methods tend to fail if the initial guess is poor or if singular points are encountered. These methods also fail if one or more functions become undefined (e.g. the logarithm of negative values). In Lucia and Taylor (1992) and Lucia (2000) the authors studied and reviewed the behavior of complex domain numerical methods. By considering the complex domain, it was found that improved convergence is achieved. Either real- or complex-valued solutions can be found. In Stuber, Kumar, and Barton (2010) the authors also comment on some attempts to enlarge the neighborhood of convergence for Newton-like methods.

The main idea of homotopy continuation methods is to gradually approach a solution of the equation set from a starting point which satisfies another (simpler) system of equations (Malinen & Tanskanen, 2010). A problem common to homotopy methods is that variable values might violate the prescribed bounds during the solution, possibly making variables to assume unphysical or

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complex values. This is particularly a problem for several chemical engineering models containing functions that may be discontinuous or become undefined in terms of real values. In order to remedy this, Paloschi (1995) and Paloschi (1998) suggested bounded homotopies, extended later by Malinen and Tanskanen (2008) and Malinen and Tanskanen (2010). Even with these modifications, a potential issue with this category of methods is the determination, in a problem independent way, of multiple solutions that lie on separate homotopy path branches (Malinen & Tanskanen, 2010).

Another class of method, known as terrain methodology, was recently proposed by Lucia and Feng (2002) and Lucia and Feng (2003) for the global solution of nonlinear models. The solution of the system of equations $\mathbf{f}$ is obtained in a least-squares sense by the minimization of $\mathbf{f}^T\mathbf{f}$. The main ideas of terrain following are based on the fact that neighboring stationary points of the least-squares function are connected along valleys under the conditions of twice continuous differentiability (Lucia and Feng, 2002). This method has been shown to be superior to homotopy-continuation for distillation examples with multiple solutions (Lucia & Yang, 2004). The method was also successfully applied in complex phase stability and phase equilibrium problems (Lucia, DiMaggio, Bellows, & Octavio, 2005). Moreover, according to Lucia and Feng (2002), it is quite possible that solutions on distinct branches of homotopy parametric curves to be connected by terrain. When compared to interval methods, the terrain methodology is apparently more suited for large scale problems. This can be inferred by comparing the number of function evaluations required for solving distillation problems in Baharev and Rév (2008), Baharev, Achterberg, and Rev (2009) and Lucia and Yang (2004). For small test problems, the interval method proposed in this work required less function evaluations than the terrain method, see Section 4.

The main attractive feature of the interval methods is the mathematical guarantees for convergence to all solutions within certain variable bounds. A similar alternative is to reformulate the nonlinear problem as an optimization problem – e.g. Maranas and Floudas (1995) and Harding and Floudas (2000) – and then apply deterministic global optimization methods like $\alpha$-BB. However, this approach may require problem reformulations and the development of convex underestimators specific to each new application (Gau & Stadtherr, 2002b).

Interval methods start with a set of intervals, one for each variable. This is a rectangle for the bivariate case and a *box* for the multi-dimensional case. Then the methods can find boxes smaller than a prescribed precision $\epsilon$ containing all solutions of nonlinear systems of equations, known as $\epsilon$-solutions. The basic idea is to apply a Newton-like method using interval arithmetic (IA) coupled with a generalized bisection (GB) strategy. Taking into account that usually we are interested only in real-valued solutions, there is no need to consider the complex domain in interval methods, unless complex solutions are sought. In recent years, interval based methods have been successfully used to solve a variety of problems in chemical engineering – e.g. Schnepper and Stadtherr (1996), Maier, Brennecke, and Stadtherr (1998), Gau and Stadtherr (2002b), Lin and Stadtherr (2004), and Lin, Gwaltney, and Stadtherr (2006) – but with the potential drawback of high computational cost. Special attention should be paid in the convergence rate and in the solution of the underlying *interval* linear problem. The alternatives for solving the interval linear problem are mainly solving a series of linear programming (LP) problems and preconditioning strategies (Baharev et al., 2009; Gau & Stadtherr, 2002b; Lin & Stadtherr, 2004).

An interesting improvement in the interval-Newton methods was originally proposed by Kolev (1998) and studied/extended later in some works (Baharev et al., 2009; Baharev & Rév, 2008; Kolev, 2004; Miyajima & Kashiwagi, 2007; Yamamura & Tanaka, 2006). The basic idea is to replace interval arithmetic (IA) by affine arithmetic (AA). AA was proposed by Stolfi and de Figueiredo (1997) in the context of reliable computing and computer graphics applications (Comba & Stolfi, 1993). The method was designed to give tighter and more informative bounds than IA in several situations where the later is known to perform poorly. Additional improvement can be achieved if AA is combined with IA in the so called mixed AA/IA method. Baharev and Rév (2008), Baharev et al. (2009), and Baharev, Kolev, and Rév (2011) have successfully used the mixed strategy in solving distillation problems.

Regarding discontinuities, most of the *globally convergent* methods assume continuity. Further, for problems with discontinuity in the vicinity of the solution, most methods may fail (Shacham & Brauner, 2002). Alternatives for solving problems with discontinuities have been reviewed by Shacham and Brauner (2002) and a method for solving problems with discontinuities was developed. Essentially, the method modify the system by algebraic manipulation, if possible. Otherwise, subspaces of the original feasible region are defined, with the discontinuities located at the subspace's boundaries. Unfortunately, the method cannot assure that all solutions will be found.

In the present work, a new mixed AA/IA interval method is proposed for finding all real $\epsilon$-solutions of systems of nonlinear equations (possibly unbounded discontinuous or which can become undefined) with bound constrained variables. Similarly to the methods of Kolev (1998) and Kolev (2004) and Baharev et al. (2009) and Baharev et al. (2011), a mixed AA/IA is used in an interval-Newton method plus generalized bisection. The new mixed AA/IA implementation can handle unbounded discontinuous functions and a special constraint propagation method is used to remove regions where undefined functions are found. Results with test functions and typical chemical engineering problems have shown that the proposed implementation is able to find all $\epsilon$-solutions and requires less computation effort than similar methods available in the literature. Further, the method automatically locate points of discontinuity and removes regions where undefined functions (in terms of real numbers) are found.

## 2. Interval-Newton methods with IA and AA

### 2.1. Brief introduction to interval and affine arithmetic

In this section a brief introduction on interval and affine arithmetic is given. It is mostly based on the excellent monograph by Stolfi and de Figueiredo (1997).

Interval arithmetic (IA), is a range-based model for numerical computation where each real quantity $x$ is represented by an interval $\overline{x} = [\overline{x}^l, \overline{x}^u]$ of floating point numbers, meaning that the *true* value of $x$ is known to satisfy $\overline{x}^l \le x \le \overline{x}^u$. Those intervals are then added, subtracted, multiplied, etc., in such a way that each computed interval is guaranteed to contain the unknown value of the quantity it represents. For instance, the addition and subtraction of two intervals $\overline{x}$ and $\overline{y}$ are computed as follows[1]:

$$\overline{x} + \overline{y} = [\overline{x}^l + \overline{y}^l, \overline{x}^u + \overline{y}^u] \quad (1)$$

$$\overline{x} - \overline{y} = [\overline{x}^l - \overline{y}^u, \overline{x}^u - \overline{y}^l] \quad (2)$$

Then, when computing with IA, for every operation $f(x, y, \ldots)$ (such as sum, product, exponential, logarithm, etc.) a corresponding *interval extension* $\overline{f}(\overline{x}, \overline{y}, \ldots)$ needs to be defined. For certain functions, determining the *exact* maxima and minima may be too difficult and an approximate interval that contains the theoretical

[1] In this work we are ignoring roundoff, overflow, and other details. Check Stolfi and de Figueiredo (1997) or Hansen and Walster (2004).