A greedy approach to transversal selection for nonlinear systems of equations

D.G. Sotiropoulos[1] and I.E. Livieris[2]

[1] Ionian University, Department of Informatics, Corfu, Greece
dgs@ionio.gr
[2] University of Patras, Department of Mathematics, Patras, Greece
livieris@math.upatras.gr

Abstract. Interval methods have been established for rigorously bounding all solutions of a nonlinear system of equations within a given region. In this paper, we introduce a new method for determining a good pivoting sequence for Gauss-Seidel method, based on a greedy algorithm, called `4M`, solving assignment problems with worst case complexity $O(n^2)$.

Key words: nonlinear systems, interval arithmetic, interval Newton methods, perfect matching, transversal.

1 Introduction and Motivation

We consider the problem of finding with certainty *all* zeros of a nonlinear continuously differentiable function $f : \mathbb{R}^n \to \mathbb{R}^n$ in a given interval vector $[x] \in \mathbb{IR}^n$ (an n-dimensional box). This problem is difficult due to its inherent computational complexity (NP-hard) and due to numerical issues involved to guarantee correctness. Interval Newton methods have been established for finding all real roots within the specified domain of a nonlinear system with both mathematical and computational certainty. In such methods, the basic idea is to apply the interval Gauss-Seidel method to the preconditioned linearized system [12]. Nowadays, the *interval Gauss-Seidel method* [5, 13] serves as a basis not only for interval Newton algorithms (see [4, Chapter 13]) but also for interval constraint algorithms [6]. However, this method is "blind" since it works in a straightforward manner, without taking account the coupling between the variables and functions. A natural question that arises is: if it is possible to dynamically accelerate the convergence rate of nonlinear Gauss-Seidel method, that still remains an open problem.

Herbort & Ratz [7] introduced the problem in their attempt to develop a new componentwise Newton operator, using a univariate Newton iteration on a unary projection of f_i onto one of the variables $x_1, \ldots, x_n$. Actually, finding such an assignment set is known as finding a *transversal* in the incidence matrix associated with the problem. Thus, a transversal may not be unique, but finding a "good" one is not a trivial problem. Sotiropoulos et al. [14] suggested to compute a transversal as a preprocessing step to interval Gauss-Seidel method for solving polynomial systems based on the structure of the equations. In recent works, Goualard [2] and Goulard & Jermann [3] investigated the impact of the selection of a transversal on the speed of convergence of interval methods based on the nonlinear Gauss-Seidel procedure. In [3], the authors concluded that it is not possible to select statically a good transversal at the beginning of the solving process, and therefore, the selection must be reconsidered dynamically at each iteration of the solving process.

In this work, we propose a greedy algorithm which determines a transversal dynamically by exploring information not only from the *incidence matrix* (static) but also from the current subregion (dynamic). The algorithm has the advantage that it does not use any first order information, in contrast to the previous proposed algorithms [7, 2, 3, 14]. From our point of view, the selection of an transversal can be seen as a *matching problem* on the bipartite graph $G = (\mathcal{F}, \mathcal{X}, E)$ associated with the the incidence matrix of the nonlinear system.

2 The greedy algorithm `4M`

Given a system of nonlinear equations of the form

$$f_i(x_1, x_2, \ldots, x_n) = 0, \quad 1 \leq i \leq n \tag{2.1}$$

where the variables $x_j,\ j = 1, \ldots, n$ are bounded by real intervals i.e. $x_j \in [x_j]$. The associated *incident matrix* $A = [a_{ij}]$ of the nonlinear system (2.1) is a zero-one matrix where a_{ij} is set to 1 if variable x_j occurs in function f_i. We represent the incidence matrix with a bipartite graph $G(\mathcal{F}, \mathcal{X}, E)$ where each vertex $f_i \in \mathcal{F}$ and $x_j \in \mathcal{X}$ corresponds to the function f_i and the variable x_j of the nonlinear system (2.1), respectively. In order to seriate the vertices of each vertex set we apply an ordering relation between them, associating a tuple, consists of information from the nonlinear system. Specifically, for each vertex $f_i \in \mathcal{F}$ we associate the tuple $\{d_G(f_i), w([f]_i)\}$ and for each vertex $x_j \in \mathcal{X}$ the tuple $\{w([x]_j), d_G(x_j)\}$.

The algorithm is iterative and requires as input only the bipartite graph $G\,(\mathcal{F}, \mathcal{X}, E)$. At each iteration, Algorithm-`4M` selects the vertex $f_i \in \mathcal{F}$ with the minimum degree. If this vertex it is not unique, we select the least of them according to the tuple of each vertex. Afterwards, it is matched with its best neighbor that is, the vertex with the biggest tuple, in $O(n^2)$. The two matched vertices are eliminated from further processing and consequently the degree of each of their neighbors is decreased by one. The edge incident to the selected vertices is inserted in the matching set $\mathcal{M}$. Further more at any iteration of this process, if any vertex in set $\mathcal{X}$ has degree equal to one then it is matched with its unique neighbor and the vertices are removed from the graph, as well. The iterations are repeated until that bipartite graph is empty, in $O(n^2)$. Finally, every edge (f_i, x_j) in $\mathcal{M}$ is sorted according to the tuple of each vertex x_j.

Every edge of set $\mathcal{M}$ determines the transversal of the nonlinear system at the current iteration. In particular, the edge $(f_i, x_j) \in \mathcal{M}$, represents the element

(i, j) of the incidence matrix, which implies, in terms of nonlinear system, that variable x_j shall be projected onto the function f_i.

We establish that the feasibility of the matching problem on the bipartite graph G ensures the existence of the perfect matching, not its uniqueness. Our proposed algorithm looks for the appropriate perfect matching among all others, nevertheless, all other existing perfect matchings don't satisfy the primitives of the greedy selection we have defined.

Lemma 1. *Suppose the bipartite graph $G(\mathcal{F}, \mathcal{X}, E)$, arising by the representation of the incidence matrix of a nonlinear system (2.1), where $\mathcal{F}$ is the set that corresponds to the functions, $\mathcal{X}$ is the set that corresponds to the variables and $E = \mathcal{F} \times \mathcal{X}$. Algorithm-`4M` achieves a perfect matching of graph G, in $O(n^2)$.*

Note that once a vertex is matched and removed from the bipartite graph, it is never revisited by the algorithm and all the other unmatched edges incident on it are removed from the graph, thus proving the correctness of the algorithm. Further, the algorithm returns a perfect match, that is because once two vertices are matched, they remain matched until the end of the process.

3 Numerical results

In this section, we introduce experimental results in order to demonstrate the accelerating of the efficiency of interval Gauss-Seidel method using our proposed algorithm as a preprocessing step (`4M`+Gauss-Seidel) and comparing it with the traditional method (Gauss Seidel) in a variate of benchmarks. The test problems have been taken from numerical [1, 8, 11] and interval analysis [7, 10] papers.

The implementation has been carried out in C++ using the C-XSC 2.0 library [9]. We present illustrative examples, highlighting the performance and the superiority of our proposed method.

Solving process		Gauss-Seidel			`4M`+Gauss-Seidel		
No.	Problem	`FcEv`	`JcEv`	`Ps`	`FcEv`	`JcEv`	`Ps`
1.	Floudas	17167	13306	3845	1351	989	345
2.	Ex.Powell	259284	168471	90805	138977	94499	44470
3.	Cyclohexane	`n/a`	`n/a`	`n/a`	44747	36017	8713
4.	Kinematics	17155	13164	3975	2340	1757	567
5.	Powell	6591088	5459059	1132028	2642	2123	517
6.	Caprasse	1520810	1329956	190815	170918	149249	21633
7.	Brown5	125092	93113	31976	20481	14959	5519
8.	Economics5	567619	474293	93321	47728	39351	8373
9.	Economics6	`n/a`	`n/a`	`n/a`	389061	336795	52262
10.	6Body	`n/a`	`n/a`	`n/a`	210983	176067	34911

Table 1 compares the results of the two solving processes applied to ten test problems. The first row denotes the method that has been used as solving process for isolating all zeros of a nonlinear system. For each test problem we list the number of function (`FcEv`) and jacobian (`JcEv`) evaluations and the number of pruning steps (`Ps`). A "`n/a`" in a column means that the solver was unable to find all the solutions of the problem within two hours. It is shown that, our proposed technique contributing in decreasing of both function and jacobian evaluations and of pruning steps.

4 Conclusion

In this paper, we have proposed a new direction of research, merging combinatorial matching theory and a greedy based technique for obtaining a maximum transversal. Our future framework will be to access our technique to interval constraint solvers and devise more advanced structure-based heuristics.

References

1. D. Bini and B. Mourrain. Handbook of polynomial systems. November 1996.
2. F. Goualard. On considering an interval constraint solving algorithm as a free-steering nonlinear gauss-seidel procedure. In *SAC '05: Proceedings of the 2005 ACM symposium on Applied computing*.
3. F. Goualard and C. Jermann. On the selection of a transversal to solve nonlinear systems with interval arithmetic. In *Procs. of the International Conference on Computational Science 2006*, volume 3991 of *Lecture Notes in Computer Science*, pages 332–339. Springer-Verlag, 2006.
4. R. Hammer, M. Hocks, U. Kulisch, and D. Ratz. *C++ Toolbox for Verified Computing I, Basic Numerical Problems: Theory, Algorithms, and Programs*. Springer-Verlag, 1995.
5. E. R. Hansen and S. Sengupta. Bounding solutions of systems of equations using interval analysis. *BIT*, 21:203–211, 1981.
6. P. Van Hentenryck, D. McAllester, and D. Kapur. Solving polynomial systems using a branch and prune approach. *SIAM J. Numer. Anal.*, 34(2):797–827, 1997.
7. S. Herbort and D. Ratz. Improving the efficiency of a nonlinear–system–solver using a componentwise newton method. Technical Report Bericht 2/1997, Institut für Angewandte Mathematik, Universität Karlsruhe (TH), 1997.
8. R. B. Kearfott. Some tests of generalized bicection. *ACM Transactions on Mathematical Software*, 13:197–220, 1987.
9. R. Klatte, U. Kulisch, C. Lawo, M. Rauch, and A. Wiethoff. *C-XSC – A C++ Class Library for Extended Scientific Computing*. Springer-Verlag, Heidelberg, 1993.
10. Van Hentenryck P. Michel L. and Deville Y. *Numerica: A Modeling Language for Global Optimization*. MIT Press, 1997.
11. K. Meintjes and A. P. Morgan. Chemical equilibrium systems as numerical test problems. *ACM TOMS*, 16(2):143–151, 1990.
12. A. Neumaier. *Interval Methods for systems of equations*. Cambridge University Press, 1990.
13. D. Ratz. *Automatische Ergebnisverifikation bei globalen Optimierungsproblemen*. PhD thesis, Universität Karlsruhe, 1992.
14. D.G. Sotiropoulos, J.A. Nikas, and T.N. Grapsa. Improving the efficiency of a polynomial system solver via a reordering technique. In *Proceedings of 4th GRACM Congress on Computational Mechanics (GRACM 2002)*, pages 970–976, 2002.