Comparing inclusion techniques on chemical engineering problems

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Abstract

Solving general nonlinear systems of equations and/or finding the global optimum of nonconvex functions constitute an important part of the everyday practice in chemical engineering. Standard methods cannot provide theoretical guarantee for convergence to a solution, cannot find multiple solutions, and cannot prove non-existence of solutions. This is the main motive to apply interval methods. Interval analysis has been applied to a wide variety of problems in chemical engineering, *e.g.* [1]. Similarly impressive results can be achieved with αBB, a fairly general global optimization method [2, 3].

Computing steady states of multistage separation processes requires solving large-scale nonlinear systems of equations. Despite of the outstanding results referred above, computation of these problems with interval arithmetic have not yet been considered in the literature, according to the authors' best knowledge. The only globally convergent methods used in this area seem to be the homotopy-continuation methods [4]. Leading edge software packages, such as [5], are also available to find zeros of nonlinear systems. Unfortunately, finding all solutions can be guaranteed only in special cases *e.g.* polynomial systems with no constraints [6].

The authors aim to compute steady states of homogeneous and heterogeneous azeotropic distillation columns with interval methods, keeping the algorithm as problem independent as possible. The results achieved so far are presented here.

Numerical evidence published in the literature, *e.g.* [7, 8], seem to indicate superiority of the linear interval approximation (LIA, $\boldsymbol{L}(x) = Ax + \boldsymbol{b}$, A is a real matrix), proposed by Kolev in a number of publications *e.g.* [9], compared to the traditional interval linear approximation (ILA, $\boldsymbol{L}(\boldsymbol{x}) = \boldsymbol{A}(\boldsymbol{x} - z) + f(z)$, $\boldsymbol{A}$ is an interval matrix) such as the interval Newton method. LIA has the following advantages over ILA when applied to root-finding. (*i*) The solution set of the LIA has a much simpler form, the hull solution is straightforward: $\boldsymbol{X} \cap -A^{-1}\boldsymbol{b}$. (*ii*) Linear programming is directly applicable to prune the current box. The automatic

computation of LIA is possible with affine arithmetic [10] which in turn (*iii*) automatically keeps track of correlation between the computed partial results yielding tighter enclosures. There is no significant difference in the computation time per iteration between LIA and ILA.
In [11] LIA and ILA are compared as linearization techniques applying them to chemical engineering problems of real complexity. The examples considered are highly structured and are full of dependency. LIA outperforms the traditional 'textbook' interval Newton algorithm (IN/GS) by an order of magnitude in the case of the studied examples. Note that *state-of-the-art* variants of the interval Newton methods, *e.g.* [12, 13], also outperform the IN/GS used for comparison. Linear programming may be preferable as pruning technique for LIA because of its robustness. Considering the conclusions of [11], the C++ class has been re-implemented, and the LP pruning method has been revised. The improvement is significant; real life medium-scale problems are successfully solved. Some of the problems used for comparison are suitable for benchmarks, they will be contributed soon.

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