A CONTRACTION BASED APPROACH FOR FLOWSHEET SOLVING STRATEGIES USING INTERVAL GLOBAL OPTIMIZATION METHODS

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Abstract

This paper investigates finding the global minima of modular flowsheet based on interval optimization. Previous work on this area has been addressed by Byrne & Bogle (2000) but results indicate it is computationally expensive. The idea of contracting intervals within modules to improve computational performance is highlighted in this paper. A modified interval Newton method with interval constraint propagation is illustrated on two simple problems. The approach was applied to the Haverly Pooling problem and the resulting efficiency is discussed. It was seen that the modified interval Newton approach saved considerable time in finding the global minimum for both simultaneous and modular formulations of the Haverly Pooling problem.

Keywords: Global optimization, Interval, Modules, Haverly Pooling problem.

1.Introduction

New methods for global optimization are continually generating interest in chemical engineering. Recent advances in deterministic global optimization methods (Neumaier-2003) of non linear constrained problems allowed us to consider a wide range of chemical engineering optimization problems.

Flowsheet optimization can provide significantly better designs at modest cost during the early stages of design. Two important distinctions are identified in formulating flowsheeting problems. In the equation-oriented formulation the flowsheet is treated as a set of mass/energy balance and constituent equations that are solved simultaneously. The alternative sequential modular approach views the flowsheet as interconnected black boxes. Local modular optimization methods have been investigated by Schmid & Biegler (1994). Both approaches have their advantages, however the modular approach has the advantage that it matches more closely to the natural structure of the flowsheet. Modular flowsheets dominate the market and are used by much of the design community. Global optima can be achieved by the application of global optimization algorithms to modular flowsheets built from generic models. Byrne & Bogle (2000) presented methods for this problem based on interval analysis.

1.1. Interval methods in global optimization

Interval methods for global optimisation are based on the branch-and-bound principle (Kearfott-1994). These methods subdivide the search interval into subintervals (branches). They use bounds for the objective function to eliminate subintervals which cannot contain a global minimizer. For a more thorough discussion see Hansen (1992). Interval arithmetic is able to provide rigorous bounds on the range of the function over the subintervals. Computation of a rigorous upper bound is less straightforward for equality-constrained problems. It is essential for branch and bound global optimization algorithms. Techniques in Kearfott (1994) highlighted procedures this area. In optimization problems, the

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number of equality constraints is different to the number of variables; since verification that a point satisfies all equality constraints (with an interval Newton method) requires a square system of equations, this problem must be resolved. In Kearfott (1996) several perturbation techniques were proposed for this problem, leading to a workable algorithm for obtaining a rigorous upper bound. Thus interval Newton methods or equivalent methods e.g. the Krawczyk method are important in branch and bound algorithms for constrained optimisation.

1.2. Influence of interval Newton method on global optimization

Interval Newton methods can be regarded as contractors. A simple example is considered below to consider the difference with and without the interval Newton contractor present in finding the global minimum. Results are shown in table 1 with a standard branch and bound global optimization algorithm (without under estimators). All the results in the table were generated using Matlab 6.1 on a Pentium III 1GHz.

Minimize X_1

s.t $(X_1)^2 + (X_2)^2 - 1 \leq 0$

$(X_1)^2 - (X_2) = 0$

Table 1

	Interval Newton Contractor Absent	Interval Newton Contractor present
CPU(Time) /sec	22	11
Number of iterations	28	9

Table 1 indicates that interval Newton contractors improve efficiency in finding the global minimum. A modified approach was applied to improve interval Newton methods to obtain feasible regions as opposed to feasible points. This idea will be explained in the next section.

1.3 Modification of the interval Newton method to obtain feasible region as opposed to feasible points

Until recently interval Newton methods hold n (variables) – m (constraints) fixed at points to obtain a square system. Hansen (2003) introduced the replacement of interval bounds for these variables. However, Hansen & Walster (2003) stated that point values are of more value than the bounds but no real analysis was discussed. However, it was clear there was a possibility of deleting and contracting regions. This is because solving a square system with interval bounds as opposed to points will produce an interval box. This indicates a feasible region over the range of interval bounds. So for simplicity a modified version of the Krawczyk method (Hansen-1992), another form of the interval Newton method, was developed. This incorporates bounds which are normally kept fixed. This modification will be explained below.

Original Krawczyk method:

i) Let y=mid(x) , FpX=interval jacobian ,Y= inverse of mid(FpX) and KX - Krawczyk operator

ii) $KX = y - Y*f(y) + (I - Y* FpX)(X-y)$

iii) $X=KX \cap X$, Interval box X produced at n-m fixed points.

f(y) is modified to incorporate intervals, known as inclusions of f(y) and is annotated as F(Y). Hence equation (ii) is changed to $KX = y - Y*F(y) + (I - Y* FpX)(X-y)$.

More variables occur than equations, so different square systems were formulated to make sure that all the variables will be contained in the square system at any one time. This is to ensure that all variables will be passed through the modified interval Newton system. Each linear square system is solved via this modified Krawcyck method; interval constraint propagation was applied prior to the system of equations to improve efficiency. The combination of these two contractors will be classed as modified contractors. The next section tests this modified method.

1.4 Testing proposed modification

The following example has been used to test the algorithm:

Minimize $-X_1$

s.t $(X_1)^3 + X_2 - (X_3)^2 = 0$

$(X_1)^2 - X_2 - (X_4)^2 = 0$

Table 2:

	Original interval Newton Method	Modified contractors
CPU(Time)/sec	165	95
Number of iterations	182	143

Table 2 illustrates that the modified Krawcyyk operator improves efficiency in finding the global minimum, when applied using a standard branch and bound algorithm.
Chemical flowsheeting engineering problems can sometimes have non-square systems in modules. So it can be proposed that the interval boxes passing through the modules can be contracted or eliminated with the modified interval Newton contractor and interval constraint propagation to enhance efficiency in finding the global minimum for modular flowsheets. This is described below.

2. Flowsheet Optimisation Methodology

Byrne & Bogle (2000) showed that the sequential modular approach can be formulated in a way suitable for interval methods. Modules are connected in the usual way but must be modified to handle interval arithmetic. A generic module requires point values or intervals for all the input streams and unit parameters and calculates the conditions for the output streams as respectively values or intervals. Due to the generic nature of modules, the internal contraction procedure postulated can be applied. The figure below illustrates this idea.

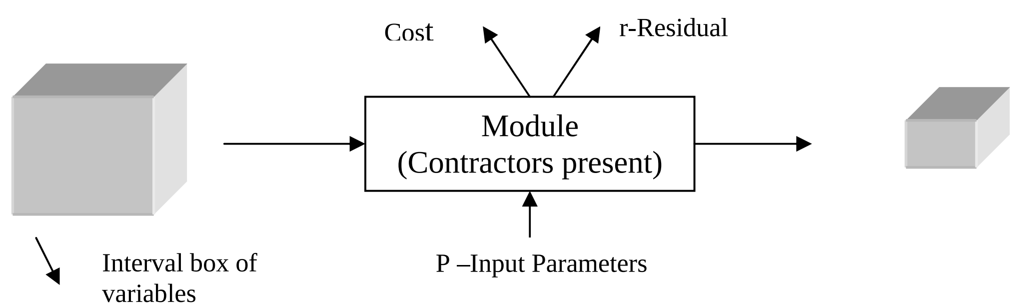

Fig 1. A Generic model which illustrates the new principle of contracting interval boxes

Modular flowsheets are constructed with generic unit modules that can provide the interval bounds, linear bounds, derivatives and derivative bounds using extended arithmetic types. Using interval analysis and automatic differentiation as the arithmetic types, lower bounding information is used for optimization in a branch and bound framework. The interval variables will be tested for validity via the equality constraints (from modules) and inequality constraints (product quality). If the intervals are not valid they will be eliminated. The interval global optimization problem is reformulated as a bound constrained linear relaxation problem. Natural extension under estimators will only be used for lower bounding information. These under-estimators and the contractors (applied to constraints occurring within the modules) proposed are combined with the interval bounded linear program to create a rigorous modified algorithm for constrained global optimization. This new proposed algorithm containing modular based contractors has been applied to a pooling problem case study described in the next section.

3. Case Study: Haverly Pooling Problem

This problem is to blend four feeds into two products to minimize the total cost. Each feed has a composition X_A , and cost c [£/(kmol h)]. Each product has a cost, required composition, and flowrate, F. The feeds are mixed to produce products that satisfy the quality requirements using mixer and splitter units to represent the blending tanks. A diagram and details of the problem can be found in Quesada & Grossmann (1995). This problem is a small scale blending problem and is non-convex. The procedure presented here could be used to obtain the global optimum of large scale non-convex blending problems by reusing a very small number of generic units (mixers, splitters, and feed and product units).
This problem has a number of local minimizers, and a global minimizer at
$F= [0, 100, 0, 0, 100, 100]^T$ with respect to $F= [F_1,F_2,F_3,F_4,F_6,F_7]$ and $X_A = 0.01$ with $f(x) = -400$.
This problem requires feeds, products, splitters and mixers. The flowrate is determined by a single input parameter and the cost by multiplying the unit cost by the flowrate. A mixer has two inputs and one output calculated by 'adding' the inputs together; in this case the cost is zero. Splitters divide one input into two outputs based on the input parameter (split

fraction) and again the cost is zero. The quality constraint placed on the two product streams become residuals in the product modules, which have one input and no outputs. The contractors will be added to the mixer and splitter module. Table 3 below indicates how the modified method finds the solution more efficiently. The original algorithm used is taken from Hansen (1992).

Table 3- Results for Haverly pooling problem

	Original Algorithm method	Modified Algorithm
CPU(Time)	No solution found within 2 hours	5min 10 secs
Number of iterations	No solution found within 2 hours	125

From table 3 it can be seen that the contractors within the module improve the efficiency significantly in finding global minima of modular constructed flowsheets. No solution was found with the original algorithm (Hansen-1992), which was allowed to run for two hours. This was due to singular matrices occurring thus making the algorithm unable to find feasible point. To find a global solution with the original algorithm, lower bounding information must be supplied with a more directed search direction (Byrne & Bogle 2000). It was deemed not necessary to input more under estimators because only the modified and the existing interval Newton method are being compared.
This case study was also run with algorithms containing just natural extension under-estimators with no contractors. The reverse was conducted i.e. just with contractors and no under-estimators to compare contractors with linear under-estimators. However no global solution was obtained within 2 hours for either method.

4. Conclusion

It can be seen that interval Newton methods are vital in finding global minima. The modification made by Hansen & Walster (2003) to the interval Newton method along with interval constraint propagation allowed significant improvements in finding the global minimum. This modification allowed us to bring the idea of the contractor within modules based on those improvements. This was applied to the Pooling problem and it was seen to significantly improve efficiency in finding global solutions in a modular flowsheet. However, it was noticed that the combination of under estimators and contractors would be needed to solve larger scale problems as no global solution was obtained when the linear under estimators and contractors were isolated and assessed individually. Future work will involve exploring these ideas and applying to further case studies, incorporating more details within the module like physical properties and to consider flowsheets containing recycles.

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