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Abstract

This paper considers the solution of systems of equations that are expressed by the two sets of equations: a global rectangular system of equations involving more variables than equations, and a set of conditional equations that are expressed as disjunctions. The set of disjunctions are given by equations and inequalities, where the latter define the domain of validity of the equations. In this way the solution of such a system is defined by variables x satisfying the rectangular equations, and exactly one set of equations for each of the disjunctions. This paper focuses mainly in the solution of systems of linear disjunctive equations. Using a convex hull representation of the disjunctions, the disjunctive system of equations is converted into an MELP problem. A sufficient condition is presented under which the model is shown to be solvable as an LP problem. The extension of the proposed method to nonlinear disjunctive equations is also discussed. The application of the proposed algorithms are illustrated with several examples.

Keywords: Disjunctive Programming, Mixed-Integer Programming

Introduction

A basic problem in Process Systems Engineering is the solution of sets of algebraic linear/nonlinear equations (Sargent, 1981). While a large body of literature has been reported on these problems, much less attention has been given to the solution of conditional models where the equations/inequalities of the unit depend on the region that they were defined. A simple example is the friction factor depending on whether the flow is laminar or turbulent Another example is when different empirical correlations for mass balance are applied over several ranges in plant capacity. Stateva and Westerberg (1983) were the first researchers to address the problem, and developed a search method based on defining differem regions d e p ^ing on the possible behavior of the unit Their method requires visiting the predefmedregk^ OIK by one until the equations of a particular region are satisfied. The extension of this solution approach with NLP techniques was performed by Zaher (1995). In a somewhat related work, Billiard and Biegler (1992) extended their iterated LP techniques for systems of equations and inequalities to structured nonsmooth functions by using a continuous and an MILP formulation for the representation of max. functions by Sahinidis and Grossmann (1991).

Disjunctive programming models that handle the conditional existence of process units in the optimization of linear synthesis problems was proposed by Raman and Grossmann (1994). Aside from showing that generalized disjunctive programming facilitates the modeling of such systems they also proposed a logic based branch and bound algorithm to solve disjunctive linear programming models. TOrkay and Grossmann (1995a) addressed nonlinear disjunctive programming models for the synthesis of process systems, and proposed two logic based MINLP solution algorithms that improve the efficiency and robustness of the solution of these problems.

In this paper, it will be shown that the solution of conditional algebraic equations can be shown to be a particular case of generalized disjunctive programming models. Based on this observation, a solution approach for systems of linear disjunctive equations is proposed. To our knowledge this is the first time that an algorithm has been proposed for linear conditional equations. The basic idea relies on using the convex hull representation for the systems of linear disjunctive equations, which gives rise to an MILP model which has the important feature that it does not involve "big-M" constraints. Sufficient conditions are given that guarantee the proposed model is solvable as a linear program. It is also shown that the solution of systems of nonlinear disjunctive equations can be achieved by extending the convex hull formulation of the disjunctions in a Newton iteration scheme. The application of the algorithms is illustrated with several examples including the mass balance of process networks in which the linear equations are a function of the ranges of component flows, and simulation of pipe networks with check valves.

Problem Formulation

Engineering design, synthesis and operation problems involving discrete choices can be modeled in the following disjunctive programming framework as shown in by Raman and Grossmann (1994):

$$
\begin{aligned}
\min\ Z = &\sum_{i\in D_k}\sum_{k\in K} c_{ik} + f(x)\\
\text{s.t.}\quad & g(x) = 0\\
&\bigvee_{i\in D_k}\begin{bmatrix} Y_{ik}\\ h_{ik}(x) = 0\\ r_{ik}(x) \le 0\\ c_{ik} = \gamma_{ik}\end{bmatrix} \quad k\in K \qquad (1)\\
&\Omega(Y) = \text{True}\\
&x \in X,\ c_{ik} \ge 0,\ Y = \{\text{True},\text{False}\}
\end{aligned}
$$

When there is no objective function in the above problem, and no logic relations between the Boolean variables, problem (1) reduces to the system of disjunctive equations:

$$
\begin{aligned}
&g(x) = 0\\
&\bigvee_{i\in D_k}\begin{bmatrix} h_{ik}(x) = 0\\ r_{ik}(x) \le 0\end{bmatrix} \quad k\in K \qquad (2)\\
&x\in X
\end{aligned}
$$

As will be shown in the next section a simple but efficient solution method can be derived for the linear case with no degrees of freedom.

Linear Systems

For the ca$e of linear equations and inequalities problem (2) is given by the following system of disjunctive equations,

$$Ax=b$$
$$\bigvee_{i\in D}\begin{bmatrix} B_{ik}x = b_{ik} \\ C_{ik}x \le d_{ik}\end{bmatrix} \quad \forall k\in K \tag{3}$$

where it is assumed that x is an n-dimensional vector, the matrix of coefficients B& is ftc* n-dimensional, and the dimension of matrix A is mxn where m = n - £Pk • Also for simplicity we assume that all the disjunctions have the same number of
keK
terms. Hence, we drop the subscript k in the set D. To our knowledge, no method has been proposed for solving problem (3).

A first important question is the existence and uniqueness of solution for (3). It is clear that there exists at least one solution $\hat{x}$ if the following condition holds:

Condition I: Existence of a solution.

3$\hat{i}$k Vk€K
such that
A$\hat{x}$ = b, B^xsbj^.andC^x^d^

where the augmented matrix [A^T, B?, B?2,..]^T is non-singular.

Furthermore, the solution is unique if all but one term in each disjunction arc not satisfied. That is,

ConditionII: CfcX>dfc Vi*$\hat{i}$, keK.

Following the treatment by Balas (1985) (see also Tdikay and Grossmaim, 1995b for derivation) the convex hull of the disjunctive system in (3) is given by the following system in which the variables x are disaggregated for each disjunction and by introducing variables yik for the terms of each disjunction:

$$\begin{aligned} &Ax = a \\ &x=\sum_i x_{ik} \quad k\in K \\ &\left.\begin{aligned} B_{ik}x_{ik} &= b_{ik}y_{ik} \\ C_{ik}x_{ik} &\le d_{ik}y_{ik}\end{aligned}\right\} i\in D,\ k\in K \\ &\sum_{i\in D} y_{ik} = 1 \quad \forall k\in K \\ &x\in X,\ yik^O \end{aligned} \tag{4}$$

The above can be formulated as an MILP model by requiring integrality of the y variables and by defining a simple objective function:

$$\begin{aligned} &\min \sum\sum y_{ik} \\ &\text{s.t.}\quad Ax = a \\ &x = I>ik \quad k e K \\ &\left.\begin{aligned} B_{ik}x_{ik} &= b_{ik}y_{ik} \\ C_{ik}x_{ik} &\le d_{ik}y_{ik}\end{aligned}\right\} i\in D,\ k\in K \\ &\sum_{i\in D} y_{ik} = 1 \quad \forall k\in K \\ &x\in X,\ yfc=0,l \end{aligned} \tag{5}$$

While the size of the model can become relatively large, the importance of (5) is that it does not involve "big-NT constraints. Furthermore, the solution of the MILP in (S) is often attained in the LP relaxation step. A sufficient condition is given by the following proposition.

~~Proposition:~~ Consider that conditions I and II are satisfied for the linear disjunctive problem in (3). Assuming that the inequalities Cikx £ djk are inactive, there exists a basic solution in the LP relaxation of (5) such that $y_{\hat{i}k}=1$, $y_{ik}=0$, $i\in D$, $k\in K$.

~~Proof:~~ The total number of variables in (S) is given by n+IDHKIn+IDIIKI corresponding to the dimensions of x, x_{ik} and y_{ik}. The total number of equations in (4) (except inequalities) is given by:

$$(n-\sum_k Pk) + n + DQ;\sum_k p_k) + K \tag{6}$$

Rearranging (6) the number of equations is:

$$2n + (D-l)\sum_k Pk + K \tag{7}$$

Hence, the number of degrees of freedom in (4) is:

$$\Phi=[IDIIKI-l]n-(D-l)X p_k+IDIIKI-K \tag{8}$$

Since n £ £ p k and IKfel, IDfc>2, it follows that (IDIIKI-l)n £ (D - l)n £ (D - l) £ p k , which in turn implies that
k k
<t> ^IDIIKI-K. Therefore, a feasible selection for a basis in (5) is to select IDIIKI-1 non-basic variables y^. Since the equations £ yik=l. ke K are included, this yields yfc=l, yik=O» ie D, *ke* K. Furthermore, the remaining non-basic variables can easily be chosen among the disaggregated variables X&, i*i. Q**ED**

It should be noted that if one or more inequalities are active at the solution, then depending on the number of disjunctions IKI, and the corresponding number of terms IDI, the arguments of the proof of the above theorem may or may not apply. Hence, in that case the likelihood of solving the MILP as an LP is generally decreased.

Illustrative Example 1:

Consider the following system of linear disjunctive equations shown in Fig.l:

$$u + v = 2$$
$$\begin{bmatrix} v = u \\ u \le 1 \end{bmatrix} \vee \begin{bmatrix} v = u + 1 \\ v \le 1 \end{bmatrix} \qquad (9)$$

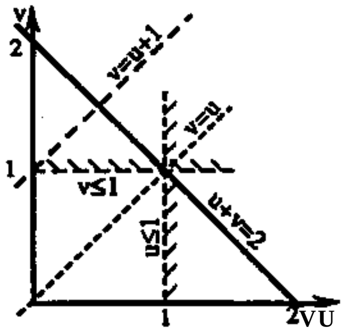

Fig.l. System of Linear Disjunctive Equations in Example 1.

It is seen from Fig.l. **that** only **the** left side of **the** disjunction satisfies **the** system at u=l **and** v=L **The system** of disjunctive **equations** in **(9) arc formulated with the MILP convex hull formulation of (5) as follows:**

$$\begin{aligned} \min\ & Z » y_1 + y_2 \\ \text{s.L}\ & u + v = 2 \\ & U = Ui + U2 \\ & v \text{ a } vj + V2 \\ & v_1 = u_1 \\ & u_1 \le y_1 \\ & v_2 = u_2 + y_2 \\ \\ & Yl + Y2 * 1 \\ & u,ui,U2,v,vi,v_2 \text{^}0,\ yi,y2=0,l \end{aligned} \qquad (10)$$

The problem is solved as a relaxed LP in 1 simplex iteration with GAMS/OSL (Brooke, et al., 1992) yielding the solution point u=l, v=l.

A straightforward approach is one in which (9) is solved with the following "big-M" formulation:

$$\begin{aligned} \min\ & Z \text{ a } yj + y_2 \\ \text{s.t.}\ & u + v = 2 \\ & -5(1 - y_1) \le v - u \le 5(1 - y_1) \\ & u \le 1 + 5(1y\text{-}i\ ) \\ & -5(1-y_2) \le v-u-1 \text{^} 5(1-y_2) \\ & v \le 1 + 5(1-y_2) \\ & yi+Y2 = 1 \\ & u,v \text{^}0,\ yi,y_2=0,l \end{aligned} \qquad (11)$$

The solution to (11) is not attained as a relaxed LP, presumably because of the presence of the big-M constraints. The LP relaxation yields the value y1=0.6, y2=0.4, u=2, v=0.

Systems of Nonlinear Disjunctive Equations

In this section we will outline the extension of the proposed method for the solution of systems of linear disjunctive equations to the case of nonlinear disjunctive equations using a Newton iteration scheme.

Consider the following system of disjunctive nonlinear equations:

$$g(x) = 0$$
$$\bigvee_{i \in D} \begin{bmatrix} h_{ik}(x) \\ r_{ik}(x) \le 0 \end{bmatrix} \quad \forall k \in K \qquad (12)$$

Linearization of the above system at any point x' is given by:

$$g(x^l) + \nabla g(x^l)^T (x - x^l) = 0$$
$$\bigvee_{i \in D} \begin{bmatrix} h_{ik}(x^l) + \nabla h_{ik}(x^l)^T (x - x^l) = 0 \\ r_{ik}(x^l) + \nabla r_{ik}(x^l)^T (x - x^l) \le 0 \end{bmatrix} \quad \forall k \in K \qquad (13)$$

Following a similar treatment as in the linear case, the convex hull representation of disjunctive system of equations in (13) is given by:

$$g(x') + \nabla g(x')^T(x-x') = 0$$
$$x = \sum_i x_{ik}$$
$$\left.\begin{array}{l}\nabla h_{ik}(x^l)^T x_{ik} = -\left[h_{ik}(x^l) - \nabla h_{ik}(x^l)^T x^l\right] y_{ik} \\ \nabla r_{ik}(x^l)^T x_{ik} \le -\left[r_{ik}(x^l) - \nabla r_{ik}(x^l)^T x^l\right] y_{ik}\end{array}\right\} \forall i, k \qquad (14)$$
$$\sum_{i \in D} y_{ik} = 1 \quad \forall k \in K$$

In order to determine a new guess from the convex hull formulation of the linearized disjunctive system of equations, an MUP problem similar to (5) will be formulated where an objective function is defined such that the summation of all binary variables y^ is to be maximized. An important difference, however; with the linear case is that linearizations of the nonlinear equations may lead to infeasibilities even if there is a solution in a given region. For this reason we introduce slack variables in the spirit of the work by Bullard and Biegler (1991) and redefine and augmented penalty function. Hence, the MILP subproblems have the form:

$$\min \; Z = \sum\sum y_{ik} + w_p(p_P + p_N) + w_q(q_P + q_N) + w_s^T s$$
$$\text{s.t.} \quad g(x') + \nabla g(x')^T(x-x') = p_P - p_N$$
$$x = \sum_i x_{ik}$$
$$\left.\begin{array}{l}\nabla h_{ik}(x^l)^T x_{ik} = -\left[h_{ik}(x^l) - \nabla h_{ik}(x^l)^T x^l\right] y_{ik} + q_P - q_N \\ \nabla r_{ik}(x^l)^T x_{ik} \le -\left[r_{ik}(x^l) - \nabla r_{ik}(x^l)^T x^l\right] y_{ik} + s\end{array}\right\} \forall i, k \qquad (15)$$
$$\sum y_{ik} = 1 \quad \forall k \in K$$
$$x \in X, \; p_P, p_N, q_P, q_N, s \ge 0, \; y_{ik} = 0,1$$

The weights w_p, w_q, w_s are assumed to be selected so as to be sufficiently large (e.g., 1000 times the lagrange multipliers as in Viswanathan and Grossmann, 1990).

The Newton solution algorithm consists then of the following steps:

L Set /=1, select tolerance e (e.g. &S10"^4), set step reduction factor a (e.g. a=0.25), select initial point x', and set initial error ϕ ∞.

2. Linearize the system of equations at the point x^l as in (13).

3. Formulate and solve the MILP problem in (IS) to determine new values x^{l+1} of the continuous variables.

4. Determine the error of the function values ϕ^{l+1} as follows:

V=abs(g(x'))+abs(h_{ik}(x') y_{ik}^l)+r

where r = abs($r_{ik}(x^l)\, y_{ik}^l$) if $r_{ik}(x^l)>0$

r = 0 otherwise

a) If ^ f t , stop.

b) If V+t>tf, set x^{/+/}=x'+a(x^{/+/}-x'). Set /=/+/, go to step 2.

c) If <^{/+7}≤<t/, set $x^M=x^l$, set /=/+7, go to step 2.

Illustrative Example 2:

Consider the following system of nonlinear disjunctive equations that is shown in Fig.2:

$$u + v = 2$$
$$\begin{bmatrix} v = (u + \sqrt{2})^2 \\ v \le 1 \end{bmatrix} \vee \begin{bmatrix} v = u^2 \\ u \ge 0.5 \end{bmatrix} \qquad (16)$$

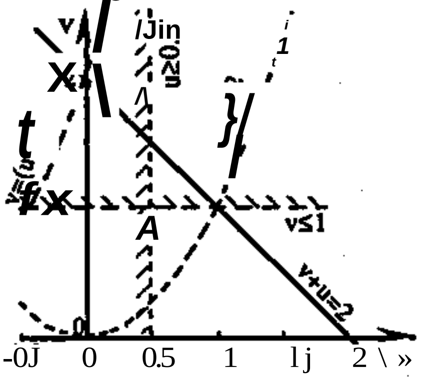

Fig.2. System of Nonlinear Disjunctive Equations in **Example** 2.

Applying the proposed procedure with a tolerance of t=\0^A the problem is solved in 13 iterations starting from the initial point (0,0).

Examples

In this section we present larger examples to illustrate the application of the proposed methods.

Example 3: Linear Process Simulation Problem

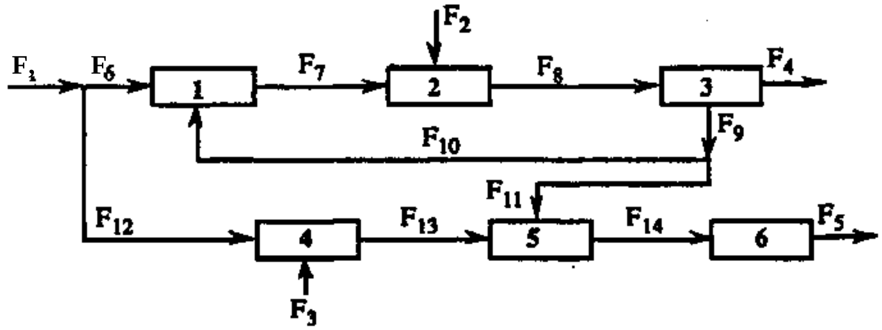

Fig.3. Flowsheet of the Linear Process Simulation Problem.

In this problem, there are 6 processing units with multiple input/output streams as shown in Fig.3. Each unit has three operating regions with different equations depending on their primary product flowrate as shown in Table 1. Fixing Fi to 47.5, the disjunctive model consists of 13 variables, 2 global linear equations and 6 disjunctions each consisting of 3 terms with one or more equations. The MILP corresponding to (5) consists of 18 0-1 variables, 66 continuous variables and 89 equations. The problem was solved in 38 iterations with GAMS/OSL and only S nodes are visited were examined in the branch and bound search requiring a total CPU time of 0.43 seconds on an IBM RS6000/530. The same problem is solved in 158 iterations and 38 nodes in 1.32 seconds with the "big-M" formulation.

Table 1. Material balance equations for units in Example 2.

Unit	Main Prod	Interval	LB	UB	Mass Balance Coefficients	
1	Fr	1	0	50	F_6: 1.10	F_{10}:0.05
		2	50	80	1.15	0.10
		3	80	150	1.20	0.20
2	Fg	1	0	50	F_2:0.50	F_7: 0.80
		2	50	100	0-47	0.75
		3	100	150	045	0.70
3	F4	1	0	50	F_g: 1.70	F_9: 0.67
		2	50	no	1.80	0.70
		3	no	180	1.87	0.75
4	Fis	1	0	50	F_3: 1.18	F_{12}:0.23
		2	50	90	1.15	0.25
		3	90	140	1.10	030
5	Fl4	1	0	40	F_u:0.37	F_{13}:1.20
		2	40	80	035	125
		3	80	130	030	130
6	F_5	1	0	20	F_{14}:1.15	
		2	20	45	1.10	
		3	45	75	1.02	

Example 4: Nonlinear Systems of Equations

The following system of disjunctive nonlinear equations were considered in this example:

$$
\begin{gathered}
x_1 + x_2 = 14 \\
\begin{bmatrix} x_1 = (x_2)^2 \\ x_1 \le 6 \end{bmatrix} \vee \begin{bmatrix} x_1 = (x_2 + \sqrt{3})^2 \\ x_1 \ge 6 \end{bmatrix} \\
\begin{bmatrix} x_2 = \sqrt{x_3 + 2} \\ x_2 \le 2 \end{bmatrix} \vee \begin{bmatrix} x_2 = \sqrt{x_3} \\ x_2 \ge 2 \end{bmatrix} \\
\begin{bmatrix} x_3 = (x_4 + 1)^2 \\ x_3 \le 2 \end{bmatrix} \vee \begin{bmatrix} x_3 = (x_4 + 2)^2 \\ x_3 \ge 2 \end{bmatrix}
\end{gathered}
\qquad (17)
$$

Using as a starting point x=(l,1,1,1) and a tolerance of e=10*^{4}, the algorithm converged to the solution x=(12.2343,1.7657,l.l 177,0.0572) in 4 iterations requiring 1.1 seconds with GAMS/OSL on an IBM RS6000/530.

Example 5: Pipe Network

Consider the pipe network described in Bullard and Biegler (1992), consisting of 22 nodes, 38 pipes and 5 check valves as shown in Fig. 4. The pipe network can be modeled by the following system of disjunctive equations:

Hy =

$$\sum_j Q_{ij} \quad \_ \, \sum_j Q_{ji} = w_i \qquad \text{Vnodei}$$

$$H_{ij} = K\,\text{sign}(Q_{ij})Q_i^2 \qquad \text{Varcs i, j without valve}$$

$$\begin{bmatrix} KQ_{ij}^2 = 0 \\ Hij \leq 5 \end{bmatrix} \vee \begin{bmatrix} KQJ\text{-}Hy \\ H_{ij} \geq \delta \end{bmatrix} \qquad \text{Varcs i, j with valve} \qquad (18)$$

Qij^O Varcs i, j with valve

where 5 is a small tolerance

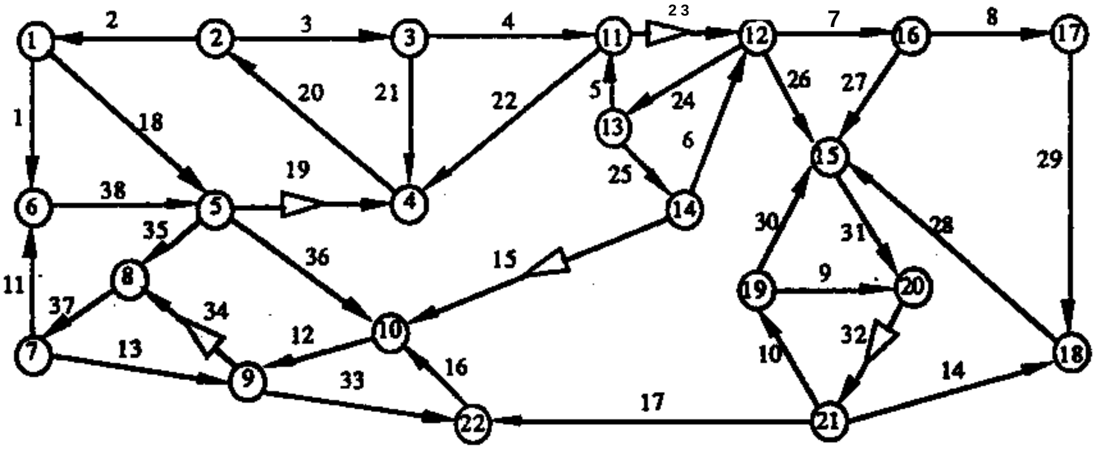

Fig.4. Pipeline example with five check valves.

Applying the proposed method with a tolerance of e=10*^{4}$_t$ convergence is achieved in 10 iterations requiring 3.8 CPU seconds with GAMS/OSL on an IBM RS6000/530 workstation. The progress of iterations is summarized in Table 2.

Table 2. Summary of iterations for pipe network example.

Iteration	Initial	1	2	3	4	5	6	7	8	9	10
Error	34.96303	8.47843	2.10858	0.53012	0.13250	0.03312	0.00828	0.00207	0.00051	0.00012	0.00003

Conclusions

This paper has addressed the solution of algebraic disjunctive equations. For the linear case, it has been shown that the problem can be solved as an MILP problem that is often solvable as an LP. The extension to the nonlinear case has also been considered although no theoretical guarantee of convergence was given. The effectiveness of the proposed methods has been illustrated with several example problems.

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