On Numerical Stability of Relaxations of Generalized Disjunctive Programs

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Abstract

In this paper we present an approach that guarantees equally tight, if not tighter, continuous relaxations of mixed-integer (non)linear programs obtained by the reformulation of Generalized Disjunctive Programs than those obtained by the Hull Reformulation. The approach allows to solve cases where the the functions are not defined at a particular point or even over a larger part of the domain of the global variables. The numerical difficulties are avoided by the translation of variables. An algorithm is presented that optimizes the values of the non-zero points to which the disaggregated variables are driven when the corresponding binary variables are zero. The different MINLP reformulations obtained, i.e., the proposed reformulation, Big-M reformulation, and Hull reformulation, are discussed and compared in terms of their efficiency based on the results of numerical studies.

**Keywords**: Generalized Disjunctive Programming, Mixed-Integer Nonlinear Programming, Continuous Relaxation, Hull Reformulation, Big-M.

* 1. Introduction

This Generalized Disjunctive Programming (GDP) paradigm finds applications in various fields of engineering where decisions involve simultaneous continuous and discrete interactions. It was introduced as an alternative representation of the Mixed-Integer Nonlinear Programming (MINLP) model (Türkay and Grossmann, 1996; Lee & Grossmann, 2000; Grossmann and Lee, 2003). Although the GDP framework provides a higher-level representation of the relationships between the discrete and continuous aspects of a model, solving these models directly is not straightforward. Commonly, a reformulation of GDP into its MINLP counterpart is used. This can be achieved by either the Big-M reformulation (BMR) or Hull Reformulation (HR). The latter generally provides tighter continuous relaxation of the obtained MINLP (Lee and Grossmann, 2000); however, at an expense of increased model size. In addition, if a constraint *r*(*x*) ≤ 0 in a disjunction of a GDP is nonlinear, it requires the introduction of the perspective function *yr*(*x*/*y*), where *y* is a binary variable, or its numerically more stable approximation, Eq. 1, (Sawaya and Grossmann, 2007).

 (1)

One of the downsides is that either of the perspective function formulations introduces additional nonlinear terms for each linear term originally present in *r*(*x*). To avoid this, Bogataj and Kravanja (2018) introduced a reformulation that preserves the nonlinear functions in their original form. The reformulation is based on the translation of variables introduced by Ropotar and Kravanja (2009). So far, however, the continuous relaxations obtained by HR have generally been tighter.

In this work we focus on reformulation of nonlinear GDPs that contain problematic functions that are undefined either at a single point or over a larger part of the domain of global variables. The most common examples of such functions in engineering are logarithmic and rational functions, the simples being 1/*x*.

* 1. Proposed reformulation

The proposed GDP to MINLP reformulation addresses three goals. The first goal is to provide a reformulation that avoids numerical difficulties that arise when one or more constraints in the disjunctive terms are undefined at a particular point or over a larger part of the domain of global variables. The second goal is to provide a reformulation that preserves the form of the local constraints. The third and final goal is to provide a reformulation that guarantees a tight continuous relaxation of the resulting MINLP. To keep the derivation short, let us consider the following problem (GDP), which consists of an objective function *f*(**x**), a global constraint *g*(**x**) and a disjunction with two terms containing local constraints *r*1(**x**) and *r*2(**x**).

 (GDP)

The proposed Mixed-Integer Reformulation (MIR) follows the general idea of HR. However, three major exceptions are noticeable. First, the local constraints are expressed with disaggregated variables **x**D without the use of the perspective function. Second, the bounding constraints on disaggregated variables (Eqs. 2–3) are augmented to fix disaggregated variables to predetermined non-zero values **x**F if *yj*= 0, and allow them to take any value between the lower and upper bounds if *yj* =1. Third, the aggregation constraint (Eq. 4) is augmented so that the value *x*F*i,j* is subtracted from the value of the corresponding disaggregated variable if y*j* = 0.

 (MIR)

* 1. Illustrative Example

The example considered in this work is a convex nonlinear GDP example composed of a quadratic objective function, and a single disjunction with three terms (GDP-E). The optimal solution to the problem is *Z* = 6.8237, **x** = (3.7069, 4.1506), **Y**= (*False, True, False*). The problematic constraints within each term are those with logarithmic functions.

 (GDP-E)

* 1. Numerical results

*Big-M reformulation (BMR):* The most important thing when applying the BMR is to determine the appropriate values of Big-M parameters. They should be large enough to make a particular constraint redundant when *y* = 0, so that the entire feasible region of the problem is preserved. At the same time, they should be small enough to ensure a tight continuous relaxation of the problem. A common approach is to maximize the value of each constraint *r*(**x**) ≤ 0, s.t. **x**LO ≤ **x** ≤ **x**UP by which the following Big-M parameters *Mj,k* = (141,1, 491,2, 142,1, 82,2, 113,1, 44.753,2), where *j* = 1, 2 , 3 is the term in disjunction and   
*k* = 1, 2 is index of a constraint in the particular term of the disjunction. Note, however, that the constraints containing logarithmic functions are not easily subjected to this approach. For example, in constraint *r*1,1(**x**), the term –log(*x*1) approaches ∞ as *x*1 approaches 0, and becomes the dominant term in the constraint, thus making the Big-M parameter seemingly infinite. To avoid this, the Big-M parameter was determined by bounding the critical variable to the *δ*-vicinity (*δ =* 10*–*9) of a point at which the function is undefined. Nevertheless, solving the problem using BMR when the domains of problematic constraints do not coincide leads to reduction of feasible region and potential cut-off of the optimal solution. In the given example, a solution *Z* = 13.5812, **x** = (6.1253, 2.0981), **y**= (0, 0, 1) was identified as optimal. The reason is that no matter how large the Big-M parameters associated with the critical functions are, the only part of the feasible region in which all the critical functions are defined is when *x*1 ≥ 6.0000 + *δ.*

*Modified Hull Reformulation (MHR):* The HR (Lee and Grossmann, 2000) requires that the continuous variables assume the value 0 if a disjunctive term is not selected, i.e., *y* = 0. Therefore, it is required that all constraints in disjunctions are defined at 0. This is clearly a difficulty in the given example. To overcome this problem, we propose a modified formulation of the perspective function (Eq. 5). The bounding constraints on the disaggregated variables and the aggregating constraint are the same as in MIR. Eq. 5 is an extension of the one proposed by Sawaya (2006) and allows continuous variables to take values different than 0 when *y* = 0. It is also easy to show the reformulation is identical to the HR when parameter *x*F is 0.

 (5)

The GDP-E was formulated as an MINLP using BMR, MHR (*ε =*10–6) and the proposed MIR. First, apart from the BMR, the models were solved with 10,000 uniformly distributed values of the parameter *x*F per disjunctive term. All *x*F values were feasible points. The distribution of the obtained objective functions is shown in Figure 1. The results show that the values of *x*F clearly affect the tightness of the continuous relaxation in both MINLP reformulations, indicating that neither reformulation yields a strict hull relaxation. While MIR leads to tighter relaxations (3.850 ≤ *Z*R ≤ 5.085) compared to the MHR (3.466 ≤ *Z*R ≤ 3.527), the deviation around the mean value is significantly lower in the latter case. We attribute the “looseness” of the MHR to the effect of the last term in Eq. 5, which acts as a considerably large Big-M parameter for small *ε* and large *x*F values.

|  |
| --- |
|  |
| (a) |
|  |
| (b) |

**Figure 1:** Distribution of objective function values obtained from 10,000 randomly selected *x*F points: (a) MIR, (b) MHR.

Second, each of the 10,000 *x*F values were optimized with the goal of obtaining the tightest possible continuous relaxation of the MINLP problem. The optimization was based on an algorithm that iterates between two nonlinear problems (NLPs). The first NLP is relaxed MINLP with respect to MHR or MIR. Note that the problem is convex if GDP is convex. The second NLP corresponds to its nonconvex derivative, in which the aggregating constraint is replaced by Eq. 6 and the bounding constraints on disaggregated variables are omitted. The algorithm iterates between the two NLPs and resets the value of the parameters *x*F to the current solution (values of the disaggregated variables) of the optimization problem. The algorithm terminates once the difference between the values of the objective functions is less than tolerance (e.g. 10–5).

 (6)

The proposed algorithm was used to obtain the values of the *x*F parameters shown in Table 1. Regardless of the initial random value, the same optimal values were obtained in all 10,000 cases. Note that none of the values listed in Table 1 correspond to the optimal solution of the GDP problem or to the minimum of a particular disjunction with respect to the objective function. The values of the objective functions when solving the continuous relaxation of the corresponding MINLPs are 3.6604 for MHR and 5.1928 for MIR. Thus, in both cases, the continuous relaxation is tightened. The optimization of the *x*F parameters took on average 1 pass (2 NLPs) in the case of MIR and 3 passes (6 NLPs) in the case of MHR. As a sidenote, the optimal values of the *x*F parameters can also be determined by iteratively solving the convex, relaxed MINLP alone. In our experience, however, up to 20 NLPs must be solved before the algorithm terminates. This is not problematic for the small example considered in this paper but can contribute significantly to the solution time of larger problems.

**Table 1:** Values of optimal *x*F parameters.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **MHR** | | | | | | |
| ***x*F*i,j*** | *x*F1,1 | *x*F1,2 | *x*F1,3 | *x*F2,1 | *x*F2,2 | *x*F2,3 |
|  | 0.811 | 0.989 | 4.156 | –0.932 | 5.000 | 2.012 |
| **MIR** | | | | | | |
| ***x*F*i,j*** | *x*F1,1 | *x*F1,2 | *x*F1,3 | *x*F2,1 | *x*F2,2 | *x*F2,3 |
|  | 0.305 | 3.206 | 6.050 | –0.516 | 4.685 | 1.702 |

In addition to the illustrative example presented in Chapter 3, the proposed approach was tested on several examples from the literature, such as different instances of illustrative examples, e.g., Circles (Lee and Grossmann, 2000), and various instances of a Strip Packing Problem (Trespalacios and Grossmann, 2016), and Process Synthesys Problem (Türkay and Grossmann, 1996, Sawaya and Grossmann, 2007). The aim was to cover the diversity of GDPs, i.e., from purely linear GDPs to purely nonlinear GDPs. The results of these experiments show that the proposed MIR in conjunction with the proposed algorithm to optimize *x*F values provides as tight a continuous relaxation as HR, regardless of the GDP type.

* 1. Conclusions

In this paper, we have presented an approach to reformulate GDP problems into MI(N)LP problems. The strength of the proposed approach is that the points at which the local constraints in disjunctions are not defined, if such constraints exist, do not pose a numerical problem. According to the results obtained, it provides at least as tight a continuous relaxation as HR. Moreover, the proposed approach avoids the use of the perspective function when local constraints are nonlinear; therefore, the reformulation of GDP is identical for linear and nonlinear constraints. We could argue that this simplifies the implementation of the proposed approach compared to HR. More importantly, the proposed reformulation does not introduce additional nonlinearities. A drawback of the proposed approach is that, at the time of this publication, an algorithmic approach is needed to determine the values of the *x*F parameters.

This research provided some answers and new insights into GDP to MI(N)LP reformulations. However, it also opened up several additional topics for future research. The first is to determine whether an algorithmic approach can be avoided when determining the optimal values of the *x*F parameters. Furthermore, it is tempting to answer the question whether and under which conditions the optimal values of the *x*F parameters can be used to tighten the bounds on disaggregated variables. Last but not least, future research will try to determine the role of *x*F parameters in the Logic-Based Outer Approximation algorithm, namely their potential role in providing valid and good linearization points.

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