Convex envelopes of multilinear terms: the dual approach

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1 Introduction

In the Global Optimization community that stems out of Chemical Engineering, there seems to be an ongoing race to finding the "explicit form of the convex envelopes of the k-linear terms", i.e. inequalities depending on the original (primal) problem variables. This race lately got to the point where such explicit formulæ became simply too unwieldy to be useful. Since k-linear terms have vertex polyhedral convex envelopes [6], a very natural way to describe these envelopes is to use the *dual* formulation for the convex hull of a set of points. In our talk we shall describe our computational set-up for comparing the classic primal with the new dual envelopes. By definition of convex envelope, the two formulations yield exactly the same bounds. It turns out, however, that the dual envelopes can be solved more efficiently than the primal ones.

2 The setting

We consider the multilinear Mixed-Integer Nonlinear Program (MINLP) formulation:

$$\left.\begin{array}{rrcl} \min_x & g_o(x) & & \\ \forall 1 \le i \le m & g_i(x) & \le & 0 \\ \forall 0 \le i \le m & g_i(x) & = & \sum_{\ell \in L_i} c_{i\ell} T_\ell(x_{K_\ell}) f_{i\ell}(x) + \hat{f}_i(x) \\ \exists Z \subseteq \{1,\ldots,n\} \forall j \in Z & x_j & \in & \mathbb{Z} \\ & x^L \le x & \le & x^U \end{array}\right\} \tag{1}$$

where $x \in \mathbb{R}^n$ are decision variables, $x^L, x^U \in \mathbb{R}^n$ are given variable bounds, L_i is a set indexing the multilinear terms in the i-th constraint, $c_{i\ell} \in \mathbb{R}$, K_ℓ is a set indexing the variables occurring in the ℓ-th multilinear term T_ℓ, $f_{i\ell}, \hat{f}_i : \mathbb{R}^n \to \mathbb{R}$.

Several applications are in this class, e.g. pooling and blending, multilinear least squares, distance geometry. Problems (1) can be solved to global optimality using the spatial Branch-and-Bound (sBB) algorithm, which requires the (automatic) construction of a convex relaxation [2]. This relaxation involves replacing each multilinear term T_ℓ with a new *linearizing variable* w_ℓ, and ensuring that

$$(x, w_\ell) \in B = \mathrm{conv}(\{w_\ell = T_\ell(x_{K_\ell}) \mid x^L \le x \le x^U\}). \tag{2}$$

3 Convex envelopes of multilinear terms

Consider a k-linear term T_ℓ with $k = |K_\ell|$. Because of vertex polyhedrality, (2) are enforced by means of adjoining linear inequalities to the formulation. Whenever x^L, x^U are assigned numerical values, the actual constraints implying (2) can be worked out by software such as PORTA [3] for any k. The challenge is to find out formulæ which explicitly mention the *symbols*

x^L, x^U, and which yield the linear inequalities for (2) on replacing such symbols with the given bound values. For $k = 2$, the *McCormick's envelopes* [4] imply (2) using 4 inequalities. For $k = 3$, Meyer and Floudas [5] worked out 10 cases (depending on bound signs and other factors) with 12 inequalities each: as such, implementing Meyer and Floudas' work computationally is a significant hurdle. We believe that even though the next step ($k = 4$) were to be solved, it would border on practical uselessness out of sheer size. It turns out that just *one* case for $k = 4$, that of nonnegative bounds, was recently worked out [1], and it contains 44 inequalities. The dependency of the number of inequalities on k is $O(2^k)$, with a definitely positive multiplying factor that empirically looks like $O(k)$.

Because it is defined over the hyperrectangle H given by $x^L_{K_\ell} \le x_{K_\ell} \le x^U_{K_\ell}$, the graph of T_ℓ is a pointed hypersurface homotopic to H. The first k components of each of its extreme points $P = \{p_1, \ldots, p_{2^k}\} \subseteq \mathbb{R}^{k+1}$ are the vertices of H, and the last component is the k-linear product of the previous components. We define

$$\forall i \le 2^k \; d_i = \left(\left\lfloor \frac{i-1}{2^{k-j}} \right\rfloor \bmod 2 \mid j \in K_\ell \right) \quad \wedge \quad \forall j \in K_\ell \; b_j(0) = x^L_j \;\wedge\; b_j(1) = x^U_j,$$

i.e. for all $i \le 2^k$, we have $p_i = (b_j(d_{ij}) \mid j \in K_\ell)$. Having listed the extreme points P of B, we add 2^k new variables $\lambda_i \ge 0$. Then the vectors $x \in B$ can be described as follows:

$$\forall j \in K_\ell \; x_j = \sum_{i \le 2^k} \lambda_i b_j(d_{ij}) \quad \wedge \quad w_\ell = \sum_{i \le 2^k} \lambda_i \prod_{j \in K_\ell} b_j(d_{ij}) \quad \wedge \quad \sum_{i \le 2^k} \lambda_i = 1. \qquad (3)$$

It is well known that the projection of the (x, w_ℓ, λ)-set (3) on (x, w_ℓ) is precisely B. The dual envelopes adjoin *precisely* 2^k nonnegative variables and $k + 1$ constraints to (1).

4 Results and outlook

Our computational results are consistent with the size difference between $2^k + k + 1$ new entities of the dual envelopes and the apparent $O(k2^k)$ new entities of the primal envelopes: our most remarkable result is that dual formulations are better than primal formulations in practice. This also means that global optimizers working on sBB (the senior author of this paper among them) have been managing convex relaxations the wrong way for decades. As a further point, our work also settles the "race" mentioned above for all values of k in an elegant way.

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