Relaxations of multilinear convex envelopes: dual is better than primal

Alberto Costa¹, Leo Liberti¹

¹LIX, École Polytechnique, Palaiseau, France

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- Definitions
- Multilinear terms
- Applications

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Outline



- Definitions
- Multilinear terms
- Applications

2 Relaxations

- Primal relaxation
- Dual relaxation

Outline



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3 Results

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Outline



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Definitions Multilinear terms Applications

Where are we?



- Definitions
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2 Relaxations

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- Dual relaxation

3 Results



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Definitions Multilinear terms Applications

Convex sets



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Definitions Multilinear terms Applications



- Let $S \subseteq \mathbb{R}^n$ be non-empty
- \bullet Any convex set containing S is a convex relaxation of S

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Definitions Multilinear terms Applications

Convex sets

- Let $S \subseteq \mathbb{R}^n$ be non-empty
- Any convex set containing S is a **convex relaxation** of S
- $\bullet\,$ The convex hull $\operatorname{conv} S$ of S is the intersection of all convex relaxations of S



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Definitions Multilinear terms Applications

Convex functions

• Let $C \subseteq \mathbb{R}^n$ be convex and compact

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Definitions Multilinear terms Applications

Convex functions

- Let $C \subseteq \mathbb{R}^n$ be convex and compact
- $\bullet~ \mbox{Let}~ f: C \rightarrow \mathbb{R}$ be lower semicontinuous

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Definitions Multilinear terms Applications

Convex functions

- Let $C \subseteq \mathbb{R}^n$ be convex and compact
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- Any convex function underestimating *f* is a **convex** relaxation of *f*

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Definitions Multilinear terms Applications

Convex functions

- Let $C \subseteq \mathbb{R}^n$ be convex and compact
- $\bullet~ {\rm Let}~ f: C \to \mathbb{R}$ be lower semicontinuous
- Any convex function underestimating f is a ${\bf convex}$ relaxation of f
- The **convex envelope** $\operatorname{conv} f$ of f is the pointwise supremum of all convex underestimators of f



Definitions Multilinear terms Applications

Definitions

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Definitions Multilinear terms Applications

Definitions

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Definitions Multilinear terms Applications

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- The function $w(x) = x_1 x_2 \cdots x_k$ is a multilinear term

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Definitions Multilinear terms Applications

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Definitions Multilinear terms Applications

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- The function $w(x) = x_1 x_2 \cdots x_k$ is a multilinear term
- If k-1 vars are fixed, w is a linear function of 1 var
- Smallest nontrivial case: $w(x) = x_1 x_2$ (bilinear term)



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Definitions Multilinear terms Applications

Some applications

 Process synthesis in chemical engineering (e.g., Haverly's pooling problems [Haverly; ACM SIGMAP Bull., 1978])

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Definitions Multilinear terms Applications

Some applications

- Process synthesis in chemical engineering (e.g., Haverly's pooling problems [Haverly; ACM SIGMAP Bull., 1978])
- Molecular Distance Geometry Problem (MDGP) [Liberti et al.; ITOR, 2008 JOGO, 2009 ITOR, 2010 JOGO, 2011 OPTL, 2011]

Definitions Multilinear terms Applications

Some applications

- Process synthesis in chemical engineering (e.g., Haverly's pooling problems [Haverly; ACM SIGMAP Bull., 1978])
- Molecular Distance Geometry Problem (MDGP) [Liberti et al.; ITOR, 2008 JOGO, 2009 ITOR, 2010 JOGO, 2011 OPTL, 2011]
- Multilinear Least-Squares (MLLS) [Paatero; JCGS, 1999]

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Definitions Multilinear terms Applications

Haverly's pooling problem



Find oil routing minimizing costs and satisfying mass+sulphur balance, quantity and quality demands

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Definitions Multilinear terms Applications

Haverly's pooling problem



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Definitions Multilinear terms Applications

Haverly's pooling problem



Find oil routing minimizing costs and satisfying mass+sulphur balance, quantity and quality demands

Decision variables: input quantities x, routed quantities y, percentage p of sulphur in

pool Sulphur balance: $3x_{11} + x_{21} = p(y_{11} + y_{12})$ Quality demands (blend 1): $py_{11} + 2y_{21} \le 2.5(y_{11} + y_{21})_{\text{max}} + y_{21} \ge 3.3$

Definitions Multilinear terms Applications

Molecular Distance Geometry

• Known set of atoms V, determine 3D structure

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Definitions Multilinear terms Applications

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Definitions Multilinear terms Applications

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Definitions Multilinear terms Applications

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Definitions Multilinear terms Applications

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Continuous quartic formulation:

$$\min_{x} \sum_{\{i,j\} \in E} (||x^{i} - x^{j}||^{2} - d_{ij}^{2})^{2}$$

involves quadrilinear terms

Definitions Multilinear terms Applications

Multilinear Least Squares

- Decision variables x_1, \ldots, x_n
- Sampled data d_1, \ldots, d_m
- Theoretical model:

$$\forall i \leq m \quad d_i = \sum_{\ell \in L_i} \left(\prod_{j \in J_\ell} x_j \right)$$

where $L_\ell \subseteq \{1, \ldots, n\}$ for all ℓ

- Minimize error $Q_p = \|d (\sum_{\ell \in L_i} \prod_{j \in J_\ell} x_j \mid i \le m)\|_p$, where $p \in \mathbb{N} \cup \{\infty\}$
- $\bullet\,$ With $1 \text{ or } \infty\,$ norms, get multilinear terms

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Primal relaxation Dual relaxation

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- 2 Relaxations
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Primal relaxation Dual relaxation

Relaxing problems having multilinear terms

Two ways to relax multilinear terms are presented and compared:

Primal relaxation Dual relaxation

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Primal relaxation Dual relaxation

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- Primal relaxation
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Primal relaxation Dual relaxation

Primal relaxation

• For the general case, convex envelopes for multilinear terms are available explicitly in function of x^L, x^U for k=2,3 and partly k=4

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Primal relaxation Dual relaxation

Primal relaxation

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- They consist of sets of constraints to be adjoined to the Mathematical Programming formulation
Primal relaxation Dual relaxation

Primal relaxation

- For the general case, convex envelopes for multilinear terms are available explicitly in function of x^L, x^U for k=2,3 and partly k=4
- They consist of sets of constraints to be adjoined to the Mathematical Programming formulation
- No further variables are needed

Primal relaxation Dual relaxation

Bilinear terms: McCormick's inequalities

• Let $W = \{(w, x_1, x_2) \mid w = x_1 x_2 \land (x_1, x_2) = [x^L, x^U]\}$, then conv(W) is given by:

$$\begin{array}{rcl} w & \geq & x_1^L x_2 + x_2^L x_1 - x_1^L x_2^L \\ w & \geq & x_1^U x_2 + x_2^U x_1 - x_1^U x_2^U \\ w & \leq & x_1^L x_2 + x_2^U x_1 - x_1^L x_2^U \\ w & \leq & x_1^U x_2 + x_2^L x_1 - x_1^U x_2^L \end{array}$$

 Stated [McCormick; MP, 1976], proved [Al-Khayyal, Falk; MOR, 1983]

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McCormick's envelopes



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Special case: Fortet's linearization

If x_1 and x_2 are binary variables, the McCormick's inequalities lead to the Fortet's inequalities [Fortet; RFR0, 1960]:

$$w \geq 0$$

$$w \geq x_2 + x_1 - 1$$

$$w \leq x_1$$

$$w \leq x_2$$

The resulting reformulation is an exact linearization as shown in [Liberti; RAIRO-RO, 2009]

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Trilinear case

It is not as easy as bilinear convex relaxation:

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• the number of constraints is greater than 4

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Primal relaxation Dual relaxation

Trilinear case

It is not as easy as bilinear convex relaxation:

- the number of constraints is greater than 4
- there are several cases, depending on sign of bounds of the variables: $x_i^L x_i^U \ge 0$ [Meyer, Floudas; 2003]; mixed case [Meyer, Floudas; JOGO, 2004]

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Primal relaxation Dual relaxation

Trilinear case

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- the number of constraints is greater than 4
- there are several cases, depending on sign of bounds of the variables: $x_i^L x_i^U \ge 0$ [Meyer, Floudas; 2003]; mixed case [Meyer, Floudas; JOGO, 2004]
- there are further conditions to check

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Primal relaxation Dual relaxation

Example (1): $x_1^U, x_2^U, x_3^U \le 0$

Permute variables x_1 , x_2 and x_3 such that:

$$\begin{array}{rcl} x_1^U x_2^L x_3^L + x_1^L x_2^U x_3^U &\leq & x_1^L x_2^U x_3^L + x_1^U x_2^L x_3^U \\ x_1^U x_2^L x_3^L + x_1^L x_2^U x_3^U &\leq & x_1^U x_2^U x_3^L + x_1^L x_2^L x_3^U \end{array}$$

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Primal relaxation Dual relaxation

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Permute variables x_1 , x_2 and x_3 such that:

$$\begin{array}{rcl} x_1^U x_2^L x_3^L + x_1^L x_2^U x_3^U &\leq & x_1^L x_2^U x_3^L + x_1^U x_2^L x_3^U \\ x_1^U x_2^L x_3^L + x_1^L x_2^U x_3^U &\leq & x_1^U x_2^U x_3^L + x_1^L x_2^L x_3^U \end{array}$$

Lower envelope:

$$\begin{array}{lll} w & \geq & x_2^L x_3^L x_1 + x_1^L x_3^L x_2 + x_1^L x_2^L x_3 - 2x_1^L x_2^L x_3^L \\ w & \geq & x_2^U x_3^U x_1 + x_1^U x_3^U x_2 + x_1^U x_2^U x_3 - 2x_1^U x_2^U x_3^U \\ w & \geq & x_2^L x_3^U x_1 + x_1^L x_3^U x_2 + x_1^U x_2^L x_3 - x_1^L x_2^L x_3^U - x_1^U x_2^L x_3^U \\ w & \geq & x_2^U x_3^L x_1 + x_1^U x_3^L x_2 + x_1^L x_2^U x_3 - x_1^U x_2^U x_3^L - x_1^L x_2^U x_3^L \\ w & \geq & \mathbf{c_1} x_1 + x_1^U x_3^L x_2 + x_1^U x_2^L x_3 + x_1^L x_2^U x_3^U - \mathbf{c_1} x_1^L - x_1^U x_2^U x_3^L - x_1^U x_2^L x_3^U \\ w & \geq & \mathbf{c_2} x_1 + x_1^L x_3^U x_2 + x_1^L x_2^U x_3 + x_1^L x_2^U x_3^U - \mathbf{c_1} x_1^L - x_1^U x_2^U x_3^L - x_1^U x_2^L x_3^U \\ \end{array}$$

where
$$\mathbf{c_1} = \frac{x_1^U x_2^U x_3^L - x_1^L x_2^U x_3^U - x_1^U x_2^L x_3^L + x_1^U x_2^L x_3^U}{x_1^U - x_1^L}$$
 and
 $\mathbf{c_2} = \frac{x_1^L x_2^L x_3^U - x_1^U x_2^L x_3^L - x_1^L x_2^U x_3^U + x_1^L x_2^U x_3^L}{x_1^L - x_1^U}$

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Primal relaxation Dual relaxation

Example (2): $x_1^U, x_2^U, x_3^U \le 0$

Upper envelope:

w	\leq	$x_2^L x_3^L x_1 + x_1^U x_3^L x_2 + x_1^U x_2^U x_3 - x_1^U x_2^U x_3^L - x_1^U x_2^L x_3^L$
w	\leq	$x_2^U x_3^L x_1 + x_1^L x_3^L x_2 + x_1^U x_2^U x_3 - x_1^U x_2^U x_3^L - x_1^L x_2^U x_3^L$
w	\leq	$x_2^L x_3^L x_1 + x_1^U x_3^U x_2 + x_1^U x_2^L x_3 - x_1^U x_2^L x_3^U - x_1^U x_2^L x_3^L$
w	\leq	$x_2^U x_3^U x_1 + x_1^L x_3^L x_2 + x_1^L x_2^U x_3 - x_1^L x_2^U x_3^U - x_1^L x_2^U x_3^L$
w	\leq	$x_{2}^{L}x_{3}^{U}x_{1} + x_{1}^{U}x_{3}^{U}x_{2} + x_{1}^{L}x_{2}^{L}x_{3} - x_{1}^{U}x_{2}^{L}x_{3}^{U} - x_{1}^{L}x_{2}^{L}x_{3}^{U}$
w	\leq	$x_2^U x_3^U x_1 + x_1^L x_3^U x_2 + x_1^L x_2^L x_3 - x_1^L x_2^U x_3^U - x_1^L x_2^L x_3^U.$

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Primal relaxation Dual relaxation

Quadrilinear terms

The convex envelope is not known explicitly for quadrilinear terms

- Combine bilinear and trilinear envelope [Cafieri, Lee, Liberti; JOGO, 2011]
- Convex envelope for some cases presented in [Balram; M.Sc. Thesis, 2019] (e.g., when x_1^L , x_2^L , x_3^L , $x_4^L \ge 0$, then 44 constraints are generated)

Primal relaxation Dual relaxation

Tighter relaxations by associativity

Write $w = x_1 x_2 x_3 x_4$ as:

- **1** $(x_1x_2)x_3x_4$ (tri(bi,1,1))
- **2** $(x_1x_2x_3)x_4$ (bi(tri,1))
- **3** $(x_1x_2)(x_3x_4)$ (bi(bi(1,1),bi(1,1)))
- ($(x_1x_2)x_3$) x_4 (bi(bi(bi(1,1),1),1))

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Primal relaxation Dual relaxation

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- **3** $(x_1x_2)(x_3x_4)$ (bi(bi(1,1),bi(1,1)))
- $((x_1x_2)x_3)x_4$ (bi(bi(bi(1,1),1),1))

Apply bilinear/trilinear envelopes, get different relaxations for w: which one is tightest?

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Primal relaxation Dual relaxation

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Theorem

Choose smallest number of compositions ((1)-(2) are better than (3)-(4))

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Primal relaxation Dual relaxation

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Apply bilinear/trilinear envelopes, get different relaxations for w: which one is tightest?

Theorem

Choose smallest number of compositions ((1)-(2) are better than (3)-(4))

Some empirical indications on choosing (1) or (2) depending on bounds $\langle \Box \rangle \langle \overline{\Box} \rangle$

Primal relaxation Dual relaxation

Beyond quadrilinear terms

 envelopes for multilinear terms larger than quadrilinear: not known explicitly

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Primal relaxation Dual relaxation

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- envelopes for multilinear terms larger than quadrilinear: not known explicitly
- software as PORTA can compute the convex hull of a given set of points in \mathbb{R}^n

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Primal relaxation Dual relaxation

Beyond quadrilinear terms

- envelopes for multilinear terms larger than quadrilinear: not known explicitly
- software as PORTA can compute the convex hull of a given set of points in \mathbb{R}^n
- Balram's thesis reports a similar procedure to compute the convex hull (but less refined)

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Primal relaxation Dual relaxation

Dual relaxation: preliminaries

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• Consider the 2^k point set P:

$$\{ \begin{array}{c} (x_1^L, \dots, x_{k-1}^L, x_k^L), \\ (x_1^L, \dots, x_{k-1}^L, x_k^U), \\ (x_1^L, \dots, x_{k-1}^U, x_k^L), \\ (x_1^L, \dots, x_{k-1}^U, x_k^L), \\ \dots, \\ (x_1^U, \dots, x_{k-1}^U, x_k^L), \\ (x_1^U, \dots, x_{k-1}^U, x_k^L), \\ (x_1^U, \dots, x_{k-1}^U, x_k^L), \end{array}$$

(i.e., all combinations of lower/upper bounds) • Let $w(x) = \prod_{i \leq k} x_i$: lift P to (x, w) space, get $P_W \subseteq \mathbb{R}^{k+1}$

$$\forall \bar{x} \in P \quad (\bar{x}, w(\bar{x})) \in P_W$$

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Primal relaxation Dual relaxation

Dual representation of a point set

• Convex hull of $P = \{p_1, \ldots, p_m\} \subseteq \mathbb{R}^n$ is given by $x \in \mathbb{R}^n \mid$:

$$\exists \lambda \in \mathbb{R}^m \left(x = \sum_{i \le m} \lambda_i p_i \land \sum_{i \le m} \lambda_i = 1 \land \forall i \le m \; (\lambda_i \ge 0) \right)$$

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Primal relaxation Dual relaxation

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 $\bullet \Leftrightarrow x \text{ is a convex combination of points in } P$

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Primal relaxation Dual relaxation

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- $\bullet \, \Leftrightarrow x$ is a convex combination of points in P
- Can express points in P_W in function of x,w,x^L,x^U and of added (dual) variables λ for any k

Primal relaxation Dual relaxation

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$$\exists \lambda \in \mathbb{R}^m \left(x = \sum_{i \le m} \lambda_i p_i \land \sum_{i \le m} \lambda_i = 1 \land \forall i \le m \; (\lambda_i \ge 0) \right)$$

- $\bullet \, \Leftrightarrow x \text{ is a convex combination of points in } P$
- Can express points in P_W in function of x,w,x^L,x^U and of added (dual) variables λ for any k
- Automatically get explicit convex envelopes for multilinear terms

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Primal relaxation Dual relaxation

Dual envelopes of multilinear terms

• We compute the *i*-th point $p_i \in P$ in $O(2^k)$ as follows:

$$\begin{aligned} \forall i \leq 2^k \qquad & d_i = \left(\left\lfloor \frac{i-1}{2^{k-j}} \right\rfloor \mod 2 \mid j \leq k \right) \\ \forall j \leq k \qquad & b_j(0) = x_j^L \ \land \ b_j(1) = x_j^U \end{aligned}$$

i.e. for all $i \leq 2^k$, we have $p_i = (x_j^{L/U?} \mid j \leq k) = (b_j(d_{ij}) \mid j \leq k)$

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 $\bullet~$ We add 2^k new variables $\lambda \geq 0$ and k+1 new constraints:

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• The projection of this feasible region on (x, w) is conv(W)

Primal relaxation Dual relaxation

Example: bilinear term

Using a matrix representation, we have:

$$\begin{bmatrix} \lambda_1 & \lambda_2 & \lambda_3 & \lambda_4 \end{bmatrix} \cdot \begin{bmatrix} x_1^L & x_2^L \\ x_1^L & x_2^U \\ x_1^U & x_2^L \\ x_1^U & x_2^L \end{bmatrix} = \begin{bmatrix} x_1 & x_2 \end{bmatrix}$$

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Primal relaxation Dual relaxation

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Primal relaxation Dual relaxation

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$$\begin{array}{rcl} x_1 &=& \lambda_1 x_1^L + \lambda_2 x_1^L + \lambda_3 x_1^U + \lambda_4 x_1^U \\ x_2 &=& \lambda_1 x_2^L + \lambda_2 x_2^U + \lambda_3 x_2^L + \lambda_4 x_2^U \\ w &=& \lambda_1 x_1^L x_2^L + \lambda_2 x_1^L x_2^U + \lambda_3 x_1^U x_2^L + \lambda_4 x_1^U x_2^U \\ \sum_{i \leq 4} \lambda_i &=& 1 \end{array}$$

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Where are we?



- Definitions
- Multilinear terms
- Applications

2 Relaxations

- Primal relaxation
- Dual relaxation

3 Results



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Comparison between relaxations

Primal envelopes	Dual envelopes
Original variables only	2^k added variables
$O(2^k)$ added constraints	k+1 added constraints

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4	[Balram] 44	16
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Primal envelopes constraints: apparent growth like $k2^k$

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Primal envelopes constraints: apparent growth like $k2^k$

 $O(k2^k)$ vs. 2^k might yield CPU improvements

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Experimental set-up

- $\bullet\,$ Generate random multilinear NLPs P
 - linear, bilinear, trilinear terms
 - nonseparable
- Generate primal convex LP relaxation R_P
- Generate dual convex LP relaxation Λ_P
- Solve R_P, Λ_P using CPLEX, compare CPU times
- To "get a feel" about how R_P, Λ_P might perform in BB, add integrality constraints on primal variables, get MILP relaxations R'_P, Λ'_P
- Solve R'_P, Λ'_P using CPLEX, compare CPU times

Instance set

- 2500 random instances
- # variables $n \in \{10, 20\}$
- n = 10:
 - # bilinear terms $\beta \in \{0, 10, 13, 17, 21, 25, 29, 33\}$
 - # trilinear terms $\tau \in \{0, 10, 22, 34, 46, 58, 71, 83\}$
- n = 20:
 - $\beta \in \{0, 20, 38, 57, 76, 95, 114, 133\}$
 - $\tau \in \{0, 20, 144, 268, 393, 517, 642, 766\}$
- 16 instances for each parameter combination yielding multilinear NLPs (and then MINLPs after imposing integrality on some variables)
- $\bullet\,$ Variable bounds chosen at random, magnitude 1.0×10^1










MILP relaxation test, n = 10





MILP relaxation test, n = 20



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Conclusion

Considerations

• Dual relaxation outperforms the primal when the number of variables increases

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- Dual relaxation is more stable (empirically CPU time increases proportionally to instance size) than primal for MILP
- These are preliminary results
- Using dual relaxation within spatial Branch-and-Bound could improve computational times

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