Quadratization-based methods for solving unconstrained polynomial optimization problems

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joint work with S. Elloumi, A. Lazare, D. Porumbel

MIP 25

Conservatoire National des arts et Métiers - Cédric

Presentation of the problem and literature

The unconstrained polynomial optimization problem

$$
(\mathrm{P}) \quad \begin{cases} \min & F(x) = \displaystyle\sum_{\alpha \in \Gamma_d^n} \mathtt{m}_\alpha x^\alpha \\ \text{s. t.} & 0 \le x_i \le 1 \qquad\qquad \forall i \in \mathcal{C} \\ & x_j \in \{0, 1\} \qquad\qquad \forall j \in \mathcal{I} \end{cases}
$$

- n variables x_i, and $\mathcal{C} \cup \mathcal{I} = \{1, \ldots n\}$
- $F(x)$ is a polynomial of degree d

  $\Gamma_d^n = \{\alpha \in \mathbb{N}^n \,:\, \displaystyle\sum_{i=1}^{n} \alpha_i \le d\}$, $\alpha \in \mathbb{N}^n$ with α_i the power of x_i

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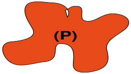
Challenge : combination of the integrality of some of the variables and the non-convexity of polynomial $F(x)$.
Our aim : Compute tight convex lower bounds of (P).

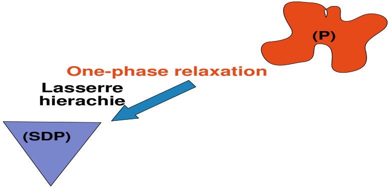
Literature: exact solution method



Standard approach:

1. Compute relaxations tight and/or easy to solve
2. Tighten relaxation or perform branch-and-bound

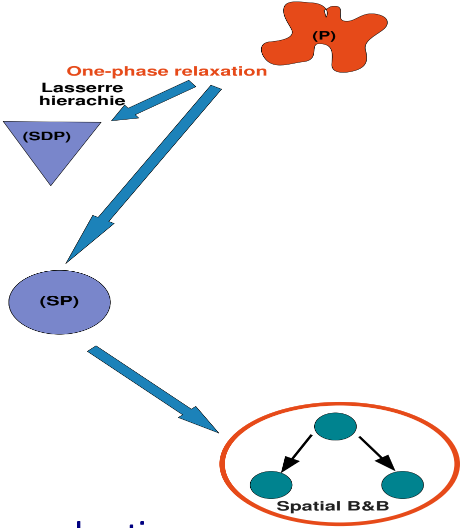
Literature: exact solution method



One-phase relaxation

SDP hierarchy of relaxations [Lasserre, 03]

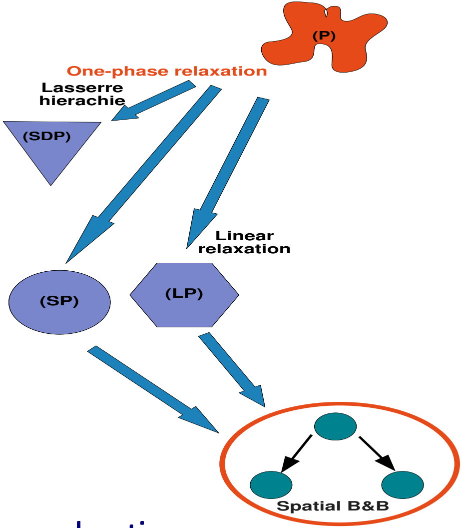
Literature: exact solution method



One-phase relaxation

Separable under-estimators [Buchheim, D'Ambrosio, 16]

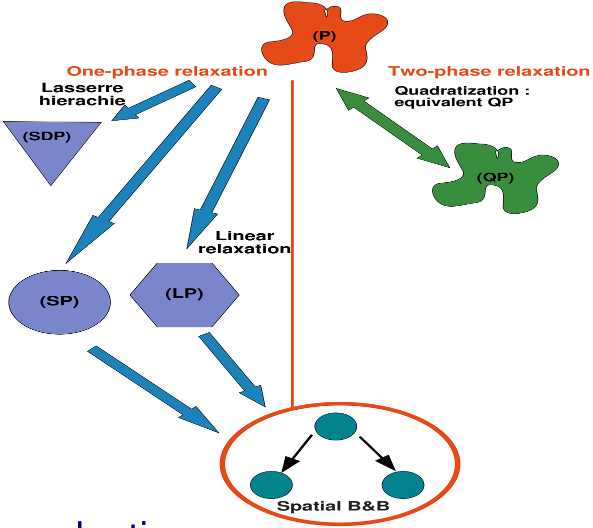
Literature: exact solution method



One-phase relaxation

Standard linearization (enriched by cutting planes)h [DelPia, Walter 22]

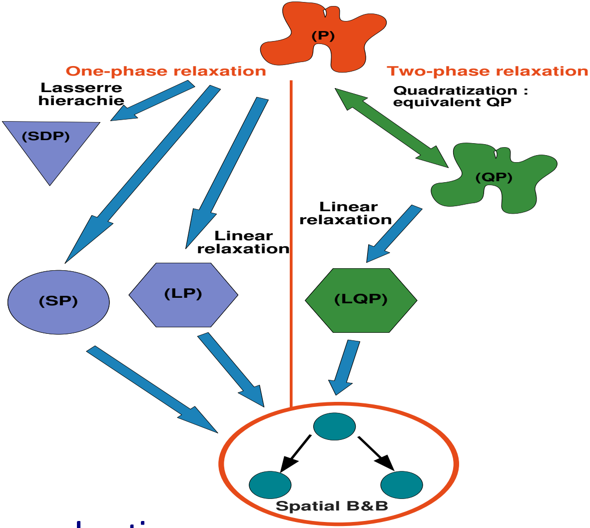
Literature: exact solution method



Two-phase relaxation

Phase 1: quadratization methods [Crama 17][Buchheim, Rinaldi 07]

Literature: exact solution method



Two-phase relaxation

Phase 1: quadratization methods [Crama 17][Buchheim, Rinaldi 07]

Phase 2: Standard linearization [McCormick, 76]

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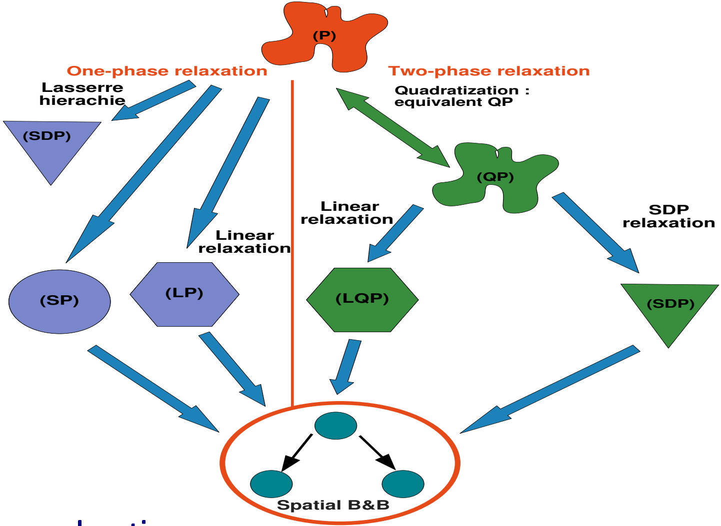
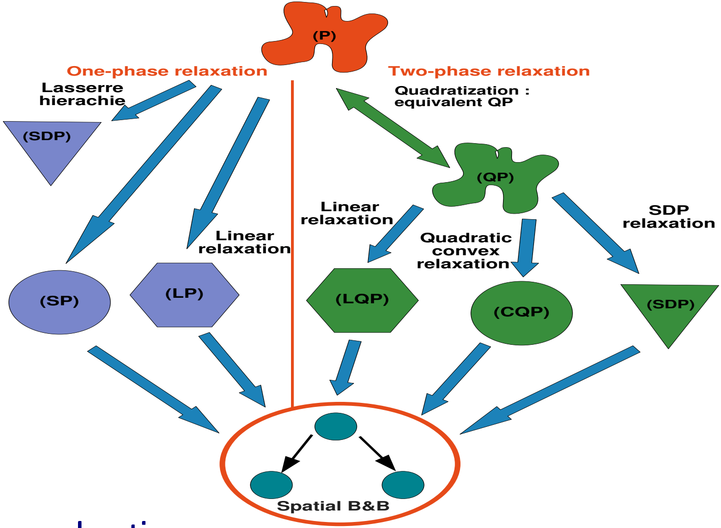


Two-phase relaxation

Phase 1: quadratization methods [Crama 17][Buchheim, Rinaldi 07]

Phase 2: SDP relaxations [Anstreicher, 09]

Literature: exact solution method

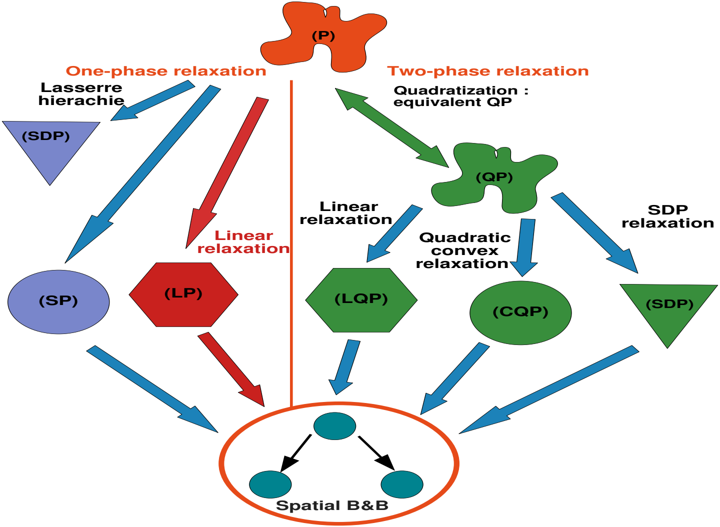


Two-phase relaxation

Phase 1: quadratization methods [Crama 17][Buchheim, Rinaldi 07]

Phase 2: Quadratic Convex Reformulation: PQCR [L., Elloumi, Lazare 21]

Outline of the presentation



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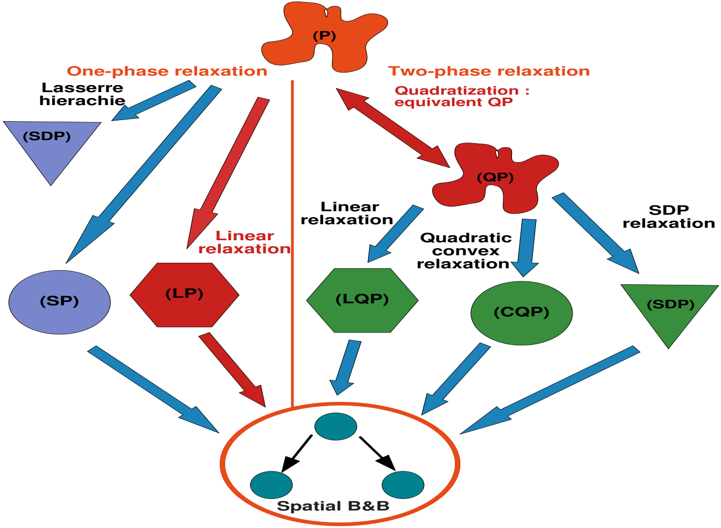

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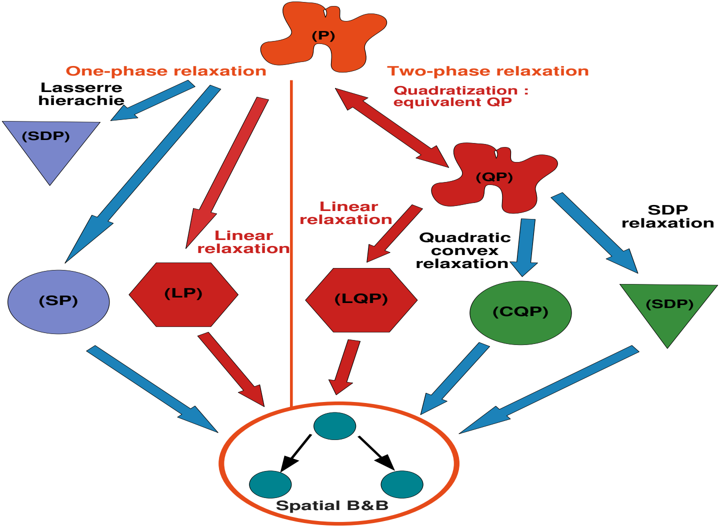

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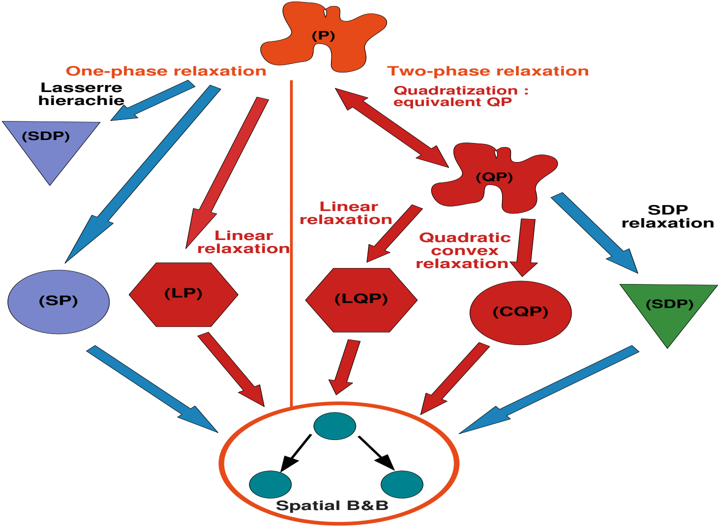

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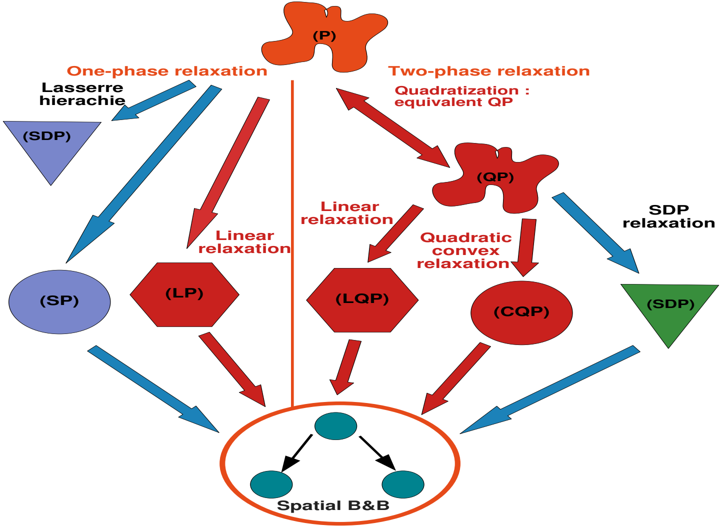
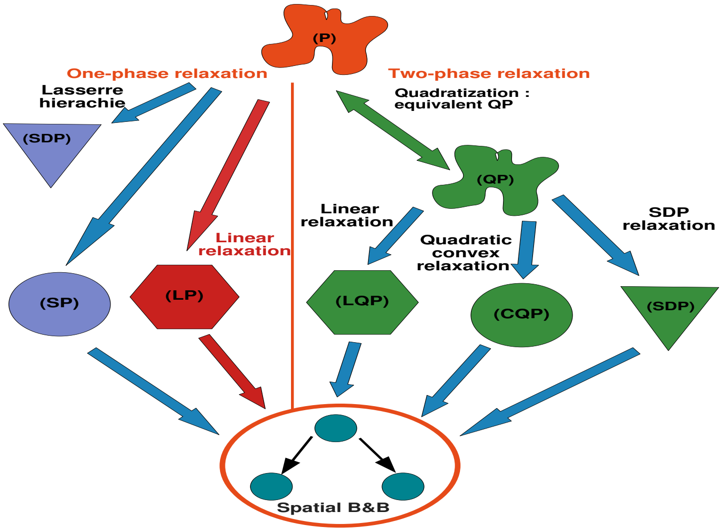


Comparaison of the approaches from the bound point of view

Computing a linear relaxation of (P)



How to compute a linear relaxation ?

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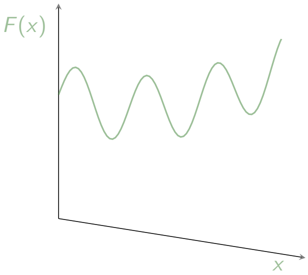

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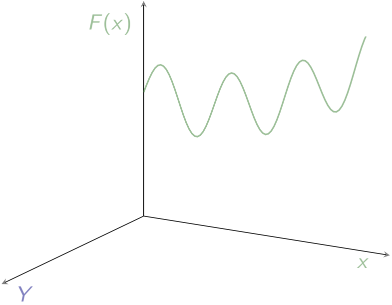
Add auxiliary variables Y_α that model the monomials x^α: $Y_\alpha = x^\alpha$



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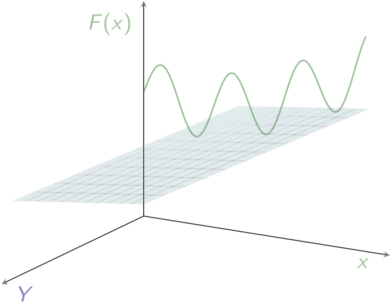

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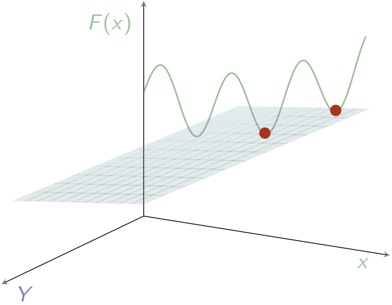


$$Y_\alpha = x^\alpha \Longleftrightarrow \mathcal{L}\begin{cases} Y_\alpha \le x_i \quad \text{if } \alpha_i \neq 0 \\ Y_\alpha \ge \displaystyle\sum_i x_i + \sum_i \alpha_i - 1 \\ Y_\alpha \ge 0 \end{cases}$$

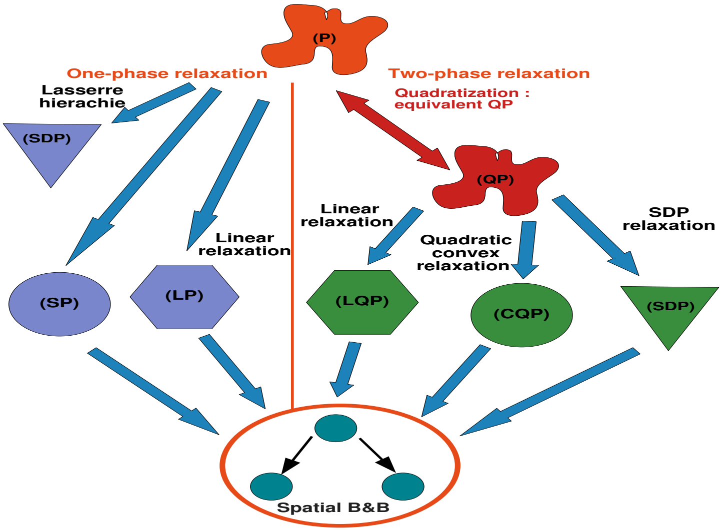
Remark: $\Longleftrightarrow$ for binary variables.

Toy example : size and initial gap comparison

10 continuous variables, 100 monomials, optimal value $= -6.00$

	(LP)
Nb aux var	100
Nb cont	465
Root LB	-16.3
Root gap	172.4

Quadratization schemes and quadratic reformulations



Definition : Quadratization schemes

Decompose each monomial with a ***quadratization scheme*** $\mathcal{S}$

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$$\underbrace{x_1 x_2 x_3 x_4}_{z_1} x_5$$

$$\downarrow$$

$$x_5$$

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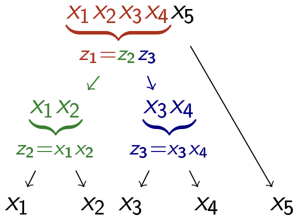

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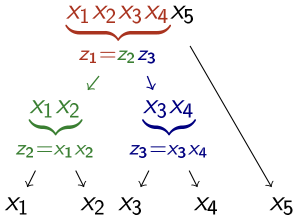

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$\Longrightarrow$ Easy to build (QP) a quadratic reformulation of (P)

$$(P)\begin{cases} \min \ x_1x_2x_3x_4x_5 \\ 0 \leq 1 \leq u_i \ \ i \in \mathcal{C} \\ x_j \in \{0,1\} \ \ j \in \mathcal{I} \end{cases} \qquad \Leftrightarrow (QP)\begin{cases} \min \ \ z_1x_5 \\ z_1 = z_2z_3 \\ z_2 = x_1x_2 \\ z_3 = x_3x_4 \\ 0 \leq x_i \leq 1 \ \ i \in \mathcal{C} \\ x_j \in \{0,1\} \ \ j \in \mathcal{I} \end{cases}$$

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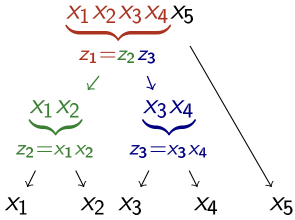

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Quadratic reformulation of (P)

Given a ***quadratization scheme*** $\mathcal{S}$

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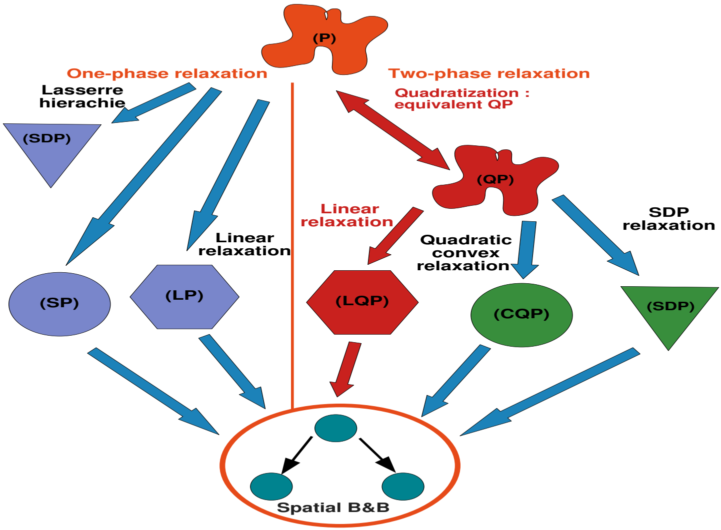
But is still hard to solve:

- $z >> x$: potentially large number of auxiliary variables
- Objective function $f(z)$ is still non convex
- Constraint set $z \in \mathcal{S}$, $z_j \in \{0,1\}$ $j \in \mathcal{I}$ is a non-convex set.

Convexification by linearization



Linearization of the constraints

- Binary constraints:
  if $\mathcal{I} \neq \emptyset$, $z_j \in \{0, 1\}$ $j \in \mathcal{I}$ $\xrightarrow{\text{relax}}$ $z_j \in [0, 1]$.

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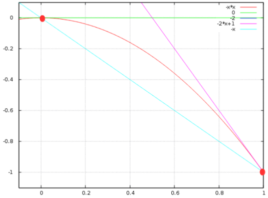
- Linearization of constraints of the quadratization scheme:
  $z \in \mathcal{S} \quad \xrightarrow{\text{relax}} \quad z \in \mathcal{L}$

$$\left\{\begin{array}{l} z_k = x_i x_j \\ \ell_i \leq x_i \leq u_i \\ \ell_j \leq x_j \leq u_j \end{array}\right. \xrightarrow{\text{relax}} \mathcal{L}\left\{\begin{array}{l} z_k \leq u_j x_i + \ell_i x_j - u_j \ell_i \\ z_k \leq u_i x_j + \ell_j x_i - u_i \ell_j \\ z_k \geq u_j x_i + u_i x_j - u_i u_j \\ z_k \geq \ell_j x_i + \ell_i x_j - \ell_i \ell_j \end{array}\right.$$

McCormick envelopes [McCormick 76]



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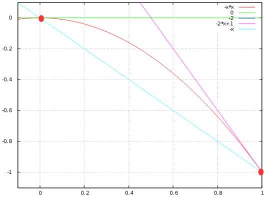
$$\left\{ \begin{array}{l} z_k = x_i x_j \\ x_i \in \{0,1\} \\ x_j \in \{0,1\} \end{array} \right. \iff \mathcal{L} \left\{ \begin{array}{l} z_k \leq x_i \\ z_k \leq x_j \\ z_k \geq x_i + x_j - 1 \\ z_k \geq 0 \end{array} \right.$$

Standard linearization [Fortet 59]



Remark: the equivalence holds if x_i or x_j are binary variables.

Linearization of the objective function

$$(P) \Leftrightarrow (QP_{\mathcal{S}}) \begin{cases} \min \ \langle Q, zz^\top \rangle + c^\top z \\ z \in \mathcal{S} \\ 0 \leq z_i \leq 1 \ i \in \mathcal{C} \\ z_j \in \{0,1\} \ j \in \mathcal{I} \end{cases}$$

- Add auxiliary variables Y that model the products $zz^\top$

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$(LQP_{\mathcal{S}})$ is a linear relaxation of (P) with auxiliary variables z and Y

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Theorem If $\mathcal{S}$ is disjoint, we have $v(LQP_{\mathcal{S}}) \ge v(LP)$.

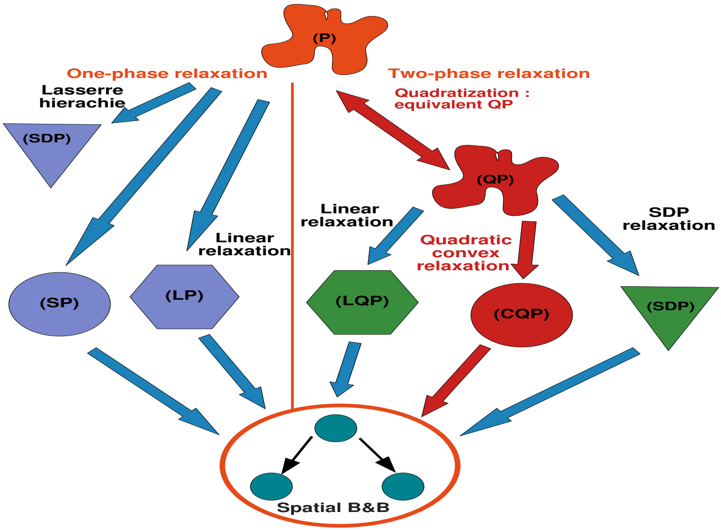
(disjoint : the intersection of the 2 sets of a decomposition is empty)

Toy example : size and initial gap comparison

10 continuous variables, 100 monomials, optimal value $= -6.00$

	(LP)	$(LQP_{\mathcal{S}})$
Nb aux var	100	225
Nb cont	465	675
Root LB	-16.3	-12.9
Root gap	172.4	114.7

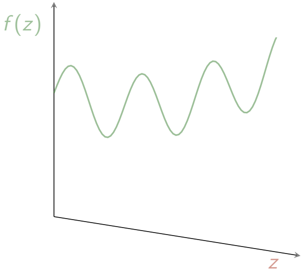
Convexification by Quadratic Convex Relaxation



What is Quadratic Convex Relaxation ?

We have $f(z) = \langle Q, zz^\top \rangle + c^\top z$ with Q indefinite

Goal: perturb Q while keeping the value of $f(z)$



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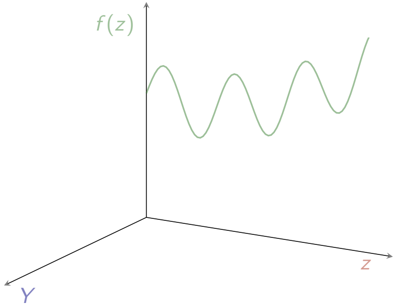
$$f_\phi(z, Y) = f(z) + \langle \phi, zz^\top - Y \rangle$$

1. Add variable $Y = zz^T$
2. Add a matrix parameter ϕ



What is Quadratic Convex Relaxation ?

We have $f(z) = \langle Q, zz^\top \rangle + c^\top z$ with Q indefinite

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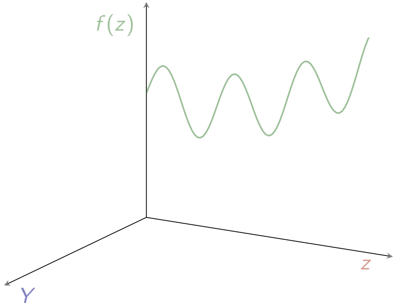

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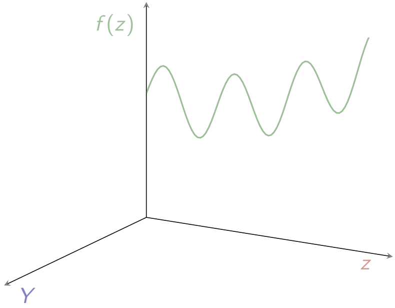

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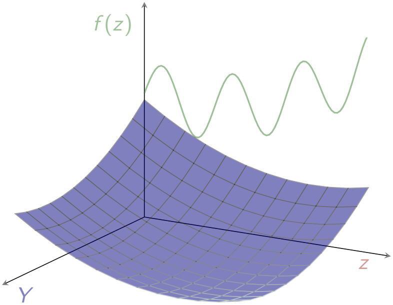

Choose ϕ such that $Q + \phi \succeq 0$,
e.g. $\phi = \mathrm{diag}(-\lambda_{min}(Q))$.

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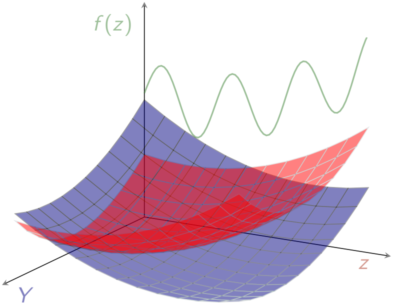

Compute ϕ such that

i. $Q + \phi \succeq 0$

ii. the bound is tight

$\Longrightarrow$ use SDP optimization

$$
(SDP) \begin{cases} \min \ \langle Q, Z \rangle + c^T x \\ (z, Z) \in \mathcal{L} \leftarrow \phi \\ Z - zz^\top \succeq 0 \end{cases}
$$

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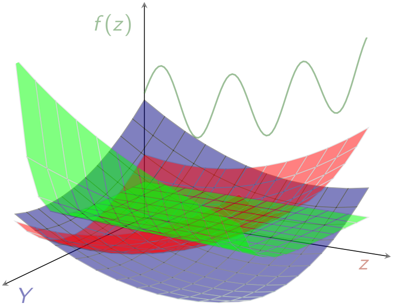

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To improve the bound:
add quadratic cuts to SDP

Use $\mathcal{S}$ to build quadratic cuts

Quadratization scheme for monomial $x_1x_2x_3x_4x_5 = z_1x_5$.

$$\mathcal{S} = \left\{z_1 = z_2z_3,\ z_2 = x_1x_2,\ z_3 = x_3x_4\right\}$$

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if $z_j \in \{0, 1\}$**:**

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if $0 \leq z_i \leq 1$**:**

- Box constraints $z_i^2 - z_i \leq 0$

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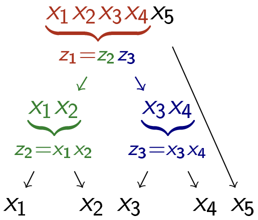
For the same monomial many 2×2 quadratization schemes:



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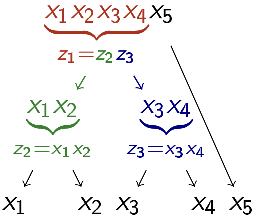

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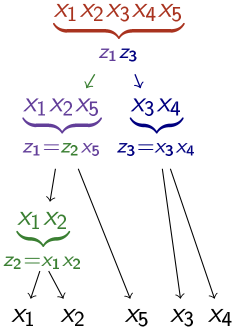

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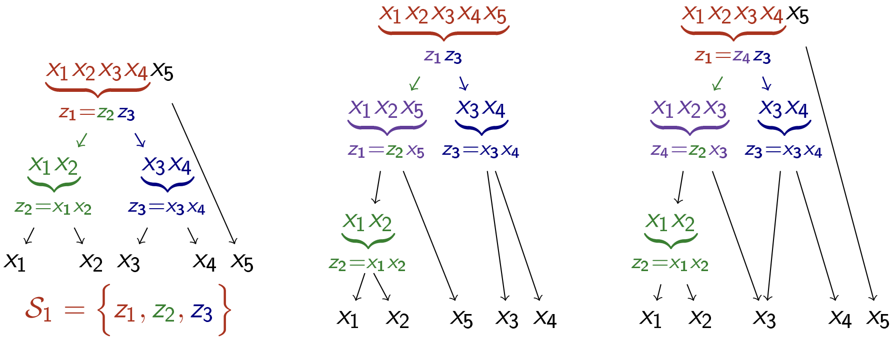

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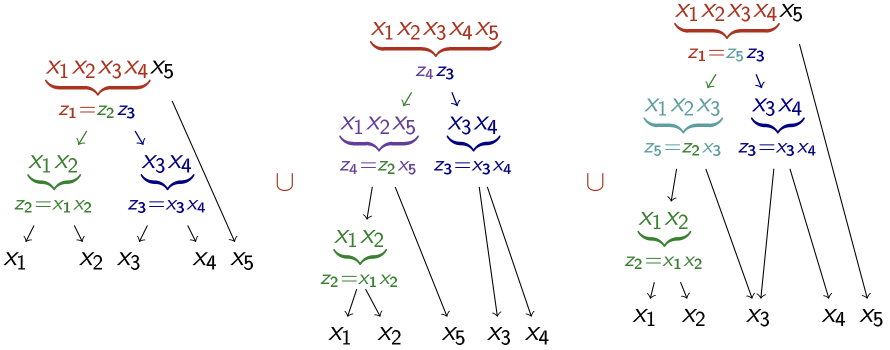
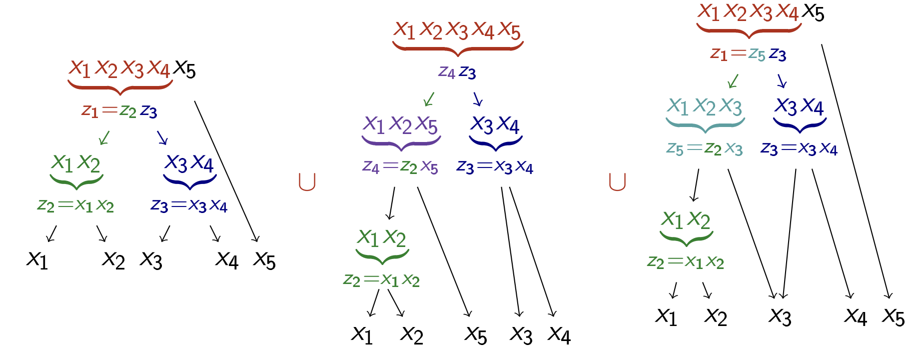


$$\mathcal{S} = \cup_{k=1}^{K} \mathcal{S}_k = \left\{ z_1, z_2, z_3, z_4, z_5 \right\}$$

- **Our idea** use K quadratization schemes: $\mathcal{S} = \cup_{k=1}^{K} \mathcal{S}_k$
  $\Longrightarrow$ **generate more quadratic cuts.**

For the same monomial many 2×2 quadratization schemes:



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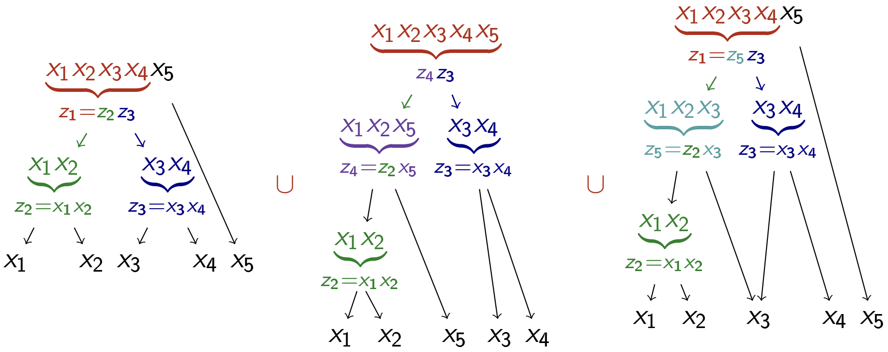

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- Objective function : $z_1 x_5 = z_4 z_3$
- Other quadratic cuts: $z_2 z_3 = z_5 x_4$ (represent monomial $x_1 x_2 x_3 x_4$)

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(P)\begin{cases} \min \sum_{\alpha \in \Gamma_d^n} \mathtt{m}_\alpha x^\alpha \\ \ell_i \leq x_i \leq u_i \;\; i \in \mathcal{C} \\ x_j \in \{0,1\} \;\; j \in \mathcal{I} \end{cases} \xrightarrow{relax} (CQP_{\mathcal{S}})\begin{cases} \min \;\; f(z) = \langle Q, zz^\top \rangle + c^\top z \\ z \in \mathcal{L} \\ (x, Y) \in \mathcal{L} \\ \langle D_r, Y \rangle + d_r^\top z \leq 0 \\ 0 \leq z_i \leq 1 \;\; i \in \mathcal{C} \cup \mathcal{I} \end{cases}
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- Valid equalities $\langle A_r, zz^\top \rangle + a_r^\top z = 0$
  $\rightarrow$ we will use them to convexify the objective function

Convexification of the objective function

Given a parameter γ, add quadratic cuts $\langle A_r, zz^\top \rangle + a_r^\top z = 0$ to $f_\phi(z, Y)$.

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\end{aligned}
$$

If $\left(Q + \sum_{r=1}^{m} \gamma_r A_r + \phi\right)$ is SDP then $f_{\gamma,\phi}(z, Y)$ is a convex function

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Compute (γ^*, ϕ^*) leading to the tightest bound :

$$(LB) : \left\{ \max_{(Q + \sum \gamma_r A_r + \phi) \succeq 0} v(P_{\mathcal{S},\gamma,\phi}) \right\}$$

$\Longrightarrow$ Use Semidefinite programming to solve (LB)

Solving (LB) with Semidefinite programming

$$
(CQP_{\mathcal{S},\gamma,\phi})\begin{cases}
\min \ f_{\gamma,\phi}(z, Y) \\
z \in \mathcal{L} \\
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\ell_i \leq z_i \leq u_i \ i \in \mathcal{C} \cup \mathcal{I}
\end{cases}
\qquad
(SDP)\begin{cases}
\min \ \langle Q, Z\rangle + c^T x \\
\langle D_r, Z\rangle + d_r^\top z \leq 0 \\
\langle A_r, Z\rangle + a_r^\top z = 0 \\
(z, Z) \in \mathcal{L} \\
Z - zz^\top \succeq 0
\end{cases}
$$

Solving (LB) with Semidefinite programming

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- Let γ, ϕ_1 and ϕ_2 the dual variables of (SDP)

Solving (LB) with Semidefinite programming

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- Let γ, ϕ_1 and ϕ_2 the dual variables of (SDP)

Theorem We have $v(LB) = v(SDP) = v(CQP_{\mathcal{S},\gamma^*,\phi^*=\phi_1^*+\phi_2^*})$ where $\gamma^*, \phi^* = \phi_1^* + \phi_2^*$ are the optimal dual variables to (SDP)

To sum up: an exact algorithm to solve (P)

`Polynomial Quadratic Convex Reformulation` - mixed-integer case

Phase 1: Generate K schemes of $F(x)$, and get $\mathcal{S} = \cup_{k=1}^{K} \mathcal{S}_k$

PQCR for the mixed-case [L., Porumbel 25]

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i. Build quadratic cuts: $\langle D_r, zz^\top \rangle + d_r^\top z \leq 0$ and $\langle A_r, zz^\top \rangle + a_r^\top z = 0$

ii. Solve (SDP) to compute the best parameters γ^*, and ϕ^*

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Phase 3: Solve (P) by a spatial B&B based on the solution of $(CQP_{\mathcal{S},\gamma^*,\phi^*})$

PQCR for the mixed-case [L., Porumbel 25]

Toy example : size and initial gap comparison

10 continuous variables, 100 monomials, optimal value $= -6.00$

	(LP)	$(LQP_{\mathcal{S}})$	$(CQP_{\mathcal{S},\gamma^*,\phi^*})$			
			$K=1$	$K=2$	$K=3$	$K=4$
Nb aux var	100	225	336	364	455	1042
Nb cont	465	675	1003	1108	1544	4291
Root LB	-16.3	-12.9	-6.7	-6.6	-6.3	-6.0
Root gap	172.4	114.7	11.6	9.9	5.2	0.0

Preliminary computational results

Comparison initial gaps (in %)

100 instances of 10 continuous variables

Each line is an average over 10 instances

# mon.	(LP)	$(LQP_{\mathcal{S}})$	$(CQP_{\mathcal{S},\gamma^*,\phi^*})$			
			$K=1$	$K=2$	$K=3$	$K=4$
10	6.6	6.5	2.3	1.8	1.4	1.2
20	11.4	7.3	1.6	1.5	0.7	0.5
30	54.0	39.8	12.4	10.1	6.6	4.6
40	74.6	52.9	13.2	12.2	5.7	3.2
50	81.4	56.2	10.3	7.4	3.6	2.0
60	114.2	76.7	14.8	13.1	8.6	4.3
70	153.9	106.4	19.9	17.7	9.1	4.5
80	140.9	93.4	13.3	11.7	7.2	3.7
90	139.7	89.8	8.3	7.1	3.2	1.1
100	62.9	35.7	0.5	0.1	0.1	0.1

- Quadratic Convex relaxation significantly tighter
- The more K increases, the more we close the gap

Conclusion and perspectives

Conclusions et perspectives

Conclusions

- An exact 3-phases algorithm that handles continuous variables
- Allows to use several quadratization schemes.
- Encouraging first computational results

  $\rightarrow$ Tighten the bound obtained by compared approaches

Future work

- Use conic bundle to accelerate the solution of (SDP)
- Improve the implementation of the B&B
- Handling problems with constraints

$(CQP_{\mathcal{S},\gamma^*,\phi^*})$ - # vars and # cont

100 instances of 10 continuous variables

Each line is an average over 10 instances

# mon.	$K=1$		$K=2$		$K=3$		$K=4$	
	# var	# cont	# var	# cont	# var	# cont	# var	# cont
10	66	80	79	108	120	229	167	330
20	121	198	142	255	215	605	324	910
30	160	299	188	399	271	857	440	1,396
40	206	461	230	558	323	1,131	560	1,990
50	233	579	273	763	354	1,258	649	2,393
60	261	696	292	838	382	1,370	731	2,797
70	280	796	313	942	400	1,421	796	3,089
80	301	836	334	987	432	1,519	912	3,621
90	326	974	360	1,112	456	1,581	992	3,980
100	200	526	232	656	301	931	600	2,243

- Same family of quadratizations ($K=1,2,3$) small increase of the size
- For $K=4$ incremental quadratization clearly increases the size.