# Reformulations in Mathematical Programming

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# Summary of Talk

- Motivation
- Definitions and results
- Symmetry-breaking “narrowing” example
- Applications and perspectives

# Existing definitions

- "Problem $Q$ is a reformulation of $P$": what does it mean?
- Definition in Mathematical Programming Glossary: *Obtaining a new formulation $Q$ of a problem $P$ that is in some sense better, but equivalent to a given formulation*. **Trouble:** vague.
- Definition by H. Sherali [private communication]: *bijection between feasible sets, objective function of $Q$ is a monotonic univariate function of that of $P$*. **Trouble:** condition on feasible sets bijection is too restrictive
- Definition by P. Hansen [Audet et al., JOTA 1997]: *$P, Q$ opt. problems; given an instance $p$ of $P$ and $q$ of $Q$ and an optimal solution $y^*$ of $q$, $Q$ is a reformulation of $P$ if an optimal solution $x^*$ of $p$ can be computed from $y^*$ within a polynomial amount of time*. **Trouble:** ignores feasible / locally optimal solutions

# Motivation 1

Widespread use of nonlinear modelling

- Solution methods for nonlinear models are not as advanced as for linear ones
- Modelling many real-life problems as linear is innatural / difficult
- Practitioners cannot solve nonlinear models and are not always able to model linearly
- $\Rightarrow$ Inhibits spreading of mathematical programming / optimization techniques in non-specialist industrial settings

# Motivation 2

Solving large-scale NLPs/MINLPs

- Solution methods for nonlinear models are not as advanced as for linear ones (again)
- Instead of solving the original (nonlinear) model, can attempt to reformulate it to a linear one
- The reformulation should be *automatic* (i.e. transparent for the user)

# Motivation 3

Efficiency/choice of solution algorithms

- Most general purpose solution algorithms compute optima *by means* of the formulation
- Different formulations influence algorithmic behaviour
  1. In BB, alter (tighten) the bound
  2. In VNS, define different (more advantageous) neighbourhoods
- Reformulation may allow the use of a different general purpose solver (e.g. finding feasible solutions for tightly constrained MILPs by reformulation to LCPs [Di Giacomo et al., JOC 2007])

# Current status and needs

- Google search:

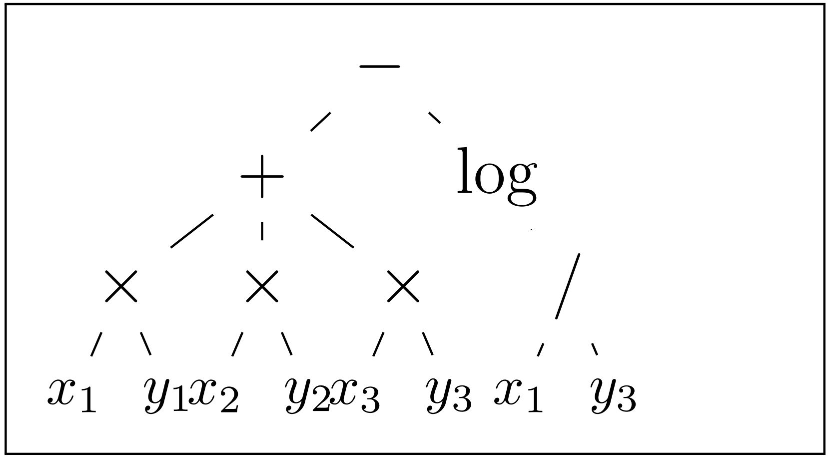
  `reformulation "mathematical programming"`

  yields 419,000 hits ⇒ everyone uses them
- No satisfactory definitions, no general theoretical results (how do we combine simple reformulations into a more complicated one? what is the size/solution difficulty of the complex reformulation?), no reformulation-based literature review, no software!
- Need for:
  1. *reformulation theory*
  2. *list of elementary reformulations*
  3. *reformulation software*
- Develop a **reformulation systematics** (under way)

# Definitions

- Mathematical expressions as $n$-ary *expression trees*

$$\sum_{i=1}^{3} x_i y_i - \log(x_1/y_3)$$



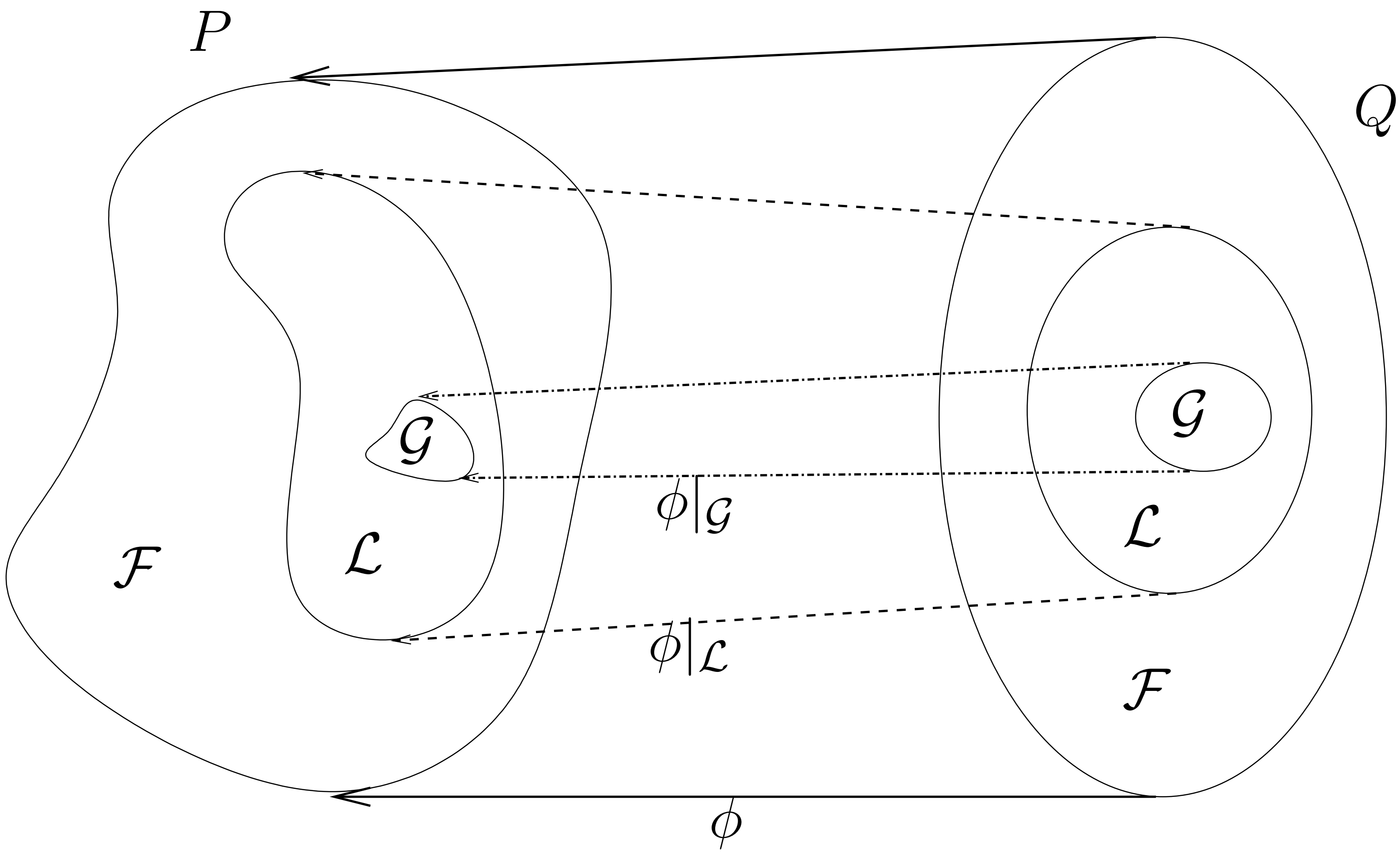

- A *formulation* $P$ is a 7-tuple $(\mathcal{P}, \mathcal{V}, \mathcal{E}, \mathcal{O}, \mathcal{C}, \mathcal{B}, \mathcal{T})$ =(parameters, variables, expression trees, objective functions, constraints, bounds on variables, variable types)
- Constraints are encoded as triplets $c \equiv (e, s, b)$ ($e \in \mathcal{E}$, $s \in \{\leq, \geq, =\}$, $b \in \mathbb{R}$)
- $\mathcal{F}(P) =$ feasible set, $\mathcal{L}(P) =$ local optima, $\mathcal{G}(P) =$ global optima

# Auxiliary problems

If problems $P, Q$ are related by a computable function $f$ through the relation $f(P, Q) = 0$, $Q$ is an *auxiliary problem* with respect to $P$.

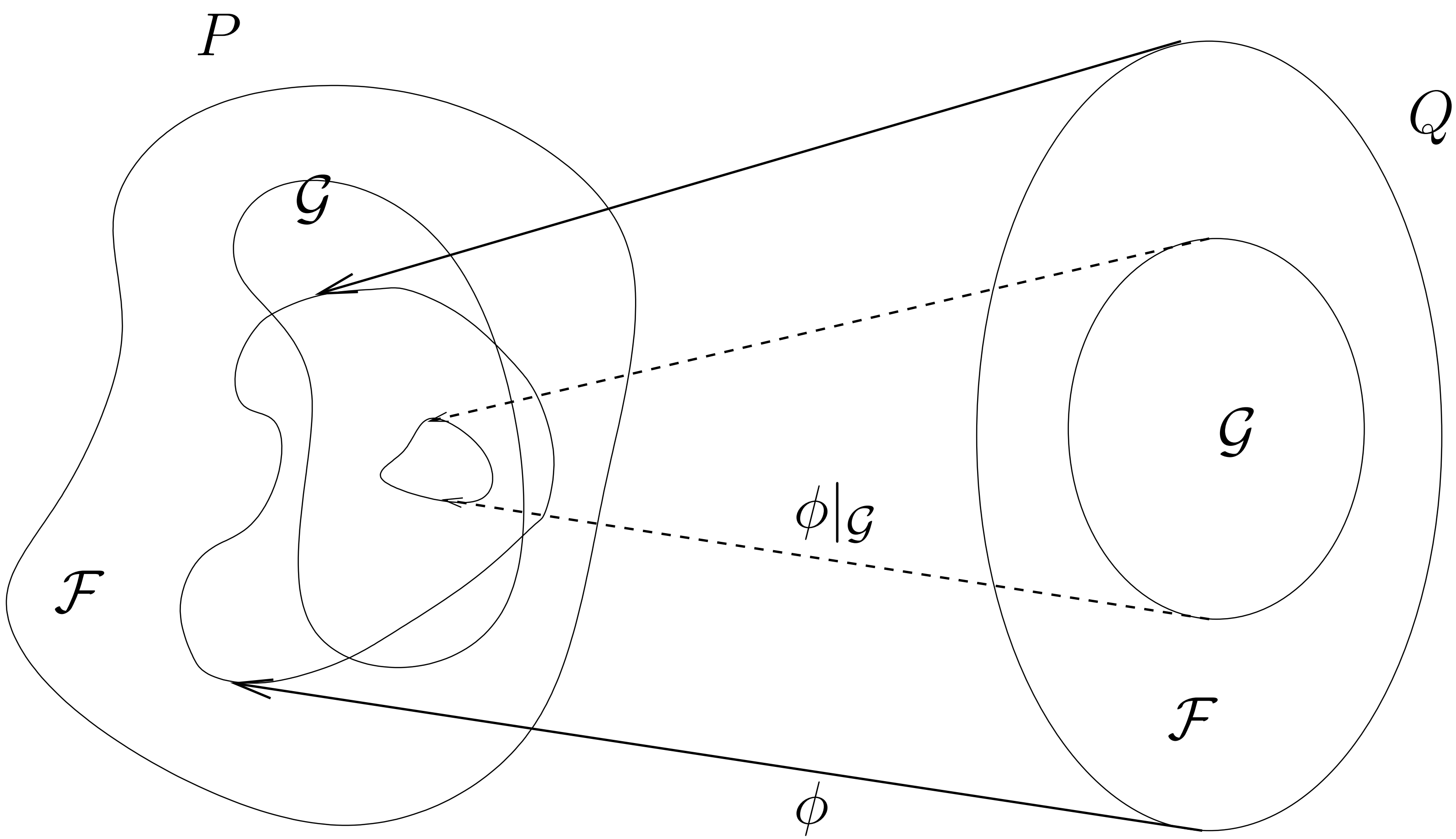
- **Opt-reformulations**: preserve all optimality properties
- **Narrowings**: preserve some optimality properties
- **Relaxations**: drop constraints / bounds / types
- **Approximations**: formulation $Q$ depending on a parameter $k$ such that "$\lim_{k\to\infty} Q(\varepsilon)$" is an opt-reformulation, narrowing or relaxation

# Opt-reformulations




*Main idea*: if we find an optimum of $Q$, we can map it back to the same type of optimum of $P$, and for all optima of $P$, there is a corresponding optimum in $Q$.

# Narrowings




*Main idea*: if we find a global optimum of $Q$, we can map it back to a global optimum of $P$. There may be optima of $P$ without a corresponding optimum in $Q$.

# Relaxations

A problem $Q$ is a relaxation of $P$ if $\mathcal{F}(P) \subseteq \mathcal{F}(Q)$.

# Approximations

$Q$ is an *approximation* of $P$ if there exist: (a) an auxiliary problem $Q^*$ of $P$; (b) a sequence $\{Q_k\}$ of problems; (c) an integer $k' > 0$; such that:

1. $Q = Q_{k'}$
2. $\forall f^* \in \mathcal{O}(Q^*)$ there is a sequence of functions $f_k \in \mathcal{O}(Q_k)$ converging uniformly to $f^*$;
3. $\forall c^* = (e^*, s^*, b^*) \in \mathcal{C}(Q^*)$ there is a sequence of constraints $c_k = (e_k, s_k, b_k) \in \mathcal{C}(Q_k)$ such that $e_k$ converges uniformly to $e^*$, $s_k = s^*$ for all $k$, and $b_k$ converges to $b^*$.

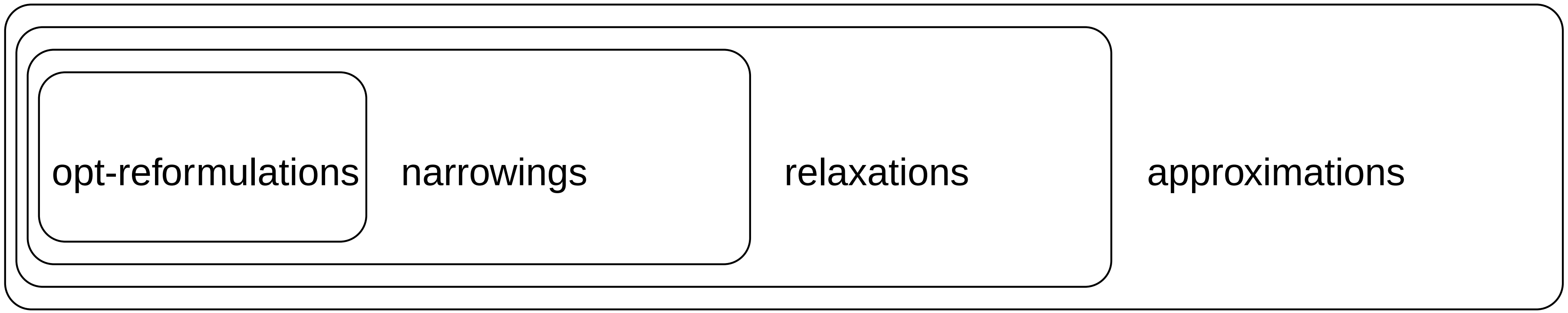
There can be approximations to opt-reformulations, narrowings, relaxations.

$Q_1, Q_2, Q_3, \ldots Q_{k'}, \ldots \longrightarrow Q^*$ ⟨auxiliary problem of⟩ $P$

approximation of $P$

# Fundamental results

- Opt-reformulation, narrowing, relaxation, approximation are all transitive relations
- *An approximation of any type of reformulation is an approximation*
- A reformulation consisting of opt-reformulations, narrowings, relaxations is a relaxation
- *A reformulation consisting of opt-reformulations and narrowings is a narrowing*
- A reformulation consisting of opt-reformulations is an opt-reformulation



# The SymmBreak2 narrowing 1/7

- SymmBreak2 motivating example
- Consider the mathematical program $P$ (a covering problem instance):

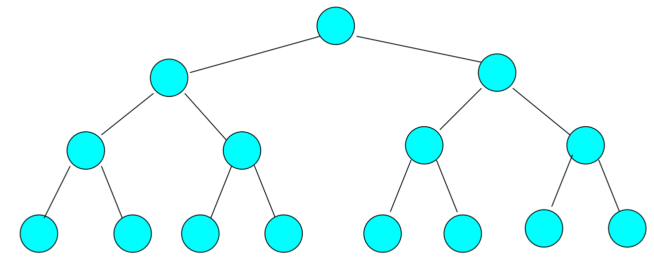
$$\left.\begin{array}{rrcl} \min & \sum\limits_{\substack{i\le 2\\ j\le 3}} x_{ij} & & \\ \forall i\le 2 & \sum\limits_{j\le 3} x_{ij} & \ge & 1 \\ \forall j\le 3 & \sum\limits_{i\le 2} x_{ij} & \ge & 1 \\ & x & \in & \{0,1\}^6 \end{array}\right\} \left\{\begin{array}{lcccccccc} \min & x_{11} & +x_{12} & +x_{13} & +x_{21} & +x_{22} & +x_{23} & & \\ & x_{11} & +x_{12} & +x_{13} & & & & \ge & 1 \\ & & & & x_{21} & +x_{22} & +x_{23} & \ge & 1 \\ & x_{11} & & & +x_{21} & & & \ge & 1 \\ & & x_{12} & & & +x_{22} & & \ge & 1 \\ & & & x_{13} & & & +x_{23} & \ge & 1 \end{array}\right.$$

- The set of optimal solutions is $\mathcal{G}(P) =$

$$\{(0,1,1,1,0,0),\quad (1,0,0,0,1,1),\quad (0,0,1,1,1,0),$$
$$(1,1,0,0,0,1),\quad (1,0,1,0,1,0),\quad (0,1,0,1,0,1)\}$$

# The SymmBreak2 narrowing 2/7

- The group $G^*$ of automorphisms of $\mathcal{G}(P)$ is $\langle(1,4)(2,5)(3,6),(1,5)(2,4)(3,6),(1,4)(2,6)(3,5)\rangle \cong D_{12}$
- For all $x^* \in \mathcal{G}(P)$, $Gx^* = \mathcal{G}(P) \Rightarrow \exists$ essentially *one* solution in $\mathcal{G}(P)$
- This is **bad** for Branch-and-Bound techniques: many branches will contain (symmetric) optimal solutions and therefore will not be pruned by bounding $\Rightarrow$ *deep and large BB trees*




- If we knew $G^*$ in advance, we might add constraints eliminating (some) symmetric solutions out of $\mathcal{G}(P)$
- ... in other words, look for a *narrowing* of $P$
- Can we find $G^*$ (or a subgroup thereof) *a priori*?
- What constraints provide a valid narrowing of $P$ excluding symmetric solutions of $\mathcal{G}(P)$?

# The SYMMBREAK2 narrowing 3/7

- The cost vector $c^{\mathsf{T}} = (1,1,1,1,1,1)$ is fixed by all (column) permutations in $S_6$
- The vector $b = (1,1,1,1,1)$ is fixed by all (row) permutations in $S_5$
- Consider $P$'s constraint matrix:

$$\begin{pmatrix} 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 \end{pmatrix}$$

- Let $\pi \in S_6$ be a column permutation such that $\exists$ a row permutation $\sigma \in S_5$ with $\sigma(A\pi) = A$
- Then permuting the variables/columns in $P$ according to $\pi$ does not change the problem formulation

# The SymmBreak2 narrowing 4/7

- For a packing or covering problem with $c = \mathbf{1}_n$ and $b = \mathbf{1}_m$,

$$G_P = \{\pi \in S_n \mid \exists \sigma \in S_m \, (\sigma A \pi = A)\} \tag{1}$$

  is called the *problem symmetry group* of $P$

- In the example above, we get $G_P \cong D_{12} \cong G^*$

  Thm.

  For a covering/packing problem $P$, $G_P \leq G^*$.

- Result can be extended to all MILPs [Margot02, Margot03, Margot07]
- Extension to MINLPs under way using expression trees encodings

# The SymmBreak2 narrowing 5/7

Thm.

Assume:

- $P$ is a BLP
- $\exists x^* \in \mathcal{G}(P)$ with $1 \le |\text{supp}(x^*)| \le n-1$;
- $|G_P| > 1$.

Let $\gamma = (\gamma_1, \ldots, \gamma_k)$ with $k > 1$ be a cycle in the disjoint cycle representation of $\pi \in G_P$. Then adjoining the constraints:

$$\forall 2 \le j \le k \quad x_{\sigma_1} \le x_{\sigma_k} \tag{2}$$

to $P$ results in a strict narrowing $Q$ of $P$ (i.e. one s.t. $|\mathcal{G}(Q)| < |\mathcal{G}(P)|$).

# The SymmBreak2 narrowing 6/7

- *Good news*: there are automatic ways to find permutations in $G_P$

  | |
  |---|
  | One formulates an auxiliary mathematical program the solution of which encodes $\pi \in G_P$ (incidentally if $\pi = e$ this proves $G_P = \{e\}$) |

- *Bad news*: the CPU time required to find permutations of $G_P$ is prohibitively high (for now)
- *Good news*: once some $\pi \in G_P$ is known, adding constraints (2) for the longest disjoint cycle of $\pi$ yields a narrowing $Q$ computationally as tractable as $P$
- *Bad news*: there is an element of arbitrary choice in (2), namely that $x_{\sigma_1}$ is a minimum element within $x[\sigma]$
- …found no way (yet) to eliminate this arbitrary choice without adding more variables to $Q$

# The SymmBreak2 narrowing 7/7

Very preliminary computational results on a small set of instances (some from MILPLib, some from Margot's website):

| *Instance* | *Group* | $\lvert\gamma\rvert$ | BBn($P$) | BBn($Q$) |
|---|---|---|---|---|
| `enigma` | $C_2$ | 2 | 3321 | **269** |
| `jgt18` | $C_2 \times S_4$ | 6 | **573** | 1300 |
| `oa66234` | $S_3$ | 2 | 0 | 0 |
| `oa67233` | $C_2 \times S_4$ | 6 | 6 | **0** |
| `oa76234` | $S_3$ | 2 | 0 | 0 |
| `ofsub9` | $C_3 \times S_7$ | 21 | 1111044 | **980485** |
| `stein27` | $((C_3 \times C_3 \times C_3) \ltimes PSL(3,3)) \ltimes C_2$ | 24 | **1084** | 1843 |
| `sts27` | $((C_3 \times C_3 \times C_3) \ltimes PSL(3,3)) \ltimes C_2$ | 26 | 1317 | **968** |

**Results are promising but not exciting**

**Need to improve narrowing efficacy**

# Other applications

- RcLin opt-reformulation: applied in (L., 4OR, 2007) to the Graph Partitioning Problem (GPP), the Multiprocessor Scheduling Problem with Communication Delays (MSPCD) and the Quadratic Assignment Problem (QAP): CPU improvement 2 Orders of Magnitude (OMs)
- RRLTRelax relaxation:
  1. used in (L. &Pantelides, JOGO, 2006) to drastically tighten the convex relaxation of pooling and blending problems from the oil industry: sBB nodes improvements 2-5 OMs
  2. use in (Lavor et al., EPL, 2007 and L. et al., DAM, accepted) to be able to compute molecular orbitals solving Hartree-Fock systems by sBB (impossible without it)
- InnerApprox approximation: found feasible solutions of a large-scale (25-50K bin vars/constrs) convex MINLP occurring in a sphere covering problem arising in the configuration of gamma-ray radiotherapy units (using CPLEX)

# Perspectives

- Principal Investigator for the Automatic Reformulation Search (ARS) project funded by ANR, and part of a WP in the EU project "Morphex": extend the reformulation library and implement a prototype of the automatic reformulation software

- Reformulation techniques offer high didactical value when teaching modelling courses

- My bet: successful algorithms for large scale MINLPs will *have* to employ automatic reformulation techniques to some extent

- My regret: there is a widespread belief that reformulations are "just" modelling tricks, and to dismiss them as implementation details, even though computational results improvements due to reformulations are major.

# The end

Thank you