Developing spatial branch & bound solvers

For mixed-integer nonlinear optimization

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EPSRC EP/P016871/1

2021/06/23

Outline

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Definition: Mixed-integer nonlinear optimization (MINLP)[1]

Grossmann and Sargent [1979]

This class of problem is very difficult to solve, and no general method yet exists for its efficient solution.

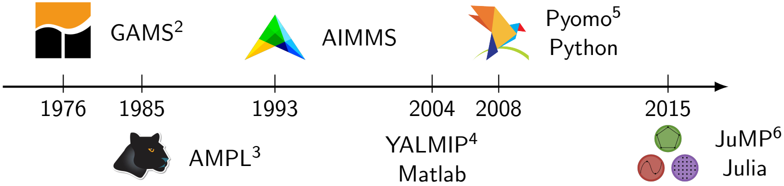
$$
\begin{aligned}
\min_{\mathbf{x}\in X,\, \mathbf{y}\in Y} \quad & f(\mathbf{x}, \mathbf{y}) && \longleftarrow \text{Objective function} \\
\text{s.t.} \quad & \mathbf{h}(\mathbf{x}, \mathbf{y}) = \mathbf{0} && \longleftarrow \text{Equality constraints} \\
& \mathbf{g}(\mathbf{x}, \mathbf{y}) \leq \mathbf{0} && \longleftarrow \text{Inequality constraints} \\
& \mathbf{x} \in \left[\mathbf{x}^{\mathrm{L}}, \mathbf{x}^{\mathrm{U}}\right] \subset \mathbb{R}^{n_x} && \longleftarrow \text{Continuous variable bounds} \\
& y \in \{0, 1\}^{n_y} && \longleftarrow \text{Binary variables}
\end{aligned}
$$

Assumptions

$f, \mathbf{h}, \mathbf{g} \in \mathcal{C}^2$

[1] Grossmann and Biegler [2004], Floudas and Gounaris [2009], Bussieck and Vigerske [2010], D'Ambrosio and Lodi [2011], Belotti et al. [2013], Boukouvala et al. [2016]

How can we represent MINLP?



Many MINLP solvers also have dedicated interfaces

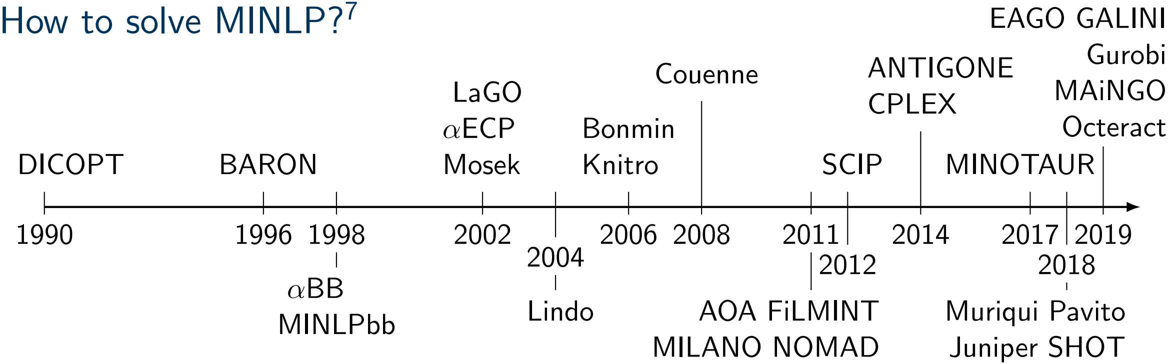
Mosel for FICO Xpress, ZIMLP for SCIP [Koch, 2004], etc.

General purpose mathematical software with MINLP connections

Excel, Matlab, R, . . .

[2]Brooke et al. [1997], [3]Fourer et al. [1993], [4]Löfberg [2004], [5]Hart et al. [2017], [6]Dunning et al. [2017]

How to solve MINLP?[7]



[7] α**BB** Adjiman et al. [1998a] • α**ECP** Westerlund and Pörn [2002] • **ANTIGONE** Misener and Floudas [2014] • **AOA** Hunting [2011] • **Baron** Tawarmalani and Sahinidis [2005] • **Bonmin** Bonami et al. [2008] • **Couenne** Belotti et al. [2009] • **CPLEX** Bonami et al. [2016] • **DICOPT** Viswanathan and Grossmann [1990] • **EAGO** Wilhelm and Stuber [2017] • **FilMINT** Abhishek et al. [2010] • **GALINI** • **Gurobi** • **Juniper** Kröger et al. [2018] • **Knitro** Byrd et al. [2006] • **LaGO** Nowak et al. [2003] • **LINDO** Gau and Schrage [2004] • **MAiNGO** Najman and Mitsos [2019] • **MILANO** Benson [2011] • **MINLPbb** Fletcher and Leyffer [1998] • **Minotaur** Mahajan et al. [2017] • **Mosek** • **Muriqui** Melo et al. [2018] • **NOMAD** Le Digabel [2011] • **Octeract** • **Pavito** Coey et al. [2020] • **SBB** GAMS • **SCIP** Vigerske and Gleixner [2018] • **SHOT** Lundell et al. [2018]

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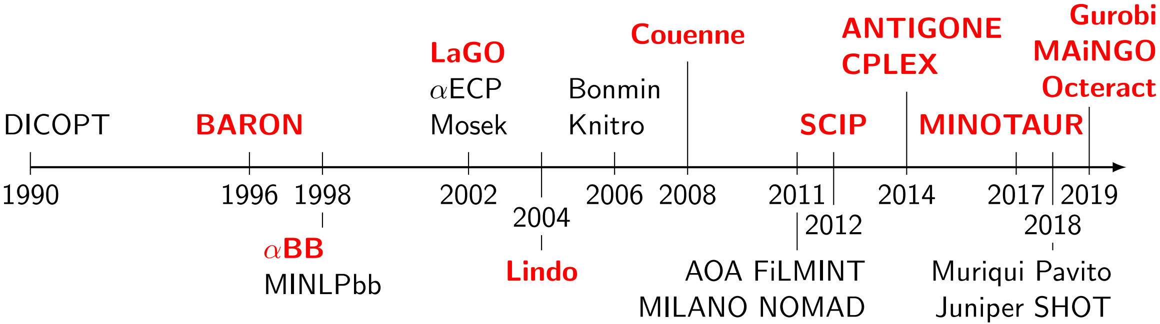

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Situating mixed-integer nonlinear optimization (MINLP)

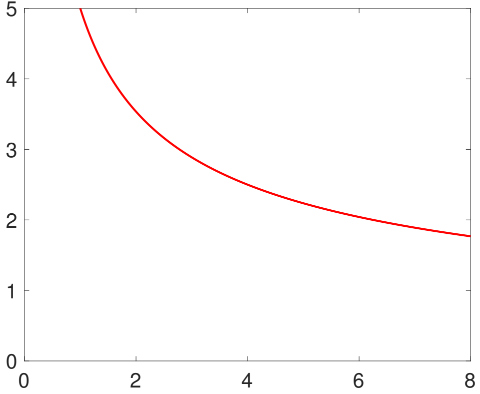
Prerequisites

Mixed-integer linear optimization • Nonlinear optimization • Convexity • Branch & bound

Connections to other work

- **Synomyn** Deterministic global optimization [Floudas and Gounaris, 2009]
- **Subclass** Convex MINLP [Kronqvist et al., 2019]
- **Classification** If computations exact, *complete methods* reach global optimum within a given tolerance in finite time [Neumaier, 2004]
  - *Asymptotically complete* methods reach a global optimum given infinite run time, e.g. Bayesian optimization [Jones et al., 1993]
  - *Rigorous* methods work despite rounding errors [Kearfott, 1996]

What is challenging here?[8]



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$$-1 \cdot x_1^3 + x_2 \leq 0$$

$$(x_1 - 7)^3 + x_2 \leq 0$$

$$-1 \cdot (x_1 - 4)^2 - x_2 \leq -4$$

Required solver elements

Structure detection • Relaxations • Variable bounds • Branching decisions • Primal heuristics

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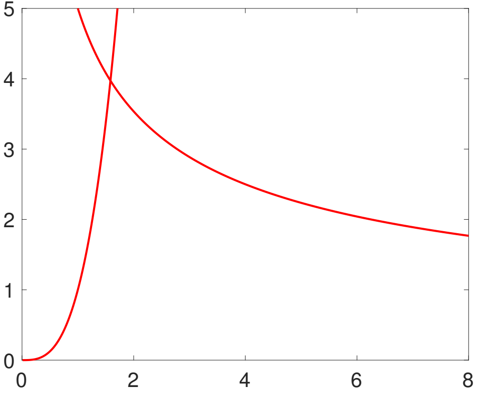

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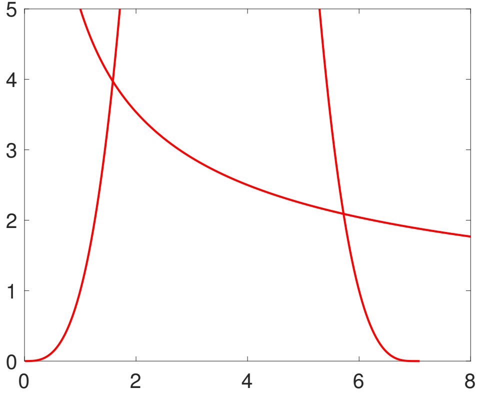

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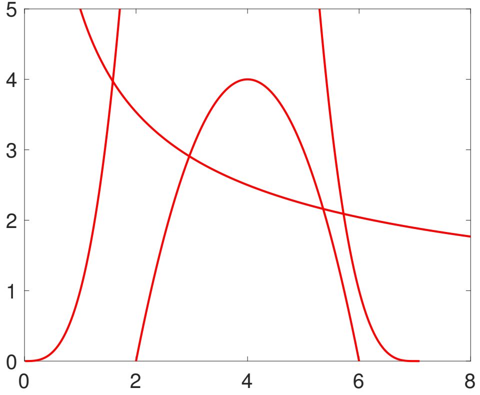

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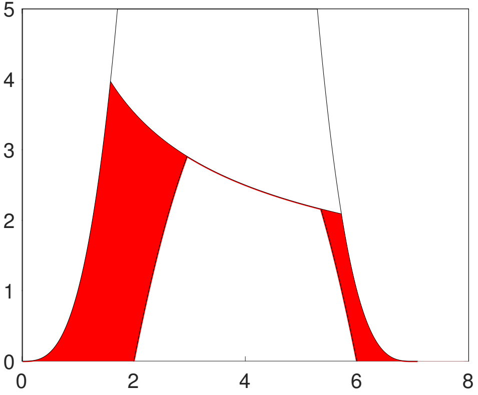

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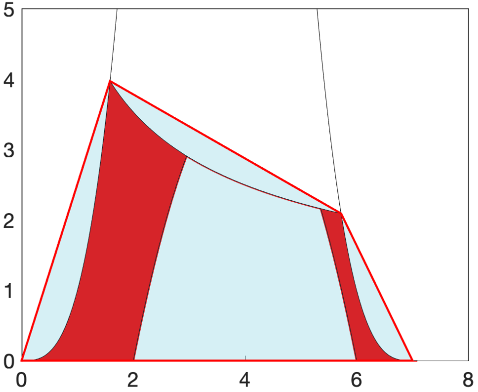

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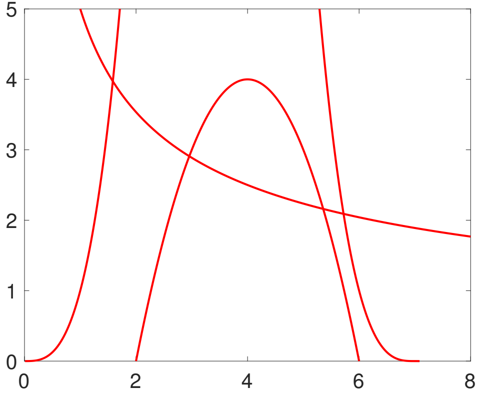

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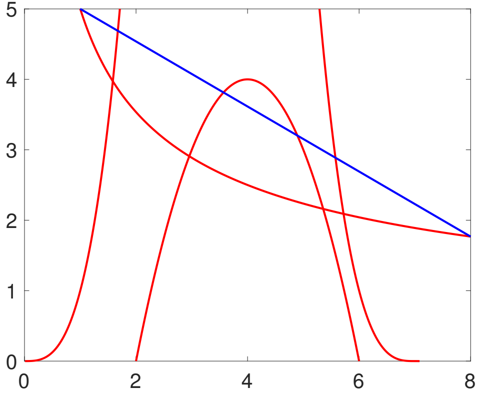

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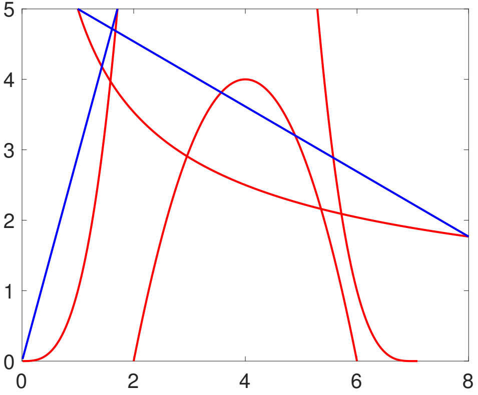

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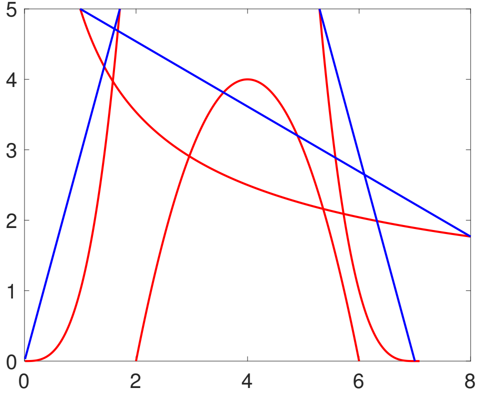

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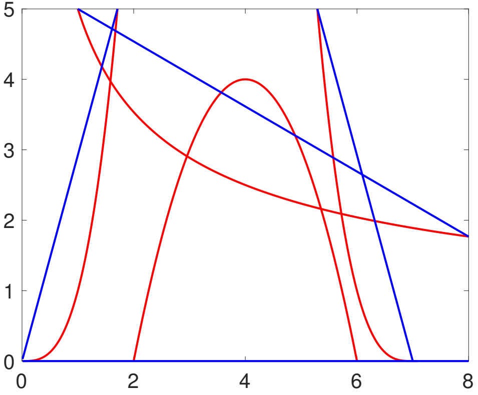

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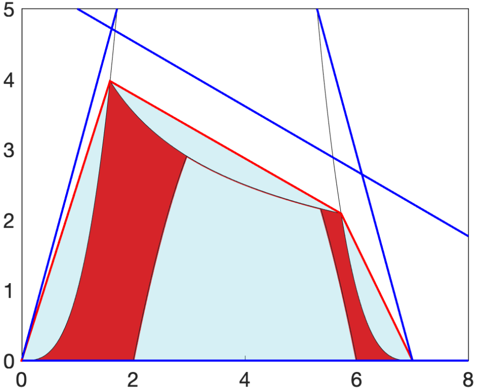

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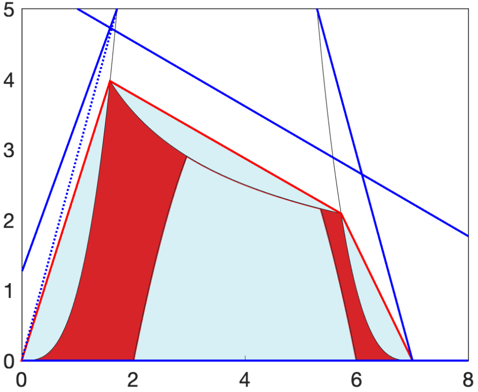

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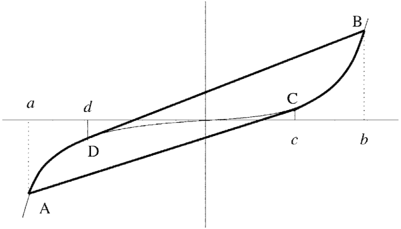

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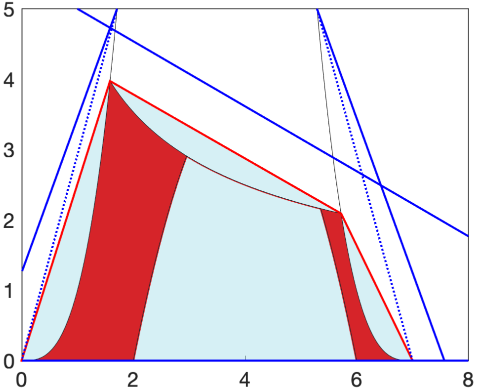

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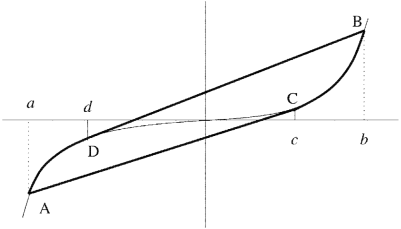

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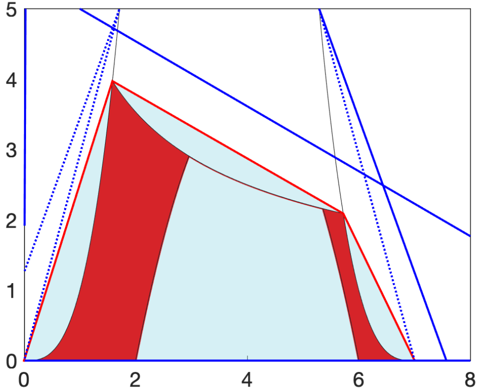

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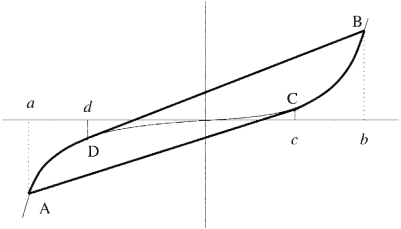

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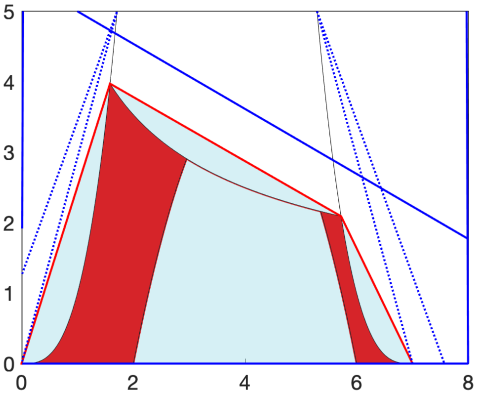

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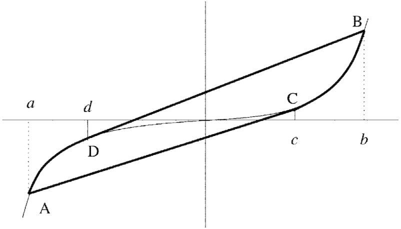

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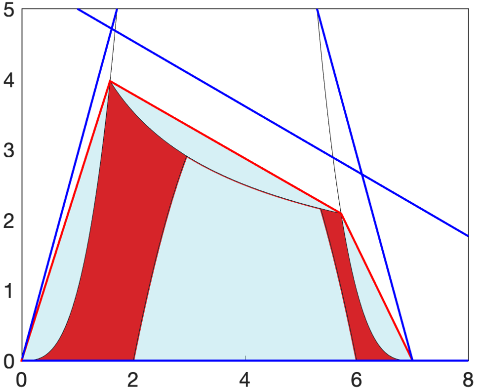

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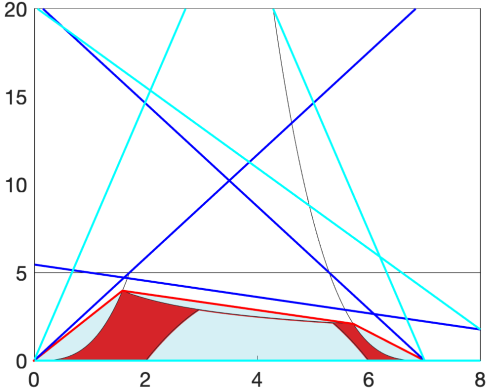

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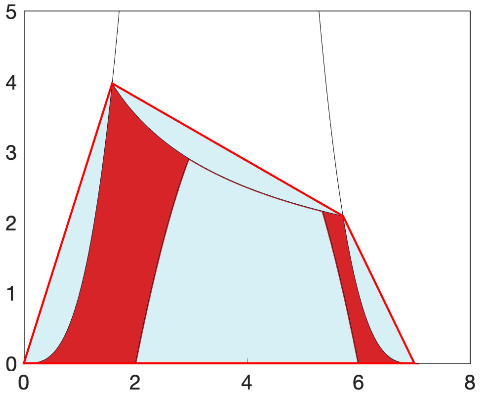

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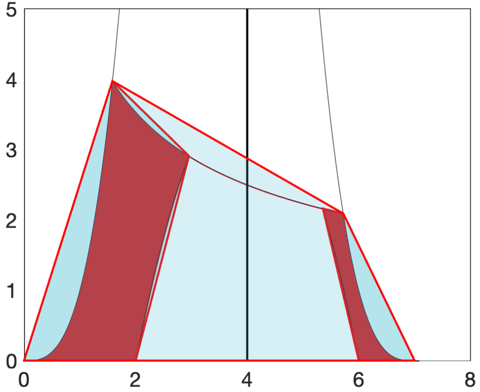

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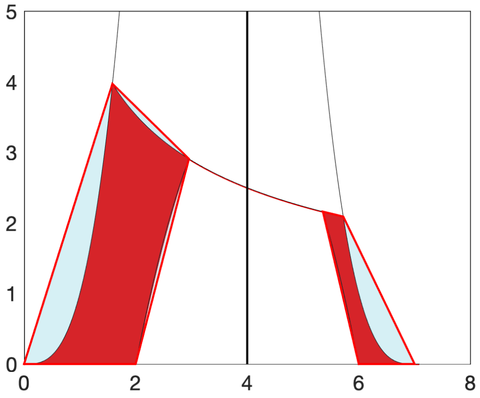

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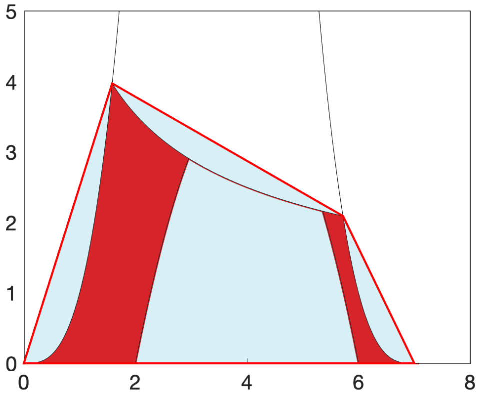
(x_1 - 7)^3 \quad & +x_2 \le 0 \\
-1 \cdot (x_1 - 4)^2 \quad & -x_2 \le -4
\end{aligned}
$$

Required solver elements

Structure detection • Relaxations • Variable bounds • Branching decisions • Primal heuristics

[8] Androulakis et al. [1995], Sahinidis [1996], Liberti and Pantelides [2003], Belotti [2013], Nguyen et al. [2018]

What is challenging here?[8]



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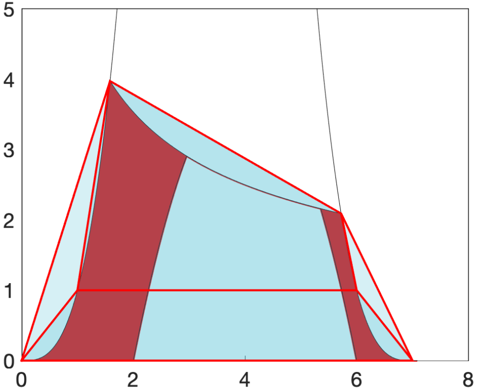

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\begin{aligned}
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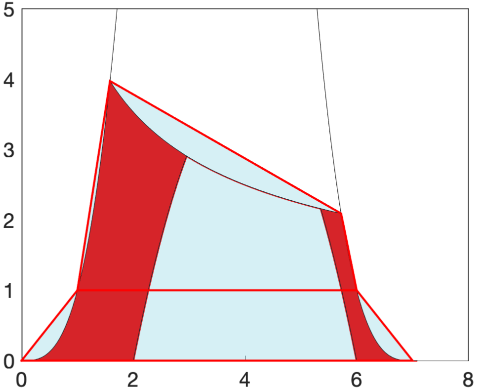

$$-\sqrt{\frac{25}{x_1}} + x_2 \le 0$$

$$-1 \cdot x_1^3 + x_2 \le 0$$

$$(x_1 - 7)^3 + x_2 \le 0$$

$$-1 \cdot (x_1 - 4)^2 - x_2 \le -4$$

Required solver elements

Structure detection • Relaxations • Variable bounds • Branching decisions • Primal heuristics

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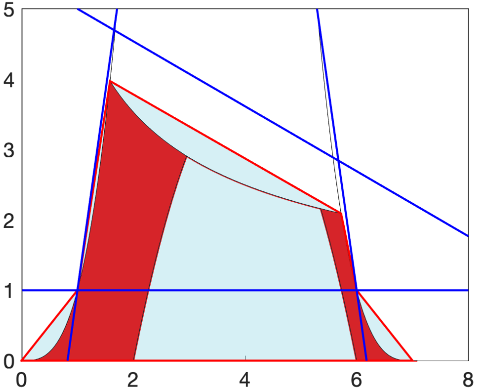

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\begin{aligned}
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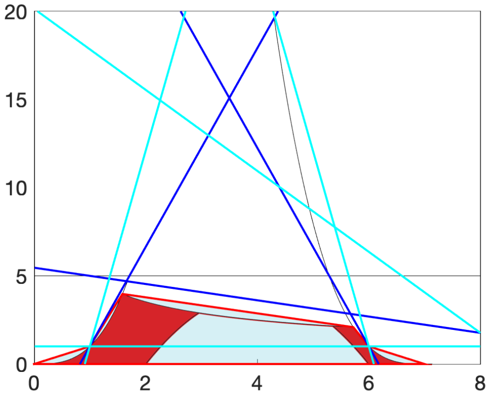

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Structure detection • Relaxations • Variable bounds • Branching decisions • Primal heuristics

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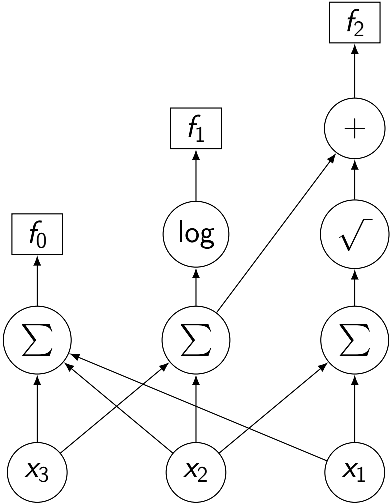
Outline

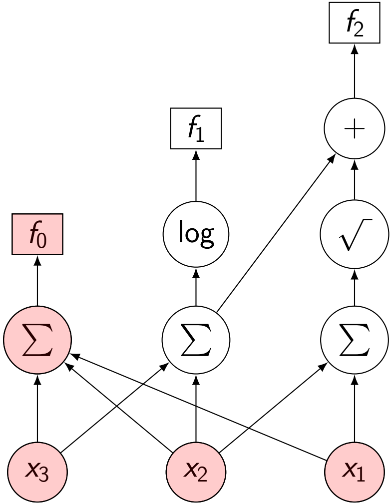
Data structures: Directed acyclic graph[9]



$$
\begin{aligned}
\min_{x_1,x_2,x_3} \quad & x_1 + x_2 + x_3 \\
\text{s.t.} \quad & \log(x_2 - x_3) \geq 0 \\
& x_2 - x_3 + \sqrt{x_1 + x_2} \leq 2 \\
& \mathbf{x} \in \left[\mathbf{x}^{\mathrm{L}}, \mathbf{x}^{\mathrm{U}}\right]
\end{aligned}
$$

[9] Smith and Pantelides [1999], Belotti et al. [2009], Liberti et al. [2010], Liberti [2012], Misener and Floudas [2014], Vigerske and Gleixner [2018], Ceccon et al. [2020]

Data structures: Directed acyclic graph[9]



$$\begin{aligned} \min_{x_1,x_2,x_3} \quad & \mathbf{x_1} + \mathbf{x_2} + \mathbf{x_3} \\ \text{s.t.} \quad & \log(x_2 - x_3) \geq 0 \\ & x_2 - x_3 + \sqrt{x_1 + x_2} \leq 2 \\ & \mathbf{x} \in \left[\mathbf{x}^{\mathrm{L}}, \mathbf{x}^{\mathrm{U}}\right] \end{aligned}$$

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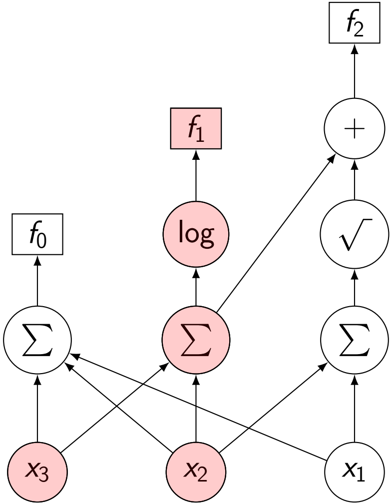
Data structures: Directed acyclic graph[9]



$$\begin{aligned} \min_{x_1,x_2,x_3} \quad & x_1 + x_2 + x_3 \\ \text{s.t.} \quad & \log(\mathbf{x_2} - \mathbf{x_3}) \geq \mathbf{0} \\ & x_2 - x_3 + \sqrt{x_1 + x_2} \leq 2 \\ & \mathbf{x} \in \left[\mathbf{x}^{\mathrm{L}}, \mathbf{x}^{\mathrm{U}}\right] \end{aligned}$$

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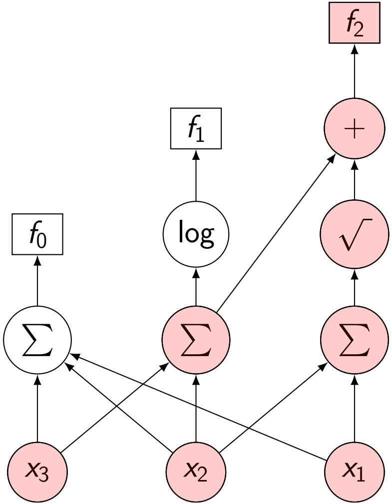

$$\begin{aligned} \min_{x_1,x_2,x_3} \quad & x_1 + x_2 + x_3 \\ \text{s.t.} \quad & \log(x_2 - x_3) \geq 0 \\ & \mathbf{x_2 - x_3 + \sqrt{x_1 + x_2} \leq 2} \\ & \mathbf{x} \in \left[\mathbf{x}^{\mathrm{L}}, \mathbf{x}^{\mathrm{U}}\right] \end{aligned}$$

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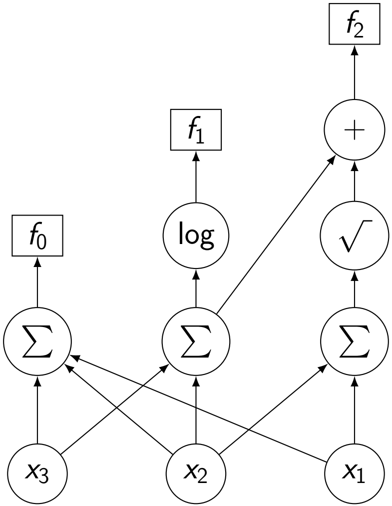
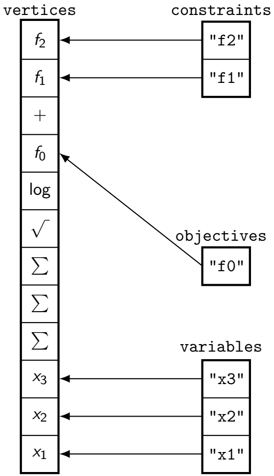
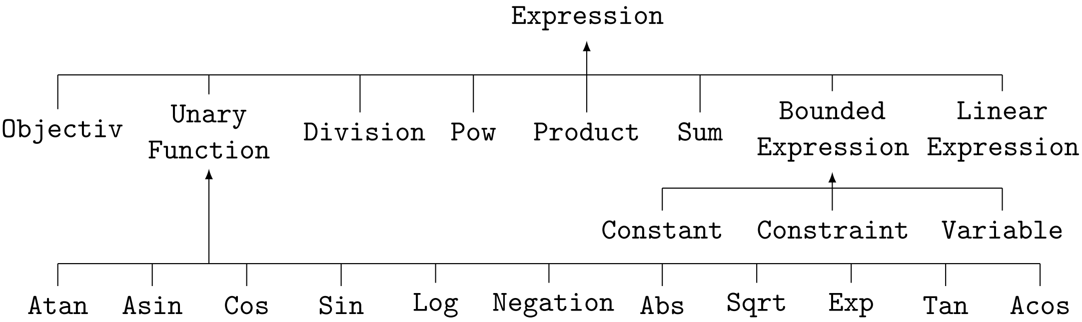




DAG may store vertices in vector, e.g. by depth.

[9] Smith and Pantelides [1999], Belotti et al. [2009], Liberti et al. [2010], Liberti [2012], Misener and Floudas [2014], Vigerske and Gleixner [2018], Ceccon et al. [2020]

Data structures: Hard-coded expression types



[10] Maranas and Floudas [1997], Ceria and Soares [1999], Lee and Grossmann [2000], Meyer and Floudas [2003, 2004], Frangioni and Gentile [2006], Aktürk et al. [2009], Anstreicher and Burer [2010], Cafieri et al. [2010], Hijazi et al. [2013], Ballerstein and Michaels [2014], Vielma et al. [2017], Speakman and Lee [2017]

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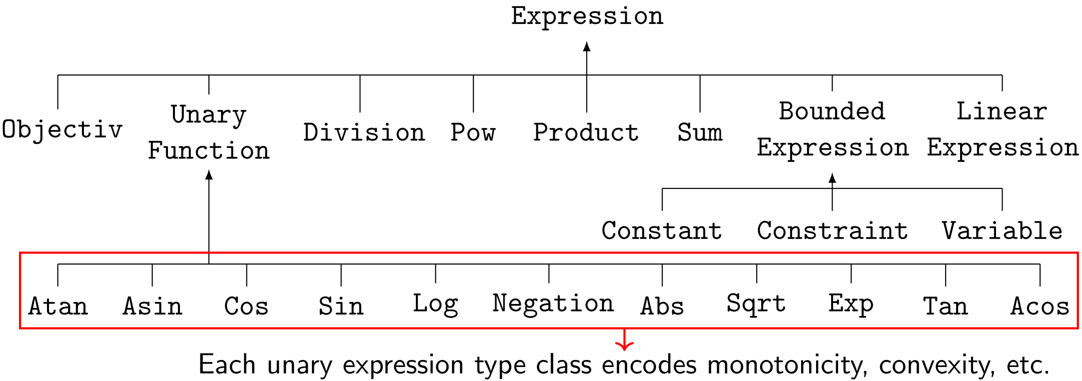

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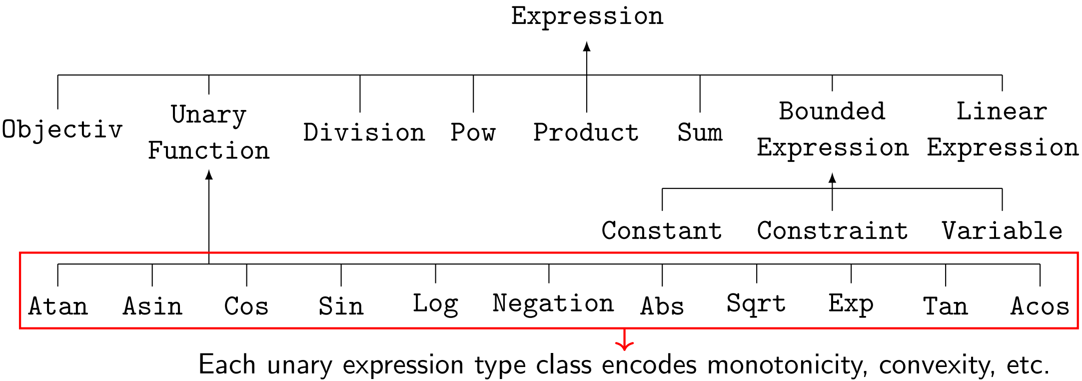
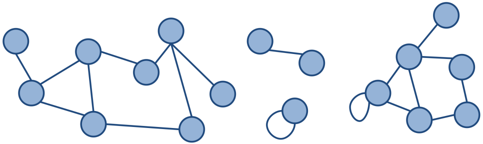


We can hard-code additional rules[10]

Indicator • Second-order cone • Signomial • {Tri-,Quadri-}linear

[10] Maranas and Floudas [1997], Ceria and Soares [1999], Lee and Grossmann [2000], Meyer and Floudas [2003, 2004], Frangioni and Gentile [2006], Aktürk et al. [2009], Anstreicher and Burer [2010], Cafieri et al. [2010], Hijazi et al. [2013], Ballerstein and Michaels [2014], Vielma et al. [2017], Speakman and Lee [2017]

Data structures: Undirected [weighted] graph



$$\min_{\mathbf{x},\mathbf{X}} \quad Q_0 \bullet \mathbf{X} + c_0^T \mathbf{x} + b_0$$

$$Q_k \bullet \mathbf{X} + c_k^T \mathbf{x} \leq b_k \; \forall k \in K$$

$$\mathbf{X} = \mathbf{x}\mathbf{x}^T$$

$$\mathbf{x} \in \left[\mathbf{x}^{\mathrm{L}}, \mathbf{x}^{\mathrm{U}}\right]$$

Quadratic $G(V, E)$

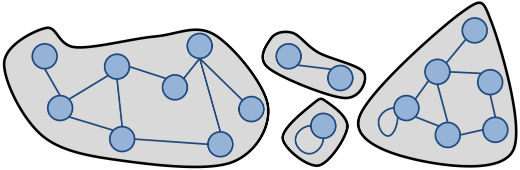
- V Vertex $\implies$ Variable
- E Edge $\implies$ Bilinear term
- [Weight $\implies$ Coefficient]

$$V = \{ \quad 1, 2, \ldots, N\}$$

$$E = \{ \quad \{i, j\} \in V \times V \mid i > j, \; \exists k \in K \text{ s.t. } Q_{ij}^{(k)} \neq 0\}$$

$$12 \cdot x_1^2 - 6 \cdot x_1 \cdot x_2 + 6 \cdot x_2^2 - 6.3 \cdot x_3^2 + x_4^2$$

Data structures: Undirected [weighted] graph



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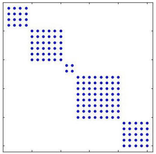

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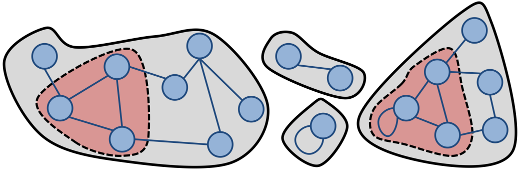
$$\underbrace{12 \cdot x_1^2 - 6 \cdot x_1 \cdot x_2 + 6 \cdot x_2^2}_{MT1} - \underbrace{6.3 \cdot x_3^2}_{MT2} + \underbrace{x_4^2}_{MT3}$$

Data structures: Undirected [weighted] graph



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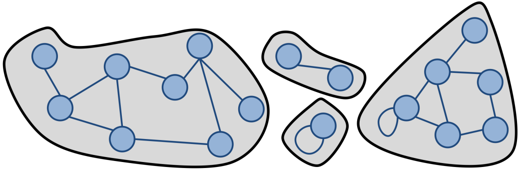
Data structures: Undirected [weighted] graph



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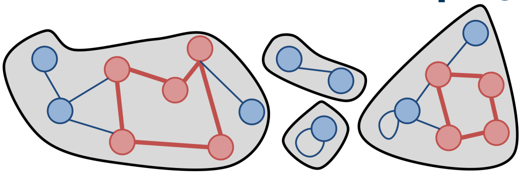

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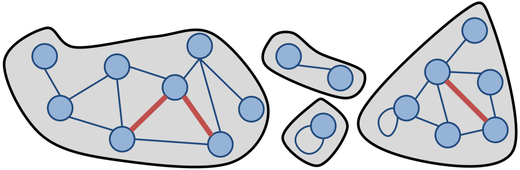
Strengthening with chordal extensions[11]

[11] Fukuda et al. [2001], Nakata et al. [2003], Baltean-Lugojan et al. [2018], Eltved et al. [2019], [12] Bao et al. [2015], Del Pia and Khajavirad [2018], Del Pia et al. [2018]

Data structures: Undirected [weighted] graph



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Strengthening with chordal extensions[11]

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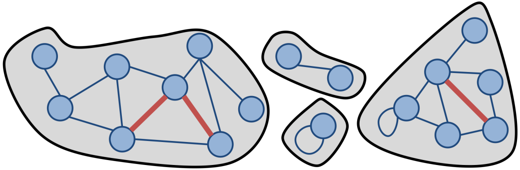
Data structures: Undirected [weighted] graph



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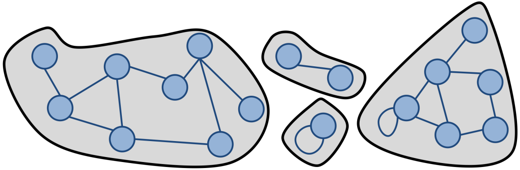
Strengthening with chordal extensions[11]

Extension to multilinear polynomials[12]

Use a hypergraph to allow an edge to join any number of vertices

[11]Fukuda et al. [2001], Nakata et al. [2003], Baltean-Lugojan et al. [2018], Eltved et al. [2019], [12]Bao et al. [2015], Del Pia and Khajavirad [2018], Del Pia et al. [2018]

Data structures: Undirected [weighted] graph[13]



Quadratic $G(V, E)$

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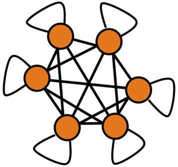
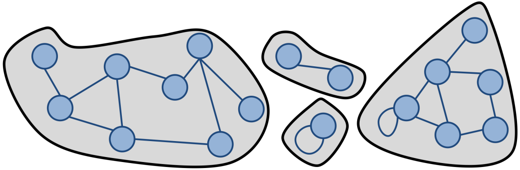
Common patterns



[13] Misener and Floudas [2012, 2013], Misener et al. [2015]

Data structures: Undirected [weighted] graph[13]



Quadratic $G(V, E)$

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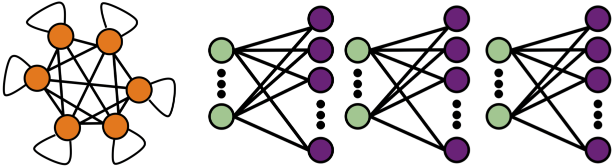
Common patterns



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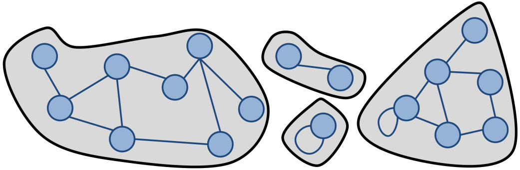

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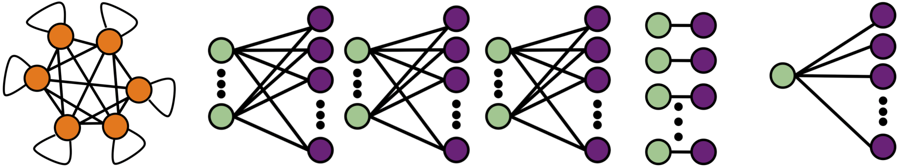


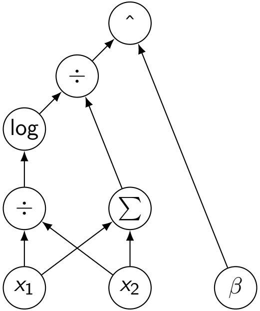
[13] Misener and Floudas [2012, 2013], Misener et al. [2015]

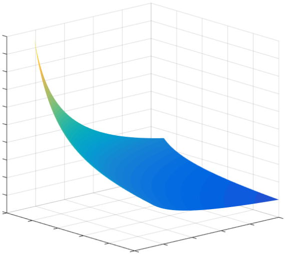
Outline

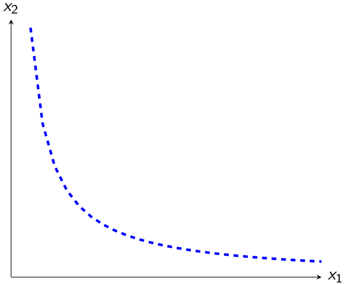
Convex substructures in heat recovery networks

Logarithmic mean temperature difference concave if $-1 \leq \beta \leq 0$ and convex if $\beta \geq 0$ [14]:

$$\text{RecLMTD}^{\beta}(x_1, x_2) = \begin{cases} \left(\frac{\ln(x_1/x_2)}{x_1 - x_2}\right)^{\beta} & x_1 \neq x_2, \\ 1/x_1^{\beta} & x_1 = x_2, \end{cases} \qquad x_1, x_2 \in \mathbb{R}_+, \beta \geq -1.$$







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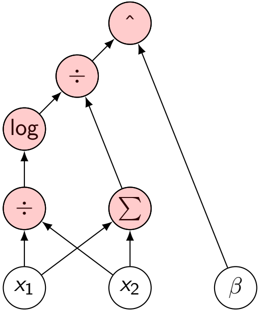

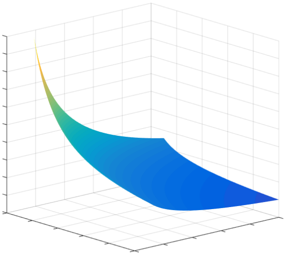

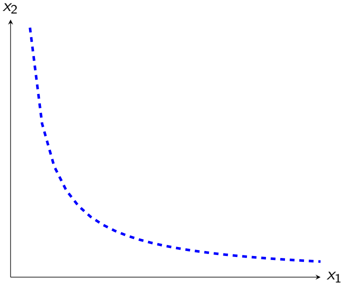

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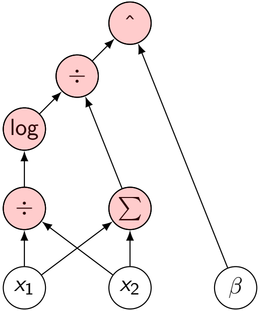

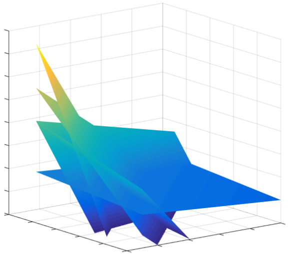

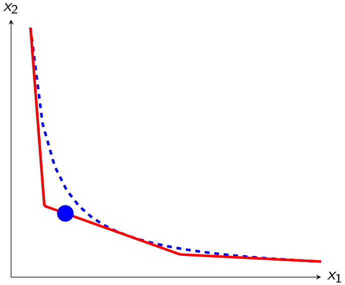

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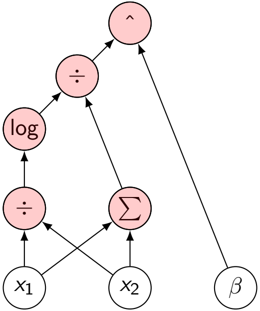

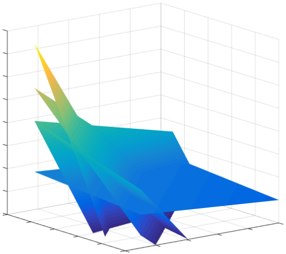

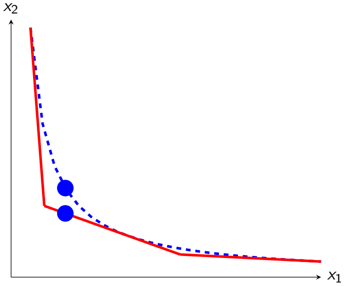

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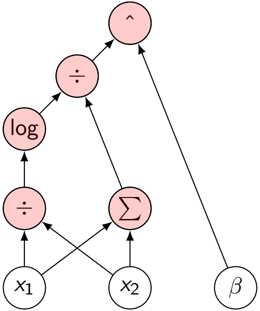

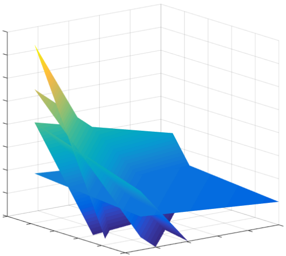

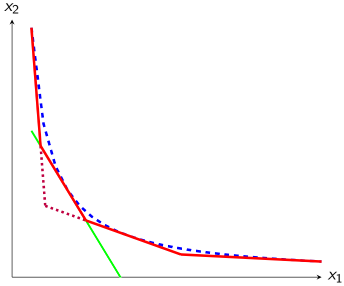

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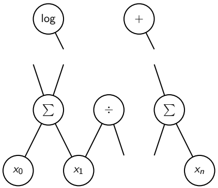
Automatic convexity detection

Tree-walking rules [Fourer et al., 2010]

Recursively apply convexity rules to expression trees:

$$k = g_1 \circ g_2, g_1 \text{ convex \& nondecreasing}, g_2 \text{ convex} \implies k \text{ convex}$$



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Hessian computation [Nenov et al., 2004]

Compute *Hessian sign* with Automatic Differentiation

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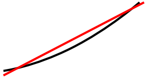

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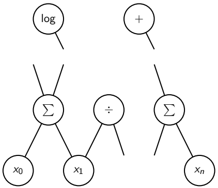

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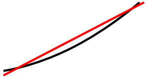

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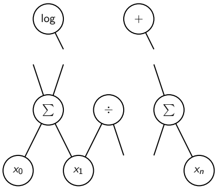

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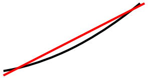

Solver software strategies

Assume functions are convex (DICOPT, SHOT) • Tag functions as convex (BARON) • Automatic detection (ANTIGONE, BARON, SCIP)

Automatic convexity detection is brittle

Missing hard-coded rule? Get factorable programming decomposition

$$\mathrm{RecLMTD}^{\beta}(x_1, x_2) = \left(\frac{\ln\left(x_1/x_2\right)}{x_1 - x_2}\right)^{\beta} \xrightarrow[\text{form}]{\text{factored}} \begin{cases} v_1 = x_1/x_2 \\ v_2 = \ln v_1 \\ v_3 = x_1 - x_2 \\ v_4 = v_3/v_2 \\ v_5 = v_4^{\beta} \end{cases}$$

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Legacy code assumes different numerical strategies [15]

$$\mathrm{RecLMTD}^{\beta}(x_1, x_2) \approx \left(\frac{\ln\left(x_1/(x_2 + \epsilon)\right)}{x_1 - x_2}\right)^{\beta}$$

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Problems are *convex by construction* [Grant and Boyd, 2008]

Impose a set of conventions or rules:

- Atom library holds convex functions,
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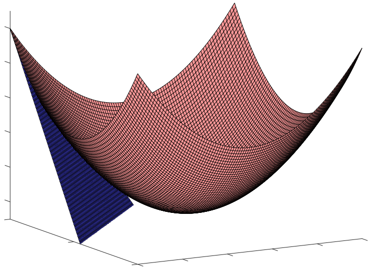

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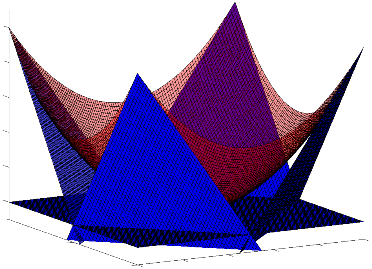

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- GitHub: `https://github.com/cog-imperial/suspect`
- SUSPECT extends convexity and monotonicity detection with a plugin-based architecture
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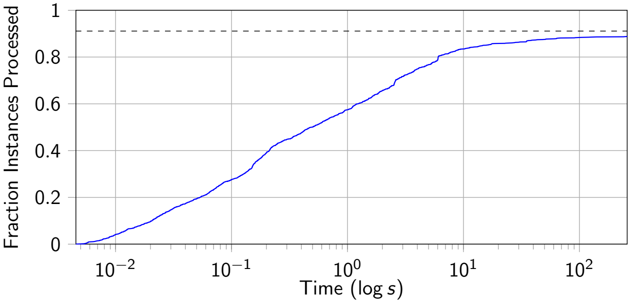

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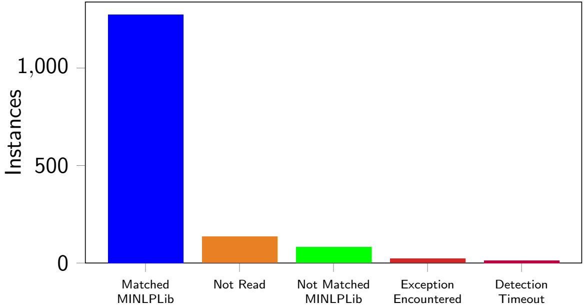

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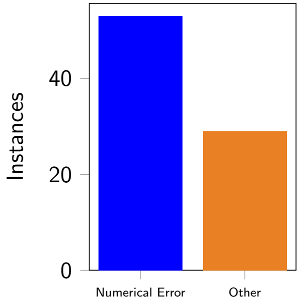

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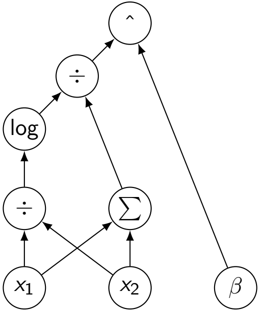

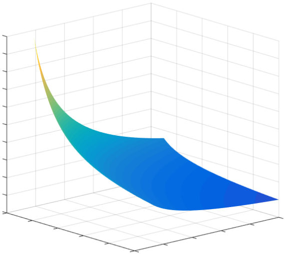

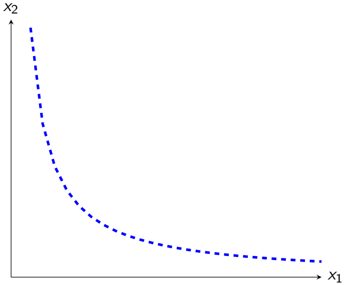

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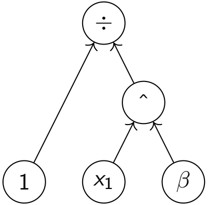

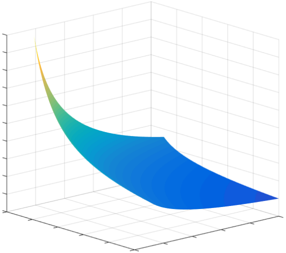

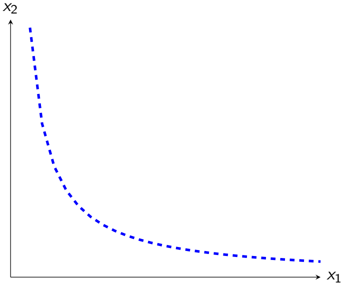

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Extending SUSPECT: Example[19]

1. Register the detector using `setuptools` entry points in `setup.py`

```
setup(entry_points={
  'suspect.convexity_detection':
  ['rec_lmtd=rec_lmtd_detector.RecLMTDDetector']
})
```

2. Subclass `suspect.ext.ConvexityDetector` and register rules

```
class RecLMTDDetector(ConvexityDetector):
    def register_rules(self):
        return [
            RecLMTDRule(),
            RecRule(),
        ]
```

3. Implement rules returning `Convexity` & `Monotonicity` information if known, `None` otherwise

[19] Ceccon et al. [2020]

Extending SUSPECT: Example[20]

```python
class RecRule(Rule):
    root_expr = ExpressionType.Division

    def apply(self, expr, ctx):
        num, den = expr.children
        # numerator has to be 1.0
        if not num.is_constant() or exp.value != 1.0:
            return
        # denominator has to be power with beta >= -1.0
        if not den.expression_type == ExpressionType.Power:
            return
        base, expo = den.children
        if not expo.is_constant() or expo.value < -1.0:
            return
        if not base.expression_type == ExpressionType.Variable:
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        bounds = ctx.bounds(base)
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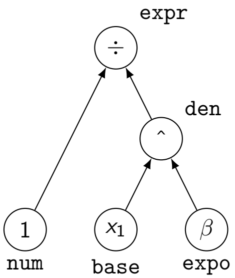

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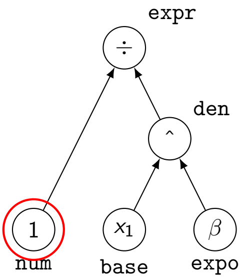

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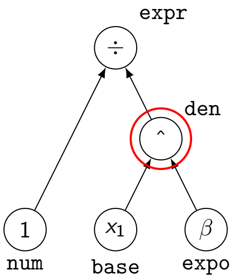

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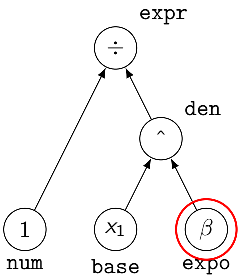
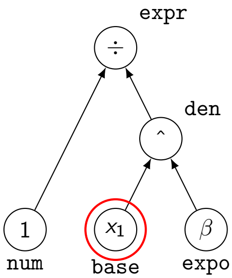


[20]Ceccon et al. [2020]

Extending SUSPECT: Example[20]

```python
class RecRule(Rule):
    root_expr = ExpressionType.Division

    def apply(self, expr, ctx):
        num, den = expr.children
        # numerator has to be 1.0
        if not num.is_constant() or exp.value != 1.0:
            return
        # denominator has to be power with beta >= -1.0
        if not den.expression_type == ExpressionType.Power:
            return
        base, expo = den.children
        if not expo.is_constant() or expo.value < -1.0:
            return
        if not base.expression_type == ExpressionType.Variable:
            return
        bounds = ctx.bounds(base)
        if bounds.is_nonnegative():
            return self._convexity_from_beta(expo.value)
```



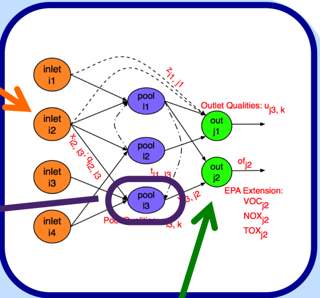
[20] Ceccon et al. [2020]

Structure beyond convexity: Pooling problem[21]

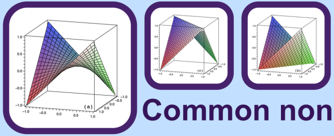
Know input species concentrations (*e.g.*, sulfur)

Variables

$$\sum_{i\in \mathrm{In}} c_{\mathrm{Sulfur},\,i}\cdot f_i = c_{\mathrm{Sulfur,\,Out}}\cdot \sum_{o\in \mathrm{Out}} f_o$$



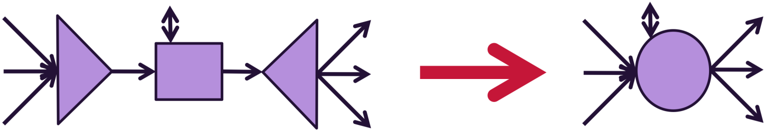
Have output species requirements (e.g., laws)



Common nonlinear term: x × y

[21] **Branching** Dey et al. [2019] • **Relaxations** Adhya et al. [1999], Karuppiah and Grossmann [2006], Meyer and Floudas [2006], Misener et al. [2011], Dey and Gupte [2015], Gupte et al. [2017], Marandi et al. [2017], Dey et al. [2020] • **Cuts** Luedtke et al. [2020] • **Formulations** Alfaki and Haugland [2013], Boland et al. [2016] • **Special structure** Visweswaran and Floudas [1990], Baltean-Lugojan and Misener [2018]

Structure beyond convexity: Local detection[22]



- Product disaggregation for convex relaxations & bounds tightening

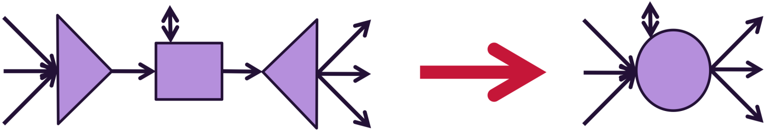
$$\mathbf{p}_{\ell,\mathbf{k}} \cdot \sum_{j \in J} \mathbf{f}_{\ell,\mathbf{j}} = \sum_{j \in J} \mathbf{p}_{\ell,\mathbf{k}} \cdot \mathbf{f}_{\ell,\mathbf{j}}$$

- Find products of linear equality equations & variables

$$\left(\sum_j a_{m,j} \cdot x_j - b_m \right) \cdot \mathbf{x_i} = \sum_j a_{m,j} \cdot x_j \cdot \mathbf{x_i} - b_m \cdot \mathbf{x_i} = 0$$

[22] Adams and Sherali [1990], Tawarmalani and Sahinidis [2002], Liberti and Pantelides [2006], Vigerske et al. [2012], Misener and Floudas [2013], Zorn and Sahinidis [2014], Misener et al. [2015]

Structure beyond convexity: Local detection[22]



Mixer
$$\begin{cases} \sum_i F_{M,i} = F_T^{IN} \\ \sum_i x_{M,i,j} \cdot F_{M,i} = x_{T,j}^{IN} \cdot F_T^{IN} \quad \forall\, j \in \{1, \ldots, J\} \end{cases}$$

Treatment
$$\begin{cases} F_T^{IN} = F_T^{OUT} \\ x_{T,j}^{IN} = \beta_{T,j} \cdot x_{T,j}^{OUT} \quad \forall\, j \in \{1, \ldots, J\} \end{cases}$$

Splitter
$$\begin{cases} F_T^{OUT} = \sum_i F_{S,i} \\ x_{T,j}^{OUT} = x_{T,i,j} \quad \forall\, i \in \{1, \ldots, I\};\; j \in \{1, \ldots, J\} \end{cases}$$

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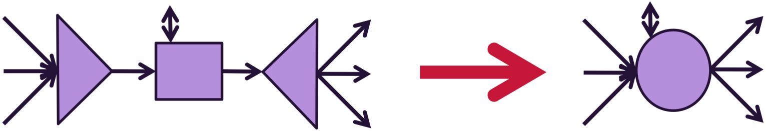

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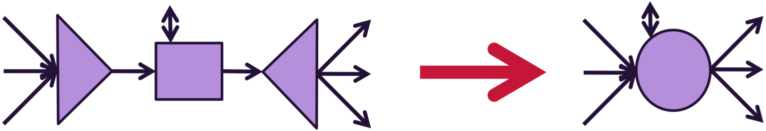
Structure beyond convexity: Local detection[22]

> 10× Speed-up for 10% of process networks

ANTIGONE, BARON, Couenne, LINDO



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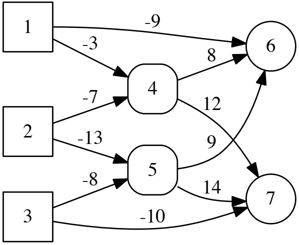
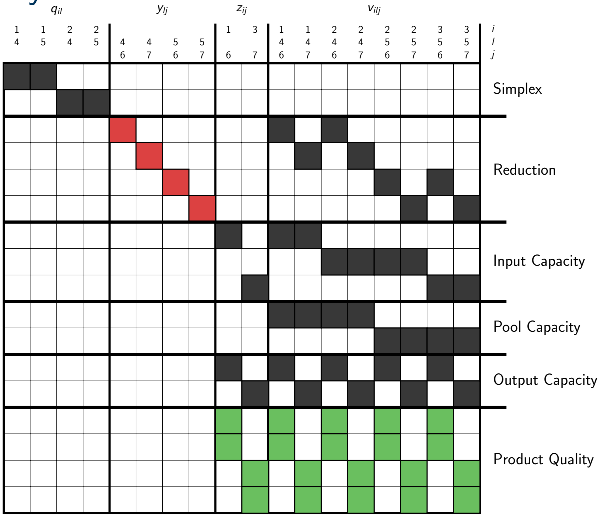
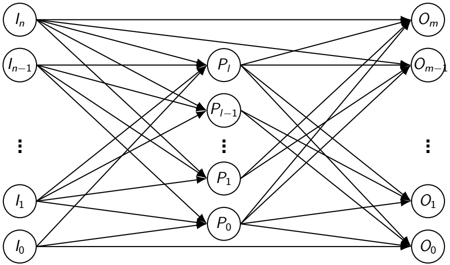
Structure beyond convexity: Global detection[23]





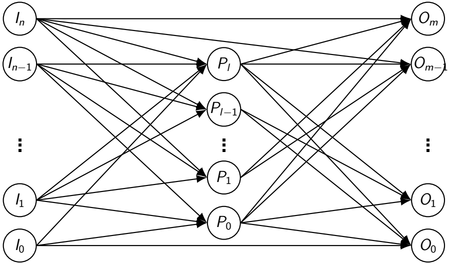
[23] Brown and Wright [1984], Bixby and Fourer [1988], Nemhauser et al. [1994], Achterberg and Raack [2010], Salvagnin [2016], Ceccon et al. [2016]

Structure beyond convexity: Disciplined programming?[24]



[24] Evans et al. [1979], Barton and Pantelides [1994], Ceccon et al. [2020]

Structure beyond convexity: Disciplined programming?[24]



Other networks

- **Gas** [Pfetsch et al., 2015, Humpola and Fügenschuh, 2015, Liers and Merkert, 2016, Bärmann et al., 2018]
- **Power** [Bienstock and Munoz, 2014, Chen et al., 2015, Kocuk et al., 2016]

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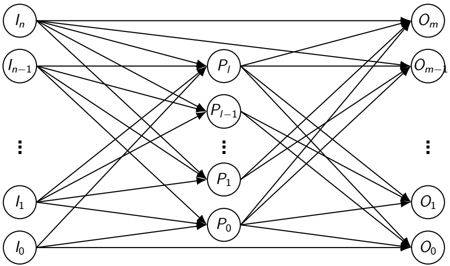

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Substructures in other important problems?

Where to go looking for interesting structures ...

- **Sustainability**, e.g. Guillén-Gosálbez and Grossmann [2010]
- **Swing adsorption** with PDEs [Hasan et al., 2012, Leperi et al., 2016]
- **Thermodynamic equilibria** [Bollas et al., 2009, Mitsos et al., 2009a, Pereira et al., 2010, Glass and Mitsos, 2017], e.g. within **distillation** [Nallasivam et al., 2016, Mertens et al., 2018]

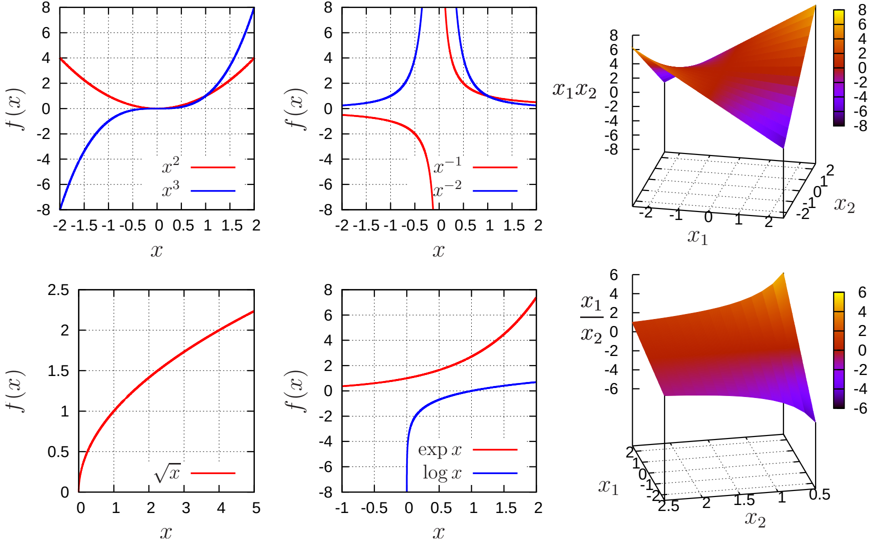
[24] Evans et al. [1979], Barton and Pantelides [1994], Ceccon et al. [2020]

Outline

Outline

Recognize and relax common functions on boxes[25]

Graphics by Benoît Chachuat



Factorable programming: Recursively compose functions

Auxiliary variable method [Smith and Pantelides, 1999]

$$\mathrm{RecLMTD}^{\beta}(x_1, x_2) = \left(\frac{\ln(x_1/x_2)}{x_1 - x_2}\right)^{\beta} \xrightarrow[\text{form}]{\text{factored}} \begin{cases} v_1 = x_1/x_2 \\ v_2 = \ln v_1 \\ v_3 = x_1 - x_2 \\ v_4 = v_3/v_2 \\ v_5 = v_4^{\beta} \end{cases}$$

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Subgradient propagation method

- **Theory** McCormick [1976], Mitsos et al. [2009b], Tsoukalas and Mitsos [2014], Stuber et al. [2015]
- **Try it out** `EAGO` `https://github.com/PSORLab/EAGO.jl` • `MAiNGO` `https://git.rwth-aachen.de/avt.svt/public/maingo`

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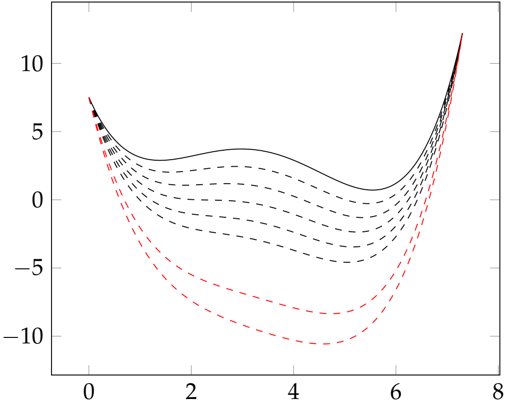
Relaxation

`MC++` `https://omega-icl.github.io/mcpp/` • `Coramin` `https://github.com/Coramin/Coramin` , used in `GALINI` `https://github.com/cog-imperial/galini`

αBB: Quadratic shift matrix



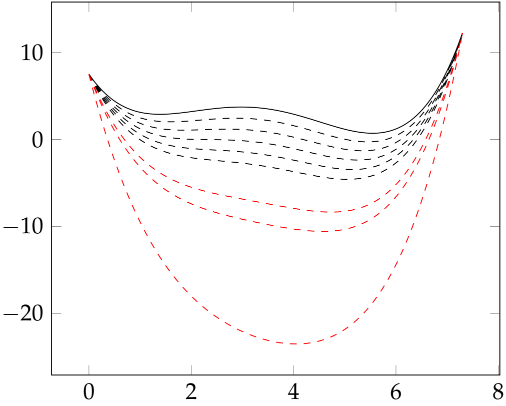
$$f^{\mathsf{CVX}}(\mathbf{x}) = f(\mathbf{x}) + \alpha \left[\mathbf{x} - \mathbf{x}^{\mathrm{L}}\right]^{\mathsf{T}} \left[\mathbf{x} - \mathbf{x}^{\mathrm{U}}\right],$$

$\alpha \implies$ shift parameter

$\mathbf{H}(\mathbf{x}) + 2\alpha\,\mathrm{I} \succeq 0, \ \forall \mathbf{x} \in \mathbf{X}$

Androulakis et al. [1995], Adjiman et al. [1998b,a], Mönnigmann [2011], Schulze Darup and Mönnigmann [2016]

αBB: Quadratic shift matrix



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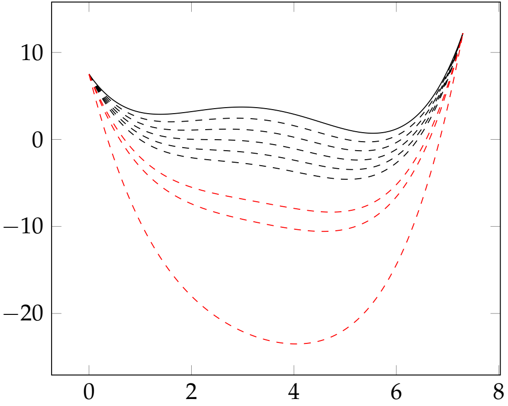

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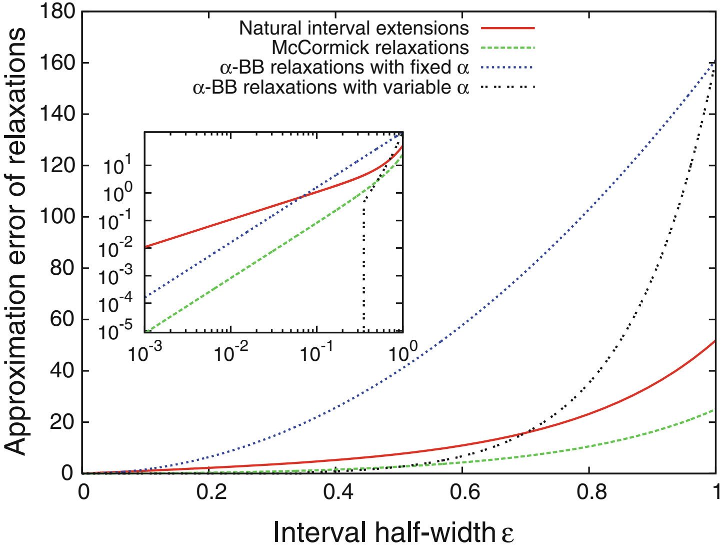
Androulakis et al. [1995], Adjiman et al. [1998b,a], Mönnigmann [2011], Schulze Darup and Mönnigmann [2016]

Other relaxation schemes ...

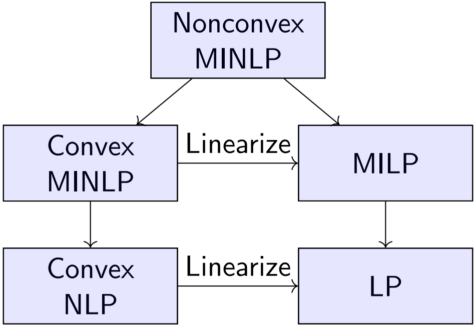
Lasserre [2001] hierarchy for polynomials, e.g. in `GloptiPoly` [Henrion and Lasserre, 2003] • Sum-of-squares and alternatives, e.g. Ahmadi and Majumdar [2019]

Goal: Use all the relaxations at once[26]



[26] Anstreicher [2009], Bompadre and Mitsos [2012]

Open engineering question: How to relax?



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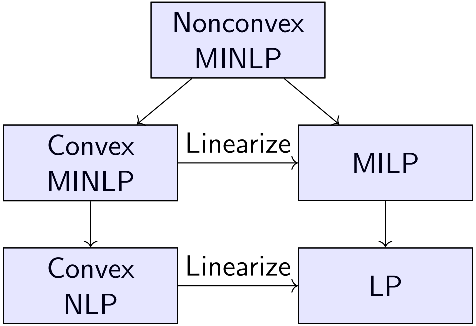
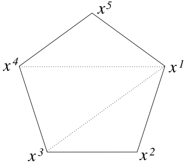


Open engineering question: Use auxiliary variables?

- **No auxiliary variables** αBB • Factorable programming with subgradient propagation,
- **Use auxiliary variables** Factorable programming with auxiliary variables • SOS-like hierarchies,
- Can I hybridize using auxiliary variables or not?
- Do I have to commit to a strategy at the root node?

Convex relaxations beyond boxes?



Edge concave

Tardella [2004], Meyer and Floudas [2006], Tardella [2008]

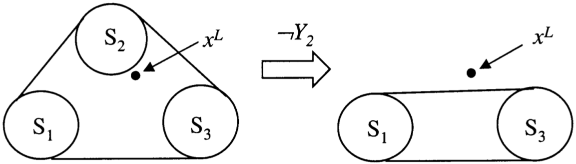
- **Intersect: quadratic & polytope** Linderoth [2005], Tawarmalani et al. [2010], Nguyen et al. [2011], Kocuk et al. [2016], Davarnia et al. [2017], Rahman and Mahajan [2019], Li and Vittal [2018], Santana and Dey [2018], Dey et al. [2019], Anstreicher et al. [2020]
- **Intersect: 2 quadratics** Burer and Kılınç-Karzan [2017], Modaresi and Vielma [2017]
- **Regions** Khajavirad and Sahinidis [2013], Tawarmalani et al. [2013]
- **Intersect: Bivariate function & polytope** Locatelli [2018]

What do we need to integrate into generic solvers?

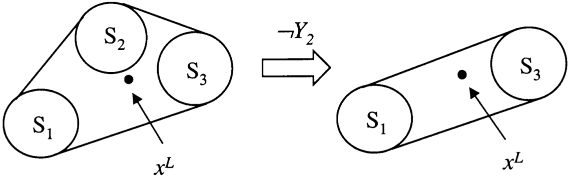
More relaxations • Generic data structures [Kvasnica et al., 2004]

Outline

One branch may not exclude the current relaxation![27]



a) Partitionable set



b) Non-partitionable set

[27] Lee and Grossmann [2000]

How shall we branch?

Integer variables

- Integrate directly into a MIP solver?
  - SCIP [Vigerske and Gleixner, 2018] • CPLEX [Bonami et al., 2016]
- Leave the discrete variables to a state-of-the-art MIP solver?
  - BONMIN [Bonami et al., 2008] • ANTIGONE [Misener and Floudas, 2014]
- Effectively develop a MIP solver together with the MINLP solver?
  - BARON [Tawarmalani and Sahinidis, 2005] • Couenne [Belotti et al., 2009]

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Continuous variables

- On the original problem variables?
- In a reduced space?
  - Concave [Phillips and Rosen, 1988] • Bilinear [Sherali and Alameddine, 1992] • Difference of convex [Horst and Van Thoai, 1994] • Factorable MINLP [Epperly and Pistikopoulos, 1997] • Flowsheets [Bongartz and Mitsos, 2017]
- In a lifted space?

How shall we branch?

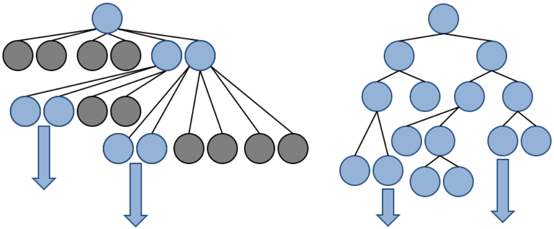
$$\begin{aligned} \min_{\mathbf{x}_1,\mathbf{x}_2} \quad & f^{\text{cvx}}(\mathbf{x}_1,\mathbf{x}_2) \\ & g_1^{\text{cvx}}(\mathbf{x}_1,\mathbf{x}_2) + \textstyle\sum_i g_{2,i}^{\text{cvx}}(\mathbf{x}_1)\cdot g_{3,i}^{\text{noncvx}}(\mathbf{x}_2) + g_4^{\text{noncvx}}(\mathbf{x}_2) \le 0 \\ & \mathbf{x}_1 \in \left[\mathbf{x}_1^{\mathrm{L}},\, \mathbf{x}_1^{\mathrm{U}}\right] \\ & \mathbf{x}_2 \in \left[\mathbf{x}_2^{\mathrm{L}},\, \mathbf{x}_2^{\mathrm{U}}\right] \end{aligned}$$

Only need to branch on the $\mathbf{x}_2$ variables!

Continuous variables

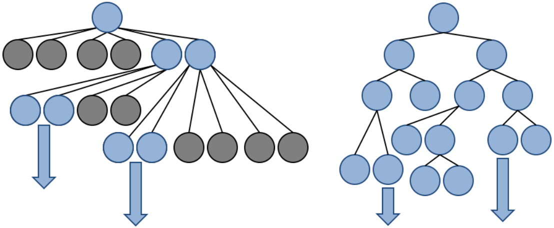
- On the original problem variables?
- In a reduced space?
  - Concave [Phillips and Rosen, 1988] • Bilinear [Sherali and Alameddine, 1992] • Difference of convex [Horst and Van Thoai, 1994] • **Factorable MINLP** [Epperly and Pistikopoulos, 1997] • Flowsheets [Bongartz and Mitsos, 2017]
- In a lifted space?

Reliability branching[28]

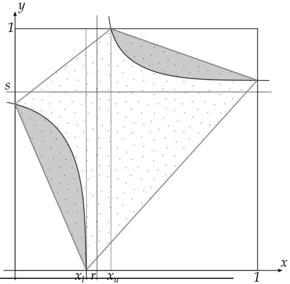


[28] Achterberg et al. [2005], Belotti et al. [2009], Misener and Floudas [2014], Vigerske and Gleixner [2018]

Reliability branching[28]



Get disjunction [Dey et al., 2019]



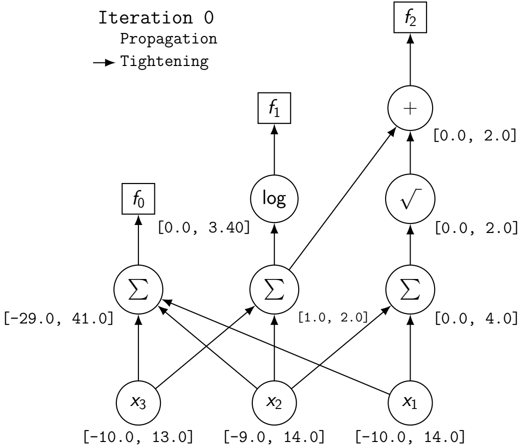
Outlook

Get disjunctions • Branch on constraints • Improve relaxations & bounds tightening

[28] Achterberg et al. [2005], Belotti et al. [2009], Misener and Floudas [2014], Vigerske and Gleixner [2018]

Outline

Feasibility & optimality-based bounds tightening[29]

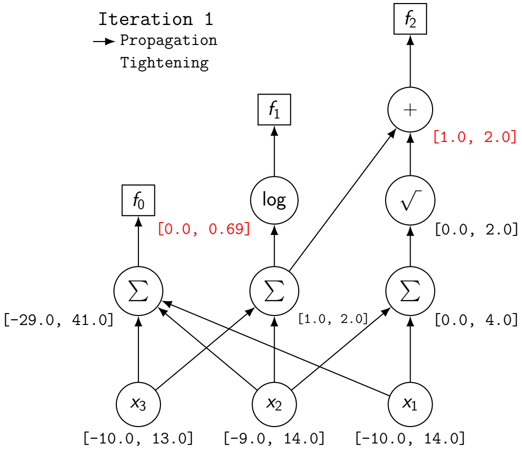


Outlook

Major accomplishments enabled generic solver software • New challenge: tighten more than variables

[29] Ryoo and Sahinidis [1996], Zamora and Grossmann [1999], Belotti et al. [2009], Belotti [2013], Gleixner et al. [2017], Puranik and Sahinidis [2017a,b]

Feasibility & optimality-based bounds tightening[29]



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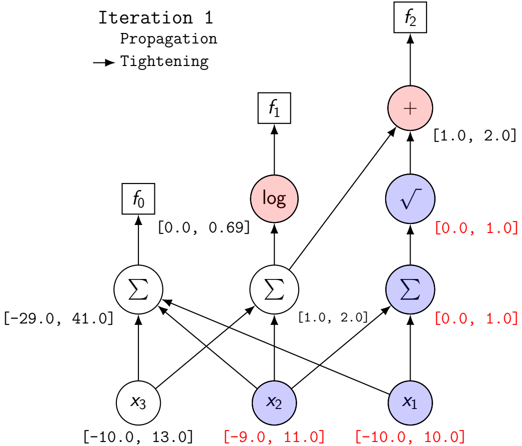
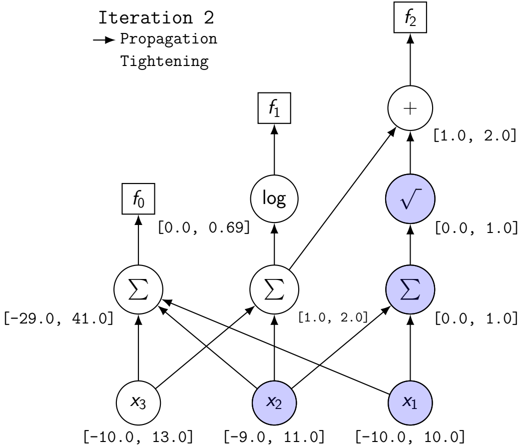


Outlook

Major accomplishments enabled generic solver software • New challenge: tighten more than variables

[29] Ryoo and Sahinidis [1996], Zamora and Grossmann [1999], Belotti et al. [2009], Belotti [2013], Gleixner et al. [2017], Puranik and Sahinidis [2017a,b]

Feasibility & optimality-based bounds tightening[29]



Outlook

Major accomplishments enabled generic solver software • New challenge: tighten more than variables

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Outline

Primal Heuristics: Overview

Ask the Jedi Masters . . .

- Fischetti and Lodi [2010]
- Berthold [2014] says to *fail fast*

Machine learning for heuristics [Bengio, Lodi, and Prouvost, 2018]

- **Offline learning** to decide a selection of heuristics [Khalil et al., 2017]
- **Online learning** to chose a heuristic [Hendel, 2018] or guide local search [Shylo and Shams, 2018]
- **Specific problem classes** [Bello et al., 2016, Hottung et al., 2020, Hu et al., 2018, Fischetti and Fraccaro, 2019, Kool et al., 2019]

Outline

RLT & SDP relaxations

Anstreicher [2009]

$$\begin{aligned} \min_x \quad & x^T Q x + c^T x \\ & Ax \le b, \\ \\ & x \in [0,1]^N \end{aligned}$$

- $X_{ij} = X_{ji}$,
- $Q \bullet X$ is the matrix inner product $Q \bullet X = \sum_{i,j=1}^{N} Q_{ij} \cdot X_{ij}$,
- RLT $\equiv$ Reformulation linearisation technique.
- SDP $\equiv$ Semidefinite programming,

RLT & SDP relaxations

Anstreicher [2009]

$$\begin{aligned} \min_x \quad & Q \bullet X + c^T x \\ & Ax \leq b, \\ & X = xx^T \\ & x \in [0,1]^N \\ & X \in [0,1]^{N \times N} \end{aligned}$$

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& x \in [0,1]^N \\
& X \in [0,1]^{N\times N}
\end{aligned}
\quad \Rightarrow \quad
\begin{aligned}
\min_x \quad & Q \bullet X + c^T x \\
& Ax \le b, \\
& \mathbf{X_{ij} - x_i - x_j \ge -1} \\
& \mathbf{X_{ij} - x_i \le 0} && \textbf{RLT relaxation} \\
& \mathbf{X_{ij} - x_j \le 0} \\
& X \succeq xx^T && \text{SDP relaxation} \\
& x \in [0,1]^N \\
& X \in [0,1]^{N\times N}
\end{aligned}
$$

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RLT & SDP relaxations

Anstreicher [2009]

$$
\begin{array}{llcll}
\min\limits_x & Q \bullet X + c^T x & \Rightarrow & \min\limits_x & Q \bullet X + c^T x \\
& Ax \leq b, & & & Ax \leq b, \\
& X = xx^T & & & \mathbf{X_{ij} - x_i - x_j \geq -1} \\
& x \in [0,1]^N & & & \mathbf{X_{ij} - x_i \leq 0} \quad \textbf{RLT relaxation} \\
& X \in [0,1]^{N \times N} & & & \mathbf{X_{ij} - x_j \leq 0} \\
& & & & \mathbf{X \succeq xx^T} \quad \textbf{SDP relaxation} \\
& & & & x \in [0,1]^N \\
& & & & X \in [0,1]^{N \times N}
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RLT & SDP to RLT & PSD

Sherali and Fraticelli [2002], Qualizza et al. [2012]

$$\begin{aligned}
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RLT & SDP to RLT & PSD

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- RLT $\equiv$ Reformulation linearization technique.
- SDP $\equiv$ Semidefinite programming,

Cutting plane method for RLT & PSD

Sherali and Fraticelli [2002], Qualizza et al. [2012]

$$\min_x \quad Q \bullet X + c^T x$$
$$Ax \leq b,$$
$$\mathbf{X_{ij} - x_i - x_j \geq -1}$$
$$\mathbf{X_{ij} - x_i \leq 0}$$
$$\mathbf{X_{ij} - x_j \leq 0}$$
$$\mathbf{v} \begin{bmatrix} 1 & x^T \\ x & X \end{bmatrix} \mathbf{v^T} \geq \mathbf{0} \quad \forall \mathbf{v} \in \mathbb{R}^{\mathbf{N+1}}$$
$$x \in [0,1]^N$$
$$X \in [0,1]^{N \times N}$$

- **Solve RLT only**, get $\tilde{X}, \tilde{x}$
- Add other polyhedral cuts, e.g. **triangle inequalities, edge-concave cuts,** $\{0, 1/2\}$**-cuts**
- Eigendecomposition on $\begin{bmatrix} 1 & \tilde{x}^T \\ \tilde{x} & \tilde{X} \end{bmatrix}$ yields t negative eigenvalues.
  - If $t = 0$, terminate.
  - If $t \geq 1$, add cuts $\mathbf{v_k} \begin{bmatrix} 1 & x^T \\ x & X \end{bmatrix} \mathbf{v_k^T} \geq \mathbf{0} \ \forall \mathbf{k} = \mathbf{1}, \ldots, \mathbf{t}$

Other cuts to integrate ...

Frangioni and Gentile [2006], Bao et al. [2009], Misener et al. [2015], Bonami et al. [2016], Baltean-Lugojan and Misener [2018], Del Pia et al. [2018]

Outline

Challenges [with some ideas] . . .

- **Data structures**
  - Move beyond boxes [Kvasnica et al., 2004] • Trade-off between recognition & disciplined programming? [Ceccon et al., 2020]
- **Convex relaxations**
  - Move beyond boxes [Slide 34] • How many auxiliary variables to introduce? • Manage symmetry [Müller et al., 2020]
- **Branching**
  - Get disjunctions [Dey et al., 2019] • Managing integers • Branch on constraints • Learning [Lodi and Zarpellon, 2017, Dilkina et al., 2017]
- **Bounds tightening**
  - Incorporate multiple constraints [Belotti, 2013] • Tighter integration with convex relaxations or branching?
- **Integrating machine learning** [Bengio, Lodi, and Prouvost, 2018]

Challenges [with some ideas] . . .

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My questions . . .

What is missing on this list? • Anything here already easy to manage?

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