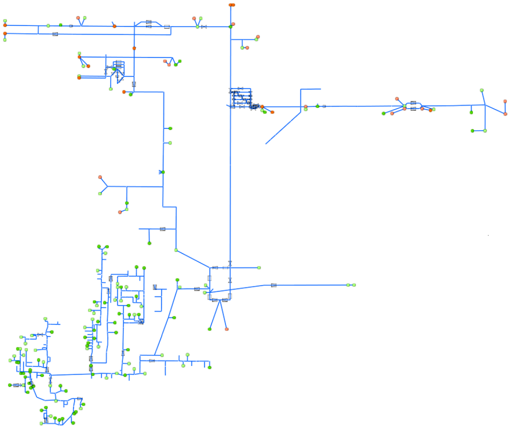
Gas Network Topology Optimization

Energy Networks Group

Zuse Institute Berlin



Given: Gas network $G = (V, A)$

- ▷ nodes
  - ▶ sources
  - ▶ sinks

    $\rightarrow$ specified gas flow
  - ▶ innodes
- ▷ pipes

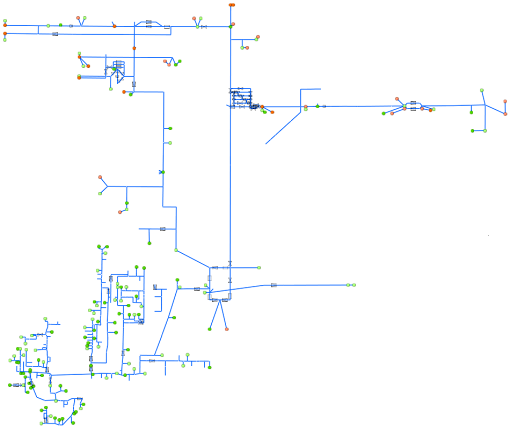
  resistors

  $\rightarrow$ nonlinear
- ▷ valves

  control valves

  compressor stations

  $\rightarrow$ binary variables
- ▷ MINLP-model



Given:

▷ Infeasible scenario

Goal:

▷ Feasibility due to cost optimal loop extensions

▷ loops = building new pipes in parallel to existing ones

Loop impact:

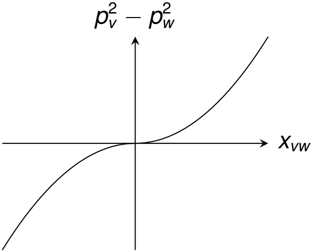
▷ Reduce pressure loss / more flow along a pipe

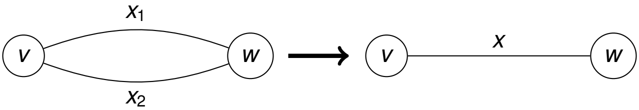
Weymouth equation $$p_v^2 - p_w^2 = \underbrace{\frac{L_{vw} C_{vw}}{D_{vw}^5}}_{\alpha_{vw}} x_{vw}|x_{vw}|$$

p_v, p_w inlet & outlet pressure

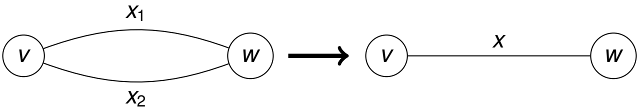
$\alpha_{vw} > 0$ weymouth constant

x_{vw} flow





$$p_v^2 - p_w^2 = \alpha x_1 |x_1|$$
$$p_v^2 - p_w^2 = \beta x_2 |x_2|$$



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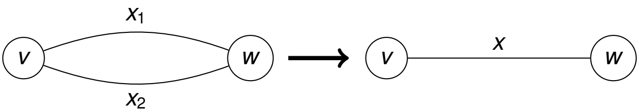
Transformation to an equivalent single equation for the aggregated flow $x = x_1 + x_2$:

$$p_v^2 - p_w^2 = \gamma x |x|$$



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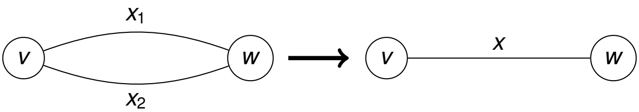
Since $\alpha, \beta > 0$, we know that $\text{sign}(x_1) = \text{sign}(x_2) = \text{sign}(x)$,

$$\alpha x_1^2 = \beta x_2^2 = \gamma x^2$$



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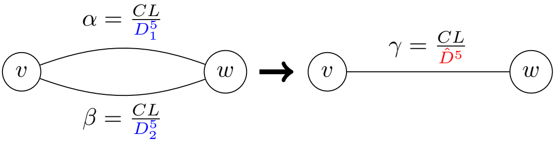
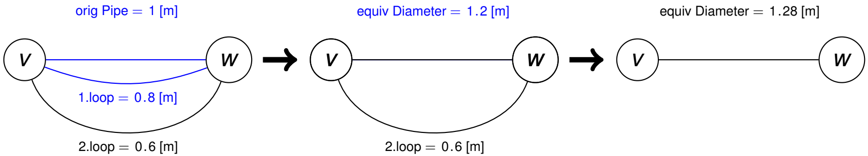
$$\alpha x_1^2 = \beta x_2^2 = \gamma x^2$$

$$\Rightarrow \quad \boxed{\gamma = \frac{\beta\alpha}{\left(\sqrt{\beta} + \sqrt{\alpha}\right)^2}}$$

Calculate an equivalent diameter of two parallel pipes:



$$\gamma = \frac{\beta\alpha}{\left(\sqrt{\beta} + \sqrt{\alpha}\right)^2} \Rightarrow \boxed{\hat{D} = \left(D_1{}^{5/2} + D_2{}^{5/2}\right)^{2/5}}$$


orig Pipe = 1 [m]
v
w
1.loop = 0.8 [m]
2.loop = 0.6 [m]
equiv Diameter = 1.2 [m]
v
w
2.loop = 0.6 [m]
equiv Diameter = 1.28 [m]
v
w

Diameters

Given:

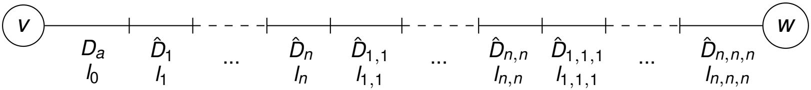
- ▷ Pipe with original diameter D_a
- ▷ Diameter candidates $\{D_1, \ldots, D_n\}$

Calculation of equivalent diameters:

$$\hat{D}_i := eq(D_a, D_i) = \boxed{\left(D_a^{5/2} + D_i^{5/2}\right)^{2/5}} \qquad i \in \{1, ..., n\}$$

$$\hat{D}_{i,j} := eq(\hat{D}_i, D_j) \qquad i, j \in \{1, ..., n\}$$

$$\hat{D}_{i,j,k} := eq(\hat{D}_{i,j}, D_k) \qquad i, j, k \in \{1, ..., n\}$$



Possible diameter allocation of a looped pipe.

$$l_i \in [0, 1]$$

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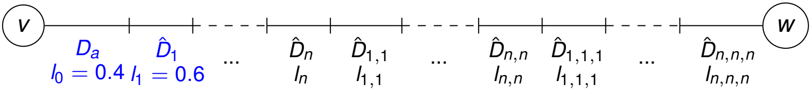


Possible diameter allocation of a looped pipe.

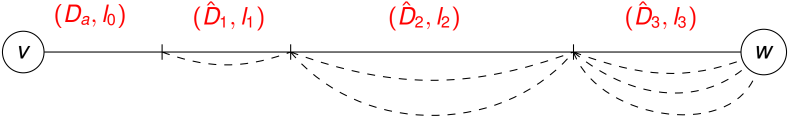
$$l_i \in [0, 1]$$

Given:

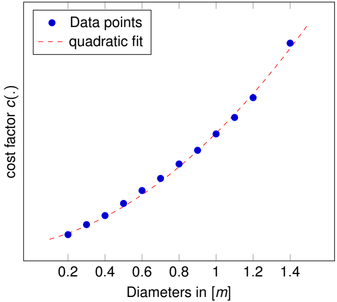
- Pipe with original diameter D_a
- Special case: Diameter candidates $\{D_a\}$

Calculation of equivalent diameters:

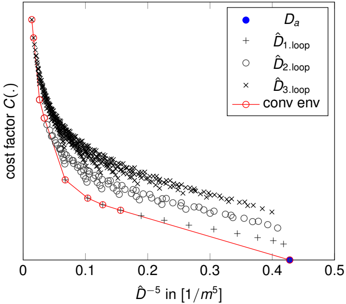
$\hat{D}_1 := eq(D_a, D_a)$	single loop
$\hat{D}_2 := eq(\hat{D}_1, D_a)$	double loops
$\hat{D}_3 := eq(\hat{D}_2, D_a)$	triple loops
$\hat{D}_k := eq(\hat{D}_{k-1}, D_a) = \boxed{(k+1)^{2/5}\, D_a}$	k loops



$l_i \in [0, 1]$



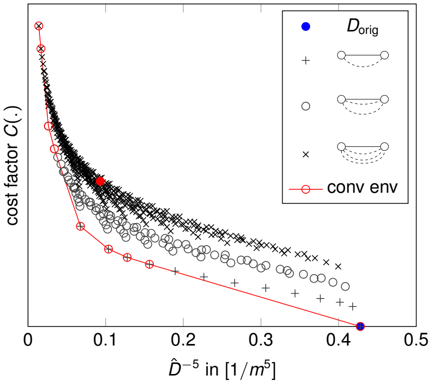
Diameter Candidates



“Lower Part“ of Convex Hull

Fujiwara, O. & Dey, D., "Two Adjacent Pipe Diameters at the Optimal Solution in the Water Distribution Network Models", *Water Resources Research*, Vol. 23, Nr.8, p. 1457-1460, 1987.

Original pipe diameter $D_a = 1.185$ [m]



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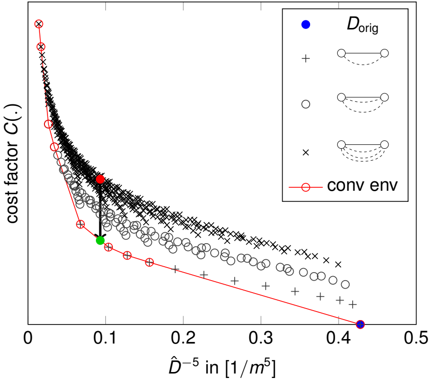
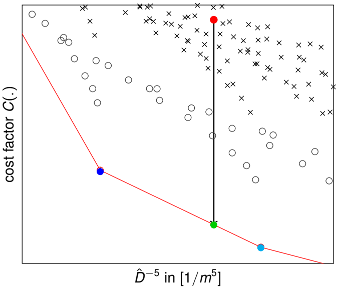
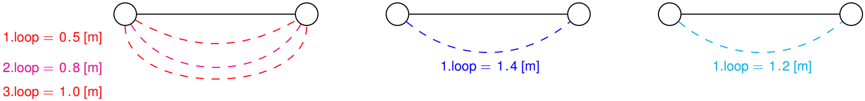




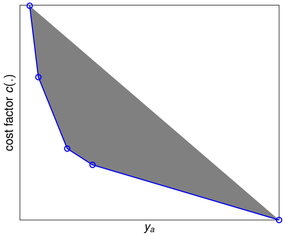


$$\Rightarrow \quad 3592\ [€/m] \quad > \quad \underbrace{0.3 \cdot 2485\ [€/m] + 0.7 \cdot 1919\ [€/m]}_{=2083\ [€/m]}$$

$$\min_{l,x,y,\Delta} \sum_{i=1}^{k} l_{a,i} \underbrace{L_a c\left(\hat{D}_{a,i}\right)}_{\text{const}}$$

$$\text{s.t. } y_a = L_a C \left(\frac{l_0}{D_a^5} + \sum_{i=1}^{k} \frac{l_{a,i}}{\hat{D}_{a,i}^5} \right)$$

$$\Delta_a = y_a \, x_a |x_a| \text{ and } \sum_{i=0}^{k} l_{a,i} = 1, \;\; l_{a,i} \in [0, 1]$$



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$$\min_{c,x,y,\Delta} c_a L_a$$

$$\text{s.t. } c_a \geq s_i y_a + t_i \quad \forall i$$

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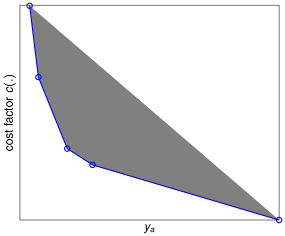

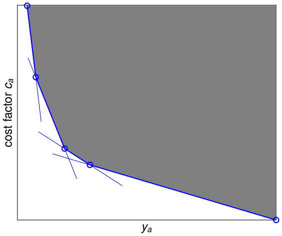

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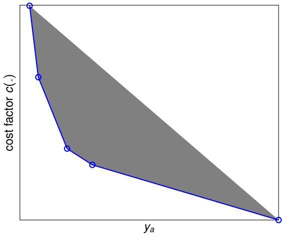

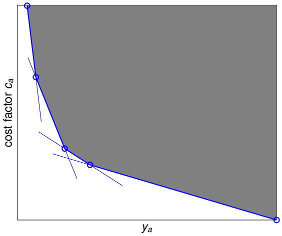

Observation: ▷ same LP-relaxation

▷ same variables as branching candidates

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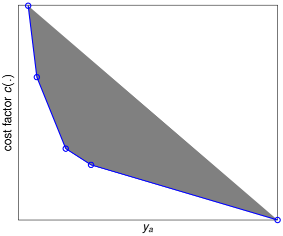

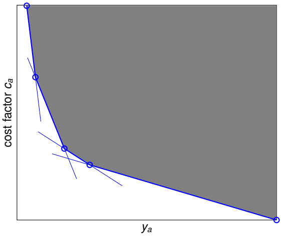

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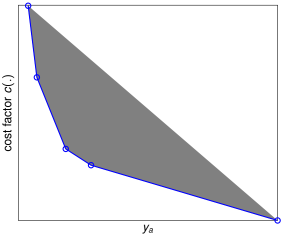
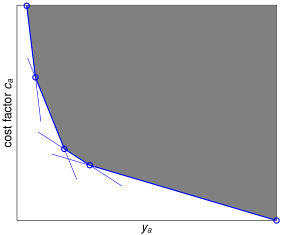
$$f(y_a, x_a) = y_a\, x_a\, |x_a|$$





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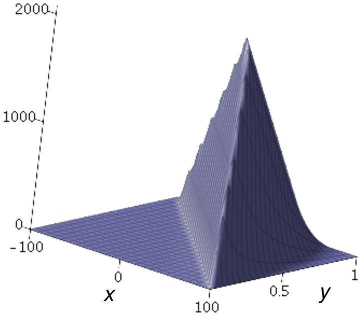
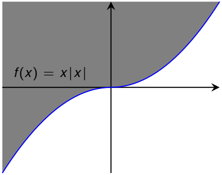


Difference between the convex envelope and the convex underestimator generated by SCIP for $f(x, y) = y\,x\,|x|$

Let $f\colon D \to \mathbb{R}$ with $D \subseteq \mathbb{R}^n$ convex and compact. The epigraph of f is defined by the set

$$\mathrm{epi}_D f = \{(x,\mu) |\ x \in D, \mu \in \mathbb{R}, \mu \geqslant f(x)\}.$$



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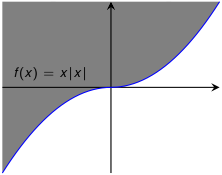
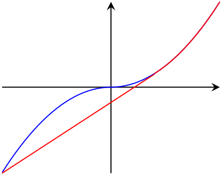


The convex envelope of a nonconvex function $f\colon D \to \mathbb{R}$ over $D \subseteq \mathbb{R}^n$ is given by the tightest convex underestimator of f:

$$\text{conv}_D[f](x) = \sup\{\ \eta(x) \mid \eta(y) \leqslant f(y)\ \ \forall y \in D, \eta\colon D \to \mathbb{R} \text{ convex}\}.$$



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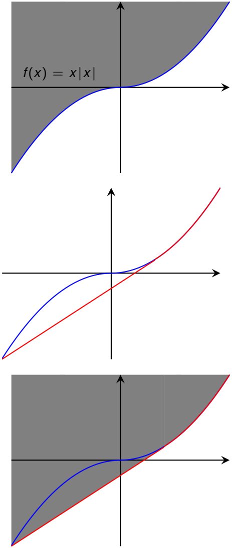

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$\rightsquigarrow$ leads to solving a nonlinear and nonconvex problem:

$$\begin{aligned} \text{conv}_D[f](x) = \min \mu \\ \text{s.t.} \quad \sum_k \lambda_k x_k = x \\ \sum_k \lambda_k f(x_k) = \mu \\ \sum_k \lambda_k = 1 \\ \lambda_k \geq 0 \text{ and } x_k \in D \ \forall k \end{aligned}$$

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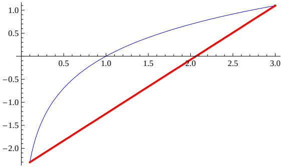
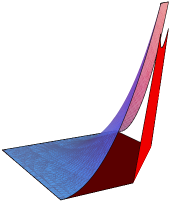
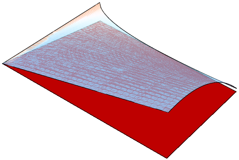
But convex envelopes are known for several cases, e.g.

concave functions | 1-convex $f(x,y) = x^2 \cdot y^2$ | $f(x,y) = -\sqrt{x} \cdot y^2$







Techniques to generate convex underestimators:

- Nonlinearities are given as factorable functions

Factorable functions

- Recursive sum of products of univariate functions
- Reduce to simple cases by introducing new variables and equations for subexpressions

Example

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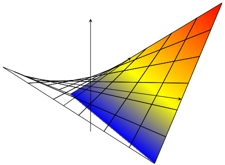
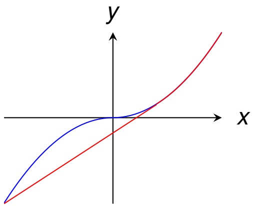
$y \cdot w$

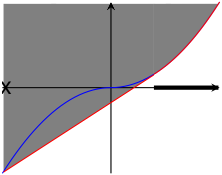


$x \cdot |x|$



The generating set of the convex envelope of f over a compact and convex set D is defined by

$$\mathcal{G}_D(f) := \{x \in D \mid (x, \text{conv}_D[f](x)) \text{ is an extreme point of conv}\,(\text{epi}_D f)\}.$$



$$f(x,y) = xy, \quad x \in [\underline{x}, \overline{x}], \quad y \in [\underline{y}, \overline{y}]$$

$$(\overline{x} - x)(\overline{y} - y) \geq 0$$
$$\Rightarrow xy \geq \overline{x}y + x\overline{y} - \overline{x}\,\overline{y}$$

$$(x - \underline{x})\left(y - \underline{y}\right) \geq 0$$
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Convex envelope of $f(x,y) = xy$:

$$\mathrm{conv}_D[f](x,y) =$$
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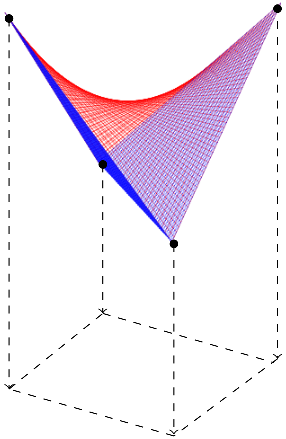

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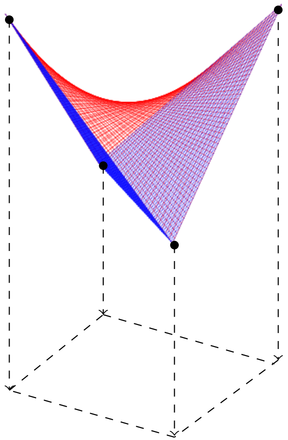

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Generating set: $\mathcal{G}_D(f) = ?$

Generating Set - Example McCormick

Convex envelope of $f(x, y) = xy$:

$\text{conv}_D[f](x, y) =$

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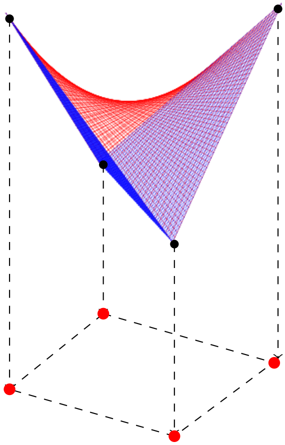

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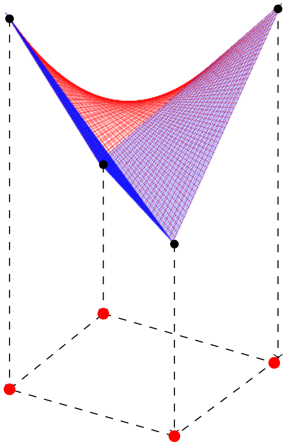
Theorem, ***Tawarmalani and Sahinidis, 2002***

Let $f\colon D \to \mathbb{R}$, with $D \subseteq \mathbb{R}^n$ compact and convex. If there exists a segment $l_x \subseteq D$ that contains x in its relative interior, i.e. $x \in \mathrm{ri}\,(l_x \cap D)$, and f is concave over $\mathrm{ri}\,(l_x \cap D)$, then $x \notin \mathcal{G}_D(f)$.



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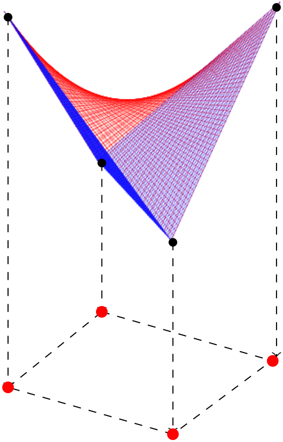

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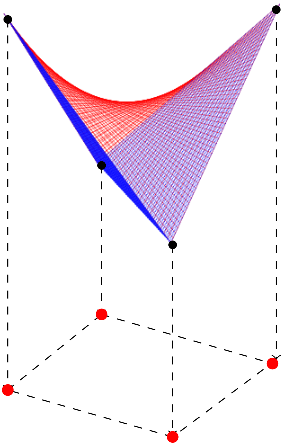
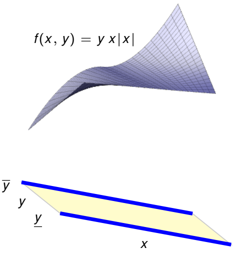


Convex envelope is <u>vertex polyhedral</u>, if

- its epigraph is polyhedral
- its vertices correspond to the vertices of the domain

$$f\colon (x, y) \mapsto y\,x|x|$$



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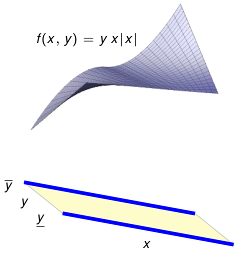

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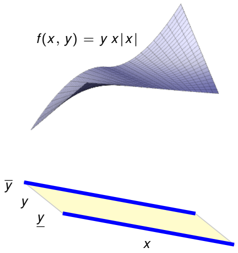

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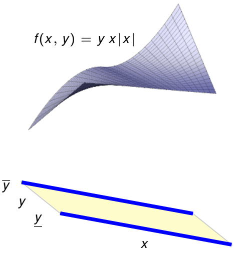
Let $f: D \to \mathbb{R}$, with $D \subseteq \mathbb{R}^n$ compact and convex. If there exists a segment $l_x \subseteq D$ that contains x in its relative interior, i.e. $x \in \text{ri}\,(l_x \cap D)$, and f is concave over $\text{ri}\,(l_x \cap D)$, then $x \notin \mathcal{G}_D(f)$.

Observation:
Generating set $\mathcal{G}_D(f)$ is subset of y boundary

Theorem

Let $f\colon D \subset \mathbb{R}^n \to \mathbb{R}$ and A be a subset of D.
Then $\operatorname{conv}(\operatorname{epi}_D f) = \operatorname{conv}(\operatorname{epi}_A f)$ if and only if $\mathcal{G}_D(f) \subseteq A$.



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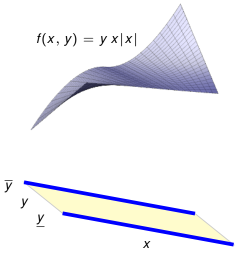
$$\operatorname{conv}(\operatorname{epi}_D f) = \operatorname{conv}(\operatorname{epi}_{D_{\underline{y}} \cup D_{\overline{y}}} f)$$



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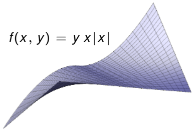

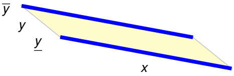

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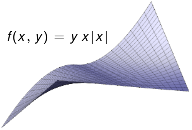

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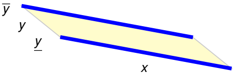

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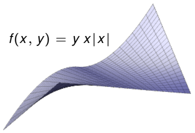

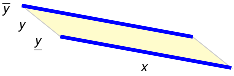

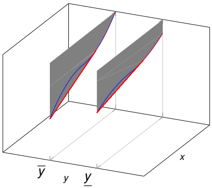

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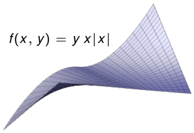
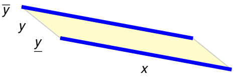
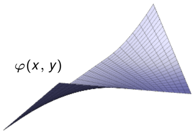




$$
\mathrm{conv}(\mathrm{epi}_D f) = \mathrm{conv}(\mathrm{epi}_{D_{\underline{y}}} \varphi \cup \mathrm{epi}_{D_{\overline{y}}} \varphi)
$$

$$
\varphi(x, y) = \begin{cases} yx^2 & x \geq \beta \underline{x} \\ 2\beta \underline{x} x y - (\beta \underline{x})^2 y & x < \beta \underline{x}, \end{cases}
$$



Remember: $\text{conv}_D[f](x, y) = \min\{\mu |\ (x, y, \mu) \in \text{conv}(\text{epi}_D f)\}$

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$$(x,y,\mu) \in \text{conv}(\text{epi}_{D_{\underline{y}}}\varphi \cup \text{epi}_{D_{\overline{y}}}\varphi) \Leftrightarrow$$

$$(x,y,\mu) = (1-\lambda)(x_1,\underline{y},\mu_1) + \lambda(x_2,\overline{y},\mu_2)$$

$$\lambda \in [0,1], x_1, x_2 \in [\underline{x},\overline{x}], \mu_1 \geq \varphi(x_1,\underline{y}), \mu_2 \geq \varphi(x_2,\overline{y})$$

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$$\begin{aligned}
\min_{x_1,x_2}\ & (1-\lambda)\varphi(x_1,\underline{y}) + \lambda\varphi(x_2,\overline{y}) \\
\text{s.t. } & (1-\lambda)x_1 + \lambda x_2 = x \\
& (1-\lambda)\underline{y} + \lambda\overline{y} = y \\
& \lambda \in [0,1] \\
& (x_1,x_2) \in [\underline{x},\overline{x}]^2
\end{aligned}$$

$$\min_{x_1, x_2} (1-\lambda)\varphi(x_1, \underline{y}) + \lambda\varphi(x_2, \overline{y})$$
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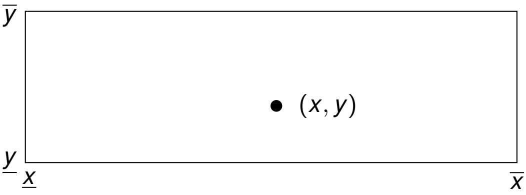

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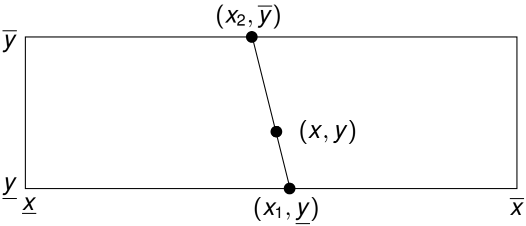

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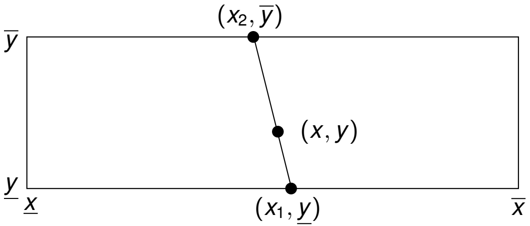

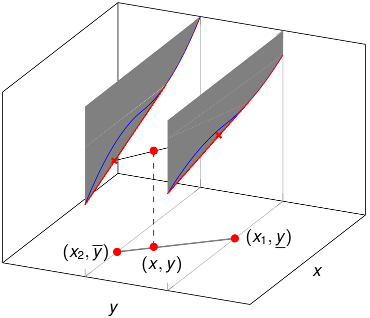

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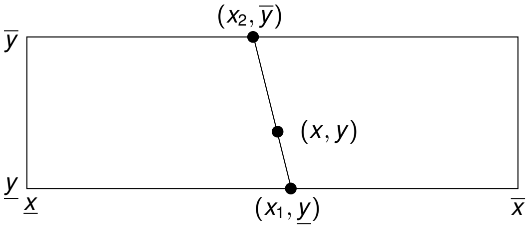

Using $x_2 = t_{x,y}(x_1)$, we can rewrite it to a 1-dim the optimization problem:

$$\min_{x_1} (1-\lambda_y)\varphi(x_1, \underline{y}) + \lambda_y\varphi(t_{x,y}(x_1), \overline{y})$$
$$\text{s.t. } \underline{x} \le x_1 \le \overline{x}$$
$$\underline{x} \le t_{x,y}(x_1) \le \overline{x}$$

Optimization Problem is of the form:

$$\begin{aligned} &\min \; F(x_1) \\ &\text{s.t. } a \leq x_1 \leq b \end{aligned} \tag{1}$$

with

$$F(x_1) = (1 - \lambda_y)\varphi(x_1, \underline{y}) + \lambda_y \varphi(t_{x,y}(x_1), \overline{y})$$

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Remark:

$F(x_1)$ is convex $\Rightarrow$ the solution of Problem 1 is $F(\text{mid}(a, b, x^*))$

Note: ▷ $\text{mid}(x_1, x_2, x_3)$ selects the middle value of three given scalars

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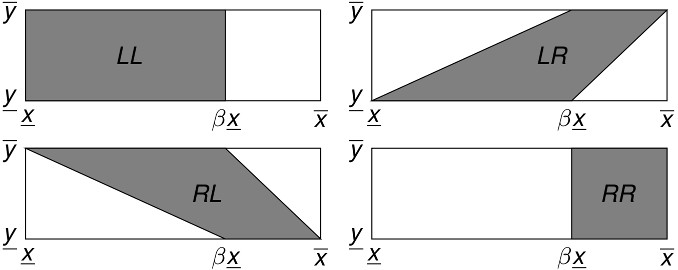
$F(x_1)$ is coercive, i. e., $\lim_{x_1 \to \infty} F(x_1) = \infty$ and $\lim_{x_1 \to -\infty} F(x_1) = \infty$
$\Rightarrow$ $F(x_1)$ has a global minimum

▷ It can be shown that the global minimum of $F(x_1)$ is unique

Solution

To compute the minimum, we solve equation $F^{'}(x_1) = 0$.



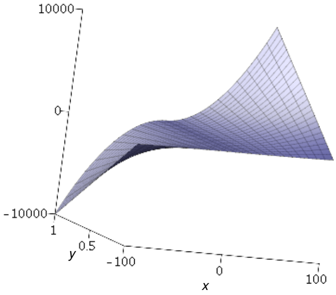
sol: x^*_{RL} if $t_{x,y}(x^*_{LR}) \leq \beta\underline{x}$

sol: x^*_{RR} if $t_{x,y}(x^*_{RR}) \geq \beta\underline{x}$

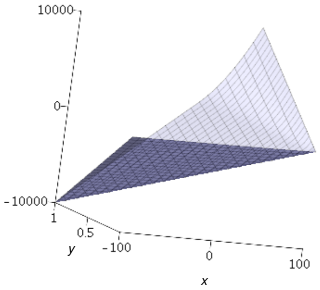
$$\text{conv}_D[f](x,y) = \begin{cases} F(\text{mid}(a,b,x^*_{RL})) & \text{if } t_{x,y}(x^*_{RL}) \leq \beta\underline{x} \\ F(\text{mid}(a,b,x^*_{RR})) & \text{otherwise} \end{cases}$$

Solution:

$$\text{conv}_D[f](x,y) = F(\min\{b, \max\{x^*_{RL}, x^*_{RR}\}\})$$



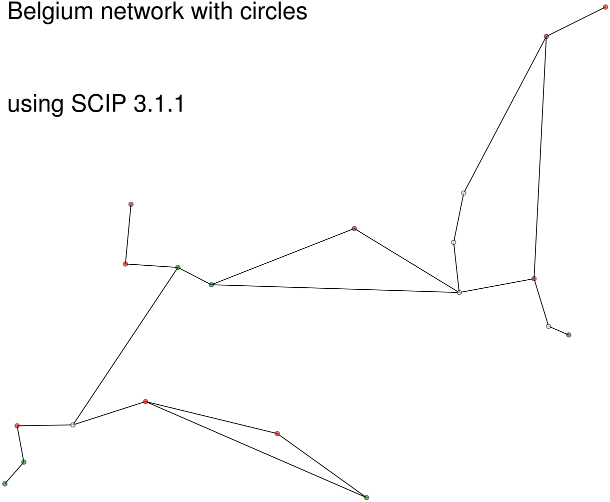
(a) $f(x, y) = y\, x\, |x|$

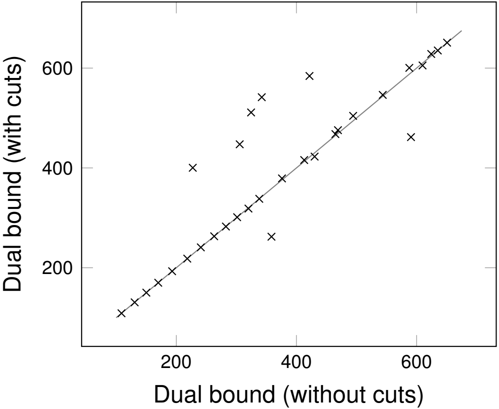


(b) $\text{conv}_D[f](x, y)$

Belgium network with circles

using SCIP 3.1.1





1h runtime
average dual bound improvement with cuts: 11%

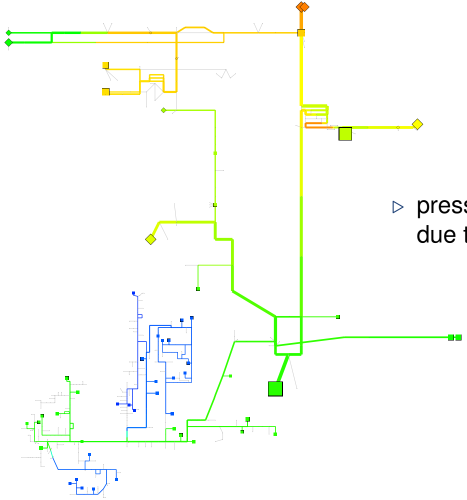
- We presented two equivalent models for optimal gas network expansion planning with continuous loop lengths, where
  - parallel pipes are represented by one “symbolic” pipe using equivalent diameters,
  - equivalent diameters correspond to extreme points of the “lower” part of the convex hull

- We showed basic ideas that might help to find the convex envelope of a nonconvex function,
  - such as using the generating set to simplify the resulting optimization model
- As an example, we calculated the convex envelope of the nonconvex function $f(x, y) = y\,x\,|x|$ that arises in the presented network expansion models

Thank you!

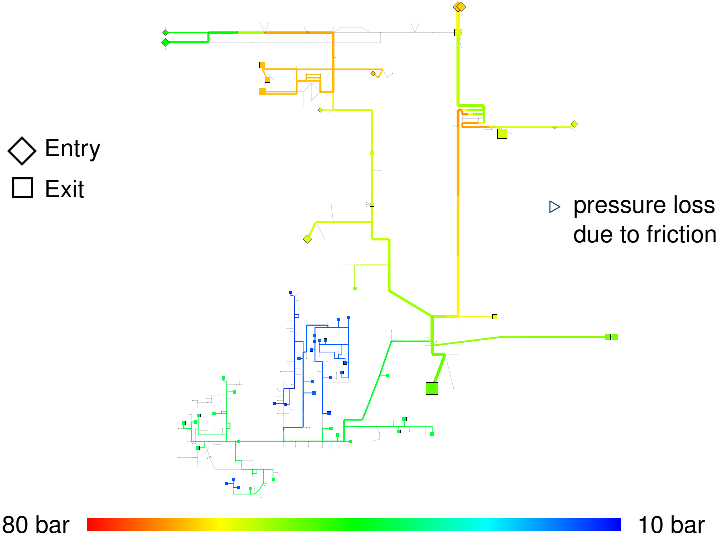
Ralf Lenz <lenz@zib.de>

◇ Entry
□ Exit

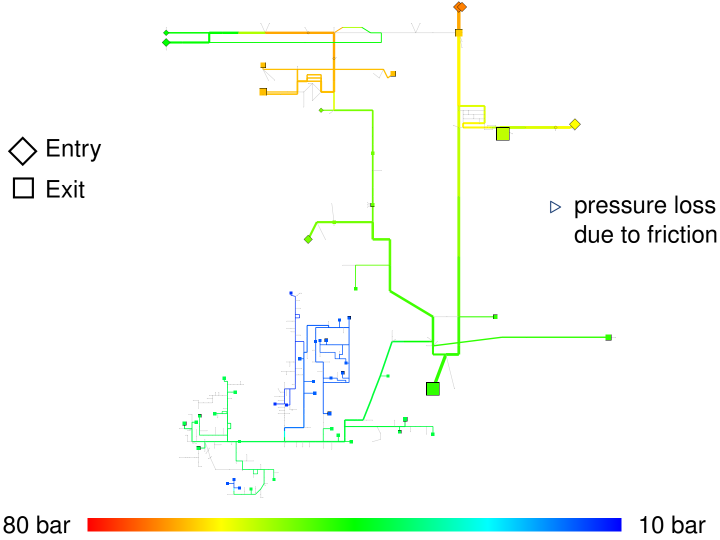


▷ pressure loss due to friction

80 bar — 10 bar



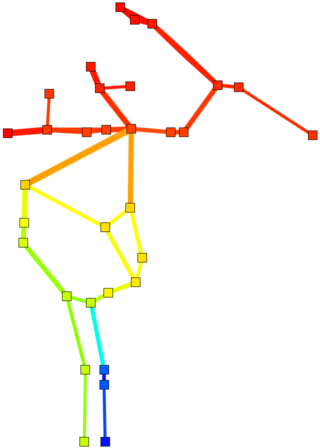
▷ pressure loss due to friction

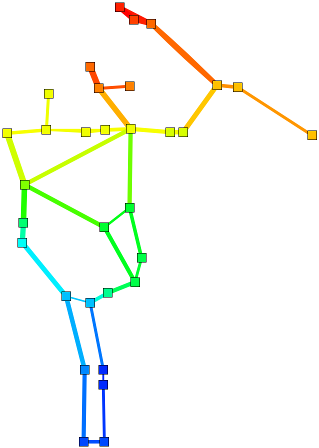


- pressure loss due to friction

▷ pressure loss due to friction

- The pressure distribution changes when adding network elements:


original network


extended network

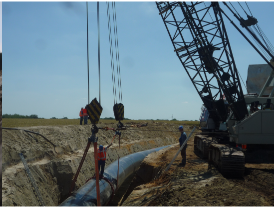



Pipeline – Compressor – Control Valve – Valve

Building Cost

- € 0.5 - 2.5 million per km pipeline
- € 2.6 - 8.9 million per new control valve
- € 17 - 41 million per additional compressor
- € 35 - 78 million per new compressor station





Topology Optimization Problem

Given:
- ▷ a detailed description of a gas network
- ▷ a nomination specifying amounts of gas flow at entries and exits
- ▷ a list of candidates of network extension

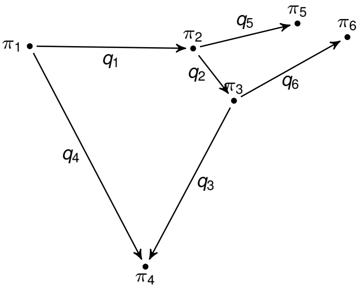
Task: Find
- ▷ cost-optimal selection of network extensions
- & settings for active devices (valves, control valves, compressors)
- & values for physical parameters of the network that comply with
  - gas physics
  - legal and technical limitations

- A gas transportation network is modeled by a directed graph

$$G = (V, A).$$

- Arc types:
  - passive: pipelines
  - active: compressors, control valves, valves

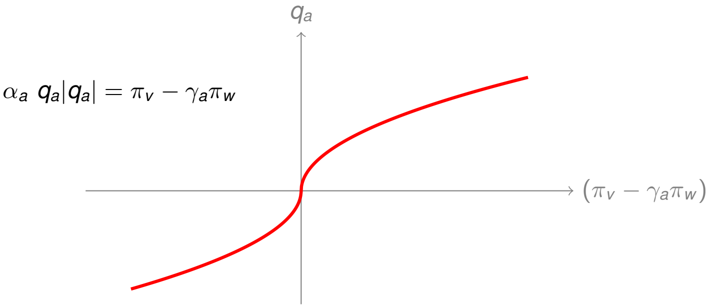
- Variables:



q_a flow for each arc $a \in A$

π_v, p_v (squared) pressure for each node $v \in V$

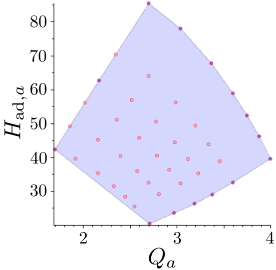
▷ The flow q_a of pipe $a \in A$ is restricted by the non-convex equation:



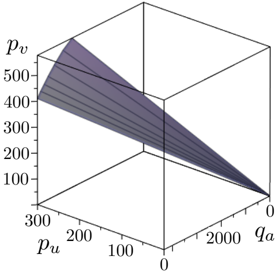
▷ **pressure loss due to friction**

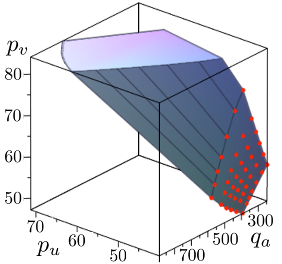
▷ $\alpha_a \sim \frac{L}{D^5}$ is a constant for pipe a, depending on its length L, diameter D, height and physical gas constants.

- A compressor $a = (v, w) \in A$ is described by three **operation modes**:
  - *Closed*: arc a is deleted ($q_a = 0$)
  - *Bypass*: arc a is contracted, endnodes v and w are identified ($p_v = p_w$)
  - *Active*: flow and pressures are restricted by linear inequalities ($A_a \, (q_a, p_v, p_w)^T \leq b_a$)



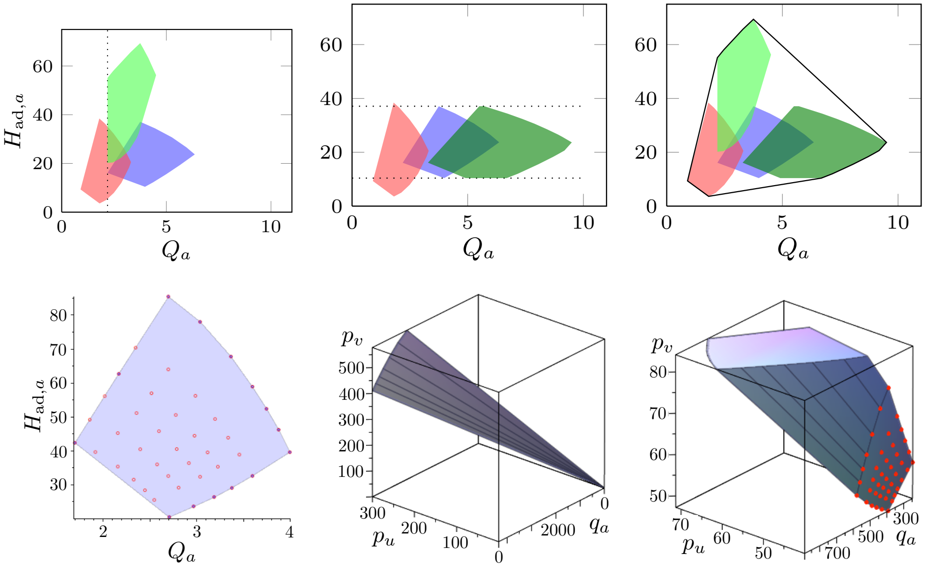
$H_{ad,a} \sim p_w / p_v$, $Q_a \sim q_a / p_v$





polytope

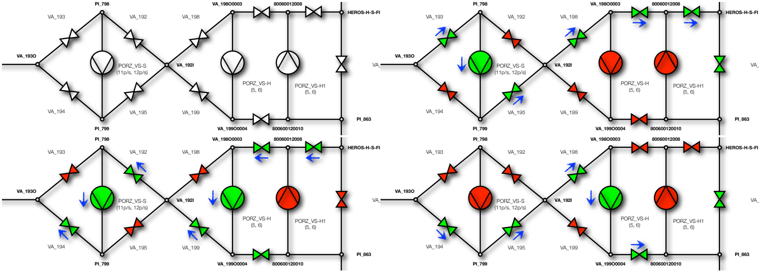
- A control valve is modeled similarly to a compressor.
- A valve can only be *closed* or in *bypass*.



$H_{ad,a} \sim p_w/p_v$, $Q_a \sim q_a/p_v$

polytope

▷ Due to **symmetry** and **technical limitations** only a subset of the potential configurations corresponds to real operation modes.



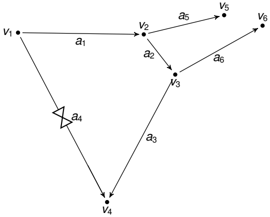
▷ An extended gas transportation network is modeled by a **directed multigraph**

$$G = (V, A_X).$$

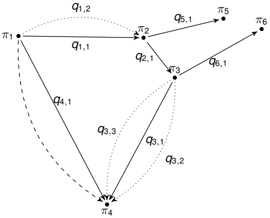
▷ The extended graph contains

- all original arcs,
- additional arcs for active elements,
- additional arcs for loops,
- additional arcs for extensions.

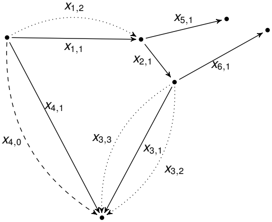
original network



extended network



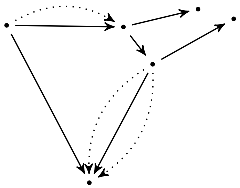
variables q, π



variables x

$$\min \sum_{(a,i)\in A_X} c_{a,i} x_{a,i}$$

$$
\begin{aligned}
\text{s.t.} \quad & x_{a,i} = 1 \Rightarrow \alpha_{a,i} q_{a,i} |q_{a,i}|^{k_a} - \beta_{a,i} y_{a,i} - (\pi_v - \gamma_a \pi_w) = 0 && \forall\, (a,i) = (v,w,i) \in A_X,\, i \neq 0, \\
& x_{a,i} = 1 \Rightarrow A_a \left(q_{a,i}, p_v, p_w\right)^T \leqslant 0 && \forall\, (a,i) = (v,w,i) \in A_X,\, i \geq 2, \\
& x_{a,i} = 0 \Rightarrow q_{a,i} = 0 && \forall\, (a,i) \in A_X,\, i \neq 0, \\
& \sum_{i:(a,i)\in A_X} x_{a,i} = 1 && \forall\, a \in A, \\
& \sum_{\substack{w,i:(v,w,i)\in A_X, \\ i\neq 0}} q_{v,w,i} - \sum_{\substack{w,i:(w,v,i)\in A_X, \\ i\neq 0}} q_{w,v,i} = d_v && \forall\, v \in V, \\
& p_v |p_v| - \pi_v = 0 && \forall\, v \in V, \\
& \underline{\pi}_v \leqslant \pi_v \leqslant \overline{\pi}_v && \forall\, v \in V, \\
& \underline{q}_{a,i} \leqslant q_{a,i} \leqslant \overline{q}_{a,i} && \forall\, (a,i) \in A_X, \\
& \underline{y}_{a,i} \leqslant y_{a,i} \leqslant \overline{y}_{a,i} && \forall\, (a,i) \in A_X, \\
& x_{a,i} \in \{0,1\} && \forall\, (a,i) \in A_X, \\
& x \in \mathcal{X}.
\end{aligned}
$$

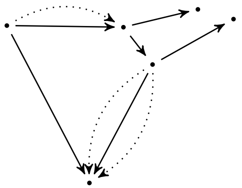


$k_a = 2$ for pipes; $k_a = 1$, $\alpha_a = 0$ for active arcs

$$\min \sum_{(a,i)\in A_X} c_{a,i} x_{a,i}$$

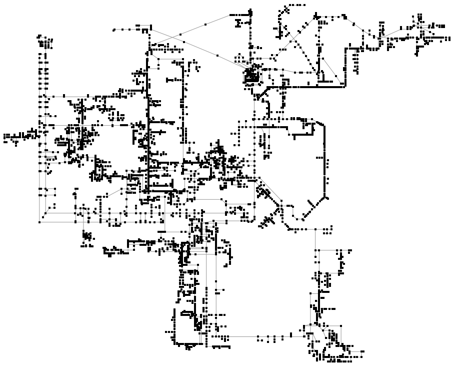
s.t.

	$x_{a,i} = 1 \Rightarrow \alpha_{a,i} q_{a,i} \lvert q_{a,i} \rvert^{k_a} - \beta_{a,i} y_{a,i} - (\pi_v - \gamma_a \pi_w) = 0$	(selected) pipelines
	$x_{a,i} = 1 \Rightarrow A_a \left(q_{a,i}, p_v, p_w\right)^T \leqslant 0$	(active) compressors / control valves
	$x_{a,i} = 0 \Rightarrow q_{a,i} = 0$	closed / non-selected elements
	$\sum_{i:(a,i)\in A_X} x_{a,i} = 1$	pipe / operation mode selection
	$\sum_{w,i:(v,w,i)\in A_X, i\neq 0} q_{v,w,i} - \sum_{w,i:(w,v,i)\in A_X, i\neq 0} q_{w,v,i} = d_v$	flow conservation
	$p_v \lvert p_v \rvert - \pi_v = 0$	(squared) pressure coupling
	$\underline{\pi}_v \leqslant \pi_v \leqslant \overline{\pi}_v$	bounds
	$\underline{q}_{a,i} \leqslant q_{a,i} \leqslant \overline{q}_{a,i}$	bounds
	$\underline{y}_{a,i} \leqslant y_{a,i} \leqslant \overline{y}_{a,i}$	bounds
	$x_{a,i} \in \{0, 1\}$	binary variables
	$x \in \mathcal{X}.$	subnetwork operation modes

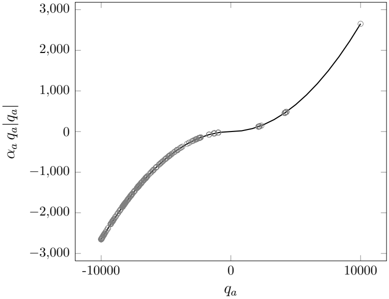


$k_a = 2$ for pipes; $k_a = 1$, $\alpha_a = 0$ for active arcs

- Large-scale network provided by Open Grid Europe GmbH
- Size:
  - 4165 nodes
  - 3983 pipes
  - 308 valves
  - 12 compressors
  - 121 control valves
- nominations: 30
- feasibility problem
- timelimit: 4h
- Computational results:



Baron			Antigone			SCIP		
feas	infeas	time limit	feas	infeas	time limit	feas	infeas	time limit
-	3	27	-	28	2	1	-	29



positions with cutting planes during branch and bound

- Consider the **domain relaxation** of the ATP:

$$\min_{\Delta_v \geqslant 0, v \in V} \sum_{v \in V} \Delta_v + \sum_{a \in A'} (\Delta_a + \|\tilde{\Delta}_a\|) \quad \text{s. t.}$$

$$
\begin{aligned}
\text{s. t.} \qquad & \alpha_a q_a |q_a|^{k_a} - \beta_a y_a - (\pi_v - \gamma_a \pi_w) = 0 && \forall\, a = (v, w) \in A', \\
& A_a (q_a, p_v, p_w)^T - \tilde{\Delta}_a \leq b_a && \forall\, a = (v, w) \in A', \\
& \sum_{w:(v,w) \in A'} q_{v,w} - \sum_{w:(w,v) \in A'} q_{w,v} = d_v && \forall\, v \in V, \\
& p_v |p_v| - \pi_v = 0 && \forall\, v \in V, \\
& \underline{y}_a \leq y_a \leq \overline{y}_a && \forall\, a \in A', \\
& q_a - \Delta_a \leqslant \overline{q}_a && \forall\, a \in A', \\
& q_a + \Delta_a \geqslant \underline{q}_a && \forall\, a \in A', \\
& \pi_v - \Delta_v \leqslant \overline{\pi}_v && \forall\, v \in V, \\
& \pi_v + \Delta_v \geqslant \underline{\pi}_v && \forall\, v \in V, \\
& \Delta \geq 0.
\end{aligned}
$$

- Consider the domain relaxation as a parametric NLP ($\tilde{p} = 0$)

$$\begin{aligned} & \min f(z) \\ \text{s.t.} \quad & g(z) - \tilde{p} \leqslant 0 \end{aligned}$$

  and a KKT point (z^*, λ^*) fulfilling

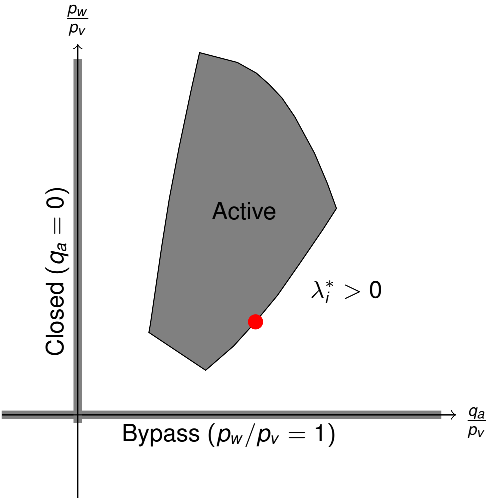
$$\begin{aligned} \nabla_z \mathcal{L}(z, \lambda) = 0, \\ \lambda \geqslant 0, \;\; g(z) - \tilde{p} \leqslant 0, \;\; \lambda\,(g(z) - \tilde{p}) = 0, \end{aligned}$$

  where $\mathcal{L}$ denotes the Lagrange function.

- When f, g are $\mathcal{C}^2$ it follows from Fiacco and Ishizuka (1990)

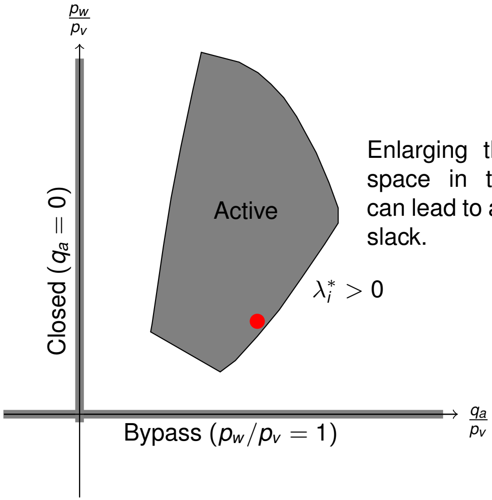
$$\frac{\partial f}{\partial \tilde{p}_i} = -\lambda_i^*.$$

- Consider a solution of the domain relaxation and focus on active arcs.



- Depending on the active constraints and slack values of this solution, change between the physical states *bypass*, *closed* or *active*.

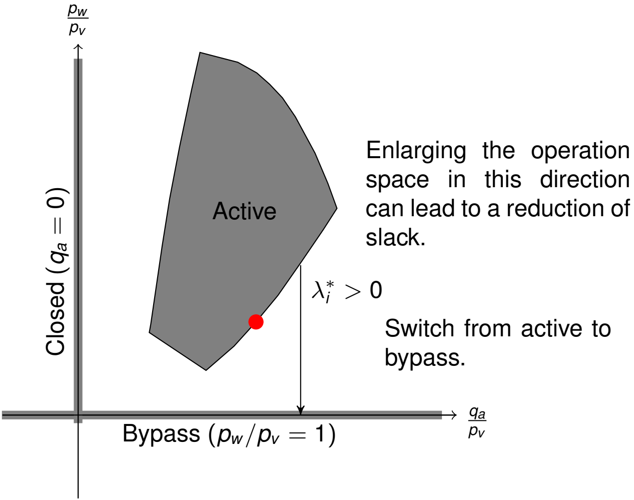
- Consider a solution of the domain relaxation and focus on active arcs.



Enlarging the operation space in this direction can lead to a reduction of slack.

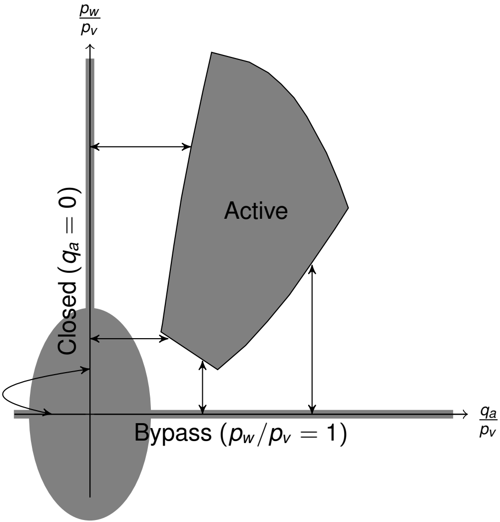
- Depending on the active constraints and slack values of this solution, change between the physical states *bypass*, *closed* or *active*.

- Consider a solution of the domain relaxation and focus on active arcs.



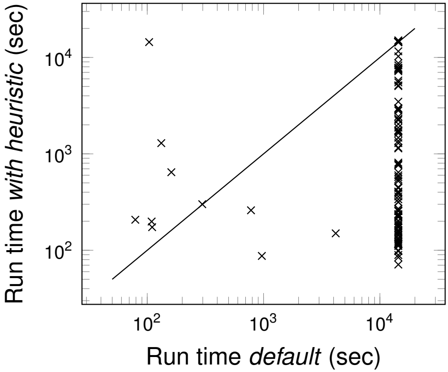
- Depending on the active constraints and slack values of this solution, change between the physical states *bypass*, *closed* or *active*.

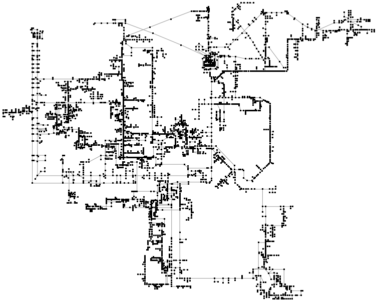
- Consider a solution of the domain relaxation and focus on active arcs.



- Depending on the active constraints and slack values of this solution, change between the physical states *bypass*, *closed* or *active*.

network	nominations	BARON	ANTIGONE	SCIP default	SCIP with heuristic
version 1	30	-	-	4	30
version 2	30	-	-	4	18
version 3	30	-	-	1	18
version 4	30	-	-	-	17
version 5	30	-	-	1	18





- Assume the network consists of **pipelines and valves only**.
- Fixing all discrete decisions yields the **passive transmission problem (PTP)**:

$$\exists\, q, \pi, p$$

$$\begin{aligned}
\text{s. t. } \alpha_a q_a |q_a|^{k_a} - \tilde{\beta}_a - (\pi_v - \gamma_a \pi_w) &= 0 && \forall\, a = (v, w) \in A', \\
\sum_{w:(v,w)\in A'} q_{v,w} - \sum_{w:(w,v)\in A'} q_{w,v} &= d_v && \forall\, v \in V, \\
p_v |p_v| - \pi_v &= 0 && \forall\, v \in V, \\
\pi_v &\leqslant \overline{\pi}_v && \forall\, v \in V, \\
\pi_v &\geqslant \underline{\pi}_v && \forall\, v \in V, \\
q_a &\leqslant \overline{q}_a && \forall\, a \in A', \\
q_a &\geqslant \underline{q}_a && \forall\, a \in A'.
\end{aligned}$$

It holds $\underline{y}_a = \overline{y}_a$ and $\tilde{\beta}_a := \beta_a \underline{y}_a$.

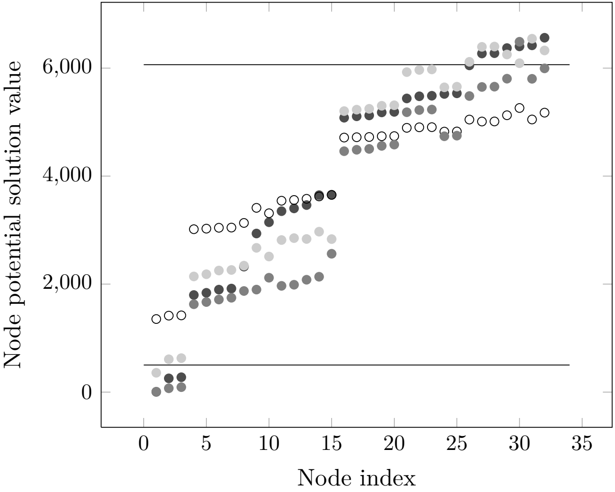
Theorem (H. and Fügenschuh 2013, Collins et al. 1978, Maugis 1977)

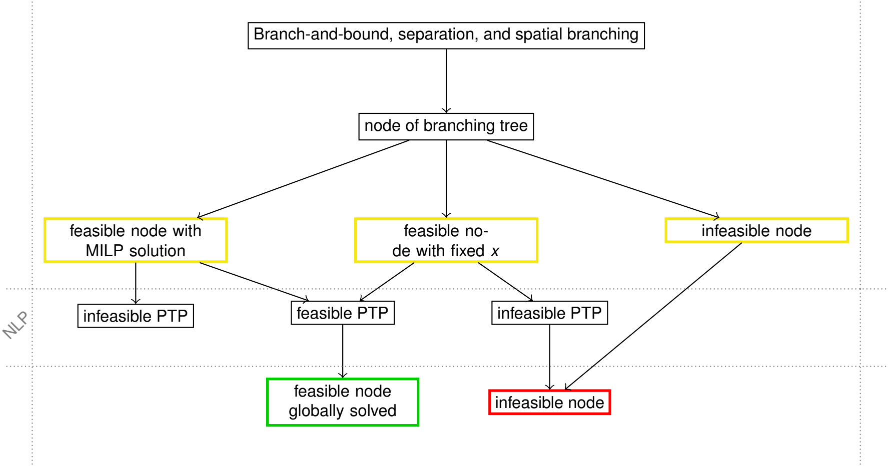
*The **domain relaxation of the PTP** is a **feasible** and **convex** continuous optimization problem:*

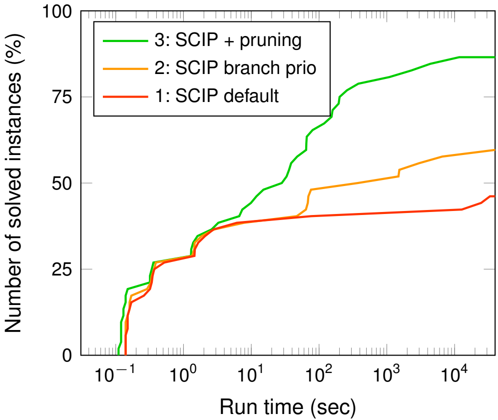
$$\min_{\Delta_v \geqslant 0, v \in V} \sum_{v \in V} \Delta_v$$

$$\begin{aligned}
s.t. \quad & \alpha_a q_a |q_a|^{k_a} - (\pi_v - \gamma_a \pi_w) = 0 && \forall\, a = (v,w) \in A', \\
& \sum_{w:(v,w)\in A'} q_{v,w} - \sum_{w:(w,v)\in A'} q_{w,v} = d_v && \forall\, v \in V, \\
& \pi_v - \Delta_v \leqslant \overline{\pi}_v && \forall\, v \in V, \\
& \pi_v + \Delta_v \geqslant \underline{\pi}_v && \forall\, v \in V, \\
& q_a - \Delta_a \leqslant \overline{q}_a && \forall\, a \in A', \\
& q_a + \Delta_a \geqslant \underline{q}_a && \forall\, a \in A', \\
& \Delta \geq 0.
\end{aligned}$$

- Squared pressure values for a test network with 2 valves, 4 discrete settings, no flow bounds:




Branch-and-bound, separation, and spatial branching
node of branching tree
feasible node with MILP solution
feasible no-de with fixed x
infeasible node
NLP
infeasible PTP
feasible PTP
infeasible PTP
feasible node globally solved
infeasible node



Strategies

1. SCIP default
2. SCIP default with branching priorities
3. SCIP with domain relaxation and node classification

- Strategies
  1. SCIP default
  2. SCIP default with branching priorities
  3. SCIP with domain relaxation and node classification

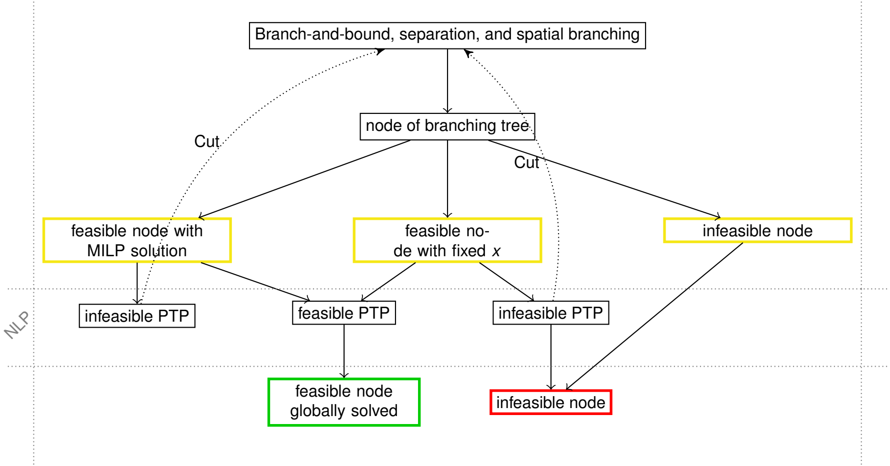
- Benchmark set: Networks containing only pipes and valves

- Solved instances

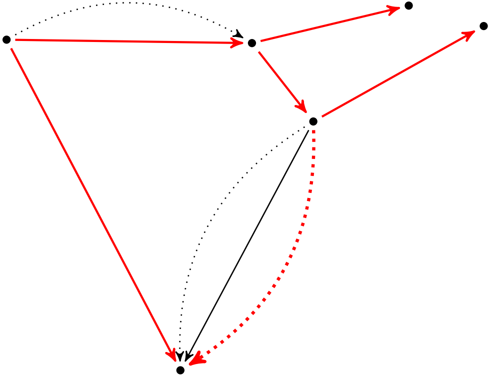
strategy	1	2	3	all
solved instances	24	30	45	52

- Means

	solved(30) time [s]	solved(30) nodes	incomp.(1) gap [%]
strategy 2	25.9	1,038	15
strategy 3	7.2	147	15
shifted geom. mean	−72 %	−86 %	0 %


Branch-and-bound, separation, and spatial branching
node of branching tree
Cut
Cut
feasible node with MILP solution
feasible no-de with fixed x
infeasible node
NLP
infeasible PTP
feasible PTP
infeasible PTP
feasible node globally solved
infeasible node

- Consider a network consisting of pipes only while different pipe diameters are available and no flow bounds on the arcs are imposed.



- Consider a network consisting of pipes only while different pipe diameters are available and no flow bounds on the arcs are imposed.
- For the **domain relaxation** of the PTP (without flow bounds and $\gamma_a = 1$)

$$\min_{\Delta_v \geqslant 0, v \in V} \sum_{v \in V} \Delta_v \quad \text{s. t.}$$

$$\begin{aligned}
&[\mu_a] && \overbrace{\alpha_a q_a |q_a|^{k_a} - \tilde{\beta}_a}^{\Phi_a(q_a)} - (\pi_v - \pi_w) = 0 && \forall\, a = (v, w) \in A', \\
&[\mu_v] && \sum_{w:(v,w)\in A'} q_{v,w} - \sum_{w:(w,v)\in A'} q_{w,v} = d_v && \forall\, v \in V, \\
&[\lambda_v^+] && \pi_v - \Delta_v \leqslant \overline{\pi}_v && \forall\, v \in V, \\
&[\lambda_v^-] && \pi_v + \Delta_v \geqslant \underline{\pi}_v && \forall\, v \in V,
\end{aligned}$$

- the Lagrange dual multipliers are denoted by (μ, λ).

▷ The dual variables of a KKT point $(q^*, \pi^*, \Delta^*, \mu^*, \lambda^*)$ fulfill

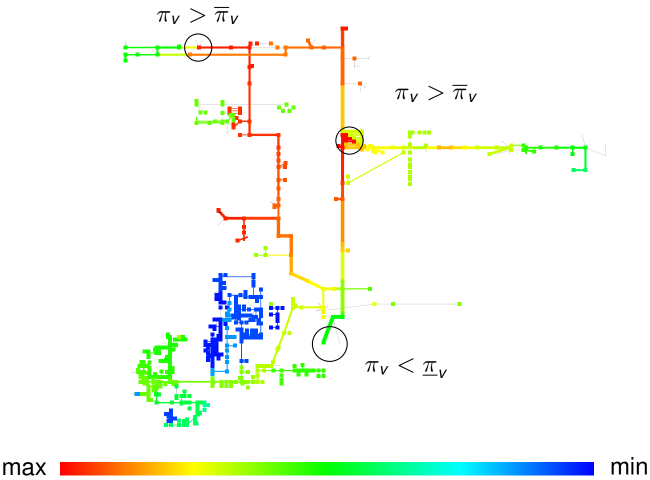
$$\mu_a \frac{d\Phi_a}{dq_a}(q_a) = \mu_v - \mu_w \qquad \forall\, a = (v, w) \in A',$$

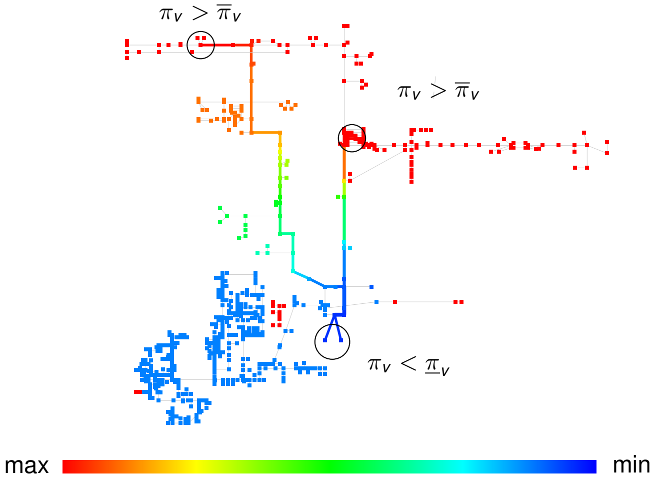
$$\sum_{w:(v,w)\in A'} \mu_{(v,w)} - \sum_{w:(w,v)\in A'} \mu_{(w,v)} = \lambda_v^+ - \lambda_v^- \qquad \forall\, v \in V,$$

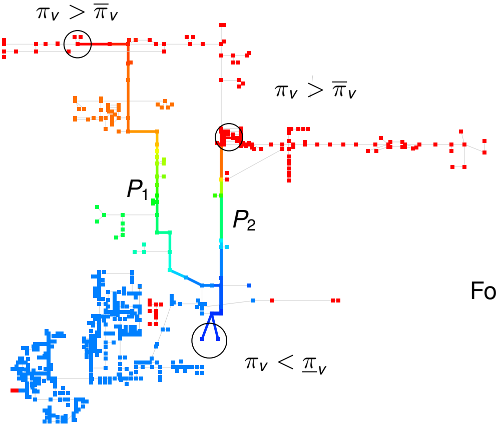
$$0 \le \lambda_v^+ \begin{cases} = 0 & \pi_v < \overline{\pi}_v \\ \le 1 & \pi_v = \overline{\pi}_v \\ = 1 & \pi_v > \overline{\pi}_v \end{cases} \qquad 0 \le \lambda_v^- \begin{cases} = 0 & \pi_v > \underline{\pi}_v \\ \le 1 & \pi_v = \underline{\pi}_v \\ = 1 & \pi_v < \underline{\pi}_v . \end{cases} \qquad \forall\, v \in V,$$

which are part of the KKT conditions.

▷ This is a system of the **same structure**.


$\pi_v > \overline{\pi}_v$
$\pi_v > \overline{\pi}_v$
$\pi_v < \underline{\pi}_v$
max
min


$\pi_v > \overline{\pi}_v$
$\pi_v > \overline{\pi}_v$
$\pi_v < \underline{\pi}_v$
max
min



For the s_1-t_1-path P_1 it holds

$$\sum_{a=(v,w)\in A'(P_1)} \overbrace{(\pi_v - \pi_w)}^{\Phi_a(q_a)} = \pi_{s_1} - \pi_{t_1}$$

$$\leq \overline{\pi}_{s_1} - \underline{\pi}_{t_1}$$

For the s_2-t_2-path P_2 it holds

$$\sum_{a=(v,w)\in A'(P_2)} \overbrace{(\pi_v - \pi_w)}^{\Phi_a(q_a)} = \pi_{s_2} - \pi_{t_2}$$

$$\leq \overline{\pi}_{s_2} - \underline{\pi}_{t_2}$$

Setting

$$\sum_{w:a=(v,w)\in A'} \mu_a^* - \sum_{w:a=(w,v)\in A'} \mu_a^* = \lambda_v^{+,*} - \lambda_v^{-,*} \qquad \forall\, v \in V,$$

for every node $v \in V$ every feasible solution (q, π) for the PTP has to fulfill the inequality

$$\sum_{a\in A'} \mu_a^* \overbrace{\Phi_a(q_a)}^{\pi_v - \pi_w} = \sum_{v\in V} \pi_v \left(\sum_{w:a=(v,w)\in A'} \mu_a^* - \sum_{w:a=(w,v)\in A'} \mu_a^* \right) = \sum_{v\in V} \pi_v \left(\lambda_v^{+,*} - \lambda_v^{-,*} \right)$$
$$\leqslant \sum_{v\in V} \lambda_v^{+,*} \overline{\pi}_v - \lambda_v^{-,*} \underline{\pi}_v.$$

This is a **nonlinear cut** in x, q:

$$\sum_{(a,i)\in A_X, i\neq 0} \mu_a^* x_{a,i} \Phi_{a,i}(q_{a,i}) \leqslant \sum_{v\in V} \lambda_v^{+,*} \overline{\pi}_v - \lambda_v^{-,*} \underline{\pi}_v.$$

▷ Another valid inequality for the PTP in q:

$$\sum_{(a,i)\in A_X, i\neq 0} (q_{a,i} - q_a^*)\, x_{a,i}\Phi_{a,i}(q_{a,i}) \;=\; 0.$$

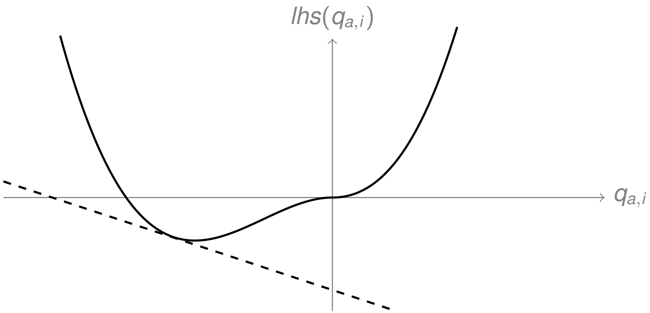
This equality is used as **regularization term**.

▷ A linear combination of both with $\zeta \in \mathbb{R}_{\geq 0}$:

$$\zeta \sum_{(a,i)\in A_X, i\neq 0} (q_{a,i} - q_a^*)\, x_{a,i}\Phi_{a,i}(q_{a,i}) + (1-\zeta) \sum_{(a,i)\in A', i\neq 0} \mu_a^*\, x_{a,i}\Phi_{a,i}(q_{a,i}) \leqslant (1-\zeta)\sum_{v\in V} (\lambda_v^{+*}\overline{\pi}_v - \lambda_v^{-*}\underline{\pi}_v).$$

Visualization of the left-hand side

$$q_{a,i} \mapsto ((1-\zeta)\mu_a^* + \zeta(q_{a,i} - q_a^*))\, x_{a,i}\Phi_{a,i}(q_{a,i}) =: lhs(q_{a,i}).$$



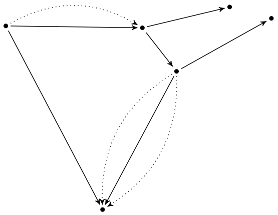
Use **linear underestimator** in $q_{a,i}$ of the form

$$q_{a,i} \mapsto \text{const}(x_{a,i}) + \left(\zeta(\pi_v^* - \pi_w^*) + (1-\zeta)(\mu_v^* - \mu_w^*)\right) q_{a,i}.$$

- Every primal solution (q, π) for the topology optimization problem has to fulfill the following inequality:

$$\zeta \sum_{(a,i)\in A', i\neq 0} (q_{a,i} - q_a^*) x_{a,i} \Phi_{a,i}(q_{a,i}) + (1-\zeta) \sum_{(a,i)\in A', i\neq 0} \mu_a^* x_{a,i} \Phi_{a,i}(q_{a,i})$$
$$\leqslant (1-\zeta) \sum_{v\in V} (\lambda_v^{+*} \overline{\pi}_v - \lambda_v^{-*} \underline{\pi}_v).$$

Here: $\zeta \in \mathbb{R}_+$, (q^*, π^*) primal solution to the domain relaxation of the PTP.



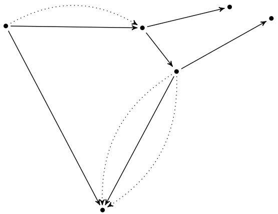
- Every primal solution (q, π) for the topology optimization problem has to fulfill the following inequality:

$$\text{const}(x) + \sum_{(a,i)=(v,w,i)\in A', i\neq 0} \left(\left(\zeta(\pi_v^* - \pi_w^*) + (1-\zeta)(\mu_v^* - \mu_w^*) \right) q_{a,i} \right)$$

$$\leq \zeta \sum_{(a,i)\in A', i\neq 0} (q_{a,i} - q_a^*) x_{a,i} \Phi_{a,i}(q_{a,i}) + (1-\zeta) \sum_{(a,i)\in A', i\neq 0} \mu_a^* x_{a,i} \Phi_{a,i}(q_{a,i})$$

$$\leqslant (1-\zeta) \sum_{v\in V} (\lambda_v^{+*} \overline{\pi}_v - \lambda_v^{-*} \underline{\pi}_v).$$

Here: $\zeta \in \mathbb{R}_+$, (q^*, π^*) primal solution to the domain relaxation of the PTP.



- Every primal solution (q, π) for the topology optimization problem has to fulfill the following inequality:

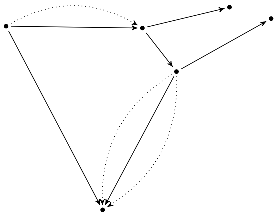
$$\text{const}(x) + \zeta \sum_{v \in V} d_v \pi_v^* + (1-\zeta) \sum_{v \in V} d_v \mu_v^*$$

$$\leq \text{const}(x) + \sum_{(a,i)=(v,w,i) \in A', i \neq 0} \left(\left(\zeta(\pi_v^* - \pi_w^*) + (1-\zeta)(\mu_v^* - \mu_w^*) \right) q_{a,i} \right)$$

$$\leq \zeta \sum_{(a,i) \in A', i \neq 0} (q_{a,i} - q_a^*) x_{a,i} \Phi_{a,i}(q_{a,i}) + (1-\zeta) \sum_{(a,i) \in A', i \neq 0} \mu_a^* x_{a,i} \Phi_{a,i}(q_{a,i})$$

$$\leqslant (1-\zeta) \sum_{v \in V} (\lambda_v^{+*} \overline{\pi}_v - \lambda_v^{-*} \underline{\pi}_v).$$

Here: $\zeta \in \mathbb{R}_+$, (q^*, π^*) primal solution to the domain relaxation of the PTP.



Theorem (H. and Fügenschuh 2013)

Let $(q^*, \pi^*, \Delta^*, \mu^*, \lambda^*)$ be a KKT point of the domain relaxation for arc set A' and let (μ, λ) be a dual transmission flow derived from this KKT point. Denote by x^* the binary values which yield the domain relaxation. Let $\zeta \in]0,1[$ such that

1. *if $\mu_a\, q_a^* > 0$, then $(1-\zeta)|\mu_a^*| < \zeta\, \gamma_{r,v}|q_a^*|$,*
2. *if $\mu_a\, q_a^* < 0$, then $(1-\zeta)\,|\mu_v^* - \mu_w^* - \lambda_a^{*+} + \lambda_a^{*-}| < \zeta\, \gamma_{r,v}|\pi_v^* - \gamma_a \pi_w^* - \tilde{\beta}_a|$,*
3. *if $\mu_a\, q_a^* = 0$, then $(1-\zeta)\,\mu_a^* = 0$*

holds for every arc $a \in A'$. Then for

$$\tilde{f}_{\zeta,q^*,\mu}(q_{a,i}, y_{a,i}) := (\zeta\, \gamma_{r,v}(q_{a,i} - q_a^*) + (1-\zeta)\mu_a)\,(\alpha_{a,i}\, q_{a,i}|q_{a,i}|^{k_a} - \beta_{a,i} y_{a,i})$$

$$\tilde{\ell}_{\zeta,\pi^*,\mu,\lambda}(q_{a,i}) := \zeta\,(\pi_v'(\pi^*) - \pi_w'(\pi^*))\, q_{a,i} + (1-\zeta)(\mu_v - \mu_w - \lambda_a^+ + \lambda_a^-)\, q_{a,i}$$

and constants $\tau_{a,i}(y_{a,i}) := \inf\{\tilde{f}_{\zeta,q^*,\mu}(q_{a,i}, y_{a,i}) - \tilde{\ell}_{\zeta,\pi^*,\mu,\lambda}(q_{a,i}) \mid \underline{q}_{a,i} \le q_{a,i} \le \overline{q}_{a,i}\}$ for each arc $(a,i) \in A_X, i \neq 0$ the inequality in binary variables x

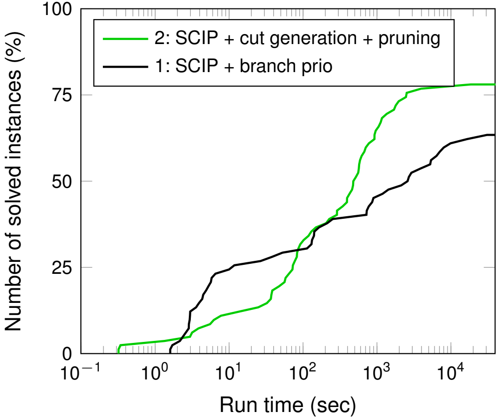
$$\sum_{\substack{(a,i)\in A_X \\ i\neq 0}} x_{a,i}\, \tau_{a,i}(y_{a,i}) \leqslant -\zeta \sum_{v\in vs} d_v \pi_v'(\pi^*)$$

$$+(1-\zeta)\left(\sum_{v\in vs}\left(\lambda_v^+\, \overline{\pi}_v - \lambda_v^-\, \underline{\pi}_v\right) + \sum_{\substack{(a,i)\in A_X \\ i\neq 0}} x_{a,i}(\lambda_a^+\, \overline{q}_{a,i} - \lambda_a^-\, \underline{q}_{a,i}) - \sum_{v\in V} d_v\, \mu_v\right)$$

$$+\zeta \sum_{a=(v,w)\in A'} x_{a,0} \max\left\{q_a^*(\overline{\pi}_v' - \underline{\pi}_w'),\, q_a^*(\underline{\pi}_v' - \overline{\pi}_w')\right\}$$

$$+(1-\zeta) \sum_{a=(v,w)\in A} x_{a,0} \max\left\{\mu_a(\overline{\pi}_v - \underline{\pi}_w),\, \mu_a(\underline{\pi}_v - \overline{\pi}_w)\right\}$$

is valid for the topology optimization problem. This inequality cuts off the PTP corresponding to the arc set A' if and only if it is infeasible. For the corresponding decision vector $x = x^*$ the violation of the inequality is greater than or equal to $(1-\zeta)$ times the optimal objective value of the domain relaxation.



Strategies

1. SCIP default with branching priorities
2. SCIP in combination with cut generation and node pruning

- Strategies
  1. SCIP default with branching priorities
  2. SCIP in combination with cut generation and node pruning

- Benchmark set: Networks containing only pipes, loops and valves

- Solved instances

strategy	1	2	all
solved instances	53	64	82

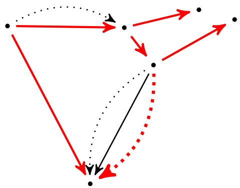
- Means

	solved(53)		incomp.(18)
	time [s]	nodes	gap [%]
strategy 1	180.0	49,219	159
strategy 2	120.0	8,681	31
shifted geom. mean	−33 %	−82 %	−81 %

▷ Fixing all discrete decisions yields the **active transmission problem (ATP)**:

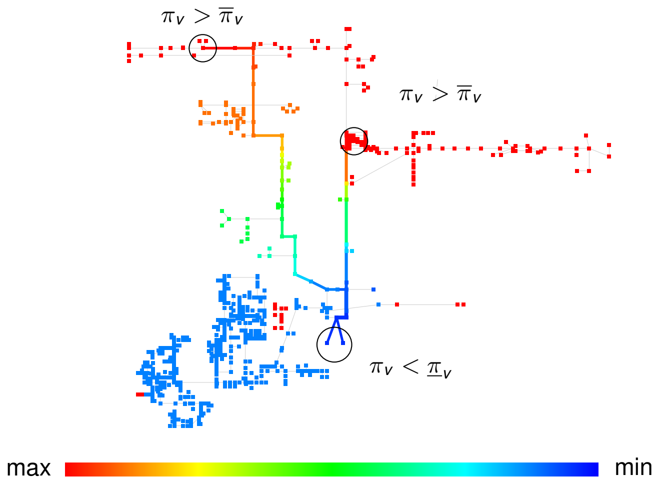
$$\exists\, q, \pi, p, y$$

$$\begin{aligned}
\text{s.t.}\quad & \alpha_a q_a |q_a|^{k_a} - \beta_a y_a - (\pi_v - \gamma_a \pi_w) = 0 && \forall\, a = (v,w) \in A', \\
& A_a\,(q_a, p_v, p_w)^T \le b_a && \forall\, a = (v,w) \in A', \\
& \sum_{w:(v,w)\in A'} q_{v,w} - \sum_{w:(w,v)\in A'} q_{w,v} = d_v && \forall\, v \in V, \\
& p_v|p_v| - \pi_v = 0 && \forall\, v \in V, \\
& \underline{y}_a \le y_a \le \overline{y}_a && \forall\, a \in A', \\
& q_a \leqslant \overline{q}_a && \forall\, a \in A', \\
& q_a \geqslant \underline{q}_a && \forall\, a \in A', \\
& \pi_v \leqslant \overline{\pi}_v && \forall\, v \in V, \\
& \pi_v \geqslant \underline{\pi}_v && \forall\, v \in V.
\end{aligned}$$



Here the set of selected arcs is denoted by $A' := \{(a,i) \in A_X : x_{a,i} = 1\}$.

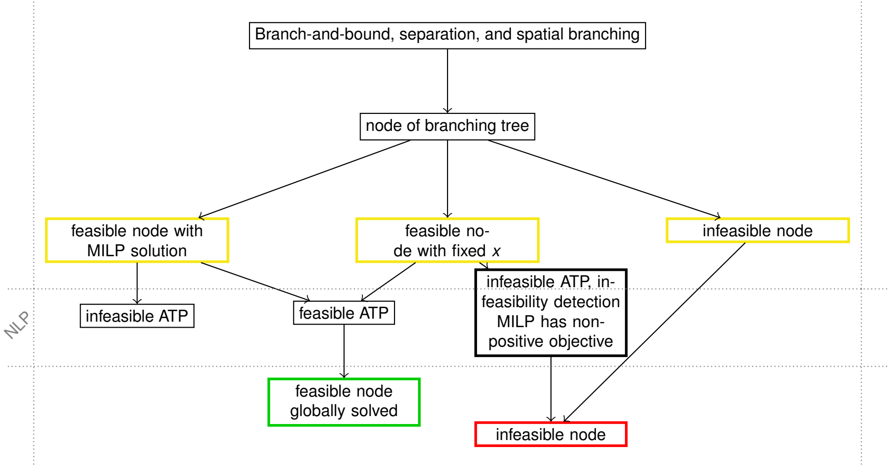
- Use domain relaxation for computing a feasible solution and visualize dual multipliers.



Theorem (H. 2015)

*If the **infeasibility detection MILP** is infeasible or has a non-positive objective value, then the active transmission problem (ATP) is infeasible.*

$$
\begin{aligned}
&\max \ z \\
\text{s.t.} \quad & \sum_{a \in \delta^+_{A'}(v)} q_a - \sum_{a \in \delta^-_{A'}(v)} q_a = d_v && \forall\, v \in V, \\
& x_v^+ - x_v^- - x_v - \kappa_v z = 0 && \forall\, v \in V, \\
& \tilde{\kappa}_a (q_a - \tilde{q}_a) > 0 \Rightarrow x_v - x_w + x_a \geq 0 && \forall\, a = (v, w) \in A', \\
& \tilde{\kappa}_a (q_a - \tilde{q}_a) = 0 \Rightarrow x_v - x_w + x_a = 0 && \forall\, a = (v, w) \in A', \\
& \tilde{\kappa}_a (q_a - \tilde{q}_a) < 0 \Rightarrow x_v - x_w + x_a \leq 0 && \forall\, a = (v, w) \in A', \\
& \alpha_a (q_a - \tilde{q}_a) > 0 \Rightarrow s_v - s_w + s_a \geq \kappa_a z && \forall\, a = (v, w) \in A', \\
& \alpha_a (q_a - \tilde{q}_a) = 0 \Rightarrow s_v - s_w + s_a = 0 && \forall\, a = (v, w) \in A', \\
& \alpha_a (q_a - \tilde{q}_a) < 0 \Rightarrow s_v - s_w + s_a \leq \kappa_a z && \forall\, a = (v, w) \in A', \\
& \underline{q}_a \leq q_a \leq \bar{q}_a && \forall\, a \in A', \\
& \underline{s}_a \leq s_a \leq \bar{s}_a && \forall\, a \in A', \\
& \underline{x}_a \leq x_a \leq \bar{x}_a && \forall\, a \in A', \\
& x_v^+ \leq \bar{x}_v^+ && \forall\, v \in V, \\
& x_v^- \leq \bar{x}_v^- && \forall\, v \in V, \\
& x_v, s_v \in \mathbb{R} && \forall\, v \in V, \\
& x_v^+, x_v^- \in \mathbb{R}_+ && \forall\, v \in V, \\
& x_a, s_a, q_a \in \mathbb{R} && \forall\, a \in A'
\end{aligned}
$$


Branch-and-bound, separation, and spatial branching
node of branching tree
feasible node with MILP solution
feasible node with fixed x
infeasible node
NLP
infeasible ATP
feasible ATP
infeasible ATP, infeasibility detection MILP has nonpositive objective
feasible node globally solved
infeasible node

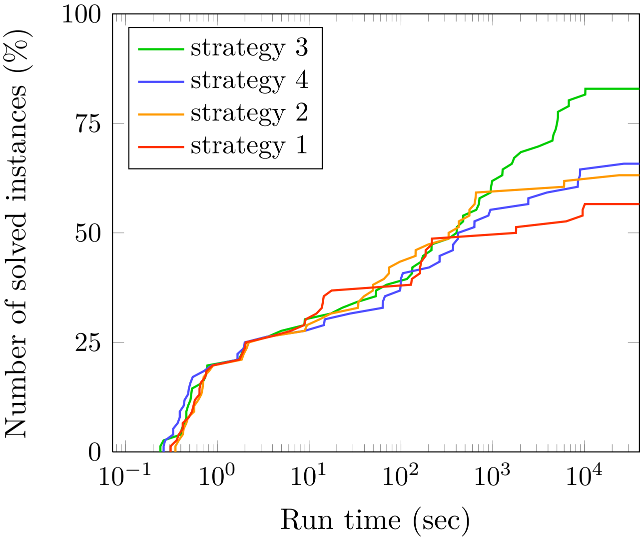
- Strategies
  1. SCIP default
  2. SCIP default with branching priorities
  3. SCIP in combination with domain relaxation for ATP and node pruning
  4. SCIP in combination with domain relaxation for ATP

- Solved instances

strategy	1	2	3	4	all
solved instances	43	48	63	50	63

- Means

	solved(48)		incomp.(3)
	time [s]	nodes	gap [%]
strategy 2	50.4	2,565	28
strategy 3	62.3	2,021	17
shifted geom. mean	23 %	−21 %	−40 %



strategy 3
strategy 4
strategy 2
strategy 1
100
75
50
25
0
Number of solved instances (%)
10^{-1}
10^{0}
10^{1}
10^{2}
10^{3}
10^{4}
Run time (sec)

- A model for the topology optimization problem was presented.
- Improvements of the solving performance of SCIP were obtained by
  - computing primal solutions heuristically,
  - pruning convex subproblems manually,
  - adding valid inequalities.
- The presented adaptations of the MINLP solver SCIP allow to improve the solving performance of large scale network operation and expansion instances.
- The methods are used by our cooperation partner.

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