Global Optimization of ODE constrained network problems

Marc Pfetsch

Joint work with: Oliver Habeck and Stefan Ulbrich

TU Darmstadt

Discrete Optimization

Supported by the SFB Transregio 154: Mathematical Modelling, Simulation and Optimization using the Example of Gas Networks

Outline

TECHNISCHE UNIVERSITÄT DARMSTADT

1 General Theory
- Abstract Model and Relaxations
- Solving Strategies

2 Application – Stationary Gas Transport
- Model
- Relaxation of the ODE

3 Implementation – for Stationary Gas Transport
- The Algorithm
- Results

Optimization Problem

TECHNISCHE UNIVERSITÄT DARMSTADT

We consider the ODE constrained optimization problem:

$$
\begin{aligned}
\min \quad & C(x, y^0, y^S, z) \\
\text{s.t.} \quad & G(x, y^0, y^S, z) \leq 0, \\
& \partial_s y(s) = f\big(s, x, y(s)\big), \qquad\qquad s \in [0, S] \qquad\qquad (\mathcal{P}_{ode}) \\
& y^0 = y(0),\ \ y^S = y(S), \\
& x \in X,\ \ y^0 \in Y^0,\ \ y^S \in Y^S,\ \ z \in Z,
\end{aligned}
$$

- Y^0, $Y^S \subset \mathbb{R}^n$ and $X \subset \mathbb{R}^k$ are polytopes and $Z \subset \mathbb{Z}^m$ is bounded.
- $C\colon X \times Y^0 \times Y^S \times Z \to \mathbb{R}$ and $G\colon X \times Y^0 \times Y^S \times Z \to \mathbb{R}^l$ are continuously differentiable and possibly nonlinear.
- Values of y only need to be known for finitely many points $y(0),\ y(S) \in \mathbb{R}^n$.
- Examples: Stationary networks (gas, water, (electricity), ...)

Idea of our Approach

- Standard approach is “Discretize then optimize”:
  discretize ODE (add N variables), use numerical approximation scheme and obtain MINLP. Solve it and possibly refine.
- Our goal: compute globally optimal solution without explicitly discretizing.
- Workhorse: good convex/concave under/over-estimators.
- Will show: Easy to construct in certain cases, e.g., gas optimization.
- Yields globally convergent solution algorithm.

Equivalent Optimization Problem

TECHNISCHE UNIVERSITÄT DARMSTADT

Equivalent reformulation with the solution mapping $F\colon (x, y^0) \mapsto y^S$:

$$\begin{aligned} \min \quad & C(x, y^0, y^S, z) \\ \text{s.t.} \quad & G(x, y^0, y^S, z) \leq 0, \\ & y^S - F\big(x, y^0\big) = 0, \\ & x \in X, y^0 \in Y^0, y^S \in Y^S, z \in Z. \end{aligned} \tag{$\mathcal{P}$}$$

Nonconvex Relaxation of $(\mathcal{P})$

TECHNISCHE UNIVERSITÄT DARMSTADT

Assume that there exist $F^\ell \colon X \times Y^0 \times \mathbb{N}^n \to \mathbb{R}^n$ and $F^u \colon X \times Y^0 \times \mathbb{N}^n \to \mathbb{R}^n$, with

$$F^\ell\big(x, y^0, N\big) \leq F\big(x, y^0\big) \leq F^u\big(x, y^0, N\big)$$

for all $x \in X$ and $y^0 \in Y^0$. Furthermore, on the polytopes $X,\ Y^0$ the functions F^ℓ and F^u converge uniformly to F for $N \to \infty,\ i = 1, \dots, n$.

This yields the relaxation

$$\begin{aligned} \min \quad & C(x, y^0, y^S, z) \\ \text{s.t.} \quad & G(x, y^0, y^S, z) \leq 0, \\ & F^\ell\big(x, y^0, N\big) \leq y^S \leq F^u\big(x, y^0, N\big), \\ & x \in X, y^0 \in Y^0, y^S \in Y^S, z \in Z. \end{aligned} \qquad (\mathcal{P}_r(N))$$

Convex Relaxation of $(\mathcal{P}_r(N))$

TECHNISCHE UNIVERSITÄT DARMSTADT

Assume that there exist

- convex underestimators $\check{C} \leq C$, $\check{G} \leq G$, and $\check{F}^\ell \leq F^\ell$
- and a concave overestimator $F^u \leq \hat{F}^u$.

Hence,

$$
\begin{aligned}
\min \quad & \check{C}(x, y^0, y^S, z) \\
\text{s.t.} \quad & \check{G}(x, y^0, y^S, z) \leq 0, \\
& \check{F}^\ell\big(x, y^0, N\big) \leq y^S \leq \hat{F}^u\big(x, y^0, N\big), \\
& x \in X, y^0 \in Y^0, y^S \in Y^S, z \in \operatorname{conv}(Z)
\end{aligned}
\qquad (\mathcal{P}_{cv}(N))
$$

is a convex relaxation of $(\mathcal{P}_r(N))$.

$\rightsquigarrow$ we can solve $(\mathcal{P}_r(N))$ with spatial branch-and-bound.

(ϵ, δ)-optimal solutions

TECHNISCHE UNIVERSITÄT DARMSTADT

Definition

A vector $(x, y^0, y^S, z) \in X \times Y^0 \times Y^S \times Z$ is (ϵ, δ)-optimal, if

- each constraint is violated by a maximum of δ
- and the objective function satisfies $C(x, y^0, y^S, z) \leq C^* + \epsilon$.

Solving Strategy

TECHNISCHE UNIVERSITÄT DARMSTADT

Goal: Find $(\epsilon, \delta_1 + \delta_2)$-optimal solution of $(\mathcal{P})$.

- Start spatial branch-and-bound with some initial $N \in \mathbb{N}^n$ and feasibility tolerance δ_1.
- Solve the convex relaxation $(\mathcal{P}_{cv}(N))$ in a node.
- Check if
$$\|F^u(x, y^0, N) - F^\ell(x, y^0, N)\|_\infty \leq \delta_2$$
holds for the current solution of the relaxation.
- Increase N if necessary, improve the under- and overestimators $\check{F}^\ell$, $\hat{F}^u$, and solve the convex relaxation again.
- Continue like in the “normal” spatial branch-and-bound algorithm.

Solving Strategy

TECHNISCHE UNIVERSITÄT DARMSTADT

Theorem

For a nested sequence of nodes $\mathcal{F}_k = X_k \times Y_k^0 \times Y_k^T \times Z_k$ *with* $\mathcal{F}_{k+1} \subseteq \mathcal{F}_k$ *let*

- $\lim_{k\to\infty} \operatorname{diam} \mathcal{F}_k = 0$
- *and the estimators become exact in the limit, i.e., the estimators converge to the original functions on* $\mathcal{F}_k$ *for* $k \to \infty$*.*

Then the solving strategy produces an $(\epsilon, \delta_1 + \delta_2)$ *feasible point of* $(\mathcal{P})$ *or shows that it is infeasible in finite time.*

Outline

TECHNISCHE UNIVERSITÄT DARMSTADT

1 General Theory
- Abstract Model and Relaxations
- Solving Strategies

2 Application – Stationary Gas Transport
- Model
- Relaxation of the ODE

3 Implementation – for Stationary Gas Transport
- The Algorithm
- Results

Model

- Gas networks are given by directed graphs $\mathcal{G} = (\mathcal{V}, \mathcal{A})$.
- The nodes are junctions of the network.
- The arcs are

(control)valves:	linear constraints with binary variables
resistors:	(non)linear constraints with indicator variables
compressors:	(here) polyhedral approximation of operating range
pipes:	ordinary differential equation

The Differential Equation

TECHNISCHE UNIVERSITÄT DARMSTADT

Stationary isothermal Euler equation with no inclination and $\frac{|v|}{c} = \frac{c|q|}{Ap} \leq 0.8$:

$$\partial_x p(x) = -\frac{\lambda c^2\, q|q|\, p(x)}{2D\left(A^2 p(x)^2 - c^2 q^2\right)} =: \phi\big(p(x), q\big).$$

Variables:

- pressure $p(x)$
- mass flow q

Constants:

- friction coefficient λ
- speed of sound c
- diameter D
- cross sectional area A
- length of the pipe L

For $q \geq 0$ the solution $p(x)$ is concave and non increasing.

Optimization Problem

TECHNISCHE UNIVERSITÄT DARMSTADT

Thus, we want to solve the following optimization problem:

$$
\begin{aligned}
\min \quad & C(p, q, z) \\
\text{s.t.} \quad & G(p, q, z) \leq 0, \\
& \partial_x p_a(x) = \phi_a\big(p_a(x), q_a\big) && \forall\, a \in \mathcal{A}_{pipe} \subseteq \mathcal{A}, \\
& p_u = p_a(0),\ p_v = p_a(L_a) && \forall\, a = (u, v) \in \mathcal{A}_{pipe}, \\
& \underline{q}_a \leq q_a \leq \overline{q}_a && \forall\, a \in \mathcal{A}, \\
& \underline{p}_u \leq p_u \leq \overline{p}_u && \forall\, u \in \mathcal{V}, \\
& z \in Z \subset \mathbb{Z}^m
\end{aligned}
$$

with spatial branch-and-bound.

Bounding Methods for Gas Transport

TECHNISCHE UNIVERSITÄT DARMSTADT

Theorem

Given a discretization $0 = x_N < x_{N-1} < \cdots < x_0 = L$ *with* $h_{i+1} = x_i - x_{i+1}$ *for* $i = 0, 1, \dots, N-1$*. If* $q \geq 0$*, bounds on* $p(0)$ *are given by the following methods:*

- ▷ *Upper bounds through the trapezoidal rule:*

$$p_0^u = p_{out}, \quad p_{i+1}^u + \tfrac{1}{2} h_{i+1} \phi\big(p_{i+1}^u, q\big) = p_i^u - \tfrac{1}{2} h_{i+1} \phi\big(p_i^u, q\big), \ \ \forall i = 0, 1, \dots, N-1.$$

- ▷ *Lower bounds through the explicit midpoint method:*

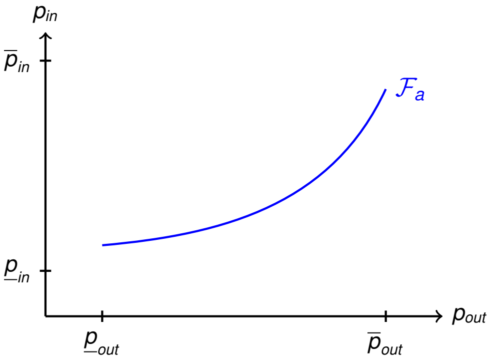
$$p_0^\ell = p_{out}, \quad p_{i+1}^\ell = p_i^\ell - h_{i+1}\, \phi\big(p_i^\ell - \tfrac{1}{2} h_{i+1}\, \phi\big(p_i^\ell, q\big), q\big), \ \ \forall i = 0, 1, \dots, N-1.$$

$\rightsquigarrow$ yields (nonconvex) relaxation of $\mathcal{F}_a$.

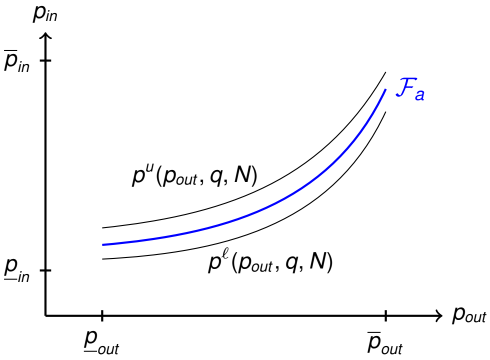
Critical property: nonnegative local truncation error.

Illustration

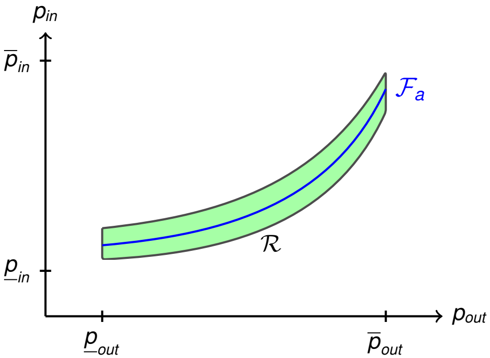
TECHNISCHE
UNIVERSITÄT
DARMSTADT



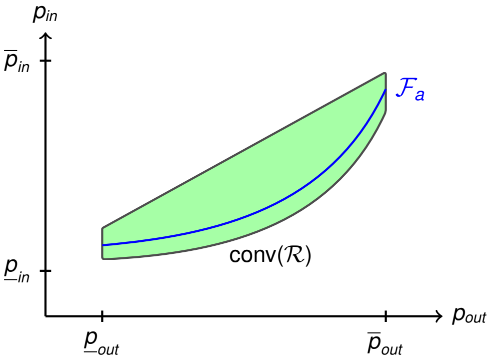
Illustration



Illustration



Illustration



Outline

TECHNISCHE
UNIVERSITÄT
DARMSTADT

1 General Theory
- Abstract Model and Relaxations
- Solving Strategies

2 Application – Stationary Gas Transport
- Model
- Relaxation of the ODE

3 Implementation – for Stationary Gas Transport
- The Algorithm
- Results

Some Informations

TECHNISCHE UNIVERSITÄT DARMSTADT

- We use the branch-and-bound framework SCIP.
- We implemented a constraint handler for the ODEs.
- Test instances are available at `http://gaslib.zib.de/`.

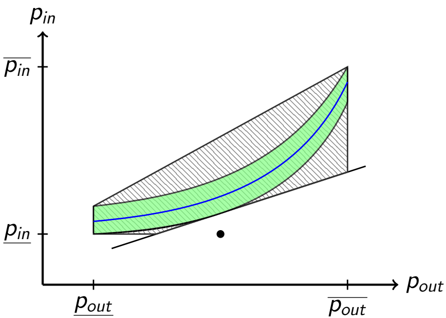
Basic Algorithm

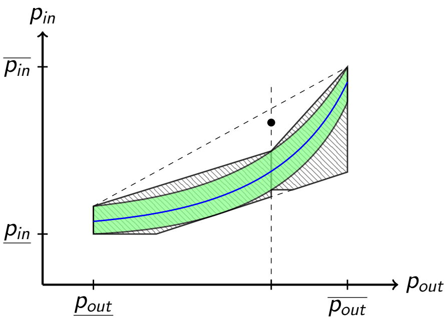
We perform the following steps in the nodes of the branch-and-bound tree:

1. Perform bound propagation (use estimators)
2. Solve LP-relaxation
3. Enforce feasibility of “most infeasible” pipe by one of the following steps:
   3.1 Fixing the direction of the flow by branching.
   3.2 Adding (parts of) the concave overestimator.
   3.3 Branching w.r.t. input pressure, output pressure or massflow.
   3.4 Adding a gradient cut (convex underestimator).
4. Resolve new LP-relaxation or choose a new node.

Illustration

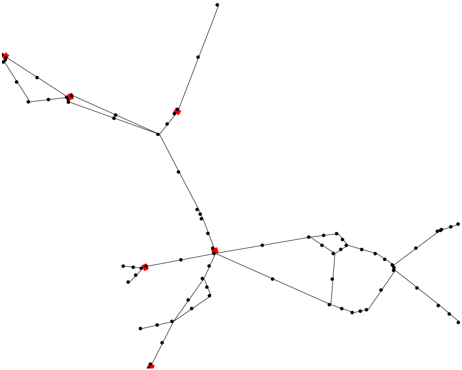
TECHNISCHE
UNIVERSITÄT
DARMSTADT





Example: GasLib-40

TECHNISCHE UNIVERSITÄT DARMSTADT



- 40 nodes
- 39 pipes
- 6 compressors
- 12 binary variables for compressors

Results

TECHNISCHE UNIVERSITÄT DARMSTADT

objective: minimize	$-\sum_{v\in\mathcal{V}} p_v$	$\sum_{v\in\mathcal{V}} q_v^{\pm} p_v$	$\sum_{a\in\mathcal{A}_{cs}} z_a$
solving time (seconds)	877.74	542.48	65.08
processed Nodes	12,444	2790	263
branchings on flow (%)	46.2	81.0	84.2
branchings on pressure (%)	52.9	0.0	8.8
branchings on binary variables (%)	0.9	19.0	7.0
leaves	5900	1412	73
cut offs by propagation	5297	1149	38
bound changes by propagation	32,444	63,317	6051
added overestimators	7362	2385	985
added underestimators	6360	4281	488

$$\delta_1 = \epsilon = 10^{-6},\ \delta_2 = 10^{-4}$$

Conclusions

Future theoretical goals:

- ▷ Extend to case with inclination.
- ▷ Include temperature?
- ▷ Transient case (much more difficult).

Future implementation issues:

- ▷ Better branching rules
- ▷ Additional primal heuristics
- ▷ Avoid cycle flows
- ▷ Cuts on binary variables
- ▷ Larger instances

Literature

TECHNISCHE
UNIVERSITÄT
DARMSTADT

O. Habeck, S. Ulbrich, and M. E. Pfetsch.
Global Optimization of ODE constrained network problems.
Preprint, TRR 154, 2017.
`opus4.kobv.de/opus4-trr154/frontdoor/index/index/docId/186`.

M. E. Pfetsch, T. Koch, L. Schewe, and B. Hiller, editors.
Evaluating Gas Network Capacities.
Society for Industrial and Applied Mathematics, Philadelphia, PA, 2015.

M. Schmidt, D. Aßmann, R. Burlacu, J. Humpola, I. Joormann, N. Kanelakis, T. Koch, D. Oucherif, M. E. Pfetsch, L. Schewe, R. Schwarz, and M. Sirvent.
GasLib – A Library of Gas Network Instances.
Data, 2: Article 40, 2017.