Mixed-integer methods for polynomial optimization and application to energy networks

Carl Eggen

University of Konstanz

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Outline

Motivation

How can climate targets be achieved in urban energy supply?

Contribution of mathematics:

Algorithms for calculating optimal energy networks

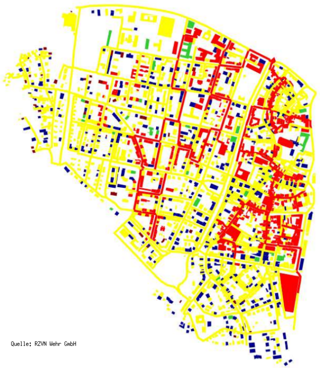


Figure 1: Example of an energy network for Konstanz

Network model [Lu21]

Minimize the total costs of energy supply considering the following aspects:

- energy sources, i.e. natural gas and electricity (soon: district heating)
- energy demand
- network expansion
- power balance
- CO_2-limit
- Renovation progress
- Nonlinear physical laws for the individual energy carriers (e.g. Ohm's law for electricity)

Optimization of the network model

The network model yields a mixed-integer nonlinear optimization problem, in short MINLP

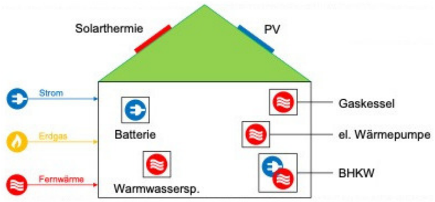


Figure 2: How should houses be supplied with energy?

- integer variables: gas pipe or district heating?
- continuous variables: How much electricity/gas/district heating needs to be supplied?

Optimization problem

The network model yields mixed-binary polynomial optimization problems (MBPOP) of the form

$$\begin{aligned} \min_{x \in \mathbb{R}^n} \ & f(x) \\ \text{s.t. } & g_j(x) \geq 0 \text{ for } j \in [m], \\ & x_i \in \{0,1\} \text{ for } i \in I, \end{aligned} \tag{MBPOP}$$

where

- $f, g_1, \ldots, g_m \in \mathbb{R}[x]$ are polynomials in $x_1, \ldots, x_n$ variables,
- $x = (x_1, \ldots, x_n)$ is the vector of variables,
- $I \subseteq [n]$ index set of binary variables in x,
- $S(g) := \{x \in \mathbb{R}^n \mid g_j(x) \geq 0\}$ is box constrained,
- $S(g,h) := \{x \in \mathbb{R}^n \mid g_j(x) \geq 0, h_i(x) = x_i(x_i - 1) = 0\}$.

For solving MBPOPs different relaxations techniques can be used.

Moment hierarchy: Reformulation [Las01; Lau09]

$$f^{\min} := \inf_{x \in S(g)} f(x) \tag{POP}$$

Rewrite (POP)

$$\inf_{x \in S(g)} f(x) = \inf_{\mu \in \mathcal{P}_{S(g)}} \int_{S(g)} f(x)\, \mu(dx)$$
$$= \inf_{\mu \in \mathcal{P}_{S(g)}} \sum_{\alpha} f_\alpha \int_{S(g)} x^\alpha\, \mu(dx) = \inf_{y \in \mathcal{M}_{S(g)}} \mathrm{vec}(f)^\top y,$$

where

$$\mathcal{P}_{S(g)} = \{\mu \text{ probability measure on } \mathbb{R}^n \mid \mathrm{supp}(\mu) \subseteq S(g)\},$$

and

$$\mathcal{M}_{S(g)} = \{y \in \mathbb{R}^{\mathbb{N}^n} \mid \exists \mu \in \mathcal{P}_{S(g)} : y_\alpha = \int_{S(g)} x^\alpha\, \mu(dx)\}.$$

Moment hierarchy: Relaxation

Lemma

If $y \in \mathbb{R}^{\mathbb{N}^n}$ is the sequence of moments of a measure μ, then $M(y) \succeq 0$. Let $g \in \mathbb{R}[x]$. If $\operatorname{supp}(\mu) \subseteq \{x \in \mathbb{R}^n \mid g(x) \geq 0\}$, then $M(gy) \succeq 0$.

Relax the constraint $y \in \mathcal{M}_{S(g)}$ by the weaker constraint of positive semidefitness of the (infinite) moment matrix $M(y)$ and localizing matrices $M(g_j y)$

$$
\begin{aligned}
f^{\text{MOM}} = \inf_{y \in \mathbb{R}^{\mathbb{N}^n}} \ & \operatorname{vec}(f)^\top y \\
\text{s.t. } & y_0 = 1, M(y) \succeq 0 \\
& M(g_j y) \succeq 0 \text{ for } j = 1, \dots, m
\end{aligned}
$$

$$f^{\text{MOM}} \leq f^{\min}$$

Moment hierarchy: Truncation

Truncating the moment matrices yields a hierarchy of SDPs

$$f_d^{\text{MOM}} = \inf_{y \in \mathbb{R}^{\mathbb{N}^n_{2d}}} \ \text{vec}(f)^\top y \qquad (\text{MOM}_d)$$

$$\text{s.t. } y_0 = 1, M_d(y) \succeq 0$$

$$M_{d-d_j}(g_j y) \succeq 0 \text{ for } j = 1, \ldots, m$$

for any $d \geq \lceil \frac{\deg(f)}{2} \rceil$ with $d_1 := \lceil \frac{\deg(g_1)}{2} \rceil, \ldots, d_m := \lceil \frac{\deg(g_m)}{2} \rceil$.

$$f_d^{\text{MOM}} \leq f_{d+1}^{\text{MOM}} \leq f^{\text{MOM}} \leq f^{\min}$$

Further properties

- **Duality:**
  The Lagrangian dual SOS_d of MOM_d uses sums of squares representations, $f_d^{\text{SOS}} \leq f_d^{\text{MOM}}$ and no duality gap, if $\text{int}(S(g)) \neq \emptyset$.
- **Convergence:**
  $\lim_{d\to\infty} f_d^{\text{SOS}} = f^{\min}$ via Putinar's Positivstellensatz from real algebraic geometry.
- **Optimality certificate:**
  If $\text{rank}\, M_d(y^d) = \text{rank}\, M_{d+1}(y^{d+1})$, then $f_d^{\text{MOM}} = f^{\min}$ holds (y^d solution of MOM_d).
- **Extracting global minimizers:**
  If rank condition is satisfied, compute finite atomic meassure for truncated moment sequence y^d.
- **Unique minimizer:**
  x^* unique solution of MBPOP, then $\lim_{d\to\infty} y_{e_i}^d = x_i^*$

Some practical problems of the moment hierarchy

- Size of matrices is proportional to $\binom{n+d}{d}$ in MOM_d (n number of variables).
- Sparsity can be exploited. But if n is big, even MOM_2 can be too large.
- In most practical application: no global optimality and no extraction of global minimizers possible.
- Even no feasible point can be extracted from solutions of MOM_d.
- **BUT**: First moments can be used as initial point for an local NLP-Solver.

Feasiblity pump: Finding feasible points

Motivation

Feasible points yield upper bounds for optimal value
$\rightarrow$ essential for a Branch-and-Bound framework

Feasibility pump: Heuristic for finding feasible points

Feasiblity pump: Basic idea [FGL05; BLS19]

Generating two sequences of points which (hopefully) converge to a feasible point, i.e.

$$x^{k,R} \to x^{\text{fea}} \leftarrow x^{k,I}$$

for $k \to \infty$ with

- $(x^{k,R})_k$ sequence of solutions of a relaxation of MBPOP with relaxed feasible set $S(g,h) \subseteq R$.
- $(x^{k,I})_k$ sequence of points fulfilling the binary condition, i.e. $x_i^{k,I} \in \{0,1\}$ for $i \in I$,

Feasiblity pump: Basic idea [FGL05; BLS19]

Generating two sequences of points which (hopefully) converge to a feasible point, i.e.

$$x^{k,R} \to x^{\mathrm{fea}} \leftarrow x^{k,I}$$

for $k \to \infty$.
Starting from a solution of a relaxation $x^{0,R}$ new points are generated by alternately

- rounding a feasible point of the relaxation and
- projecting the rounded, i.e. integral, solution onto the closest point in the relaxed feasible set R.

Feasiblity pump: Three main ingredients for $R = S(g)$

There are three main ingredients for the feasibility pump:

- **Rounding:** Rounding of $x^{k,S(g)}$ to nearest integral point $x^{k,I}$.
- **Projecting:** Solving

$$\min_{x \in S(g)} \Delta_\rho(x, x^{k,I}) := (1-\rho) \sum_{i \in I} |x_i - x_i^{k,I}| + \rho c f(x)$$

  yields $x^{k,S(g)}$ with $\rho \in [0,1]$ and $c \in \mathbb{R}_+$.
- **Perturbing:** Cycling might occur, i.e. $x^{k-l,I} = x^{k,I}$ for some $l \in \mathbb{N}$. Then perturb some of the binary entries of $x^{k,I}$.

Feasibility Pump: Basic idea

Algorithm 1 Ideal feasibility pump for MBPOP

Require: MBPOP $\equiv \min \{f(x) \mid x \in S(g),\ \forall i \in I\colon x_i \text{ binary}\}$

Ensure: a feasible solution x^{fea} (if found)

```
x^{0,S(g)} = arg min{f(x) | x ∈ S(g)}
while not termination condition do
    if x^{k,S(g)} is integer then
        return x^fea = x^{k,S(g)}
    else
        x^{k,I} = round(x^{k,S(g)})
    end if
    if cycle detected then
        perturb(x^{k,I})
    end if
    x^{k,S(g)} = arg min_{x∈S(g)} Δ_ρ(x, x^{k,I})
end while
```

$$x^{0,S(g)} = \arg\min\{f(x) \mid x \in S(g)\}$$

$$x^{k,I} = \texttt{round}(x^{k,S(g)})$$

$$x^{k,S(g)} = \arg\min_{x \in S(g)} \Delta_\rho(x, x^{k,I})$$

Feasibility pump: Basic idea

Algorithm 1 Ideal feasibility pump for MBPOP

Require: MBPOP $\equiv \min \{f(x) \mid x \in S(g),\ \forall i \in I\colon x_i \text{ binary}\}$
Ensure: a feasible solution x^{fea} (if found)

$x^{0,S(g)} = \arg\min\{f(x) \mid x \in S(g)\}$
while *not termination condition* **do**
  if $x^{k,S(g)}$ is integer **then**
    return $x^{\text{fea}} = x^{k,S(g)}$
  else
    $x^{k,I} = \texttt{round}(x^{k,S(g)})$
  end if
  if cycle detected **then**
    $\texttt{perturb}(x^{k,I})$
  end if
  $x^{k,S(g)} = \arg\min_{x \in S(g)} \Delta_\rho(x, x^{k,I})$
end while

Feasiblity Pump: Solving the NLPs

How to solve the nonconvex NLPs? Two Options:

- using a local NLP-Solver (e.g. `Ipopt`)
  BUT: only local solution, but feasible for the NLP.
- using the moment/SOS hierarchies for global optimization
  BUT: (extracted) solution of a moment relaxation is *neither* integer *nor* feasible for the NLP, but can be used as an inital point for a local NLP-Solver.

Feasiblity pump: Adaption to MBPOPs

- Moment relaxation for finding an initial feasible candidate.
- After rounding: Fix the integer variables and enforce nonlinear constraints by a local NLP-Solver.
- If local NLP-solver fails, perturb binary entries.
- Projecting: Solve moment relaxation with objective

$$\Delta_\rho(y, x^{k,l}) = (1-\rho)\sum_{i\in I} |y_{e_i} - x_i^{k,l}| + \rho c\, \mathrm{vec}(f)^\top y,$$

where y_{e_i} is the variable associated to the first moment $\int x_i d\mu$.

Feasiblity pump: Adaption to MBPOPs

Algorithm 2 Feasibility pump for MBPOP

Require: $\text{MBPOP} \equiv \min \{f(x) \mid x \in S(g),\ \forall i \in I\colon x_i \text{ binary}\},\ d$

Ensure: a feasible solution x^{fea} (if found)

get solution $y^{0,S(g,h)}$ of MOM_d

while *not termination condition* **do**

  extract solution candidate $x^{k,S(g,h)}$ from $y^{k,S(g,h)}$

  $x^{k,I} = \texttt{round}(x^{k,S(g,h)})$

  $x^{\text{fea}}, \text{stat} = \texttt{solve\_local}(\min_{x \in S(g)} \{f(x) \mid \forall i \in I : x_i = x_i^{k,I}\})$

  if stat is `LOCALLY FEASIBLE` **then**

    return x^{fea}

  else

    $\texttt{perturb}(x^{k,I})$

  end if

  get solution $y^{k,S(g,h)}$ of MOM_d with objective $\Delta_\rho(y, x^{k,I})$

end while

Numerical results

Set Up: minimal order of moment relaxation, sparsity was exploited.

- On 39 of 48 problems from the MINLPLib the FP was successful in under 100 iterations.
- Compared to `SCIP` the FP yields better and faster feasible points for some instances.
- Random perturbation makes comparison difficult!

Numerical Results: Challenging Instances from MINLPLib

Name	#variables			#constraints		
	cont.	bin.	total	linear	nonlin.	total
chp_shorttermplan1a	864	144	1008	1684	384	2068
genpooling_meyer04	63	55	118	126	15	141
ringpack_10_1	20	50	70	55	330	385
ringpack_20_1	40	175	215	210	2337	2547
ringpack_20_3	40	213	253	173	3055	3228
ringpack_30_1	60	373	433	465	7433	7898
sfacloc1_3_80	231	62	293	2146	15	2161
sfacloc1_3_90	231	30	261	406	15	421
sfacloc1_3_95	226	9	233	266	15	281
sfacloc1_4_90	293	30	323	479	15	494
sfacloc1_4_95	286	9	295	339	15	354

Table 1: Examples from `MINLPLib`

Numerical Results: Comparison to SCIP

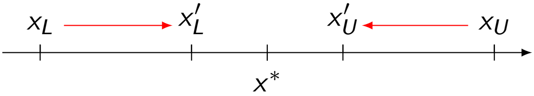
Name	FP		SCIP		
	t(s)	value	t(s)	value	#sol
chp_shorttermplan1a	52.9	331.1	**4.3**	**313.3**	1
genpooling_meyer04	**2.3**	**2.126e6**	3.5	2.279e6	1
ringpack_10_1	3.1	**-6.4**	**0.2**	-2.1	4
ringpack_20_1	**10.7**	**-30.1**	17.3	-8.9	5
ringpack_20_3	**14.4**	**-10.4**	57.2	-8.3	14
ringpack_30_1	**5.9**	**-6.3**	11.9	-2.1	4
sfacloc1_3_80	3.4	10.25	**3.0**	**9.2**	1
sfacloc1_3_90	2.7	12.3	**1.2**	**11.8**	1
sfacloc1_3_95	**0.9**	**12.7**	1.0	20.0	1
sfacloc1_4_90	3.7	**11.4**	**1.6**	16.3	1
sfacloc1_4_95	**1.6**	**11.8**	1.9	16.7	1

Table 2: Comparison to SCIP

Optimality-based bound tightening

What can we do with feasible points besides using them for upper bounds in Branch-and-Bound Algorithms?

Tightening bounds to shrink the feasible set



BENEFIT: Tighter bounds $\Longrightarrow$ lower order ?

Optimality-based bound tightening [Bel+13]

Let x^{fea} be a feasible point. Then solving

$$\begin{aligned} \min_{x\in\mathbb{R}^n} \ & -x_j \\ \text{s.t. } & f(x) \le f(x^{\mathrm{fea}}), \\ & g_j(x) \ge 0 \text{ for } j \in [m], \\ & x_i \in \{0,1\} \text{ for } i \in I, \end{aligned}$$

for $j \in [n] \setminus I$ yields tighter **lower** bound for x_j.

$$\begin{aligned} \min_{x\in\mathbb{R}^n} \ & x_j \\ \text{s.t. } & f(x) \le f(x^{\mathrm{fea}}), \\ & g_j(x) \ge 0 \text{ for } j \in [m], \\ & x_i \in \{0,1\} \text{ for } i \in I, \end{aligned}$$

for $j \in [n] \setminus I$ yields tighter **upper** bound for x_j.

Optimality-based bound tightening: A simple example

ex3_1_1 from MINLPLib:

$$
\begin{aligned}
\min_{x\in\mathbb{R}^8}\ & x_1 + x_2 + x_3 \\
\text{s.t. } & 0.0025(x_4 + x_6) \leq 1, \\
& 0.0025(x_5 + x_7 - x_4) \leq 1, \\
& 0.01(x8 - x5) \leq 1, \\
& 100x_1 - x_1x_6 + 833.33252x_4 \leq 83333.333, \\
& x_2x_4 - x_2x_7 - 1250x_4 + 1250x_5 \leq 0, \\
& x_3x_5 - x_3x_8 - 2500x_5 \leq -1250000, \\
& 100 \leq x_1 \leq 10000, 1000 \leq x_2, x_3 \leq 10000, \\
& 10 \leq x_4, x_5, x_6, x_7, x_8 \leq 1000.
\end{aligned}
$$

Optimality-based bound tightening: Numerical results

New bounds for ex3_1_1 with OBBT:

Variable	sol	orig. bounds		OBBT ($d = 1.5$)	
	x^*	x_L	x_U	x'_L	x'_U
x_1	579.19	100	10000	100	**2588.0**
x_2	1360.13	1000	10000	1000	**3488.0**
x_3	5109.92	1000	10000	**3470.0**	**5949.2**
x_4	182.01	10	1000	10	**251.3**
x_5	295.6	10	1000	**262.0**	**360.1**
x_6	217.99	10	1000	10	**390.0**
x_7	286.4	10	1000	**100.2**	**389.4**
x_8	395.6	10	1000	**362.0**	**461.2**
value	7049.25	2100.0 (0.01s)		**4569.8** (8.4s)	

Table 3: OBBT for ex3_1_1 with optimal value, value of moment relaxation of minimal order ($d = 1$) and time

Optimality-based bound tightening: Numerical results

New bounds for ex3_1_1 with OBBT:

Variable	sol	orig. bounds		OBBT ($d = 2$)	
	x^*	x_L	x_U	x'_L	x'_U
x_1	579.19	100	10000	**479.0**	**691.7**
x_2	1360.13	1000	10000	**1217.6**	**1503.5**
x_3	5109.92	1000	10000	**4967.6**	**5253.5**
x_4	182.01	10	1000	**173.0**	**190.7**
x_5	295.6	10	1000	**289.9**	**301.3**
x_6	217.99	10	1000	**209.3**	**227.0**
x_7	286.4	10	1000	**277.8**	**294.5**
x_8	395.6	10	1000	**389.9**	**401.3**
value	7049.25	2100.0 (0.01s)		**7035.5** (35.2s)	

Table 4: OBBT for ex3_1_1 with optimal value, value of moment relaxation of order $d = 2$ and time

Optimality-based bound tightening: Drawbacks

- `ex3_1_1` can be solved without OBBT to global optimality by the moment relaxation of order $d = 3$ in **0.16s**!
- OBBT is very costly (2n SDPs to solve)
- OBBT with order $d = 1.5$ is still too high for challenging problems from the MINLPLib, does not improve lower bound significantly

$\longrightarrow$ applying advanced strategies to save OBBT ?

Outlook

- Further improvement of feasibility pump and OBBT
- Development of a Branch-and-Bound algorithm with the moment/sos hierarchy as main relaxation method
- Integration of moment/sos hierarchy into existing Branch-and-Bound frameworks

Thank you!

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