On Convex Lower-Level Black-Box Constraints in Bilevel Optimization with an Application to Gas Market Models with Chance Constraints

Holger Heitsch, René Henrion, Thomas Kleinert, **Martin Schmidt**

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Overview

General Setting and Some Obstacles

Bilevel Optimization

$$\begin{aligned} \min_{x,y} \quad & F(x,y) \\ \text{s.t.} \quad & G(x,y) \leq 0 \\ & x \in \mathbb{R}^{n_x}, \quad y \in \mathbb{R}^{n_y} \\ & y \in S(x) \end{aligned}$$

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$S(x)$ is the solution set of the convex lower-level problem

$$S(x) = \arg\min_y \left\{ f(x, y) \colon g(x, y) \leq 0, \ y \in \mathbb{R}^{n_y} \right\}$$

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- NP-hard problem in general (Hansen, Jaumard, Savard 1992)
- Optimistic variant (Dempe 2002)

Black-Box Constraint in the Lower Level

A “small” extension

$$S(x) = \arg\min_{y} \left\{ f(x,y) \colon g(x,y) \le 0,\ b(y) \le 0,\ y \in \mathbb{R}^{n_y} \right\}$$

Black-Box Constraint in the Lower Level

A "small" extension

$$S(x) = \arg\min_{y} \left\{ f(x,y) : g(x,y) \le 0,\ b(y) \le 0,\ y \in \mathbb{R}^{n_y} \right\}$$

Assumption

The black-box function b is convex and for all $(x,y) \in \{(x,y) : G(x,y) \le 0,\ g(x,y) \le 0\}$ ...

1. we can evaluate the function $b(y)$,
2. we can evaluate the gradient $\nabla b(y)$,
3. the gradient is bounded, i.e., $\|\nabla b(y)\| \le K$ for a fixed $K \in \mathbb{R}$.

Some Notation & Single-Level Reformulation

- Shared constraint set

$$\Omega := \{(x, y) \colon G(x, y) \leq 0,\ g(x, y) \leq 0,\ b(y) \leq 0\}$$

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- Optimal value function of the lower level

$$\varphi(x) = \min_y \{f(x,y)\colon g(x,y),\ b(y) \le 0,\ y \in \mathbb{R}^{n_y}\}$$

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Obstacles and Pitfalls

- Main challenge: black-box constraint $b(y) \leq 0$
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  - Outer approximation (Duran, Grossmann 1986; Fletcher, Leyffer 1994)

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- Possible remedies
  - Cutting plane techniques (Kelley 1960)
  - Outer approximation (Duran, Grossmann 1986; Fletcher, Leyffer 1994)
- But: $b(y) \leq 0$ can only by satisfied up to a prescribed tolerance
- Specifying the quality of solutions via ε-δ-optimality
  - Global optimization (Locatelli, Schoen 2013)
  - Bilevel optimization (Mitsos, Lemonidis, Barton 2008)

Definition

For $\delta = (\delta_G, \delta_g, \delta_b, \delta_f) \in \mathbb{R}^{m_u+m_\ell+2}_{\geq 0}$, a point $(\bar{x}, \bar{y}) \in \mathbb{R}^{n_x} \times \mathbb{R}^{n_y}$ is called δ-feasible for the bilevel problem, if $G(\bar{x}, \bar{y}) \leq \delta_G$, $g(\bar{x}, \bar{y}) \leq \delta_g$, $b(y) \leq \delta_b$, and $f(x, y) \leq \varphi(x) + \delta_f$ hold. Moreover, for $\varepsilon \geq 0$, a point $(x^*, y^*) \in \mathbb{R}^{n_x} \times \mathbb{R}^{n_y}$ is called ε-δ-optimal for the bilevel problem, if it is δ-feasible and if $F(x^*, y^*) \leq F^* + \varepsilon$ holds, with F^* denoting the optimal objective function value of the bilevel problem.

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- A δ-feasible point $(\bar{x}, \bar{y})$ is δ_f-(δ_g, δ_b)-optimal for the lower level with fixed $x = \bar{x}$
- Assume f and g pose no challenges $\to$ choose $\delta_f = \delta_g = 0$
- Assume F and G pose no challenges $\to$ we can obtain 0-δ-optimal solutions with $\delta = (0, 0, \delta_b, 0)$

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- Consider the relaxed lower-level problem

$$\min_{y \in \mathbb{R}^{n_y}} \quad f(\bar{x}, y) \quad \text{s.t.} \quad g(\bar{x}, y) \leq 0, \; b(y) \leq \delta_b$$

- Denote the optimal value function by $\underline{\varphi}(x)$
- Relaxation property yields $\underline{\varphi}(x) \leq \varphi(x)$ for all feasible $x \in \Omega_{\text{u}}$

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- If $\underline{\varphi}(x) < \varphi(x)$ holds for any $x \in \Omega_{\mathrm{u}}$, this single-level reformulation is not a relaxation of the original single-level reformulation

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Can we hope for the δ-feasible points with $\delta = (0, 0, \delta_b, 0)$?

A “First-Relax-Then-Reformulate” Approach

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- Block-box constraint $b(y) \geq 0$ is convex
- Construct a sequence of linear outer approximations $(E^r, e^r)_{r \in \mathbb{N}}$ of the black-box constraint $b(y) \leq 0$ with the property

$$\{y \in \mathbb{R}^{n_y} : b(y) \leq 0\} \subseteq \{y \in \mathbb{R}^{n_y} : E^{r+1} y \leq e^{r+1}\} \subseteq \{y \in \mathbb{R}^{n_y} : E^r y \leq e^r\}$$

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Proposition

For every $r \in \mathbb{N}$ and every upper-level decision $x \in \Omega_{\mathrm{u}}$, it holds

$$\underline{\varphi}^r(x) \leq \underline{\varphi}^{r+1}(x) \leq \varphi(x)$$

A "First-Relax-Then-Reformulate" Approach

Modified variant of the single-level reformulation

$$
\begin{aligned}
\min_{x,y} \quad & F(x,y) \\
\text{s.t.} \quad & G(x,y) \leq 0, \quad g(x,y) \leq 0 \\
& E^r y \leq e^r \\
& f(x,y) \leq \underline{\varphi}^r(x) \\
& x \in \mathbb{R}^{n_x}, \quad y \in \mathbb{R}^{n_y}
\end{aligned}
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$$\begin{aligned} \min_{x,y} \quad & F(x,y) \\ \text{s.t.} \quad & G(x,y) \leq 0, \quad g(x,y) \leq 0 \\ & E^r y \leq e^r \\ & f(x,y) \leq \underline{\varphi}^r(x) \\ & x \in \mathbb{R}^{n_x}, \quad y \in \mathbb{R}^{n_y} \end{aligned}$$

Feasibility problem

$$\begin{aligned} \min_{x,y,s} \quad & s \\ \text{s.t.} \quad & G(x,y) \leq 0, \quad g(x,y) \leq 0 \\ & E^r y \leq e^r \\ & f(x,y) \leq \underline{\varphi}^r(x) + s \\ & x \in \mathbb{R}^{n_x}, \quad y \in \mathbb{R}^{n_y} \end{aligned}$$

Algorithm 1 "First-Relax-Then-Reformulate".

```
Choose δ_b > 0, set r = 0, s = 0, χ = ∞, E^0 = [0 ... 0] ∈ ℝ^{1×n_y}, e^0 = 0 ∈ ℝ.
while χ > δ_b or s > 0 do
    Construct E^{r+1} and e^{r+1}
    if the modified variant of the single-level reformulation is feasible then
        Solve this problem to obtain (x^{r+1}, y^{r+1}) and set s = 0.
    else if the feasibility problem is feasible then
        Solve this problem to obtain (x^{r+1}, y^{r+1}, s).
    else
        Return "The original problem is infeasible.".
    end if
    Set r ← r + 1 and χ = b(y^r).
end while
Return (x̄, ȳ) = (x^r, y^r).
```

Algorithm 2 "First-Relax-Then-Reformulate".

Choose $\delta_b > 0$, set $r = 0$, $s = 0$, $\chi = \infty$, $E^0 = [0 \dots 0] \in \mathbb{R}^{1 \times n_y}$, $e^0 = 0 \in \mathbb{R}$.
while $\chi > \delta_b$ or $s > 0$ **do**
  Construct E^{r+1} and e^{r+1}
  if the modified variant of the single-level reformulation is feasible **then**
    Solve this problem to obtain (x^{r+1}, y^{r+1}) and set $s = 0$.
  else if the feasibility problem is feasible **then**
    Solve this problem to obtain (x^{r+1}, y^{r+1}, s).
  else
    Return "The original problem is infeasible.".
  end if
  Set $r \leftarrow r + 1$ and $\chi = b(y^r)$.
end while
Return $(\bar{x}, \bar{y}) = (x^r, y^r)$.

Theorem: If Algorithm 1 terminates, then $(\bar{x}, \bar{y})$ is $(0, 0, \delta_b, 0)$-feasible for original bilevel problem.

A European Gas Market Model with Chance Constraints

Level 4 TSO cost-optimally transports the given nominations

Level 3 Traders nominate at a day-ahead market

Level 2 Traders book, i.e., sign mid- to long-term capacity contracts

Level 1 TSO announces technical capacities and booking price floors

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Grimm, Schewe, S., Zöttl (2019)

- Four-level modeling of the European entry-exit gas market
- Identification of assumptions that allow to simplify the model
- Perfect competition $\rightarrow$ reduction to a bilevel model

Bilevel Modeling Under Perfect Competition: Upper Level

$$\begin{aligned}
\max_{q^{\mathrm{TC}}, \underline{\pi}^{\mathrm{book}}, \pi, q} \quad & \varphi^{\mathrm{u}}(q^{\mathrm{nom}}, q) = \sum_{t \in T} \left(\sum_{i \in \mathcal{P}_-} \int_0^{q^{\mathrm{nom}}_{i,t}} P_{i,t}(s) \,\mathrm{d}s - \sum_{i \in \mathcal{P}_+} c_i^{\mathrm{var}} q^{\mathrm{nom}}_{i,t} \right) - \sum_{t \in T} \sum_{a \in A} c^{\mathrm{trans}}(q_{a,t}) \\
\text{s.t.} \quad & 0 \le q^{\mathrm{TC}}_u, \; 0 \le \underline{\pi}^{\mathrm{book}}_u \quad \text{for all } u \in V_+ \cup V_- \\
& \sum_{u \in V_+ \cup V_-} \sum_{i \in \mathcal{P}_u} \underline{\pi}^{\mathrm{book}}_u q^{\mathrm{book}}_i = \sum_{t \in T} \sum_{a \in A} c^{\mathrm{trans}}(q_{a,t}) \\
& (\pi, q) \in \mathcal{F}(q^{\mathrm{nom}}) \\
& (q^{\mathrm{book}}, q^{\mathrm{nom}}) \in \operatorname*{arg\,max} \{ \text{ lower-level problem } \}
\end{aligned}$$

$$
\begin{aligned}
\max_{q^{\text{book}},q^{\text{nom}}} \quad & \sum_{t \in T} \left(\sum_{i \in \mathcal{P}_-} \int_0^{q_{i,t}^{\text{nom}}} P_{i,t}(s)\,\mathrm{d}s - \sum_{i \in \mathcal{P}_+} c_i^{\text{var}} q_{i,t}^{\text{nom}} \right) - \sum_{u \in V_+ \cup V_-} \sum_{i \in \mathcal{P}_u} \underline{\pi}_u^{\text{book}} q_i^{\text{book}} \\
\text{s.t.} \quad & \sum_{i \in \mathcal{P}_u} q_i^{\text{book}} \le q_u^{\text{TC}} \quad \text{for all } u \in V_+ \cup V_- \\
& 0 \le q_{i,t}^{\text{nom}} \le q_i^{\text{book}} \quad \text{for all } i \in \mathcal{P}_- \cup \mathcal{P}_+,\ t \in T \\
& \sum_{i \in \mathcal{P}_-} q_{i,t}^{\text{nom}} - \sum_{i \in \mathcal{P}_+} q_{i,t}^{\text{nom}} = 0 \quad \text{for all } t \in T
\end{aligned}
$$

Probabilistic Extension

- In reality, exit players $i \in \mathcal{P}_-$ nominate quantities $q_{i,t}^{\text{nom}}$ without exactly knowing the actual load $\xi_{i,t}$
- Load vector $\xi = (\xi_{i,t})_{i \in \mathcal{P}_-, t \in T}$ with log-concave cumulative distribution function
- In particular: $\xi \sim \mathcal{N}(m, \Sigma)$
- Modeling assumption: the TSO imposes a fee μ on the exit players $i \in \mathcal{P}_-$ to ensure that the realized loads are covered up to a specified safety level $p \in [0, 1]$
- Joint (over all times and exit players) probabilistic constraint

$$\mathbb{P}\left(\xi_{i,t} \leq q_{i,t}^{\text{nom}} \text{ for all } i \in \mathcal{P}_-,\ t \in T\right) \geq p$$

- Log-concavity of the Gaussian distribution function implies that the log-transformed probabilistic load coverage constraint

$$h(q_-^{\text{nom}}) := \log p - \log \mathbb{P}\left(\xi_{i,t} \leq q_{i,t}^{\text{nom}} \text{ for all } i \in \mathcal{P}_-,\ t \in T\right) \leq 0$$

is convex

In iteration r, the lower-level relaxation reads

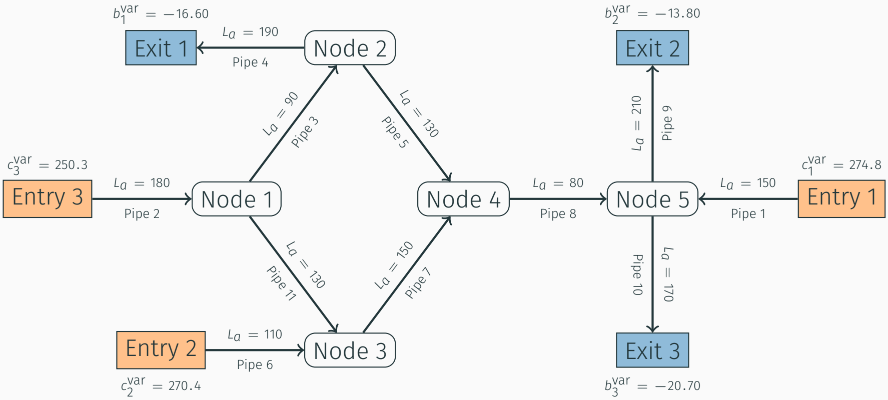
$$
\begin{aligned}
\max_{q^{\text{book}},q^{\text{nom}}} \quad & \sum_{t\in T}\left(\sum_{i\in\mathcal{P}_-}\int_0^{q_{i,t}^{\text{nom}}} P_{i,t}(s)\,\mathrm{ds} - \sum_{i\in\mathcal{P}_+} c_i^{\text{var}} q_{i,t}^{\text{nom}}\right) - \sum_{u\in V_+\cup V_-}\sum_{i\in\mathcal{P}_u} \underline{\pi}_u^{\text{book}} q_i^{\text{book}} \\
\text{s.t.} \quad & \sum_{i\in\mathcal{P}_u} q_i^{\text{book}} \le q_u^{\text{TC}}, \quad u\in V_+\cup V_- \\
& 0 \le q_{i,t}^{\text{nom}} \le q_i^{\text{book}}, \quad i\in\mathcal{P}_+\cup\mathcal{P}_-,\ t\in T \\
& \sum_{i\in\mathcal{P}_-} q_{i,t}^{\text{nom}} - \sum_{i\in\mathcal{P}_+} q_{i,t}^{\text{nom}} = 0, \quad t\in T \\
& h(q_-^j) + \nabla_{q_-^{\text{nom}}} h(q_-^j)^\top (q_-^{\text{nom}} - q_-^j) \le 0, \quad j=1,\dots,r
\end{aligned}
$$

Back to the “First-Relax-Then-Reformulate” Approach

- This lower-level problem is convex and satisfies Slater’s CQ
- Take its KKT conditions $\rightarrow$ MPCC as a single-level reformulation
- Linearize the KKT complementarity conditions using binary variables and big-Ms
- Single-level reformulation is a mixed-integer and concave maximization problem with bilinear (and thus nonconvex) equality constraints
- Can be solved with spatial branching …
- … but it’s challenging!
- See the paper for the details
  - Verification of Slater’s CQ
  - Provably correct big-Ms
  - Further quantile and other cuts
  - Further bounding techniques to obtain ex-post optimality certificates

Numerical Results

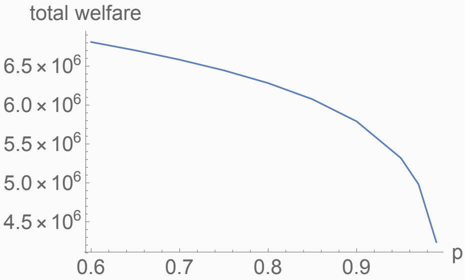
The Test Network

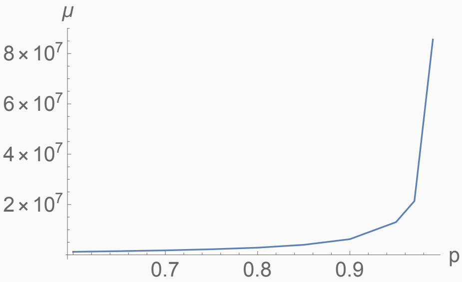


Numerical Results

	Bisection	Bounding		δ-Feasibility		Total		
p	Runtime	#Iter.	Runtime	#Iter.	Runtime	#Iter.	Runtime	Gap
0.60	12.13	32	36.80	10	28.97	42	77.9	0.001
0.65	14.15	28	32.00	16	40.71	44	86.86	0.001
0.70	11.13	26	29.70	13	39.70	39	80.53	0.001
0.75	9.04	25	28.55	6	14.19	31	51.78	0.002
0.80	7.98	25	29.06	4	6.26	29	43.3	0.005
0.85	11.08	21	24.01	3	7.41	24	42.5	0.006
0.90	11.05	23	26.34	8	27.52	31	64.91	0.017
0.95	5.96	24	27.99	6	14.14	30	48.09	0.010
0.96	7.56	22	24.56	3	4.17	25	36.29	0.011
0.97	6.94	21	23.96	4	9.20	25	40.10	0.015
0.98	4.63	25	93.68	9	106.31	34	204.62	0.032
0.99	6.96	26	29.76	10	1250.65	36	1287.37	0.187

Total Welfare and Price of Load Coverage





That's It!

SCAN ME

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- Algorithm to compute δ-feasible points
- Relevant application for chance-constrained modeling of the EU gas market
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Stay healthy!