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

A “First-Relax-Then-Reformulate” Approach

A European Gas Market Model with Chance Constraints

Numerical Results
General Setting and Some Obstacles
Bilevel Optimization

\[
\min_{x,y} \quad F(x, y) \\
\text{s.t.} \quad G(x, y) \leq 0 \\
x \in \mathbb{R}^{n_x}, \quad y \in \mathbb{R}^{n_y} \\
y \in S(x)
\]
Bilevel Optimization

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\begin{align*}
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\end{align*}
\]

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

\[
S(x) = \arg\min_y \{ f(x,y) : g(x,y) \leq 0, \quad y \in \mathbb{R}^{n_y} \}
\]

- NP-hard problem in general (Hansen, Jaumard, Savard 1992)
- Optimistic variant (Dempe 2002)
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A “small” extension

\[ S(x) = \arg \min_y \{ f(x, y) : g(x, y) \leq 0, \ b(y) \leq 0, \ y \in \mathbb{R}^n \} \]
A “small” extension

\[ S(x) = \underset{y}{\text{arg min}} \{ f(x, y) : g(x, y) \leq 0, \ b(y) \leq 0, \ y \in \mathbb{R}^n \} \]

**Assumption**

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

1. we can evaluate the function \( b(y) \),
2. we can evaluate the gradient \( \nabla b(y) \),
3. the gradient is bounded, i.e., \( \| \nabla b(y) \| \leq K \) for a fixed \( K \in \mathbb{R} \).
Some Notation & Single-Level Reformulation

• Shared constraint set

\[ \Omega := \{(x, y): G(x, y) \leq 0, \ g(x, y) \leq 0, \ b(y) \leq 0\} \]
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- Projection onto the decision space of the leader
  \[ \Omega_u := \{ x : \exists y \text{ with } (x, y) \in \Omega \} \]
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- Feasible set of the lower-level problem for a fixed leader decision \( x = \bar{x} \)
  \[ \Omega_\ell(\bar{x}) := \{y: g(\bar{x}, y) \leq 0, \ b(y) \leq 0\} \]
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• Optimal value function of the lower level

$$\varphi(x) = \min_y \{f(x,y): g(x,y), \ b(y) \leq 0, \ y \in \mathbb{R}^{n_y}\}$$
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- Single-level reformulation
  \[ \min_{x, y} \ F(x, y) \]
  \[ \text{s.t. } G(x, y) \leq 0, \ g(x, y) \leq 0, \ b(y) \leq 0 \]
  \[ f(x, y) \leq \varphi(x) \]
  \[ x \in \mathbb{R}^{n_x}, \ y \in \mathbb{R}^{n_y} \]
Obstacles and Pitfalls

- **Main challenge:** black-box constraint $b(y) \leq 0$
- **Not given explicitly** → optimality conditions are not given explicitly as well
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- **Possible remedies**
  - Cutting plane techniques (Kelley 1960)
  - Outer approximation (Duran, Grossmann 1986; Fletcher, Leyffer 1994)
Obstacles and Pitfalls

- **Main challenge**: black-box constraint \( b(y) \leq 0 \)
- **Not given explicitly** → optimality conditions are not given explicitly as well
- **Possible remedies**
  - Cutting plane techniques (Kelley 1960)
  - Outer approximation (Duran, Grossmann 1986; Fletcher, Leyffer 1994)
- **But**: \( b(y) \leq 0 \) can only be satisfied up to a prescribed tolerance
- **Specifying the quality of solutions via \( \varepsilon\)-\( \delta \)-optimality**
  - Global optimization (Locatelli, Schoen 2013)
  - Bilevel optimization (Mitsos, Lemonidis, Barton 2008)
Definition
For \( \delta = (\delta_G, \delta_g, \delta_b, \delta_f) \in \mathbb{R}_{\geq 0}^{mu+mf+2} \), a point \((\bar{x}, \bar{y}) \in \mathbb{R}^{nx} \times \mathbb{R}^{ny}\) is called \( \delta \)-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 \((x^*, y^*) \in \mathbb{R}^{nx} \times \mathbb{R}^{ny}\) is called \( \varepsilon-\delta \)-optimal for the bilevel problem, if it is \( \delta \)-feasible and if \( F(x^*, y^*) \leq F^* + \varepsilon \) holds, with \( F^* \) denoting the optimal objective function value of the bilevel problem.
\(\varepsilon, \delta\)-Optimality

**Definition**
For \(\delta = (\delta_G, \delta_g, \delta_b, \delta_f) \in \mathbb{R}^{m_u + m_e + 2}\), a point \((\bar{x}, \bar{y}) \in \mathbb{R}^{n_x} \times \mathbb{R}^{n_y}\) is called \(\delta\)-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 \(\varepsilon, \delta\)-optimal for the bilevel problem, if it is \(\delta\)-feasible and if \(F(x^*, y^*) \leq F^* + \varepsilon\) holds, with \(F^*\) denoting the optimal objective function value of the bilevel problem.

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

- Consider the relaxed lower-level problem
  $$\min_{y \in \mathbb{R}^n} f(\bar{x}, y) \quad \text{s.t.} \quad g(\bar{x}, y) \leq 0, \quad b(y) \leq \delta_b$$

- Denote the optimal value function by $\bar{\varphi}(x)$

- Relaxation property yields $\bar{\varphi}(x) \leq \varphi(x)$ for all feasible $x \in \Omega_u$

- It is not clear whether and how $\varepsilon$-$\delta$-optimality can be guaranteed

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

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- Relaxation property yields \(\bar{\varphi}(x) \leq \varphi(x)\) for all feasible \(x \in \Omega_u\)
- First-relax-then-reformulate leads to a single-level problem with \(f(x, y) \leq \bar{\varphi}(x)\)
- If \(\bar{\varphi}(x) < \varphi(x)\) holds for any \(x \in \Omega_u\), this single-level reformulation is not a relaxation of the original single-level reformulation
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0-\(\delta\)-optimal solutions with \(\delta = (0, 0, \delta_b, 0)\)?

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Can we hope for the \(\delta\)-feasible points with \(\delta = (0, 0, \delta_b, 0)\)?
A “First-Relax-Then-Reformulate” Approach
A “First-Relax-Then-Reformulate” Approach

- 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

$$\{y \in \mathbb{R}^{ny} : b(y) \leq 0\} \subseteq \{y \in \mathbb{R}^{ny} : E^{r+1}y \leq e^{r+1}\} \subseteq \{y \in \mathbb{R}^{ny} : E^ry \leq e^r\}$$
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- For a given upper-level solution $\bar{x} \in \Omega_u$ and $r \in \mathbb{N}$, the adapted lower-level problem reads

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

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- $\bar{\varphi}^r(x)$: optimal value function
- Assumption: Slater’s constraint qualification holds
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- \( \varphi^r(x) \): optimal value function
- Assumption: Slater’s constraint qualification holds

**Proposition**

For every \( r \in \mathbb{N} \) and every upper-level decision \( x \in \Omega_u \), it holds

\[
\varphi^r(x) \leq \varphi^{r+1}(x) \leq \varphi(x)
\]
A “First-Relax-Then-Reformulate” Approach

Modified variant of the single-level reformulation

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

Feasibility problem

\[
\begin{align*}
\min_{x,y,s} & \quad s \\
\text{s.t.} & \quad G(x, y) \leq 0, \quad g(x, y) \leq 0 \\
& \quad E^r y \leq e^r \\
& \quad f(x, y) \leq \varphi^r(x) + s \\
& \quad x \in \mathbb{R}^{n_x}, \quad y \in \mathbb{R}^{n_y}
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Algorithm 1 “First-Relax-Then-Reformulate”.

1: Choose $\delta_b > 0$, set $r = 0$, $s = 0$, $\chi = \infty$, $E^0 = [0 \ldots 0] \in \mathbb{R}^{1 \times ny}$, $e^0 = 0 \in \mathbb{R}$.
2: while $\chi > \delta_b$ or $s > 0$ do
3: Construct $E^{r+1}$ and $e^{r+1}$
4: if the modified variant of the single-level reformulation is feasible then
5: Solve this problem to obtain $(x^{r+1}, y^{r+1})$ and set $s = 0$.
6: else if the feasibility problem is feasible then
7: Solve this problem to obtain $(x^{r+1}, y^{r+1}, s)$.
8: else
9: Return “The original problem is infeasible.”.
10: end if
11: Set $r \leftarrow r + 1$ and $\chi = b(y^r)$.
12: end while
13: 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.
Algorithm 2 “First-Relax-Then-Reformulate”.

1: Choose $\delta_b > 0$, set $r = 0$, $s = 0$, $\chi = \infty$, $E^0 = [0 \ldots 0] \in \mathbb{R}^{1 \times ny}$, $e^0 = 0 \in \mathbb{R}$.
2: while $\chi > \delta_b$ or $s > 0$ do
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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 → reduction to a bilevel model
Bilevel Modeling Under Perfect Competition: Upper Level

$$\max_{q^U, q^W, \pi^U, \pi^W} \varphi^u(q^\text{nom}, q) = \sum_{t \in T} \left( \sum_{i \in \mathcal{P}_-} \int_0^{q^\text{nom}_{i,t}} p_{i,t}(s) \, ds - \sum_{i \in \mathcal{P}_+} c_i \varphi^\text{var}_{q^\text{nom}_{i,t}} \right) - \sum_{t \in T} \sum_{a \in \mathcal{A}} c^\text{trans}(q_{a,t})$$

s.t. $0 \leq q^U_w, 0 \leq \pi^U_w$ for all $u \in V_+ \cup V_-$

$$\sum_{u \in V_+ \cup V_-} \sum_{i \in \mathcal{P}_u} \pi^\text{book}_u q^\text{book}_i = \sum_{t \in T} \sum_{a \in \mathcal{A}} c^\text{trans}(q_{a,t})$$

$$(\pi, q) \in \mathcal{F}(q^\text{nom})$$

$$(q^\text{book}, q^\text{nom}) \in \arg \max \{ \text{lower-level problem} \}$$
Bilevel Modeling Under Perfect Competition: Lower Level

\[
\begin{align*}
\max_{q^{\text{book}, q^{\text{nom}}}} \quad & \sum_{t \in T} \left( \sum_{i \in P_-} \int_0^{q_{i,t}^{\text{nom}}} P_i(t(s)) \, ds - \sum_{i \in P_+} c_i\var q_{i,t}^{\text{nom}} \right) - \sum_{u \in V_+ \cup V_-} \sum_{i \in P_u} \pi^u_{\text{book}} q_i^{\text{book}} \\
\text{s.t.} \quad & \sum_{i \in P_u} q_i^{\text{book}} \leq q_u^{\text{TC}} \quad \text{for all } u \in V_+ \cup V_- \\
& 0 \leq q_{i,t}^{\text{nom}} \leq q_{i,t}^{\text{book}} \quad \text{for all } i \in P_- \cup P_+, \ t \in T \\
& \sum_{i \in P_-} q_{i,t}^{\text{nom}} - \sum_{i \in P_+} q_{i,t}^{\text{nom}} = 0 \quad \text{for all } t \in T
\end{align*}
\]
• 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 $\mu$ 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

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

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

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

is convex
In iteration $r$, the lower-level relaxation reads

$$
\max_{q_{\text{book}}, q_{\text{nom}}} \sum_{t \in T} \left( \sum_{i \in \mathcal{P}} \int_{0}^{q_{i,t}^{\text{nom}}} P_{i,t}(s) \, ds - \sum_{i \in \mathcal{P}_+} c_{i}^{\text{var}} q_{i,t}^{\text{nom}} \right) - \sum_{u \in V_+ \cup V_-} \sum_{i \in \mathcal{P}_u} \pi_{u}^{\text{book}} q_{i}^{\text{book}}
$$

s.t. \quad \sum_{i \in \mathcal{P}_u} q_{i}^{\text{book}} \leq q_{u}^{\text{TC}}, \quad u \in V_+ \cup V_-

\begin{align*}
0 & \leq q_{i,t}^{\text{nom}} \leq q_{i}^{\text{book}}, \quad i \in \mathcal{P}_+ \cup \mathcal{P}_- , \quad 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})^{T} (q_{\text{nom}}^{j} - q_{-}^{j}) & \leq 0, \quad j = 1, \ldots, r
\end{align*}
Back to the “First-Relax-Then-Reformulate” Approach

• This lower-level problem is convex and satisfies Slater’s CQ
• Take its KKT conditions → 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

\[
\begin{align*}
\text{Entry 1} & \quad \text{Exit 1} \\
\text{Node 2} & \quad \text{Node 3} \\
\text{Node 1} & \quad \text{Node 4} \\
\text{Node 5} & \quad \text{Entry 1} \\
\end{align*}
\]

Variables:

\[
\begin{align*}
\text{var}_1 &= 274.8 \\
\text{var}_2 &= 270.4 \\
\text{var}_3 &= 250.3 \\
\end{align*}
\]

Pipe Lengths (La):

\[
\begin{align*}
\text{Pipe 1} &: \quad \text{La} = 190 \\
\text{Pipe 2} &: \quad \text{La} = 180 \\
\text{Pipe 3} &: \quad \text{La} = 90 \\
\text{Pipe 4} &: \quad \text{La} = 190 \\
\text{Pipe 5} &: \quad \text{La} = 130 \\
\text{Pipe 6} &: \quad \text{La} = 110 \\
\text{Pipe 7} &: \quad \text{La} = 70 \\
\text{Pipe 8} &: \quad \text{La} = 80 \\
\text{Pipe 9} &: \quad \text{La} = 210 \\
\text{Pipe 10} &: \quad \text{La} = 150 \\
\text{Pipe 11} &: \quad \text{La} = 130 \\
\end{align*}
\]

Pipe Variances (b):

\[
\begin{align*}
b_1 &= -16.60 \\
b_2 &= -13.80 \\
b_3 &= -20.70 \\
\end{align*}
\]
### Numerical Results

| $p$  | Bisection | Bounding | $\delta$-Feasibility | Total |
|------|-----------|----------|-----------------------|-------|
|      | Runtime   | #Iter.   | Runtime               |       |
| 0.60 | 12.13     | 32       | 36.80                 | 77.9  |
| 0.65 | 14.15     | 28       | 32.00                 | 86.86 |
| 0.70 | 11.13     | 26       | 29.70                 | 80.53 |
| 0.75 | 9.04      | 25       | 28.55                 | 51.78 |
| 0.80 | 7.98      | 25       | 29.06                 | 43.3  |
| 0.85 | 11.08     | 21       | 24.01                 | 42.5  |
| 0.90 | 11.05     | 23       | 26.34                 | 64.91 |
| 0.95 | 5.96      | 24       | 27.99                 | 48.09 |
| 0.96 | 7.56      | 22       | 24.56                 | 36.29 |
| 0.97 | 6.94      | 21       | 23.96                 | 40.10 |
| 0.98 | 4.63      | 25       | 93.68                 | 204.62|
| 0.99 | 6.96      | 26       | 29.76                 | 1287.37|

|      | #Iter.   | Runtime   | #Iter. | Runtime | Gap   |
|------|---------|-----------|--------|---------|-------|
| 0.60 | 10      | 28.97     | 42     | 77.9    | 0.001 |
| 0.65 | 16      | 40.71     | 44     | 86.86   | 0.001 |
| 0.70 | 13      | 39.70     | 39     | 80.53   | 0.001 |
| 0.75 | 6       | 14.19     | 31     | 51.78   | 0.002 |
| 0.80 | 4       | 6.26      | 29     | 43.3    | 0.005 |
| 0.85 | 3       | 7.41      | 24     | 42.5    | 0.006 |
| 0.90 | 8       | 27.52     | 31     | 64.91   | 0.017 |
| 0.95 | 6       | 14.14     | 30     | 48.09   | 0.010 |
| 0.96 | 3       | 4.17      | 25     | 36.29   | 0.011 |
| 0.97 | 4       | 9.20      | 25     | 40.10   | 0.015 |
| 0.98 | 9       | 106.31    | 34     | 204.62  | 0.032 |
| 0.99 | 10      | 1250.65   | 36     | 1287.37 | 0.187 |
Total Welfare and Price of Load Coverage
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• Algorithm to compute $\delta$-feasible points
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Stay healthy!