Problem-based optimal scenario generation for linear two-stage stochastic programs

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Introduction

Many stochastic programming models are of the general form

$$\text{(SP)} \qquad \min\left\{ \int_{\Xi} f_0(x,\xi)P(d\xi) : x \in X,\ \int_{\Xi} f_1(x,\xi)P(d\xi) \le 0 \right\}$$

where X is a closed subset of $\mathbb{R}^m$, Ξ a closed subset of $\mathbb{R}^s$, P is a Borel probability measure on Ξ abbreviated by $P \in \mathcal{P}(\Xi)$. The functions f_0 and f_1 from $\mathbb{R}^m \times \Xi$ to the extended reals $\overline{\mathbb{R}} = [-\infty, \infty]$ are normal integrands.
For general continuous multivariate probability distributions P the evaluation of the objective or constraint functions is known to be $\#\,P$-hard in general.

Many approaches to their computational solution are based on finding a discrete probability measure P_n in

$$\mathcal{P}_n(\Xi) := \left\{ \sum_{i=1}^{n} p_i \delta_{\xi^i} : \xi^i \in \Xi,\ p_i \ge 0,\ i = 1,\ldots,n,\ \sum_{i=1}^{n} p_i = 1 \right\}$$

for some $n \in \mathbb{N}$, which approximates P at least such that the corresponding optimal values of (SP) are close. The atoms ξ^i, $i = 1,\ldots,n$, of P_n are often called scenarios in this context.

Typical integrands in linear two-stage stochastic programming models are

$$f_0(x,\xi) = \begin{cases} g(x) + \Phi(q(\xi), h(x,\xi)) & , q(\xi) \in D \\ +\infty & , \text{else} \end{cases} \quad \text{and} \quad f_1(x,\xi) \equiv 0,$$

where X and Ξ are convex polyhedral, $g(\cdot)$ is a linear function, $q(\cdot)$ is affine, $D = \{q \in \mathbb{R}^{\bar{m}} : \{z \in \mathbb{R}^r : W^\top z \leq q\} \neq \emptyset\}$ denotes the convex polyhedral dual feasibility set, $h(\cdot,\xi)$ is affine for fixed ξ and $h(x,\cdot)$ is affine for fixed x, and Φ denotes the infimal function of the linear (second-stage) optimization problem

$$\Phi(q,t) := \inf\{\langle q, y\rangle : Wy = t, y \geq 0\}$$

with $(r, \bar{m})$ matrix W.

Typical integrands f_1 appearing in chance constrained programming are

$$f_1(x,\xi) = p - \mathbb{1}_{\mathcal{P}(x)}(\xi),$$

where $p \in (0,1)$ is a probability level and $\mathbf{1}_{\mathcal{P}(x)}$ is the characteristic function of the polyhedron $\mathcal{P}(x) = \{\xi \in \Xi : h(x,\xi) \leq 0\}$ depending on x, where Ξ and h have the same properties as above.

Stability-based scenario generation

Let $v(P)$ and $S(P)$ denote the infimum and solution set of (SP). We are interested in their dependence on the underlying probability distribution P.

To state a stability result we introduce the following sets of functions and of probability distributions (both defined on Ξ)

$$\mathcal{F} = \{f_j(x,\cdot) : j = 0, 1,\ x \in X\},$$
$$\mathcal{P}_{\mathcal{F}} = \Big\{Q \in \mathcal{P}(\Xi) : -\infty < \int_{\Xi} \inf_{x \in X} f_j(x,\xi)Q(d\xi), \sup_{x \in X} \int_{\Xi} f_j(x,\xi)Q(d\xi) < +\infty, \forall j\Big\}$$

and the (pseudo-) distance on $\mathcal{P}_{\mathcal{F}}$

$$d_{\mathcal{F}}(P,Q) = \sup_{f \in \mathcal{F}} \Big| \int_{\Xi} f(\xi)(P-Q)(d\xi) \Big| \quad (P, Q \in \mathcal{P}_{\mathcal{F}}).$$

For typical applications like for linear two-stage and chance constrained models, the sets $\mathcal{P}_{\mathcal{F}}$ or appropriate subsets allow a simpler characterization, for example, as subsets of $\mathcal{P}(\Xi)$ satisfying certain moment conditions.

Proposition: We consider (SP) for $P \in \mathcal{P}_{\mathcal{F}}$, assume that X is compact and

(i) the function $x \to \int_{\Xi} f_0(x,\xi)P(d\xi)$ is Lipschitz continuous on X,

(ii) the set-valued mapping $y \rightrightarrows \left\{x \in X : \int_{\Xi} f_1(x,\xi)P(d\xi) \leq y\right\}$ satisfies the Aubin property at $(0,\bar{x})$ for each $\bar{x} \in S(P)$.

Then there exist constants $L > 0$ and $\delta > 0$ such that the estimates

$$\begin{aligned} |v(P) - v(Q)| &\leq L\, d_{\mathcal{F}}(P,Q) \\ \sup_{x \in S(Q)} d(x, S(P)) &\leq \Psi_P(L\, d_{\mathcal{F}}(P,Q)) \end{aligned}$$

hold whenever $Q \in \mathcal{P}_{\mathcal{F}}$ and $d_{\mathcal{F}}(P,Q) < \delta$. The real-valued function Ψ_P is given by $\Psi_P(r) = r + \psi_P^{-1}(2r)$ for all $r \in \mathbb{R}_+$, where ψ_P is the growth function

$$\psi_P(\tau) = \inf_{x \in X} \left\{ \int_{\Xi} f_0(x,\xi)P(d\xi) - v(P) : d(x, S(P)) \geq \tau,\ x \in X, \int_{\Xi} f_1(x,\xi)P(d\xi) \leq 0 \right\}.$$

In case $f_1 \equiv 0$ only lower semicontinuity is needed in (i) and the estimates hold with $L = 1$ and for any $\delta > 0$. Furthermore, Ψ_P is lower semicontinuous and increasing on $\mathbb{R}_+$ with $\Psi_P(0) = 0$. (Rachev-Römisch 02)

The stability result suggests to choose discrete approximations from $\mathcal{P}_n(\Xi)$ for solving (SP) such that they solve the best approximation problem

$$\text{(OSG)} \qquad \min_{P_n \in \mathcal{P}_n(\Xi)} d_{\mathcal{F}}(P, P_n)\,.$$

at least approximately. Determining the scenarios of some solution to (OSG) may be called optimal scenario generation. This optimal choice of discrete approximations is challenging and not possible in general.

It was suggested in (Rachev-Römisch 02) to eventually enlarge the function class $\mathcal{F}$ such that $d_{\mathcal{F}}$ becomes a metric distance and has further nice properties. This may lead, however, to nonconvex nondifferentiable minimization problems (OSG) for determining the optimal scenarios and to unfavorable convergence rates of

$$\left(\min_{P_n \in \mathcal{P}_n(\Xi)} d_{\mathcal{F}}(P, P_n)\right)_{n\in\mathbb{N}}.$$

Typical examples are to choose $\mathcal{F}$ as bounded subsets of some Banach space $C^{r,\alpha}(\Xi)$ with $r \in \mathbb{N}_0$, $\alpha \in (0,1]$, with convergence rate $O(n^{-\frac{r+\alpha}{s}})$.

The road of probability metrics

Motivated by linear two-stage models one may consider

Fortet-Mourier metrics:

$$\zeta_r(P,Q) := d_{\mathcal{F}_r(\Xi)}(P,Q) := \sup \left| \int_\Xi f(\xi)(P-Q)(d\xi) : f \in \mathcal{F}_r(\Xi) \right|,$$

where the function class $\mathcal{F}_r$ for $r \geq 1$ is given by

$$\mathcal{F}_r(\Xi) := \left\{ f : \Xi \mapsto \mathbb{R} : f(\xi) - f(\tilde{\xi}) \leq c_r(\xi, \tilde{\xi}), \forall \xi, \tilde{\xi} \in \Xi \right\},$$

$$c_r(\xi,\tilde{\xi}) := \max\{1, \|\xi\|^{r-1}, \|\tilde{\xi}\|^{r-1}\}\|\xi - \tilde{\xi}\| \quad (\xi, \tilde{\xi} \in \Xi).$$

Proposition: (Rachev-Rüschendorf 98)

If Ξ is bounded, ζ_r may be reformulated as transportation problem

$$\zeta_r(P,Q) = \inf \left\{ \int_{\Xi\times\Xi} \hat{c}_r(\xi,\tilde{\xi})\eta(d\xi, d\tilde{\xi}) : \pi_1\eta = P, \pi_2\eta = Q \right\},$$

where the reduced cost $\hat{c}_r$ is a metric with $\hat{c}_r \leq c_r$ and given by the minimal cost flow problem

$$\hat{c}_r(\xi,\tilde{\xi}) := \inf \left\{ \sum_{i=1}^{n-1} c_r(\xi_{l_i}, \xi_{l_{i+1}}) : n \in \mathbb{N}, \xi_{l_i} \in \Xi, \xi_{l_1} = \xi, \xi_{l_n} = \tilde{\xi} \right\}.$$

The problem of optimal scenario generation (OSG) then reads

$$\min_{P_n \in \mathcal{P}_n(\Xi)} \zeta_r(P, P_n)$$

or

$$\min_{(\xi^1,\ldots,\xi^n)\in\Xi^n} \int_\Xi \min_{j=1,\ldots,n} \hat{c}_r(\xi, \xi^j) P(d\xi).$$

The function $(\xi^1, \ldots, \xi^n) \mapsto \int_\Xi \min_{j=1,\ldots,n} \hat{c}_r(\xi, \xi^j) P(d\xi)$ is continuous on Ξ^n and has compact level sets, but is nonconvex and nondifferentiable in general. Hence, optimal scenarios exist, but their computation is difficult.

If P itself is discrete with possibly many (say $N \gg n$) scenarios and the minimization is restricted to $\Xi = \mathrm{supp}(P)$ one arrives at the optimal scenario reduction problem. This problem can be shown to decompose into finding the optimal scenario set J to remain and into determining the optimal new probabilities given J. The background is that the Fortet-Mourier metric is defined by an optimal transportation problem with fixed marginals that it has a special form if both probability measures are discrete.

Let P and Q be two discrete distributions, where ξ^i are the scenarios with probabilities p_i, $i = 1, \ldots, N$, of P and $\tilde{\xi}^j$ the scenarios and q_j, $j = 1, \ldots, n$, the probabilities of Q. Let Ξ denote the union of both scenario sets. Then

$$\begin{aligned}
\zeta_r(P,Q) &= \inf\Big\{ \int_{\Xi\times\Xi} \hat{c}_r(\xi,\tilde{\xi})\eta(d\xi,d\tilde{\xi}) : \pi_1\eta = P, \pi_2\eta = Q \Big\} \\
&= \inf\Big\{ \sum_{i=1}^{N}\sum_{j=1}^{n} \eta_{ij}\hat{c}_r(\xi_i,\tilde{\xi}_j) : \sum_{j=1}^{n}\eta_{ij} = p_i, \sum_{i=1}^{N}\eta_{ij} = q_j, \eta_{ij} \geq 0, \\
&\qquad\qquad i = 1,\ldots,N,\ j = 1,\ldots,n \Big\} \\
&= \sup\Big\{ \sum_{i=1}^{N} p_i u_i - \sum_{j=1}^{n} q_j v_j : p_i - q_j \leq \hat{c}_r(\xi_i,\tilde{\xi}_j), i = 1,\ldots,N, \\
&\qquad\qquad j = 1,\ldots,n \Big\}
\end{aligned}$$

These two formulas represent primal and dual representations of $\zeta_r(P,Q)$ and primal and dual linear programs (tranportation problems).

Now, let P and Q be two discrete distributions, where ξ^i are the scenarios with probabilities p_i, $i = 1, \dots, N$, of P and ξ^j, $j \in J$, the scenarios and q_j, $j \in J$, the probabilities of Q. Let Ξ denote the support of P.

The best approximation of P with respect to ζ_r by such a distribution Q exists and is denoted by Q^*. It has the distance

$$D_J := \zeta_r(P, Q^*) = \min_{Q \in \mathcal{P}_n(\Xi)} \zeta_r(P, Q) = \sum_{i \notin J} p_i \min_{j \in J} \hat{c}_r(\xi^i, \xi^j)$$

and the probabilities $q_j^* = p_j + \sum_{i \in I_j} p_i$, $\forall j \in J$, where $I_j := \{i \notin J : j = j(i)\}$ and $j(i) \in \arg\min_{j \in J} \hat{c}_r(\xi^i, \xi^j)$, $\forall i \notin J$ (optimal redistribution).

(Dupačová–Gröwe-Kuska–Römisch 03)

Determining the optimal scenario set J with prescribed cardinality n is, however, a combinatorial optimization problem: (metric n-median problem)

$$\min \{D_J : J \subset \{1, ..., N\}, |J| = n\}$$

The problem of finding the optimal set J of remaining scenarios is known to be $\mathcal{NP}$-hard (Kariv-Hakimi 79) and polynomial time algorithms are not available.

Reformulation of the (metric) n-median problem as combinatorial program:

$$\min \sum_{i,j=1}^{N} p_i x_{ij} \hat{c}_r(\xi^i, \xi^j) \qquad \text{subject to}$$

$$\sum_{i=1}^{N} x_{ij} = 1 \quad (j = 1, \ldots, N), \quad \sum_{i=1}^{N} y_i \leq n\,,$$
$$x_{ij} \leq y_i, \quad x_{ij} \in \{0,1\} \quad (i, j = 1, \ldots, N)\,,$$
$$y_i \in \{0,1\} \quad (i = 1, \ldots, N).$$

The variable y_i decides whether scenario ξ^i remains and x_{ij} indicates whether scenario ξ^j minimizes the $\hat{c}_r$-distance to ξ^i.

The combinatorial program can, of course, be solved by standard software. However, meanwhile there is a well developed theory of polynomial-time approximation algorithms for solving it.. The current best algorithms are local search heuristics by (Arya et al. 04) and pseudo-approximation by (Li-Svensson 16). The latter provides an approximation guarantee of $1 + \sqrt{3} + \varepsilon$.
The simplest algorithms are greedy heuristics, namely, backward (or reverse) and forward heuristics.

Starting point $(n = N-1)$: $\min_{l \in \{1,\ldots,N\}} p_l \min_{j \neq l} \hat{c}_r(\xi_l, \xi_j)$

Algorithm: (Backward reduction)

Step [0]: $J^{[0]} := \emptyset$.

Step [i]: $l_i \in \arg \min_{l \notin J^{[i-1]}} \sum_{k \in J^{[i-1]} \cup \{l\}} p_k \min_{j \notin J^{[i-1]} \cup \{l\}} \hat{c}_r(\xi_k, \xi_j)$.

$J^{[i]} := J^{[i-1]} \cup \{l_i\}$.

Step [N-n+1]: Optimal redistribution.

Starting point $(n = 1)$: $\min_{u \in \{1,\ldots,N\}} \sum_{k=1}^{N} p_k \hat{c}_r(\xi_k, \xi_u)$

Algorithm: (Forward selection)

Step [0]: $J^{[0]} := \{1, \ldots, N\}$.

Step [i]: $u_i \in \arg \min_{u \in J^{[i-1]}} \sum_{k \in J^{[i-1]} \setminus \{u\}} p_k \min_{j \notin J^{[i-1]} \setminus \{u\}} \hat{c}_r(\xi_k, \xi_j)$,

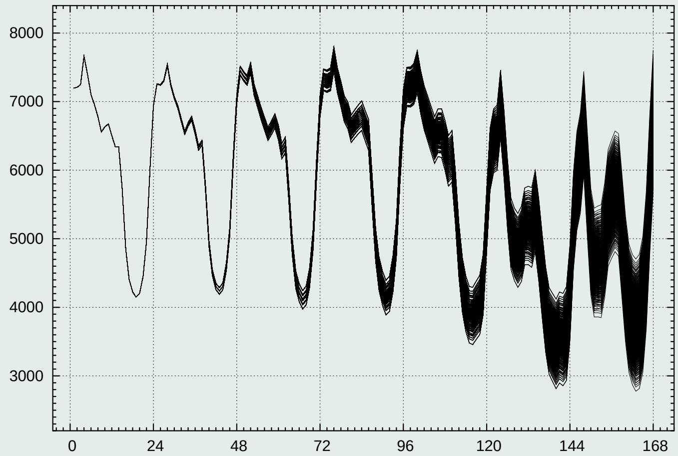
$J^{[i]} := J^{[i-1]} \setminus \{u_i\}$.

Step [n+1]: Optimal redistribution.

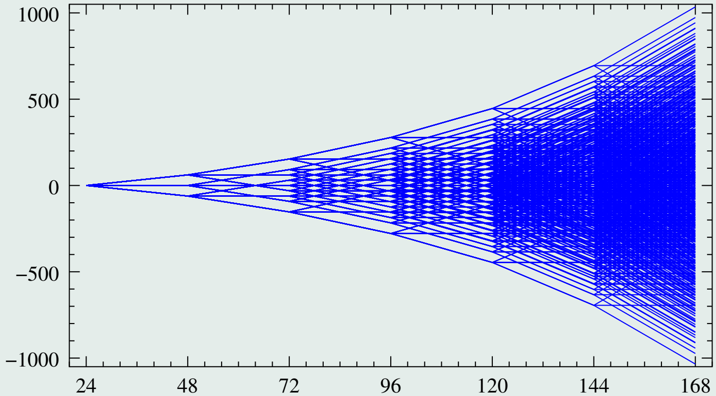
Although the approximation ratio of forward selection is known to be unbounded (Rujeerapaiboon-Schindler-Kuhn-Wiesemann 18), it worked well in many practical instances.

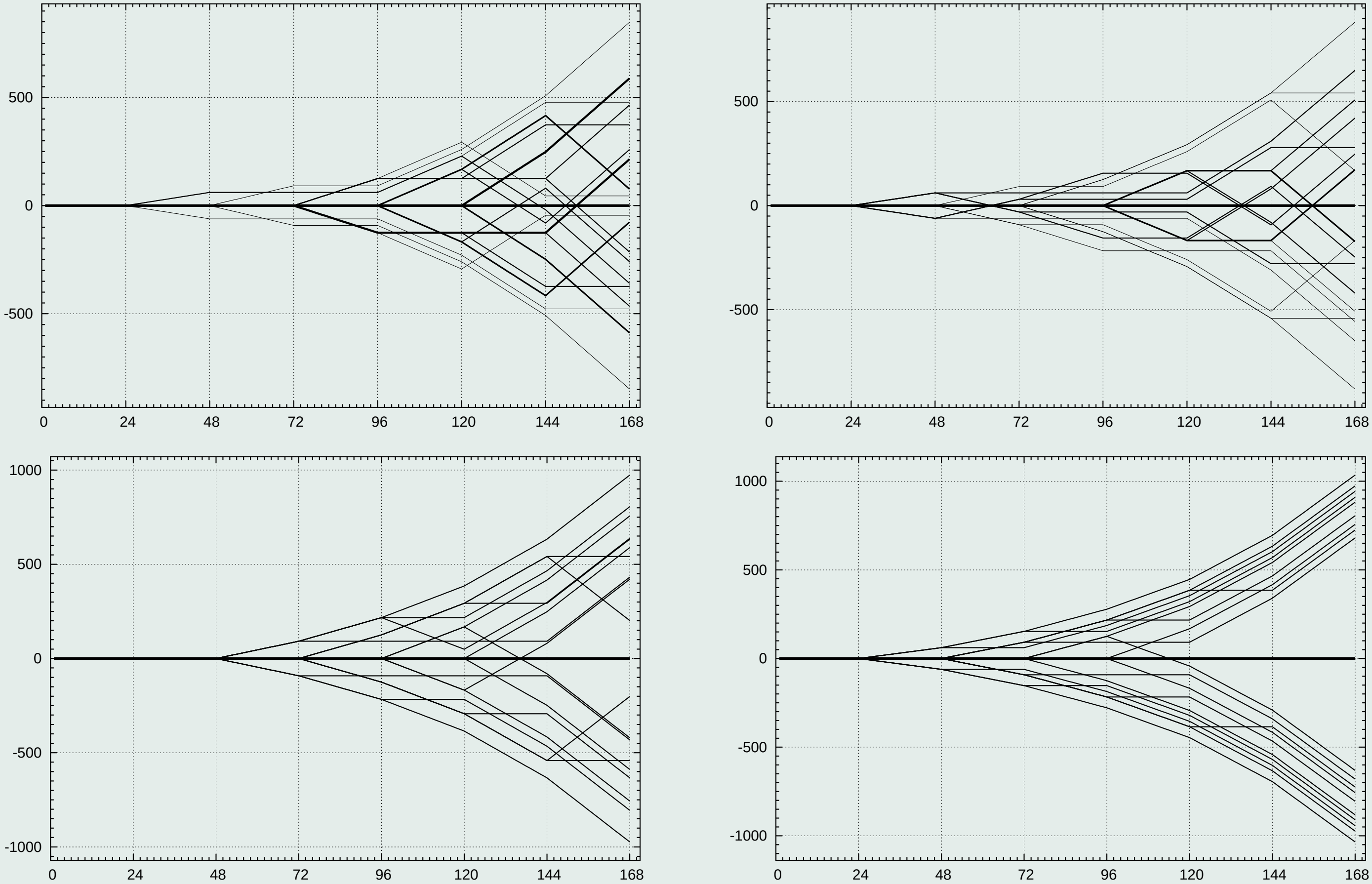
Example: (Weekly electrical load scenario tree)

Ternary load scenario tree (N=729 scenarios)



(Mean shifted) Ternary load scenario tree (N=729 scenarios)





Reduced load scenario trees obtained by forward selection with respect to the Fortet-Mourier distances ζ_r, $r = 1, 2, 4, 7$ and $n = 20$ (starting above left) (Heitsch-Römisch 07)

Problem-based scenario generation for linear two-stage models

We consider linear two-stage stochastic programs as introduced earlier and impose the following conditions:

(A0) X is a bounded polyhedron and Ξ is convex polyhedral.
(A1) $h(x,\xi) \in W(\mathbb{R}^{\bar{m}}_{+})$ and $q(\xi) \in D$ are satisfied for every pair $(x,\xi) \in X \times \Xi$,
(A2) P has a second order absolute moment.
Then the infima $v(P)$ and $v(P_n)$ are attained and the estimate

$$\begin{aligned} |v(P) - v(P_n)| &\leq \sup_{x \in X} \left| \int_{\Xi} f_0(x,\xi) P(d\xi) - \int_{\Xi} f_0(x,\xi) P_n(d\xi) \right| \\ &= \sup_{x \in X} \left| \int_{\Xi} \Phi(q(\xi), h(x,\xi)) P(d\xi) - \int_{\Xi} \Phi(q(\xi), h(x,\xi)) P_n(d\xi) \right| \end{aligned}$$

holds due to the stability result for every $P_n \in \mathcal{P}_n(\Xi)$.
Hence, the optimal scenario generation problem (OSG) with uniform weights may be reformulated as: Determine $P_n^* \in \mathcal{P}_n(\Xi)$ such that it solves the best uniform approximation problem

$$\min_{(\xi^1,\ldots,\xi^n) \in \Xi^n} \sup_{x \in X} \left| \int_{\Xi} \Phi(q(\xi), h(x,\xi)) P(d\xi) - \frac{1}{n} \sum_{i=1}^{n} \Phi(q(\xi^i), h(x,\xi^i)) \right|.$$

The class of functions $\{\Phi(q(\cdot), h(x,\cdot)) : x \in X\}$ from Ξ to $\overline{\mathbb{R}}$ enjoys specific properties. All functions are finite, continuous and piecewise linear-quadratic on Ξ. They are linear-quadratic on each convex polyhedral set

$$\Xi_j(x) = \{\xi \in \Xi : (q(\xi), h(x,\xi)) \in \mathcal{K}_j\} \quad (j = 1, \ldots, \ell),$$

where the convex polyhedral cones $\mathcal{K}_j$, $j = 1, \ldots, \ell$, represent a decomposition of the domain of Φ, which is itself a convex polyhedral cone in $\mathbb{R}^{\bar{m}+r}$.

Theorem: (Henrion-Römisch 18)
Assume (A0)–(A2). Then (OSG) is equivalent to the generalized semi-infinite program

$$\text{(GSIP)} \qquad \min_{t\geq 0, (\xi^1,\ldots,\xi^n)\in\Xi^n} \left\{ t \;\middle|\; \begin{array}{c} \frac{1}{n}\sum_{i=1}^n \langle h(x,\xi^i), z_i\rangle \leq t + F_P(x) \\ F_P(x) \leq t + \frac{1}{n}\sum_{i=1}^n \langle q(\xi^i), y_i\rangle \\ \forall (x,y,z) \in \mathcal{M}(\xi^1,\ldots,\xi^n) \end{array} \right\},$$

where the set $\mathcal{M} = \mathcal{M}(\xi^1,\ldots,\xi^n)$ and the function $F_P : X \to \mathbb{R}$ are given by

$$\mathcal{M} = \{(x,y,z) \in X \times Y^n \times \mathbb{R}^{rn} : Wy_i = h(x,\xi^i), W^\top z_i - q(\xi^i) \in Y^*, \forall i\},$$

$$F_P(x) := \int_\Xi \Phi(q(\xi), h(x,\xi)) P(d\xi).$$

The latter is the convex expected recourse function of the two-stage model.

Theorem:

Assume (A0)–(A2). Let the function h be affine and either h or q be random. Then the feasible set of (GSIP) is closed and convex. Furthermore, (GSIP) can be transformed into a (standard) linear semi-infinite program.

Example:

Assume $Y = \mathbb{R}^{\bar{m}}$ and that only q is random. Define the polyhedral convex cone $\mathcal{U} = \{u \in \mathbb{R}^r : W^\top u \leq 0\}$ and the transformation

$$t : \Xi \times \mathcal{U} \to \mathbb{R}^r, \quad t(\xi, u) = u + (W^+)^\top q(\xi),$$

where W^+ denotes the Moore-Penrose inverse of W.

Then the equivalent linear semi-infinite program is

$$\min_{\substack{t \geq 0 \\ (\xi^1,\ldots,\xi^n) \in \Xi^n}} \left\{ t \;\middle|\; \begin{array}{c} \frac{1}{n}\sum_{i=1}^{n} \langle h(x), u_i + (W^+)^\top q(\xi^i)\rangle \leq t + F_P(x) \\ F_P(x) \leq t + \frac{1}{n}\sum_{i=1}^{n} \langle q(\xi^i), y_i\rangle \\ \forall (x, y_1, \ldots, y_n, u_1, \ldots, u_n) \in X \times \mathcal{Y}(x)^n \times \mathcal{U}^n \end{array} \right\},$$

where $\mathcal{Y}(x) = \{y \in \mathbb{R}^{\bar{m}}_+ : Wy = h(x)\}$ for each $x \in X$.

We note that $F_P(x)$ can only be calculated approximately even if the probability measure P is completely known. For example, this could be done by Quasi-Monte Carlo methods with a large sample size $N > n$. Let

$$F_P(x) \approx \frac{1}{N} \sum_{j=1}^{N} \Phi(q(\hat{\xi}^j), h(x, \hat{\xi}^j))$$

be such an approximate representation of $F_P(x)$ based on a sample $\hat{\xi}^j$, $j = 1, \ldots, N$. The corresponding generalized semi-infinite program is of the form

$$\min_{t \geq 0, (\xi^1, \ldots, \xi^n) \in \Xi^n} \left\{ t \;\middle|\; \begin{array}{c} \frac{1}{n} \sum_{i=1}^{n} \langle h(x, \xi^i), z_i \rangle \leq t + \frac{1}{N} \sum_{j=1}^{N} \langle q(\hat{\xi}^j), \hat{y}_j \rangle \\ \frac{1}{N} \sum_{j=1}^{N} \langle h(x, \hat{\xi}^j), \hat{z}_j \rangle \leq t + \frac{1}{n} \sum_{i=1}^{n} \langle q(\xi^i), y_i \rangle \\ \forall (x, \hat{y}, \hat{z}) \in \mathcal{M}(\hat{\xi}^1, \ldots, \hat{\xi}^N) \\ \forall (x, y, z) \in \mathcal{M}(\xi^1, \ldots, \xi^n) \end{array} \right\}.$$

Discussion and conclusions

- What is the best possible convergence rate of

$$\min_{(\xi^1,\ldots,\xi^n)\in\Xi^n} \sup_{x\in X} \left| \int_\Xi \Phi(q(\xi),h(x,\xi))P(d\xi) - \frac{1}{n}\sum_{i=1}^{n} \Phi(q(\xi^i),h(x,\xi^i)) \right| ?$$

  Even if P is the uniform distribution on $[0,1]^s$, the integrand $\Phi(q(\cdot),h(x,\cdot))$ is not of bounded variation in the sense of Hardy and Krause on $[0,1]^s$.
  Conjecture: The Hardy-Krause variation grows polynomially in $\log n$.

- The linear semi-infinite programs appearing after transformation are very large scale and have unbounded index sets.

- Numerical experiments in cooperation with Dr. Schwientek (Uni Kaiserslautern) are in progress.

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