Scenario generation in stochastic programming with application to energy systems

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Introduction

Many stochastic programming models may be traced back to minimizing an expectation functional on some closed subset of a Euclidean space or, eventually in addition, relative to some expectation constraint. Their general form is

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

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 example, typical integrands in linear two-stage stochastic programming models are

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

where X and Ξ are convex polyhedral, $g(\cdot)$ is a linear function, $q(\cdot)$ is affine, $D = \{q \in \mathbb{R}^{\bar{m}} : \{z \in \mathbb{R}^r : W^\top z - q \in Y^\star\} \neq \emptyset\}$ 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

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

with (r, \bar{m}) matrix W and convex polyhedral cone $Y \subset \mathbb{R}^{\bar{m}}$.

Typical integrands f_1 appearing in chance constrained programming are of the form

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

where $\mathbf{1}_{\mathcal{P}(x)}$ is the characteristic function of the polyhedron $\mathcal{P}(x) = \{\xi \in \Xi : h(x,\xi) \leq 0\}$ depending on x.

For general continuous multivariate probability distributions P such stochastic optimization models (SP) are not solvable in general.

Many approaches for solving such optimization models computationally are based on discrete approximations of the probability measure P, i.e., on finding a discrete probability measure P_n in

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

for some $n \in \mathbb{N}$, which approximates P in a *suitable* way.

The atoms ξ^i , i = 1, ..., n, of P_n are often called scenarios in this context. Of course, the notion *suitable* should at least include that the distance of infima

$$|v(P) - v(P_n)|$$

becomes resonably small.

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)

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

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

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

At first sight the set $\mathcal{P}_{\mathcal{F}}$ seems to have a complicated structure. For typical applications, however, like for linear two-stage and chance constrained models, the sets $\mathcal{P}_{\mathcal{F}}$ or appropriate subsets allow a simple 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 $y \Rightarrow \{x \in X : \int_{\Xi} f_1(x,\xi) P(d\xi) \le y\}$ 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

x

$$|v(P) - v(Q)| \leq L d_{\mathcal{F}}(P,Q)$$

$$\sup_{\in S(Q)} d(x, S(P)) \leq \Psi_P(L d_{\mathcal{F}}(P,Q))$$

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

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

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

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

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. For linear two-stage models (OSG) may be reformulated as best approximation

problem for the expected recourse function or as generalized semi-infinite program which is convex in some cases (Henrion-Römisch 17).

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

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

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

Motivated by linear two-stage models one may consider **Fortet-Mourier metrics**:

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

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

$$\mathcal{F}_{r}(\Xi) := \{ f : \Xi \mapsto \mathbb{R} : f(\xi) - f(\tilde{\xi}) \le c_{r}(\xi, \tilde{\xi}), \, \forall \xi, \tilde{\xi} \in \Xi \}, \\ c_{r}(\xi, \tilde{\xi}) := \max\{1, \|\xi\|^{r-1}, \|\tilde{\xi}\|^{r-1}\} \|\xi - \tilde{\xi}\| \quad (\xi, \tilde{\xi} \in \Xi).$$

Duality holds with a transshipment problem and cost function c_r .

Proposition: (Rachev-Rüschendorf 98) If Ξ is bounded, ζ_r may be reformulated as dual transportation problem

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

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

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

Monte Carlo and Quasi-Monte Carlo methods

Monte Carlo: Let $\xi^i(\cdot)$, $i \in \mathbb{N}$, denote independent and identically distributed random vectors with common distribution P and P_n be the empirical measure

$$P_n(\cdot) = \frac{1}{n} \sum_{i=1}^n \delta_{\xi^i(\cdot)} \quad (n \in \mathbb{N})$$

defined on some probability space $(\Omega, \mathcal{A}, \mathbb{P})$. The law of large numbers implies that the sequence $(P_n(\cdot))_{n \in \mathbb{N}}$ converges \mathbb{P} -almost surely weakly to P. To study the convergence rate one considers the empirical process

$$\{\beta_n(P_n(\cdot) - P)f\}_{f \in \mathcal{F}} \ (n \in \mathbb{N})$$

indexed by a function class \mathcal{F} with sequence (β_n) , where $Qf = \int_{\Xi} f(\xi)Q(d\xi)$ for any Borel probability measure Q on Ξ . The empirical process is called bounded in probability with tail function $\tau_{\mathcal{F}}$ if for all $\varepsilon > 0$ and $n \in \mathbb{N}$ the estimate

 $\mathbb{P}(\{\beta_n d_{\mathcal{F}}(P_n(\cdot), P) \ge \varepsilon\}) \le \tau_{\mathcal{F}}(\varepsilon)$

holds. Whether the empirical process is bounded in probability, depends on the size of the class \mathcal{F} measured in terms of covering numbers in $L_2(\Xi, P)$. Typically, one has an exponential tail $\tau_{\mathcal{F}}(\varepsilon) = C(\varepsilon) \exp(-\varepsilon^2)$ and $\beta_n = \sqrt{n}$.

Quasi-Monte Carlo: The basic idea of Quasi-Monte Carlo (QMC) methods is to use deterministic points that are (in some way) uniformly distributed in $[0, 1]^s$ and to consider first the approximate computation of

$$I_s(f) = \int_{[0,1]^s} f(\xi) d\xi$$
 by $Q_{n,s}(f) = rac{1}{n} \sum_{i=1}^n f(\xi^i)$

with (non-random) points ξ^i , i = 1, ..., n, from $[0, 1]^s$.

The uniform distribution property of point sets may be defined in terms of the so-called L_p -discrepancy of ξ^1, \ldots, ξ^n for $1 \le p \le \infty$

$$d_{p,n}(\xi^1,\ldots,\xi^n) = \left(\int_{[0,1]^s} |\operatorname{disc}(\xi)|^p d\xi\right)^{\frac{1}{p}}, \quad \operatorname{disc}(\xi) := \prod_{j=1}^d \xi_j - \frac{1}{n} \sum_{i=1}^n \mathbf{1}_{[0,\xi)}(\xi^i).$$

A sequence $(\xi^i)_{i\in\mathbb{N}}$ is called uniformly distributed in $[0,1]^s$ if

$$d_{p,n}(\xi^1,\ldots,\xi^n) \to 0 \quad \text{for} \quad n \to \infty$$

There exist sequences (ξ^i) in $[0,1]^s$ such that for all $\delta \in (0,\frac{1}{2}]$

 $d_{\infty,n}(\xi^1,\ldots,\xi^n) = O(n^{-1}(\log n)^s) \quad \text{or} \quad d_{\infty,n}(\xi^1,\ldots,\xi^n) \leq C(s,\delta)n^{-1+\delta}\,.$

Using a suitable randomization of such sequences may lead to a root mean square convergence rate $\sqrt{\mathbb{E}[d_{2,n}^2(\xi^1,\ldots,\xi^n)]} \leq C(\delta)n^{-1+\delta}$ with a constant $C(\delta)$ not depending on the dimension s and $\delta \in (0,\frac{1}{2}]$.

Example: Randomly shifted lattice rule (Sloan-Kuo-Joe 02). With a random vector \triangle which is uniformly distributed on $[0, 1]^s$, we consider the randomly shifted lattice rule

$$Q_{n,s}(\omega)(f) = \frac{1}{n} \sum_{j=1}^{n} f\left(\left\{\frac{(j-1)}{n}\mathbf{g} + \Delta(\omega)\right\}\right).$$

Theorem: Let $n \in \mathbb{N}$ be prime and f belong to the weighted tensor product Sobolev space $\mathcal{W}_{2,\gamma,\min}^{(1,\dots,1)}([0,1]^s)$. Then $\mathbf{g} \in \mathbb{Z}_+^s$ can be constructed componentwise such that for each $\delta \in (0,\frac{1}{2}]$ there exists a constant $C(\delta) > 0$ with

$$\sup_{\|f\|_{\gamma} \le 1} \sqrt{\mathbb{E}} |Q_{n,s}(\omega)(f) - I_s(f)|^2 \le C(\delta) n^{-1+\delta},$$

where $C(\delta)$ increases if δ decreases, but does not depend on s if the sequence (γ_j) of coordinate weights satisfies $\sum_{j=1}^{\infty} \gamma_j^{\overline{2(1-\delta)}} < \infty$ (e.g. $\gamma_j = \frac{1}{j^3}$). Note that piecewise polynomial functions f do almost belong to $\mathcal{W}_{2,\gamma,\min}^{(1,\dots,1)}([0,1]^s)$ if its effective dimension is small (Heitsch-Leövey-Römisch 16).

Scenario reduction

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

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

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

The optimal scenario reduction problem

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

with $P \in \mathcal{P}_N(\Xi)$, N > n, can be decomposed into finding the optimal scenario set J to remain and into determining the optimal new probabilities given J.

Let P have scenarios ξ^i with probabilities p_i , i = 1, ..., N, and Q being supported by a given subset of scenarios ξ^j , $j \in J \subset \{1, ..., N\}$, |J| = n.

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: (*n*-median problem)

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

Hence, the problem of finding the optimal set J of remaining scenarios is \mathcal{NP} -hard and polynomial time algorithms are not available.

Reformulation as combinatorial program

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

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

$$x_{ij} \leq y_i, \quad x_{ij} \in \{0, 1\} \quad (i, j = 1, \dots, N),$$

$$y_i \in \{0, 1\} \quad (i = 1, \dots, N).$$

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 .

There is a well developed theory of approximation algorithms for the *n*-median problem. The current best approximation algorithm provides always an approximation guarantee of $1 + \sqrt{3} + \varepsilon$ (Li-Svensson 16).

The simplest algorithms are greedy heuristics, namely, backward (or reverse) and forward heuristics:

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

Algorithm 1: (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): $\min_{u \in \{1,...,N\}} \sum_{k=1}^{N} p_k \hat{c}_r(\xi_k, \xi_u)$

Algorithm 2: (Forward selection)

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

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 17), it worked well in many practical instances.

Example: (Weekly electrical load scenario tree)





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)

Gas network capacities and validation of nominations

(H. Heitsch, H. Leövey, R. Mirkov, I. Wegner-Specht)

We consider the gas transport network of the company Open Grid Europe GmbH (OGE). It is Germany's largest gas transport company. Such networks consist of intermeshed pipelines which are actuated and safeguarded by active elements (like valves and compressor machines). Here, we consider the stationary state of the network and the isothermal case.

Two different gas qualities are considered: H-gas and L-gas (high and low calorific gas). Both are transported by different networks.

The gas dynamics in a pipe is modeled by the Euler equations, a nonlinear system of hyperbolic partial differential equations. In the stationary and isothermal situation they boil down to nonlinear relations between pressure and flow. Together with models for the active elements, this leads to large systems of nonlinear mixed-integer equations and inequalities.

Aim: Evaluating the capacity of a gas network, validating nominations and verifying booked capacities.



Figure 1.4. German H-gas (red) and L-gas (black) network systems. The arrows indicate entry and exit nodes. Gas storages are represented by black squares. (Source: OGE.)

Statistical data and data analysis

Hourly gas flow data is available at all exit nodes of a given network for a period of eight years. Due to stationary modeling we consider the daily mean gas flow at all exit nodes. Since it depends on the daily mean temperature, we consider a daily reference temperature based on a weighted average temperature taken at different network nodes.

Due to stationary and isothermal modeling we introduce the temperature classes $(-15,-4], (-4,-2], (-2,0], \ldots, (18,20], (20,30)$ and perform a corresponding filtering of all daily mean gas flows at all exit nodes according to the daily reference temperatures. We also check that a reasonable amount of daily mean gas flow data is available for all temperature classes except for (-15,-4]. Another filtering is carried out for day classes (working day, weekend, holiday).



Examples of daily main gas flow at exit nodes as function of the temperature



Daily mean gas flow data at exit nodes with municipal power stations, with zero flow (right).



Daily mean gas flow data at exit nodes with company (left), market transition (middle), storage (right).

Univariate distribution fitting

Classes of univariate probability distributions:

- (shifted) uniform distributions
- (shifted) (log)normal distributions
- Zero gas flow appears with empirical probability p at several exit nodes. Hence, we consider the shifted probability distribution function

$$F(x) = p F^{0}(x) + (1 - p) F^{+}(x)$$



Probability distribution function of a shifted normal distribution at exit 1603

Fitting multivariate normal distributions

- Multivariate normal distributions are fitted for exit gas flows that satisfy normality tests and have significant correlations with other exit nodes, i.e., in addition to means and variances, correlations are estimated by standard estimators if sufficient data is available.
- Examples of correlation matrices:



Correlation plots for the temperature classes (10, 12] and (18, 20] in certain areas of the H-gas network.

Scenario generation

Using randomized Quasi-Monte Carlo methods we determine N samples with probability $\frac{1}{N}$ for the *s*-dimensional random vector ξ that corresponds to the random gas flows at the *s* exits of a given network. We proceed as follows:

- We determine N samples η^j of the uniform distribution on $[0, 1)^s$ using Sobol' points and perform a componentwise random scrambling of their binary digits using the Mersenne Twister. The scenarios η^j , $j = 1, \ldots, N$, combine favorable properties of both Monte Carlo and Quasi-Monte Carlo methods.
- Determine samples in \mathbb{R}^s by

$$\zeta_i^j = \Phi_i^{-1}(\eta_i^j) \quad (i = 1, \dots, s; j = 1, \dots, N)$$

using the univariate distribution function Φ_i of the *i*th component.

If a part of the components of ξ has a d-dimensional multivariate normal distribution with mean m ∈ ℝ^s and s × s covariance matrix Σ, we perform a decomposition Σ = A A^T, where the matrix A preferably corresponds to principal component analysis. Then the s-dimensional vectors

$$\xi^{j} = A \zeta^{j} + m \quad (j = 1, 2, \dots, N)$$

are suitable scenarios for this part of the random vector ξ .



Comparison of $n = 2^7$ Monte Carlo Mersenne Twister points and randomly binary shifted Sobol' points in dimension s = 500, projection (8,9)

Illustration:

N = 2340 samples based on randomized Sobol' points are generated for several hundred exits and later reduced by scenario reduction to n = 50 scenarios. The result is shown below for a specific exit where the diameters of the red balls are proportional to the new probabilities.



(Chapters 13 and 14 in Koch-Hiller-Pfetsch-Schewe 15)

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