Optimisation under Uncertainty Session 2/4

I Workshop de Otimização sob Incerteza - UFSCar

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Outline of this lecture

Introduction

Scenario trees

Generating scenario trees

Scenario (tree) generation methods

Sample Average Approximation (SAA)

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Mathematical programming models in which some of the parameters are assumed to be random variables.

It comprises the following parts:

- 1. A mathematical programming model
- 2. Deterministic parameter values
- 3. Description of the stochasticity, e.g.,
 - a known probability distribution;
 - historical data;
 - distribution properties (average, standard deviation, i.e., moments)

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The most widespread use of stochastic programs relies on scenarios:

- Lead to tractable deterministic equivalents;
- Are approximations of the original stochastic process

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A scenario tree ξ comprises sequentially observed realisations of ξ^t , for $t=1,\ldots,H$:

- \blacktriangleright $\xi = (\xi^t)_{t \in [H]}$, where (\cdot) denotes a sequence and $\xi^t \in \Xi_t$;
- ▶ a scenario is denoted $\xi_s = (\xi_s^t)_{t \in [H]}$ forming a "path" through ξ ;
- ▶ Thus, $\xi = \{\xi_s\}_{s \in [S]}$, where S is the number of scenarios.



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Example:

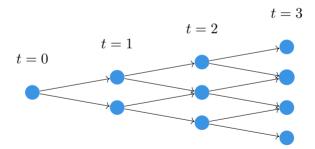


Figure: A 4-stage (lattice) scenario tree with 2 scenarios per stage. $\xi = (\xi^1, \xi^2, \xi^3)$;

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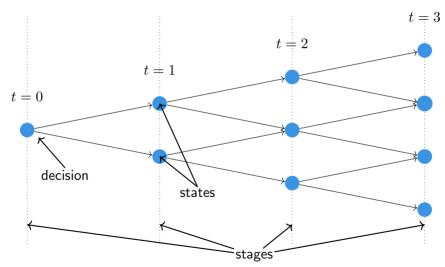
Generating scenario trees

Scenario (tree) generation methods

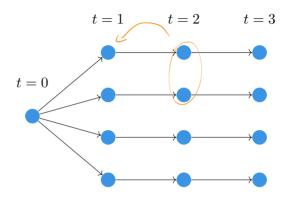
Sample Average Approximation (SAA)

Taxonomy of scenario trees

Terminology



Taxonomy of scenario trees



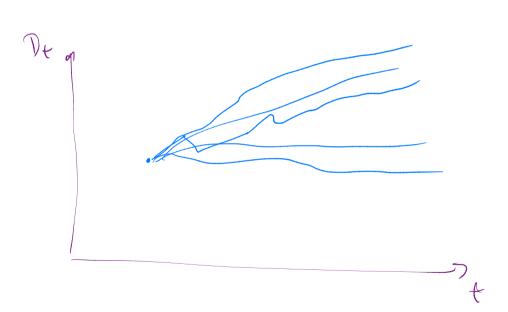
Branching indicates a decision upon arrival of new information

- ▶ No branching, no additional information;
- ► Fan trees represent multi-period 2-stage problems.

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$$\phi(t) = \frac{\epsilon'}{\epsilon_{i1}} w_{i} \beta_{i}(\epsilon') + \epsilon_{i}$$

$$\rho(M_{+}, \sigma_{\epsilon})$$



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Scenario (tree) generation method:

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Trade-off approximation quality vs. tractability

Two parameters govern the geometry of a scenario tree:

- **Depth:** number of stages *H*
- **Breadth (or width):** number of realisations per stage $|\xi^t|$

Trade-off approximation quality vs. tractability

Two parameters govern the geometry of a scenario tree:

- **Depth:** number of stages H
- **Breadth (or width):** number of realisations per stage $|\xi^t|$

The total of scenarios is $O(N^H)$ (assuming $|\xi_t| = N$ for $t \in [H]$)

- ► Larger *H* convey more adaptability to revealed information;
- ightharpoonup Larger |S| convey a more precise description of the uncertainty;
- Computational tractability issues pressure them to be as small as possible.

Most scenario generation methods seek to find trees with minimal $|\xi|$ such that representation quality requirements are observed.

Data source

Typical sources for scenarios include:

- 1. Historical data: past observations as possible future observations;
- 2. **Simulation models:** Monte Carlo, systems dynamics, agent-based and discrete event simulation;
- 3. **Expert elicitation:** typically a small number of scenarios with no possible back-testing

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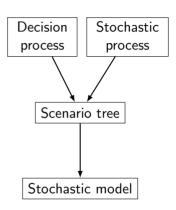
Often, a combination of the above is used:

- 1. Start from the data;
- 2. Define and fit a parametric model; (ML
- 3. Generate observations from the model.

Scenario generation and modelling

Scenario generation must be part of the modelling process

- Problem dependent;
- The method for generating scenarios is a modelling decision;
- Often overlooked in applications;
- Quality of scenarios majorly influences quality of solution ("garbage in = garbage out")



Quality measures for scenario trees

Apart from epistemic error questions, two measures must be considered when generating scenario trees:

1. Error

- Error introduced for using an approximation of the real stochastic process;
- Unlikely to be measurable, but possible to be approximated.

2. Stability

- Scenario-trees approximating the same stochastic process should yield the same solution;
- Likewise, objective function values should be stable.

Let ξ be a scenario tree representing the original stochastic process η , and $\mathcal{F}(x,\xi)=\mathbb{E}_{\xi}\left[F(x,\xi)\right]$. We are interested in understanding how well

$$\min_{x \in X} \mathcal{F}(x, \xi)$$
 approximates $\min_{x \in X} \mathcal{F}(x, \eta)$

Quality measures for scenario trees

Let ξ_k for $k=1,\ldots,n$ be a collection of alternative scenario trees generated to represent η . We have that

$$x_k^* = \arg\min_{x \in X} \mathcal{F}(x, \xi_k).$$

The approximation error [Pflug, 2001] is defined as

$$e(\eta, \xi_k) = \mathcal{F}(\arg\min_{x \in X} \mathcal{F}(x, \xi_k), \eta) - \mathcal{F}(\arg\min_{x \in X} \mathcal{F}(x, \eta), \eta)$$
$$= \mathcal{F}(x_k^*, \eta) - \min_{x \in X} \mathcal{F}(x, \eta).$$

Quality measures for scenario trees

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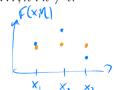
▶ Clearly, there is no way to evaluate $\min_{x \in X} \mathcal{F}(x, \eta)$.

Out-of-sample stability

We often assume that we can approximate $\mathcal{F}(x_k^{\star}, \eta)$. This allows us to

- ightharpoonup compare solution x_1^* and x_2^* ;
- compare alternative scenario generation methods;
- perform out-of-sample stability test:
 - 1. Generate a set of scenario trees $\{\xi_1, \ldots, \xi_n\}$;
 - 2. Obtain solutions x_k , $k = 1, \ldots, n$;
 - 3. Test whether $\mathcal{F}(x_k^{\star}, \eta) \approx \mathcal{F}(x_l^{\star}, \eta)$, for $k, l = 1, \dots, n : k \neq l$.





Out-of-sample stability

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Remarks:

- $e(\eta, \xi_k) \approx 0 \Rightarrow e(\eta, \xi_k) \approx e(\eta, \xi_l) \equiv \mathcal{F}(x_k^{\star}, \eta) \approx \mathcal{F}(x_l^{\star}, \eta);$
- ► The procedure above can also be used to assess scenario tree width (scenarios per stage).

In-sample stability

In-sample stability is defined as

$$\mathcal{F}(x_k^{\star}, \xi_k) \approx \mathcal{F}(x_l^{\star}, \xi_l), \text{ for } k, l = 1, \dots, n : k \neq l.$$

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In some contexts, can also be defined as

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$$||x_k^{\star} - x_l^{\star}||_p$$
, for $k, l = 1, \ldots, n : k \neq l$.

where $||\cdot||_p$ is a vector p-norm.

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- No direct connection to out-of-sample stability;
- Useful for assessing the internal stability of a random scenario generation method;
- ▶ Translates into confidence in the objective function value reported.

Final considerations

Some practical advice:

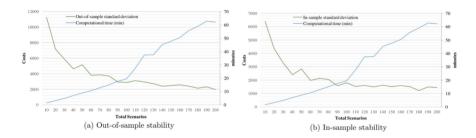
- No stability implies dependence on the scenario tree. To improve stability one can
 - 1. Consider alternative scenario generation methods
 - 2. Increase the number of scenarios
- In case approximating $\mathcal{F}(x_k^\star, \eta)$ is not feasible, cross-testing can be employed. Let

$$\overline{\mathcal{F}} = \{\mathcal{F}(x_k^{\star}, \xi_l)\}_{k,l=1,\dots,n:k\neq l}.$$

Out-of-sample stability implies that the standard deviation of $\overline{\mathcal{F}}$ is close to 0.

For a rigorous treatment of stability, check [Dupačová, 1990, Schultz, 2000, Heitsch et al., 2006].

Stability for scenario trees [Dillon et al., 2017]



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The main types of scenario-generation methods are:

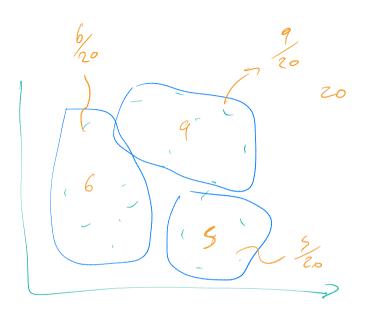
1. **Sampling:** Monte-Carlo sampling, or quasi Monte-Carlo sampling using variance reduction techniques (e.g., Sobol sequences). Combined with Sample Average Approximation (SAA).

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- Moment matching: artificially generates a set of scenarios with the same (four plus correlation, usually) moments as the desired distribution;

The main types of scenario-generation methods are:

- Sampling: Monte-Carlo sampling, or quasi Monte-Carlo sampling using variance reduction techniques (e.g., Sobol sequences). Combined with Sample Average Approximation (SAA).
- Moment matching: artificially generates a set of scenarios with the same (four plus correlation, usually) moments as the desired distribution;
- Metric-based: form smaller scenario sets whilst minimising some probabilistic distance metric. Includes clustering (k-means and related methods) and scenario reduction.



Moment matching

Build a scenario tree $(z_s,p_s)_{s\in\Xi}$ that has statistical moments $f_m(z,p)$ matching target values $M_{\rm W}^{\rm VAL}$.

- Moments extracted from the original distribution, or data;
- ► The following problem must be solved ([Høyland and Wallace, 2001]):

$$egin{aligned} \min_{z,p\geq 0} \sum_{m\in M} w_m (f_m(z,p) - M_m^{\mathsf{VAL}})^2 \ & ext{s.t.: } \sum_{j=1}^{|\Xi|} p_j = 1, \end{aligned}$$

where w_m are weights.

Remark: [Høyland et al., 2003] show how the above problem can be heuristically solved.

Metric-based methods

Probability-metric based methods use the following result [Pflug, 2001]

$$e(\eta, \xi_k) \le Kd(\eta, \xi_k)$$

where K is a (Lipschitz-related) constant and d is a Wasserstein distance between η and ξ_k . Thus, the focus is on obtaining trees that minimise d.

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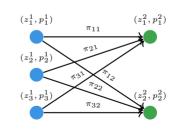
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Let $\xi^l=(z^l,p^l)\in\Xi^l$. The Wasserstein distance $d(\xi^1,\xi^2)$ is given by:

$$\begin{aligned} & \underset{\pi}{\text{min.}} & \sum_{i \in \xi^1, j \in \xi^2} ||z_i^1 - z_j^2|| \mathring{\pi}_{ij} \\ & \text{s.t.:} & \sum \pi_{ij} = p_i^1, \ \forall i \in \xi_1 \end{aligned}$$

$$\sum_{i=\ell^1}^{j\in \xi^2} \pi_{ij} = p_j^2, \ \forall j \in \xi_2.$$



Metric-based methods

1. "Clustering-like" methods:

- ► *k*-means, and variants incorporating Wasserstein distance as the metric [Condeixa et al., 2020]
- ▶ Work well in case scenarios are generated from data [Kaut, 2021];
- ▶ [Löhndorf, 2016]: Learning-based algorithms such as competitive learning and Voronoi cell sampling as alternatives to k-means.

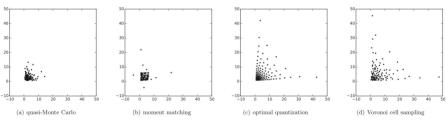


Figure: comparison of scenario generation methods ([Löhndorf, 2016])

Scenario generation methods Metric-based methods





- 2. Scenario reduction methods: Obtain ξ^2 from ξ^1 where $|\xi^2| > |\xi^1|$.
 - ▶ Based on the theory of stability of stochastic programs [Römisch, 2003]
 - Changes in the solution can be approximated using a Forter-Mourier-type metric
 - Calculation leads to a Monge-Kantorovich mass transportation problem
 - "Historical" chronology:
 - [Dupačová et al., 2003, Heitsch and Römisch, 2003]: first backward reduction and forward selection methods;
 - 2. [Heitsch and Römisch, 2007] improved versions of the heuristics;
 - 3. [Heitsch and Römisch, 2009] The above does not work for multi-stage problems. Provides a method that does.

Scenario reduction

Types of reduction algorithms. Let K be a target value for $|\xi^2|$

- ▶ Backward reduction: repeat until $|\xi^2| = K$. Start from ξ^1
 - 1. Find the scenario whose removal causes the smallest error increase
 - 2. Remove the scenario and redistribute its probability
- Forward selection: repeat until $|\xi^2| = K$. Start from $\xi^2 = \emptyset$
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Some final practical remarks:

- ▶ In [Heitsch and Römisch, 2003], their results indicate:
 - 50% of the scenarios gives 90% relative accuracy
 - 1% of the scenarios gives 50% accuracy
- **Forward selection** gives better results, but is slow for large $|\xi^1|$ and K.
- Scenred2 (GAMS) is an available implementation.

Some of my own experience

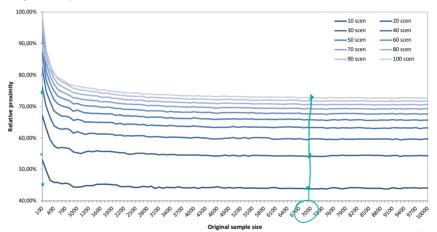


Figure: Relative accuracy for scenario reduction; x-axis is $|\xi^1|$, lines are different $|\xi^2|$. [Oliveira et al., 2016]

Some of my own experience

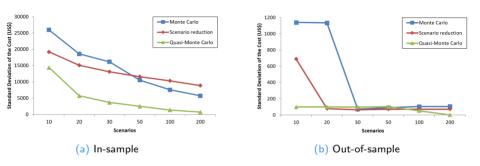


Figure: Objective function standard deviation comparing 3 alternative scenario reduction methods. Original sample had 1000 scenarios [Fernández Pérez et al., 2018]

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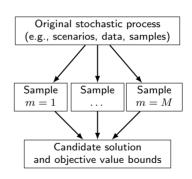
Scenario (tree) generation methods

Sample Average Approximation (SAA)

What is SAA

In the context of stochastic programming, SAA [Shapiro and Homem-de Mello, 1998] is an alternative to generating scenario trees

- Purely based on sampling;
- Monte Carlo simulation for estimating objective function bounds;
- Useful for handling large scenario sets;
- Typically, sample m size $N << |\xi|$ or $|\eta|$;
- Requires solving M problems.



SAA is based on the law of large numbers (LLN) and the central limit theorem (CLT). As such, we can

- Estimate bounds using mean values;
- Estimate confidence intervals.

f(x) is a shorthand for $\mathcal{F}(x,\xi)$.

SAA is based on the law of large numbers (LLN) and the central limit theorem (CLT). As such, we can

- Estimate bounds using mean values;
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First, let us define our notation for 2SSPs

$$z = \min_{x} f(x),$$

where:

- $f(x) = \mathbb{E}_{\xi} [F(x,\xi)]^{1}$
- $F(x,\xi) = \{c^{\top}x + Q(x,\xi) : x \in X\};$
- $X = \{x \in \mathbb{R}^n : Ax = b, x \ge 0\}.$

 $^{^{1}}f(x)$ is a shorthand for $\mathcal{F}(x,\mathcal{E})$.

Calculating a lower bounds for z

Let N be the number of samples we draw from our original stochastic process, forming the set scenario set $S=\left\{ \xi^{1},\ldots,\xi^{N}\right\} .$

Then, we can solve the sample-based approximation problem

$$\hat{z}_N = \min_{x} \left\{ \tilde{f}_N(x) = \frac{1}{N} \sum_{n=1}^{N} F(x, \xi_n) \right\}.$$
 (1)

 $^{^2}$ LLN: $\lim_{N o\infty}\mathbb{E}\left[rac{\sum_{n\equiv1}^N X_n}{N}
ight] = rac{N\overline{X}}{N} = \overline{X}$ for i.i.d. random variable X_n with mean value \overline{X} .

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 (1)

First, notice that $\tilde{f}_N(x)$ is an unbiased estimator² for f(x):

$$\mathbb{E}_{\xi}\left[\tilde{f}_{N}(x)\right] = \frac{1}{N}\mathbb{E}_{\xi}\left[\sum_{n=1}^{N}F(x,\xi_{n})\right] \xrightarrow{LLN} \frac{1}{N}(Nf(x)) = f(x). \quad \Box$$

$$\frac{^2 \text{LLN:}}{N} \lim_{N \to \infty} \mathbb{E} \left[\frac{\sum_{n=1}^N X_n}{N} \right] = \frac{N \overline{X}}{N} = \overline{X} \text{ for i.i.d. random variable } X_n \text{ with mean value } \overline{X}.$$

Calculating lower bounds for z

We now show that $\mathbb{E}[\hat{z}_N]$ is a lower bound on z:

$$\hat{\mathbf{z}}_{N} = \min_{x} \left\{ \frac{1}{N} \sum_{n=1}^{N} F(x, \xi_{n}) \right\} \leq \frac{1}{N} \sum_{n=1}^{N} F(x, \xi_{n})$$

$$\mathbb{E}_{\xi} \left[\min_{x} \left\{ \frac{1}{N} \sum_{n=1}^{N} F(x, \xi_{n}) \right\} \right] \leq \mathbb{E}_{\xi} \left[\frac{1}{N} \sum_{n=1}^{N} F(x, \xi_{n}) \right]$$

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$$\mathbb{E}_{\xi} \left[\hat{\mathbf{z}}_{N} \right] \leq \min_{x} \left\{ \mathbb{E}_{\xi} \left[\frac{1}{N} \sum_{n=1}^{N} F(x, \xi_{n}) \right] \right\} \xrightarrow{N \to \infty}$$

$$\min_{x} \left\{ \mathbb{E}_{\xi} \left[F(x, \xi) \right] \right\} = \min_{x} f(x) = \mathbf{z}. \quad \square$$

altole 2

Calculating lower bounds for z

In turn, we can approximate $\mathbb{E}\left[\hat{z}_{N}\right]$ using a sample estimate.

1. For that, we sample M scenario trees of size N:

$$\begin{cases} \xi_1^1, \dots, \xi_N^1 \end{cases}, \dots, \begin{cases} \xi_1^M, \dots, \xi_N^M \end{cases}.$$

³Again an unbiased estimator, see footnote 2.

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2. For each scenario tree, we solve

$$\hat{z}_N^m = \min_{x} \left\{ \frac{1}{N} \sum_{n=1}^N F(x, \xi_n^m) \right\}$$

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2. For each scenario tree, we solve

$$\hat{z}_N^m = \min_{x} \left\{ \frac{1}{N} \sum_{n=1}^N F(x, \xi_n^m) \right\}$$

3. We can then estimate $\mathbb{E}[\hat{z}_N]$ as

$$L_N^M = \frac{1}{M} \sum_{m=1}^M \hat{z}_N^m.$$

³Again an unbiased estimator, see footnote 2.

Statistical bounds for L_N^M

We can use the CLT to provide confidence intervals for L_N^M . A sample-estimate for $\sigma_{L_N^M}^2$ can be obtained as

$$s_{L_N^M}^2 = \frac{1}{M-1} \sum_{m=1}^M (\hat{z}_N^m - L_N^M)^2.$$

Statistical bounds for ${\cal L}_N^M$

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We can use $s^2_{L^M_N}$ to obtain an 1- α confidence interval for L^M_N :

$$\left[L_N^M - \frac{z_{\alpha/2} s_{L_N^M}}{\sqrt{M}}, L_N^M + \frac{z_{\alpha/2} s_{L_N^M}}{\sqrt{M}}\right]$$

where $z_{\alpha/2}$ is the standard normal $1 - \alpha/2$ quantile.

Calculating upper bounds for z

Let

$$\hat{x}_N^m = \operatorname*{argmin}_x \left\{ \frac{1}{N} \sum_{n=1}^N F(x, \xi_n^m) \right\}, \ \forall m \in [M].$$

Notice that $f(\hat{x}_N^m) \geq z$, $\forall m \in [M]$.

Calculating upper bounds for z

Let

$$\hat{x}_N^m = \underset{x}{\operatorname{argmin}} \left\{ \frac{1}{N} \sum_{n=1}^N F(x, \xi_n^m) \right\}, \ \forall m \in [M].$$

Notice that $f(\hat{x}_{N}^{m}) \geq z, \forall m \in [M].$

We can obtain an unbiased estimate for $f(\hat{x}_N^m)$ by

- 1. Choosing one solution $\hat{x}_N^{m'}$, $m' \in [M]$;
- 2. Sampling T scenario trees of size \overline{N} $\{\xi_1^1, \dots \xi_{\overline{N}}^1\}, \dots, \{\xi_1^T, \dots \xi_{\overline{N}}^T\}$

$$\left\{\xi_1^1,\ldots,\xi_{\overline{N}}^1\right\},\ldots,\left\{\xi_1^T,\ldots,\xi_{\overline{N}}^T\right\}$$

3. For each scenario tree t, we evaluate

$$\check{z}_{\overline{N}}^t = \frac{1}{\overline{N}} \sum_{n=1}^{\overline{N}} F(\hat{x}_N^{m'}, \xi_n^t)$$

Calculating upper bounds for z

4. We can estimate $f(\hat{x}_N^m)$ as

$$U_{\overline{N}}^{T} = \frac{1}{T} \sum_{t=1}^{T} \check{z}_{\overline{N}}^{t}.$$

Analogously, we can use the sample-estimate for $\sigma^2_{U^T_{\overline{N}}}$

$$s_{U_{\overline{N}}}^2 = \frac{1}{T-1} \sum_{t=1}^{T} (\check{z}_{\overline{N}}^t - U_{\overline{N}}^T)^2$$

to calculate the 1- α confidence interval for $U_{\overline{N}}^T$ as

$$\left[U_{\overline{N}}^T - \frac{z_{\alpha/2} s_{U_{\overline{N}}^T}}{\sqrt{T}}, U_{\overline{N}}^T + \frac{z_{\alpha/2} s_{U_{\overline{N}}^T}}{\sqrt{T}}\right].$$

In this context, an optimality gap refers to the quantity

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that
$$f(\hat{x}_N^{m'}) - \mathbb{E}[\hat{z}_N]$$

On the other hand, we know that

$$\mathbb{E}\left[\hat{z}_{N}\right] \leq z \leq f(\hat{x}_{N}^{m'}).$$

Since we have estimates for $\mathbb{E}\left[\hat{z}_N\right]\left(L_N^M\right)$ and $f(\hat{x}_N^{m'})$ $\left(U_{\overline{N}}^T\right)$, we can calculate the optimality gap estimate

$$gap(N, M, \overline{N}, T) = U_{\overline{N}}^T - L_N^M.$$

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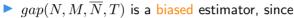
Since we have estimates for $\mathbb{E}\left[\hat{z}_N\right]$ (L_N^M) and $f(\hat{x}_N^{m'})$ (U_N^T) , we can calculate the optimality gap estimate

$$gap(N, M, \overline{N}, T) = U_{\overline{N}}^T - L_N^M.$$

Confidence intervals can also be obtained for $gap(N, M, \overline{N}, T)$ using

$$\sigma^2_{gap(N,M,\overline{N},T)} = s_{L_N^M}^2 + s_{U_{\overline{N}}}^2.$$

Some remarks on $gap(N, M, \overline{N}, T)$:

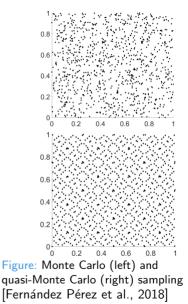


$$f(\hat{x}_N^{m'}) - \mathbb{E}\left[\hat{z}_N\right] \ge f(\hat{x}_N^{m'}) - z;$$

- As it overestimates $f(\hat{x}_N^{m'}) z$, it is still useful in practice;
- Confidence intervals for $gap(N,M,\overline{N},T)$ can be improved by reducing:
 - 1. $s_{L_N}^2$, via increasing N and M: larger N leads to larger problems, but they can be solved as M parallel problems;
 - 2. $s_{U_{\overline{N}}}^2$, via increasing \overline{N} and T; larger \overline{N} leads to more costly evaluation; solvable as T (as $\overline{N} \times T$ for 2SSPs) parallel problems.

Regarding choosing a solution $\hat{x}_N^{m'}$:

- If feasible, evaluate all distinct solutions \hat{x}_N^m for $m \in \{M\}$ and choose that with best L_N^M , $U_{\overline{N}}^T$ or $gap(N,M,\overline{N},T)$;
- Too many distinct solutions may indicate that N is too small. Perform stability analysis.
- SAA holds for non-independent sampling schemes (e.g., Latin hypercube sampling or quasi Monte Carlo). These help keep N small.



Regarding the choice of N [Oliveira and Hamacher, 2012]:

Notice that \hat{z}_N is the expected value of the random variable

$$(z_N(\xi)) = F(\hat{x}_N, \xi), \text{ where } \hat{x}_N = \operatorname*{argmin}_x \left\{ \frac{1}{N} \sum_{n=1}^N F(x, \xi_n) \right\}$$

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As such, we can estimate its sample-based variance and a $1-\alpha$ confidence interval, given by

$$s_N^2 = rac{1}{N-1} \sum_{n=1}^N (\hat{z}_N - z_N(\xi_n))^2 ext{ and } \hat{z}_N \pm rac{z_{lpha/2} s_N}{\sqrt{N}}.$$



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If we predefine a desired relative width β for the confidence interval, we can infer that

$$N \ge \frac{z_{\alpha/2} s_N}{(\beta/2)\hat{z}_N}.$$

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