Optimisation under Uncertainty
Session 2/4

I Workshop de Otimização sob Incerteza - UFSCar

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Outline of this lecture

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Introduction

Scenario trees

Generating scenario trees

Scenario (tree) generation methods

Sample Average Approximation (SAA)

Stochastic programming models

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

Stochastic programming models

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

- $\xi = (\xi^t)_{t \in [H]}$, 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:

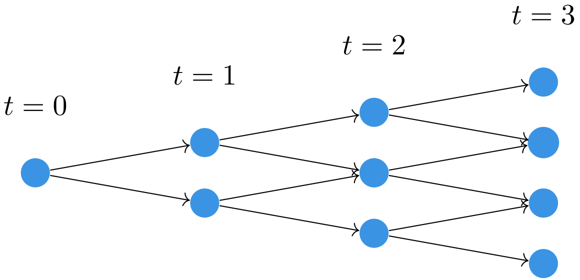

Figure: A 4-stage (lattice) scenario tree with 2 scenarios per stage. $\xi = (\xi^1, \xi^2, \xi^3)$;

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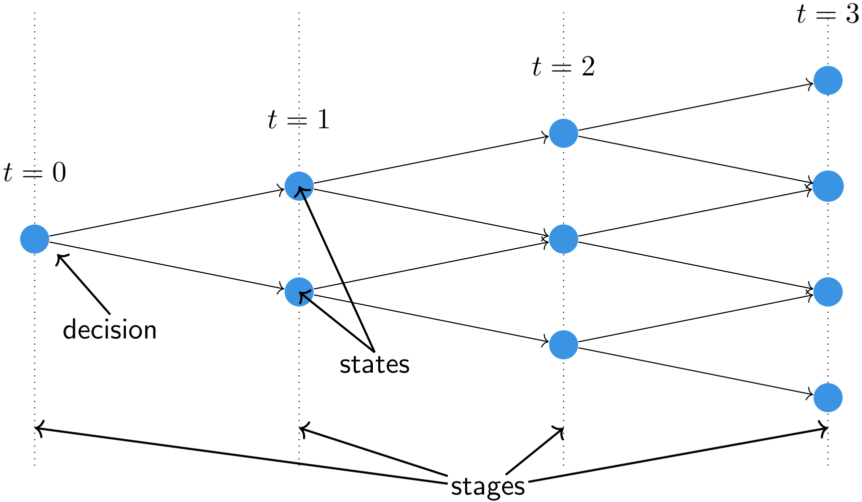
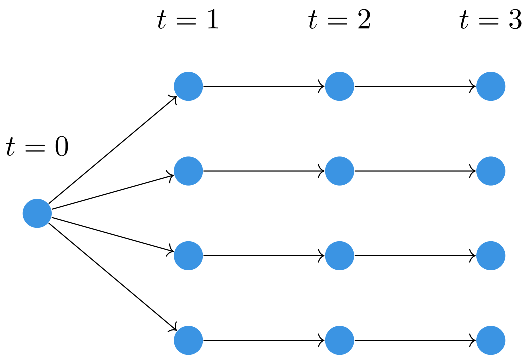
Taxonomy of scenario trees

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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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

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

- Larger H convey more adaptability to revealed information;
- 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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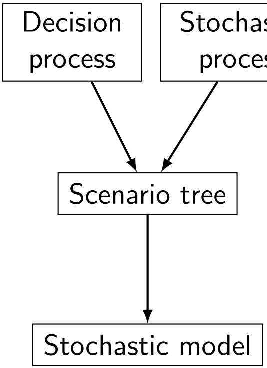
Often, a combination of the above is used:

1. Start from the data;
2. Define and fit a parametric model;
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 $\mathcal{F}(x, \xi) = \mathbb{E}_{\xi}[F(x, \xi)]$. We are interested in understanding how well

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

Quality measures for scenario trees

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

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

The approximation error [Pflug, 2001] is defined as

$$\begin{aligned} e(\eta, \xi_k) = & \ \mathcal{F}(\arg\min_{x \in X} \mathcal{F}(x, \xi_k), \eta) - \mathcal{F} \arg\min_{x \in X} \mathcal{F}(x, \eta), \eta) \\ = & \ \mathcal{F}(x_k^\star, \eta) - \min_{x \in X} \mathcal{F}(x, \eta). \end{aligned}$$

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- Calculating $\mathcal{F}(x_k^\star, \eta)$ requires evaluating the "true" objective function;
- Alternatively, Monte Carlo simulation is often employed to approximate $\mathcal{F}(x_k^\star, \eta)$;
- Clearly, there is no way to evaluate $\min_{x \in X} \mathcal{F}(x, \eta)$.

Stability for scenario trees

Out-of-sample stability

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

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

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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).

Stability for scenario trees

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In some contexts, can also be defined as

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

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.

Stability for scenario trees

Final considerations

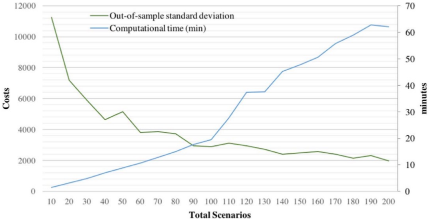
Some practical advice:

- 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

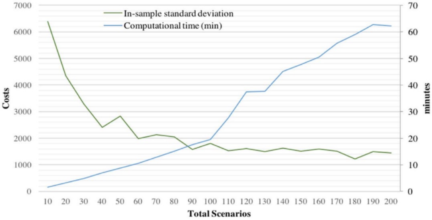
$$\overline{\mathcal{F}} = \{\mathcal{F}(x_k^\star, \xi_l)\}_{k,l=1,\dots,n:k\neq l}\,.$$

  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]



(a) Out-of-sample stability



(b) In-sample stability

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Scenario generation methods

The main types of scenario-generation methods are:

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Scenario generation methods

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).
2. **Moment matching:** artificially generates a set of scenarios with the same (four plus correlation, usually) moments as the desired distribution;
3. **Metric-based:** form smaller scenario sets whilst minimising some probabilistic distance metric. Includes clustering (k-means and related methods) and scenario reduction.

Scenario generation methods

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_m^{VAL}.

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

$$\min_{z,p \geq 0} \sum_{m \in M} w_m (f_m(z,p) - M_m^{\mathsf{VAL}})^2$$

$$\text{s.t.: } \sum_{j=1}^{|\Xi|} p_j = 1,$$

  where w_m are weights.

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

Scenario generation methods

Metric-based methods

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

$$e(\eta, \xi_k) \leq K d(\eta, \xi_k)$$

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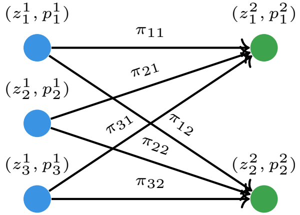
Let $\xi^l = (z^l, p^l) \in \Xi^l$. The Wasserstein distance $d(\xi^1, \xi^2)$ is given by:

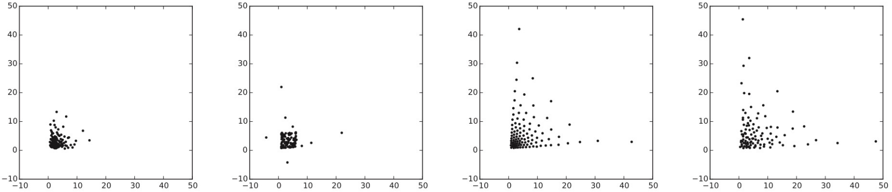
$$\begin{aligned}
\min_{\pi} \quad & \sum_{i \in \xi^1, j \in \xi^2} ||z_i^1 - z_j^2||^r \pi_{ij} \\
\text{s.t.:} \quad & \sum_{j \in \xi^2} \pi_{ij} = p_i^1, \ \forall i \in \xi_1 \\
& \sum_{i \in \xi^1} \pi_{ij} = p_j^2, \ \forall j \in \xi_2.
\end{aligned}$$



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.



(a) quasi-Monte Carlo (b) moment matching (c) optimal quantization (d) Voronoi cell sampling

Figure: comaprison 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:
  1. [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 generation methods

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.

Scenario generation methods

Some of my own experience

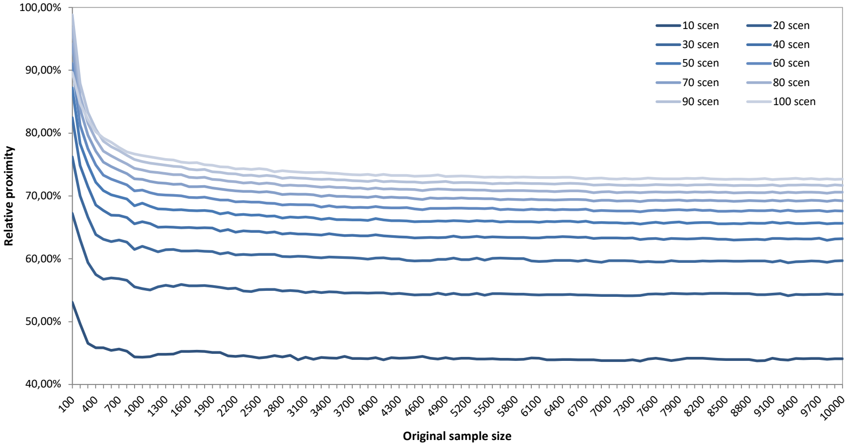
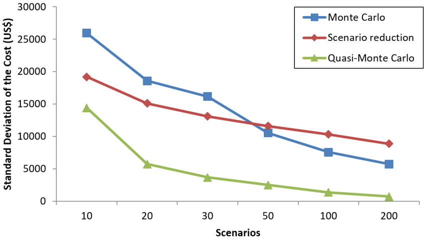


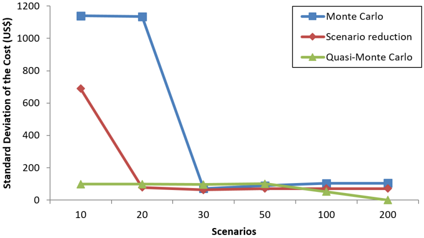
Figure: Relative accuracy for scenario reduction; x-axis is $|\xi^1|$, lines are different $|\xi^2|$. [Oliveira et al., 2016]

Scenario generation methods

Some of my own experience



(a) In-sample



(b) Out-of-sample

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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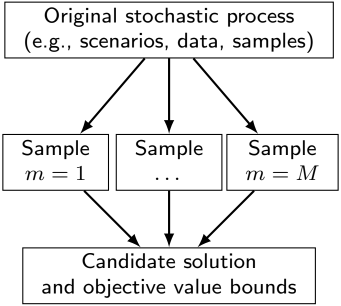
What is SAA

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.



How SAA works

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.

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

How SAA works

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

$$z = \min_x f(x),$$

where:

- $f(x) = \mathbb{E}_\xi \left[F(x, \xi)\right]$[1]
- $F(x, \xi) = \left\{c^\top x + Q(x, \xi) : x \in X\right\}$;
- $Q(x, \xi) = \text{min.}_y \left\{q(\xi)^\top y : W(\xi)y = h(\xi) - T(\xi)x, y \geq 0\right\}$;
- $X = \{x \in \mathbb{R}^n : Ax = b, x \geq 0\}$.

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

How SAA works

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 $S = \{\xi^1, \dots, \xi^N\}$.

Then, we can solve the sample-based approximation problem

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

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

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First, notice that $\tilde{f}_N(x)$ is an unbiased estimator[2] for $f(x)$:

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

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

How SAA works

Calculating lower bounds for z

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

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

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

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

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

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

How SAA works

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:

$$\left\{\xi_1^1, \dots, \xi_N^1\right\}, \dots, \left\{\xi_1^M, \dots, \xi_N^M\right\}.$$

[3] Again an unbiased estimator, see footnote 2.

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2. For each scenario tree, we solve

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

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

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

[3] Again an unbiased estimator, see footnote 2.

How SAA works

Statistical bounds for L_N^M

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

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

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

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

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

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

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

How SAA works

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

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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 $\overline{N}$

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

3. For each scenario tree t, we evaluate

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

How SAA works

Calculating upper bounds for z

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

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

Analogously, we can use the sample-estimate for $\sigma^2_{U_{\frac{T}{N}}}$

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

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

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

On estimating optimality gaps

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

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

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

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

On estimating optimality gaps

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

- $gap(N, M, \overline{N}, T)$ is a biased estimator, since

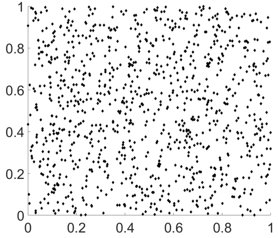
$$f(\hat{x}_N^{m'}) - \mathbb{E}\left[\hat{z}_N\right] \geq f(\hat{x}_N^{m'}) - z;$$

- 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. $s^2_{L_N^M}$, via increasing N and M: larger N leads to larger problems, but they can be solved as M parallel problems;
  2. $s^2_{U_{\overline{N}}^T}$, 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.

Final practical remarks

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.



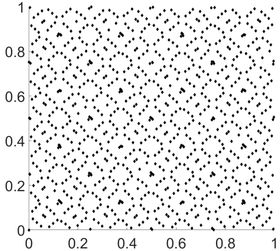


Figure: Monte Carlo (left) and quasi-Monte Carlo (right) sampling [Fernández Pérez et al., 2018]

Final practical remarks

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

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

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

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

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