

Stochastic programming & Robust optimisation

Lecture 2/4

Fabricio Oliveira

Systems Analysis Laboratory
Department of Mathematics and Systems Analysis

Aalto University
School of Science

KTH, Stockholm, Sweden
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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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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:

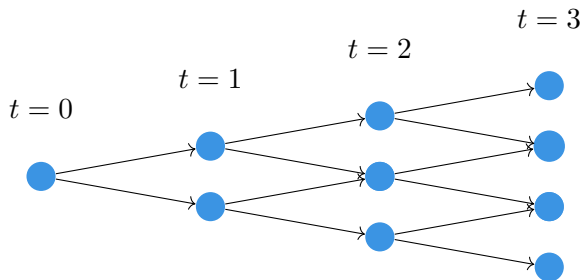


Figure: A 4-stage (**lattice**) scenario tree with 2 scenarios per stage. $\xi = (\xi^1, \xi^2, \xi^3)$;

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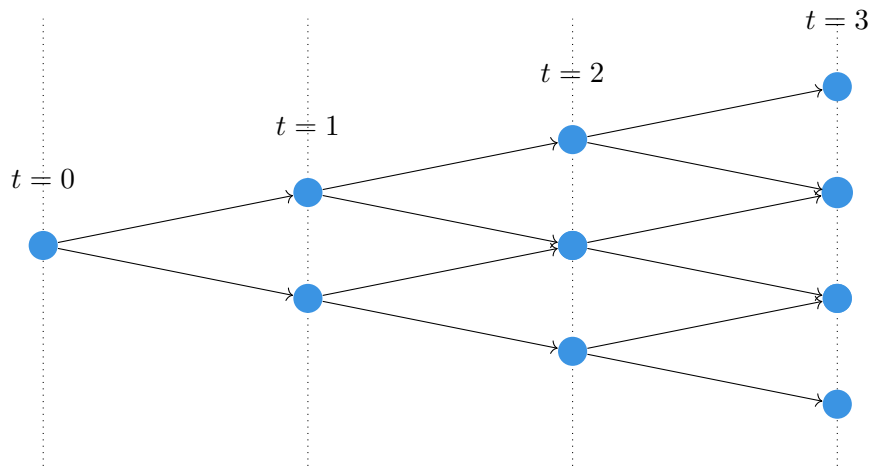
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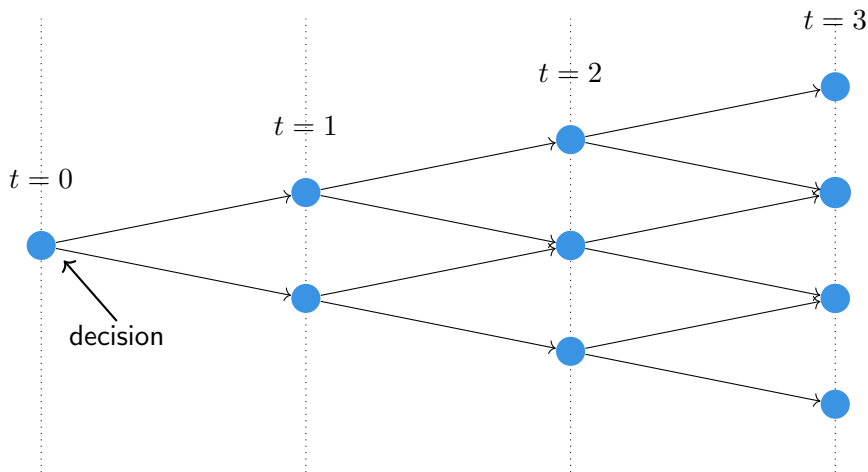
Taxonomy of scenario trees

Terminology



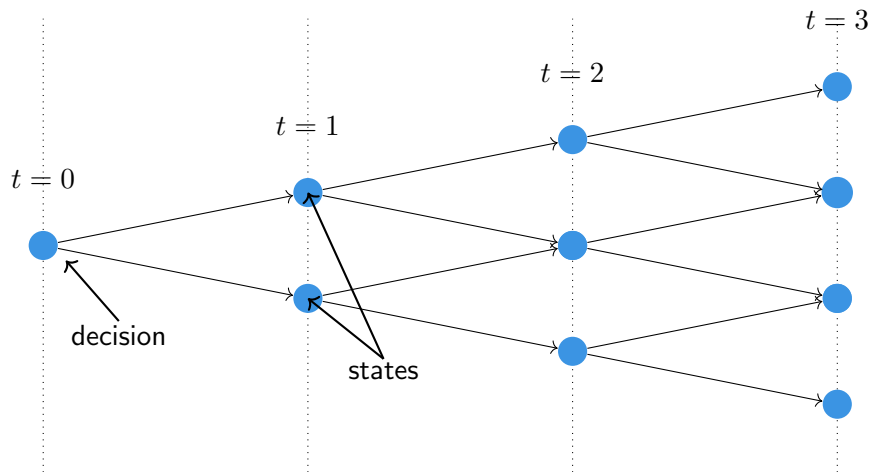
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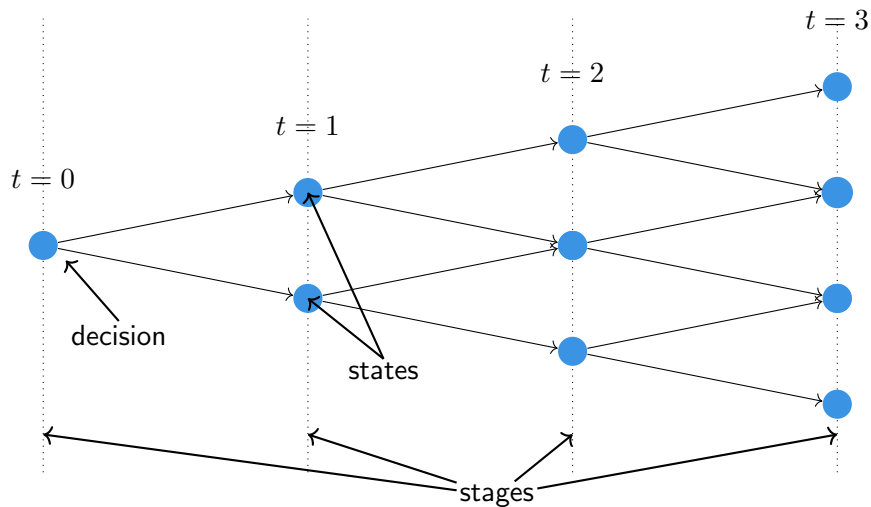
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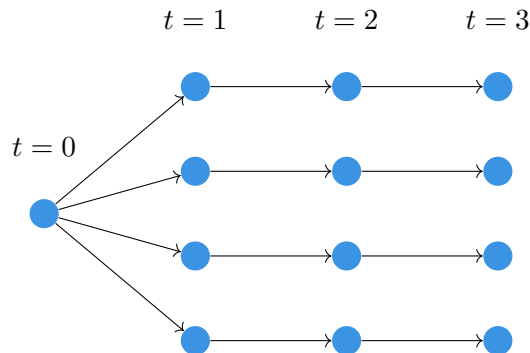


Taxonomy of scenario trees

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

Two parameters govern the geometry of a scenario tree:

- ▶ **Depth:** number of stages H
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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 (out-of-sample) testing.

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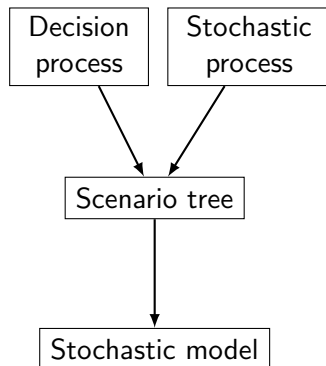
Often, a **combination** of the above is used:

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**.

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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

$$\min_x \mathcal{F}(x, \xi) \text{ approximates } \min_x \mathcal{F}(x, \eta)$$

Quality measures for scenario trees

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

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

The **approximation error** [Pflug, 2001] is defined as

$$\begin{aligned} e(\eta, \xi_k) &= \mathcal{F}(\arg \min_x \mathcal{F}(x, \xi_k), \eta) - \mathcal{F}(\arg \min_x \mathcal{F}(x, \eta), \eta) \\ &= \mathcal{F}(x_k^*, \eta) - \min_x \mathcal{F}(x, \eta). \end{aligned}$$

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- ▶ Calculating $\mathcal{F}(x_k^*, \eta)$ requires evaluating the “true” objective function;
- ▶ Alternatively, **Monte Carlo simulation** is often employed to approximate $\mathcal{F}(x_k^*, \eta)$;
- ▶ Clearly, there is no way to evaluate $\min_x \mathcal{F}(x, \eta)$.

Stability for scenario trees

Out-of-sample stability

Assume that we can **approximate** $\mathcal{F}(x_k^*, \eta)$. This allows us to

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

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Remarks:

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

Stability for scenario trees

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Stability for scenario trees

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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:

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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 $\mathcal{F}(x_k^*, \eta)$ is not feasible, cross-testing can be employed. Let

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

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

Stability for scenario trees

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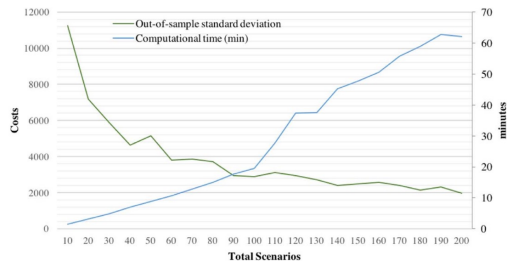
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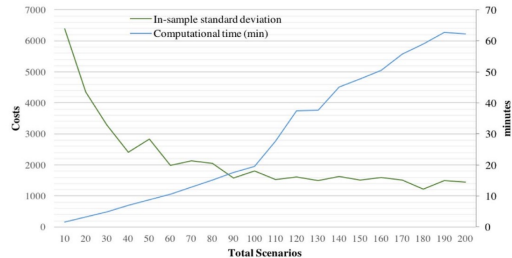
Out-of-sample stability implies that the standard deviation of $\overline{\mathcal{F}}$ is close to 0.

- ▶ 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 $\xi = \{(z_s, p_s)\}_{s \in [S]}$ that has **statistical moments** $f_m(z, p)$ matching M_m^{VAL} **target** values.

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

$$\begin{aligned} \min_{z, p \geq 0} \quad & \sum_{m \in M} w_m (f_m(z, p) - M_m^{\text{VAL}})^2 \\ \text{s.t.:} \quad & \sum_{j=1}^S p_j = 1, \end{aligned}$$

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 .

Scenario generation methods

Metric-based methods

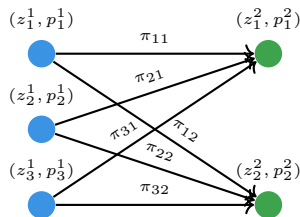
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Let $\xi^l = (z^l, p^l) \in \Xi^l$. The (p -order) Wasserstein distance $d(\xi^1, \xi^2)$ is given by:

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



Scenario generation methods

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];
- ▶ [Löhdorf, 2016]: **Learning-based algorithms** such as competitive learning and Voronoi cell sampling as alternatives to k -means.

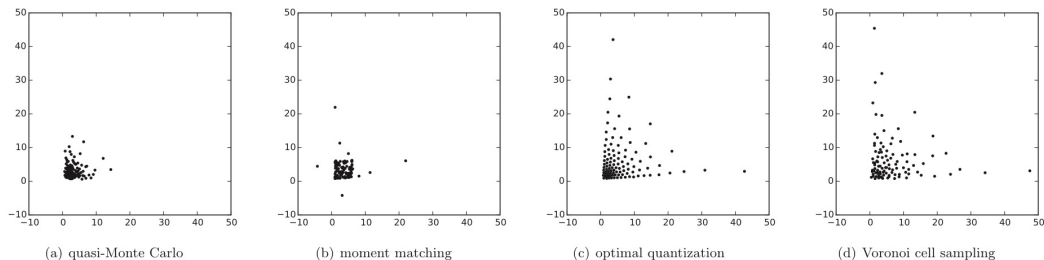


Figure: comparison of scenario generation methods ([Löhdorf, 2016])

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 Fortet-Mourier-type metric
 - Calculation leads to a Monge-Kantorovich mass transportation problem

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 - Changes in the solution can be approximated using a Fortet-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

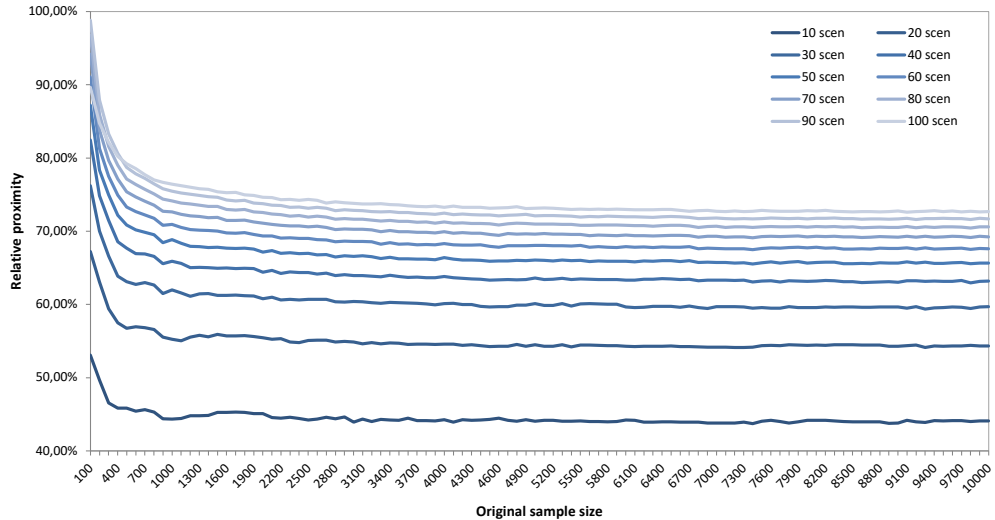
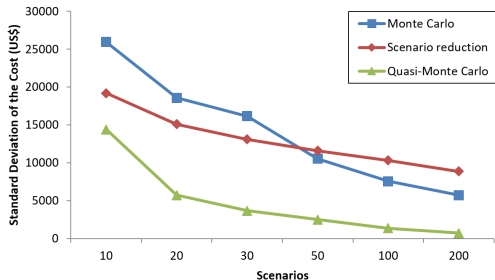


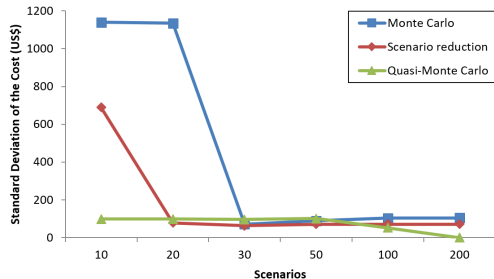
Figure: Relative accuracy for scenario reduction; x -axis is $|\xi^1|$, lines are different $|\xi^2|$.
[Oliveira et al., 2016]

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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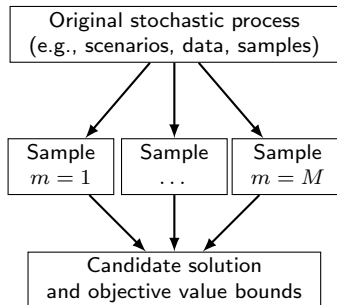
Scenario (tree) generation methods

Sample Average Approximation (SAA)

What is SAA

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

- ▶ Purely based on **sampling**;
- ▶ Monte Carlo simulation for estimating objective function bounds;
- ▶ Useful for handling **large** scenario sets;
- ▶ The sample m scenario tree size N is such that $N \ll |\xi|$ 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 $\mathcal{F}(x, \xi)$.

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First, let us define our notation for **2SSPs**

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

where:

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

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 **scenario tree** $\xi = \{\xi_1, \dots, \xi_N\}$.

Then, we can solve the **sample-based approximation** problem

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

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

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

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

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How SAA works

Calculating lower bounds for z

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

$$\begin{aligned}\hat{z}_N &= \min_x \left\{ \frac{1}{N} \sum_{n=1}^N F(x, \xi_n) \right\} \leq \frac{1}{N} \sum_{n=1}^N F(x, \xi_n) \\ \mathbb{E}_\xi \left[\min_x \left\{ \frac{1}{N} \sum_{n=1}^N F(x, \xi_n) \right\} \right] &\leq \mathbb{E}_\xi \left[\frac{1}{N} \sum_{n=1}^N F(x, \xi_n) \right] \\ \mathbb{E}_\xi [\hat{z}_N] &\leq \mathbb{E}_\xi \left[\frac{1}{N} \sum_{n=1}^N F(x, \xi_n) \right] \\ \mathbb{E}_\xi [\hat{z}_N] &\leq \min_x \left\{ \mathbb{E}_\xi \left[\frac{1}{N} \sum_{n=1}^N F(x, \xi_n) \right] \right\} \xrightarrow{N \rightarrow \infty} \\ &\quad \min_x \{ \mathbb{E}_\xi [F(x, \xi)] \} = \min_x f(x) = z. \quad \square\end{aligned}$$

How SAA works

Calculating lower bounds for z

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

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

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

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

3. We can then estimate³ $\mathbb{E}[\hat{z}_N]$ as

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

³Again an unbiased estimator, see footnote 2.

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 $\sigma_{L_N^M}^2$ can be obtained as

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

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We can use $s_{L_N^M}^2$ to obtain an **$1-\alpha$ 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

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

Under a relatively complete recourse assumption, we have that $f(\hat{x}_N^m) \geq z, \forall m \in [M]$.

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Under a relatively complete recourse assumption, we have 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 \bar{N}

$$\{\xi_1^1, \dots, \xi_{\bar{N}}^1\}, \dots, \{\xi_1^T, \dots, \xi_{\bar{N}}^T\}$$

3. For each scenario tree t , we evaluate

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

How SAA works

Calculating upper bounds for z

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

$$U_N^T = \frac{1}{T} \sum_{t=1}^T \tilde{z}_N^t.$$

Analogously, we can use the sample-estimate for $\sigma_{U_N^T}^2$

$$s_{U_N^T}^2 = \frac{1}{T-1} \sum_{t=1}^T (\tilde{z}_N^t - U_N^T)^2$$

to calculate the $1-\alpha$ confidence interval for U_N^T as

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

On estimating optimality gaps

In this context, an **optimality gap** refers to the quantity

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On the other hand, we know that

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

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

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

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

$$\sigma_{gap(N, M, \bar{N}, T)}^2 = s_{L_N^M}^2 + s_{U_N^T}^2.$$

On estimating optimality gaps

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

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

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

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 2. $s_{U_N^T}^2$, 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.

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 , $U_{\bar{N}}^T$ or $gap(N, M, \bar{N}, T)$;
- ▶ 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.

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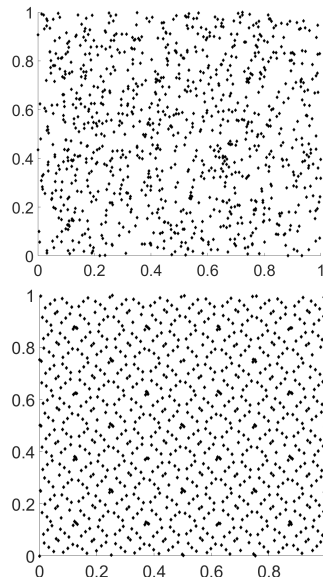


Figure: Monte Carlo (top) and quasi-Monte Carlo (bottom) sampling
[Fernández Pérez et al., 2018]

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





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

SAA example






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