# Stochastic programming & Robust optimisation

## Lecture 2/4

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# Outline of this lecture

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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 $\xi$ comprises sequentially observed realisations of $\xi^t$, for $t = 1, \ldots, H$:

- $\xi = (\xi^t)_{t \in [H]}$, 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 $\xi$;
- Thus, $\xi = \{\xi_s\}_{s \in [S]}$, where $S$ is the number of scenarios.

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**Example:**

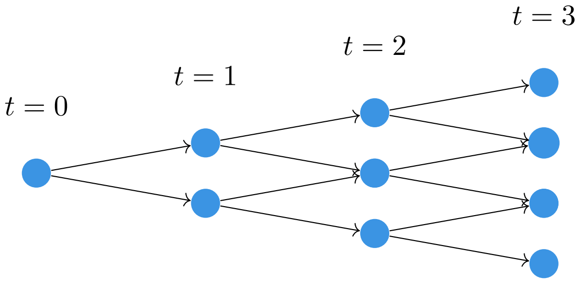


Figure: A 4-stage (lattice) scenario tree with 2 scenarios per stage. $\xi = (\xi^1, \xi^2, \xi^3)$;

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Introduction

Scenario trees

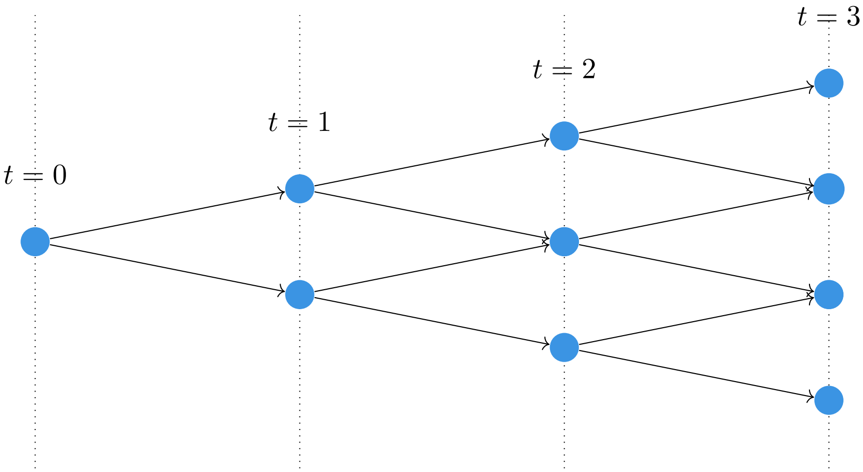
Generating scenario trees

Scenario (tree) generation methods

Sample Average Approximation (SAA)

# Taxonomy of scenario trees

## Terminology



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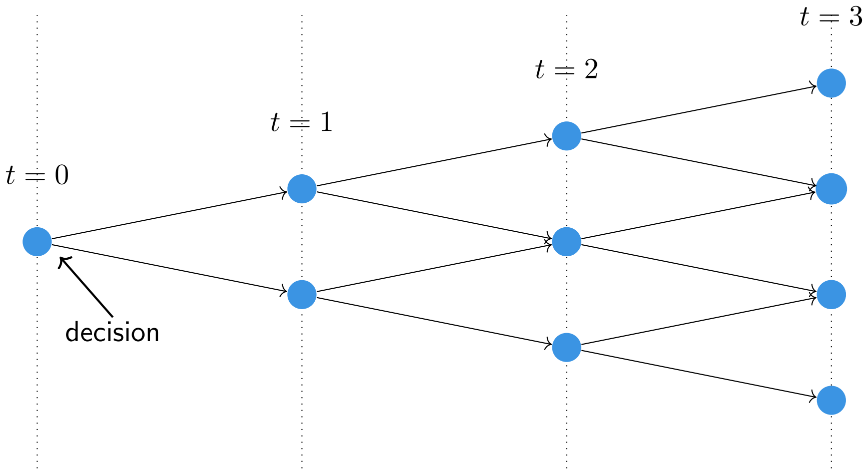

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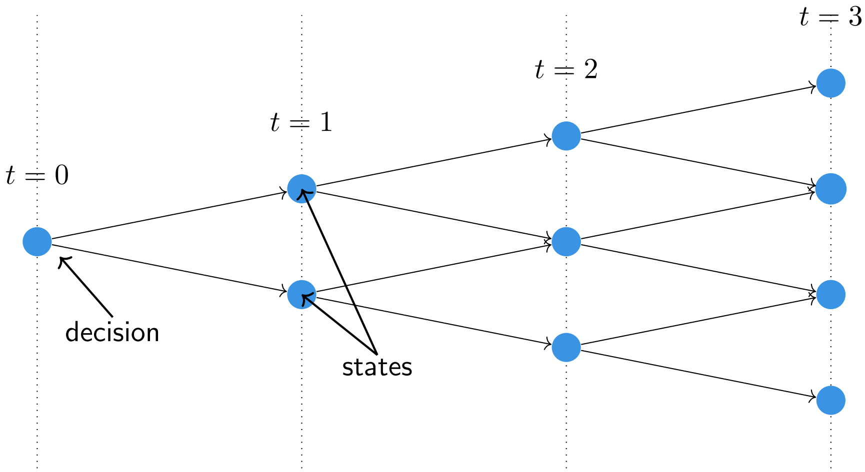

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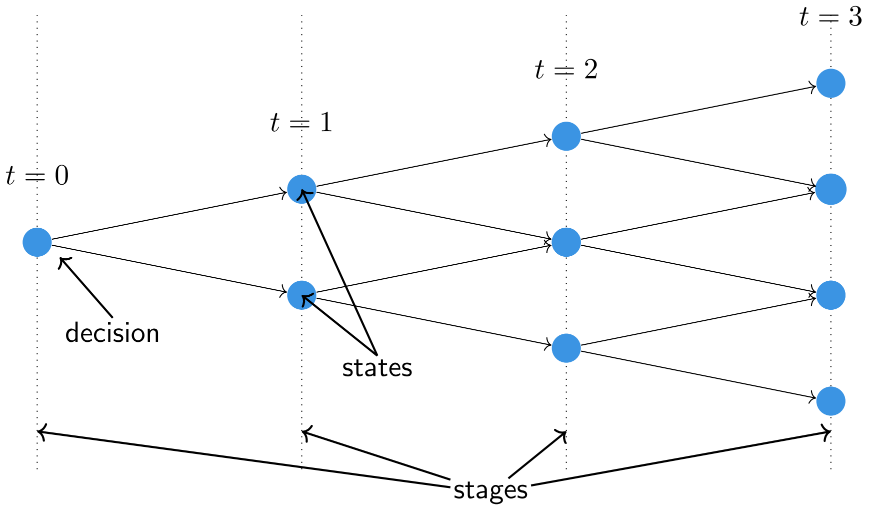

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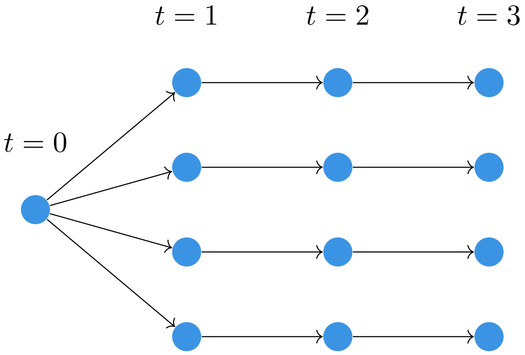


Branching indicates a decision upon arrival of new information

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

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Two parameters govern the geometry of a scenario tree:

- **Depth:** number of stages $H$
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- **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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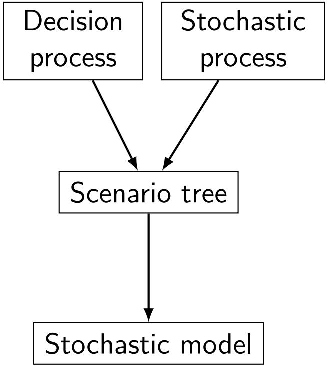
Often, a combination of the above is used:

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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   - Likewise, objective function values should be stable.

Let $\xi$ be a scenario tree representing the original stochastic process $\eta$, and $\mathcal{F}(x,\xi) = \mathbb{E}_\xi\left[F(x,\xi)\right]$. 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 $\xi_k$, for $k = 1, \dots, n$, be a collection of alternative scenario trees generated (e.g., by sampling) to represent $\eta$. We have that

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The approximation error [Pflug, 2001] is defined as

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

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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 $\min_x \mathcal{F}(x, \eta)$.

# Stability of scenario trees

## Out-of-sample stability

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

- compare solutions $x_1^\star$ 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 of scenario trees

## In-sample stability

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In some contexts, can also be defined as

$$||x_k^\star - x_l^\star||_p \approx 0, \text{ for } k, l = 1, \dots, n : k \neq l.$$

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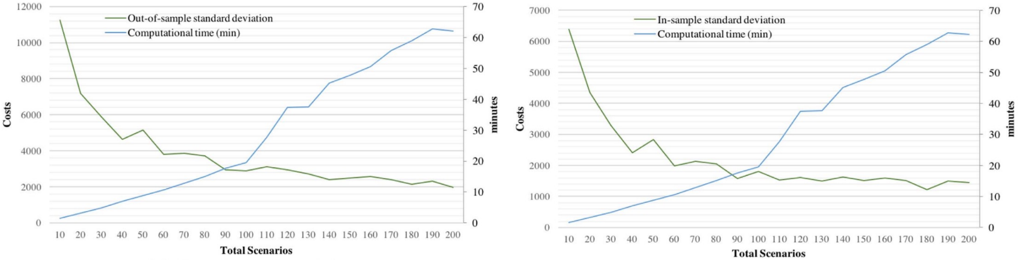
- No direct connection to out-of-sample stability;
- Useful for assessing the internal stability of a random scenario generation method;
- Translates into confidence in the objective function value reported.

# Stability of scenario trees




(a) Out-of-sample stability

(b) In-sample stability

Figure: Trade-off analysis: error v. computational time [Dillon et al., 2017]

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# Scenario generation methods

The main types of scenario-generation methods are:

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2. **Metric-based:** form smaller scenario sets whilst minimising some probabilistic distance metric. Includes clustering (k-means and related methods) and scenario reduction.
3. **Sampling:** Monte-Carlo sampling, or quasi Monte-Carlo sampling using variance reduction techniques (e.g., Sobol sequences). Combined with Sample Average Approximation (SAA).

# 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 $M_m^{\mathsf{VAL}}$ target values.

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## Moment matching

Build a scenario tree $\xi = \{(z_s, p_s)\}_{s \in [S]}$ that has statistical moments $f_m(z,p)$ matching $M_m^{\mathsf{VAL}}$ target values.

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

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

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

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 $\eta$ and $\xi_k$. Thus, the focus is on obtaining trees that minimise $d$.

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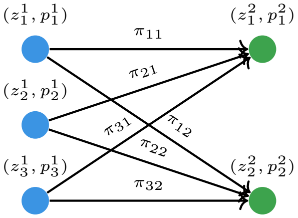
Let $\xi^l = (z^l, p^l) \in \Xi^l$. The ($p$-order) Wasserstein distance $d(\xi^1, \xi^2)$ is given by:

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



# 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];

# 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];
2. **Scenario reduction methods:** Obtain $\xi^2$ from $\xi^1$ 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 amounts to solving 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 $\xi^1$
  1. Find the scenario whose removal causes the smallest error increase
  2. Remove the scenario and redistribute its probability
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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

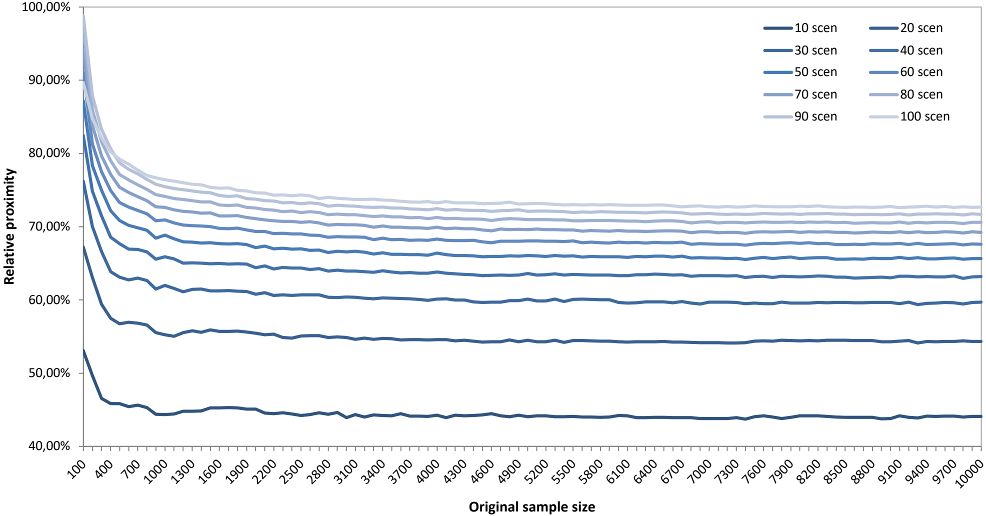


Figure: Relative accuracy for scenario reduction; $x$-axis is $|\xi^1|$, lines are different $|\xi^2|$. [Oliveira et al., 2016]

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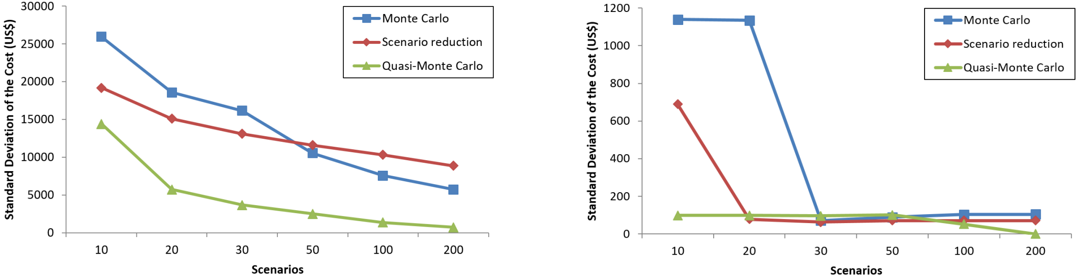


(a) In-sample (b) Out-of-sample

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

# Scenario generation methods

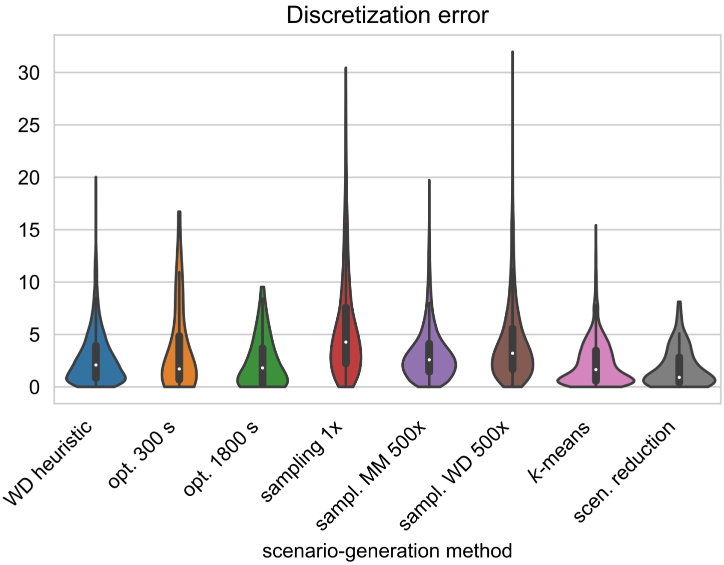


Figure: Out-of-sample error comparison of various scenario generation methods [Kaut, 2021]

# Outline of this lecture

# 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 $N << |\xi|$ or $|\eta|$;
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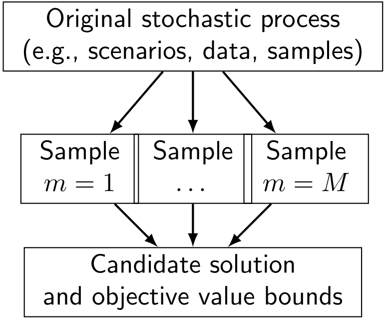

# How SAA works

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

Then, we can solve the sample-based approximation problem

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

[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 $f(x)$:

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

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

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

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\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
\end{aligned}
$$

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

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

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

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# 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 $s^2_{L_N^M}$ 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

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

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 $\overline{N}$

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

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-$\alpha$ 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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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 $\mathbb{E}\left[\hat{z}_N\right]$ ($L_N^M$) 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

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

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  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. $s^2_{U^T_{\overline{N}}}$, 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 $gap(N, M, \overline{N}, T)$;

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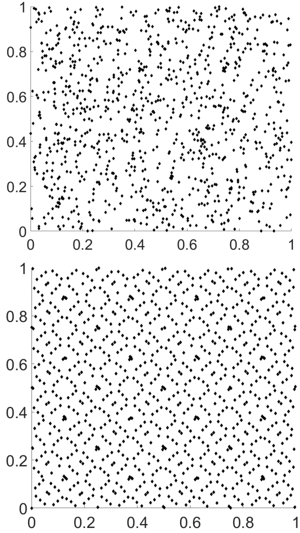


Figure: Monte Carlo (top) and quasi-Monte Carlo sampling [Fernández Pérez et al., 2018]

## 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

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

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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 $\beta$ 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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