# Scenario Generation for Stochastic Programming A Practical Introduction

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## Outline

#### Introduction to Scenario Generation Scenario Trees: What? Why? Goals of scenario generation

#### Measuring Quality of Scenario Trees Quality and how to measure it

Stability tests

#### Scenario-Generation Methods

Conditional sampling Property-matching methods "Optimal Discretization" Step-wise growing & cutting methods



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Scenario Trees: What? Why? Goals of scenario generation

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# Where Do Scenarios Come From?

A stochastic programming (SP) problem is a math. programming problem, with values of some parameters replaced by distributions.

Hence, to solve the problem, we need:

- A model describing the problem.
- Values of the deterministic (known) parameters.
- Description of the stochasticity.
  - Known distributions, described by densities and/or CDFs.
  - Historical data, i.e. a discrete sample.
  - Only some properties of the distributions, for ex. moments.

Problem: SP can handle only discrete samples of limited size, so we need to approximate the distribution. The approximation is called a scenario tree.



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Scenario Trees: What? Why? Goals of scenario generation

## Scenario Tree – Example and Terminology.



#### Terminology:

scenario is a path from the root to one leaf.

stage is a moment in time, when decisions are taken.

period is a time interval between two stages.



Scenario Trees: What? Why?

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Scenario Trees: What? Why? Goals of scenario generation

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period is a time interval between two stages.

Tree above:  $2 \times 3 \times 3 = 18$  scenarios, 4 stages, and 3 periods.



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Scenario Trees: What? Why? Goals of scenario generation

## Scenario Tree – Importance of Branching.

Why a tree, why not a "fan" like this?



- Branching = arrival of new information.
- Fan above: no new information after the first stage.
- Hence, the fan represents a two-stage problem.



## What to Do Before Scenario Generation

Prior to scenario generation, we have to:

- Decide the time discretization.
  - number of stages
  - lengths of time periods
- Know what information becomes available when, relative to the timing of decisions. This issue does not exist in the deterministic case.
- Decide the number of branches per stage.
  - Some methods will do this automatically.

Note: deep vs. wide trees - an open question...



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Scenario Trees: What? Why? Goals of scenario generation

## Sources of Data for Scenarios

- Historical data
  - Is history a good description of the future?
- Simulation based on a mathematical/statistical model
  - Parameters estimated from the real case
- Expert opinion
  - Subjective
  - Back-testing is not possible.
- Often a combination of more of the above
  - Estimate the distribution from historical data, then use a mathematical model and/or an expert opinion to adjust the distribution to the current situation.



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## Structure of a Stochastic Programming Problem





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# Structure of a Stochastic Programming Problem



- Choice of a good scenario generation method is problem-dependent.
- Scenario generation is a part of the modelling process.



## Specifics of Scenario Generation

- Scenarios are not a natural part of the problem, but a result of the method.
- Hence, neither the user nor the modeler are typically interested in scenarios and their generation.
  - Until recently, many users of stochastic programming did not pay much attention to scenario generation.
- BUT: Scenarios can influence the quality of the solution (garbage in – garbage out).
- One solution is to make scenario generation as much automatic, i.e. "invisible" to the user, as possible.



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# A Good Scenario Generation Method Should

- Be as automatic (hidden to the user) as possible.
- Influence the solution only as little as possible.
- The scenario-based solution should converge to the true optima, with increasing number of scenarios.
- ▶ Be as "good" as possible for a given number of scenarios.
- The distance from the true distribution in the statistical sense is not so important.
- What is important is problem-dependent: for example, for the classical one-period Markowitz mean-variance model, it is enough to capture means, variances, and covariances the rest is irrelevant.



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Quality and how to measure it Stability tests

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# Quality of Scenario Trees and How to Measure It

In accessing the quality, we have consider two things:

Error

- We use an approximation of the true distribution, so we are likely to find a suboptimal solution.
- Not straightforward how to measure the error.

Stability

- If we generate several scenario trees, the solutions should not vary too much.
- Stochastic programs tend to have *flat objective functions*, so we can only require stability of the objective values, not of the solutions themselves.



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## Some Notation

The original (unsolvable) problem

 $\min_{\pmb{x}\in\pmb{X}} F(\pmb{x};\tilde{\pmb{\xi}})$ 

is replaced by a scenario-based problem

$$\min_{\boldsymbol{x}\in\boldsymbol{X}} F(\boldsymbol{x};\tilde{\boldsymbol{\eta}}).$$

In the stability tests, we generate several scenario trees  $\tilde{\eta}_k$ , k = 1, ..., n, leading to solutions

$$x_k^* = \operatorname*{argmin}_{\boldsymbol{x} \in \boldsymbol{X}} F(\boldsymbol{x}; \tilde{\boldsymbol{\eta}}_k).$$



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# Error Caused by the Discretization

Pflug (2001) defines an approximation error caused by  $\tilde{\eta}_k$  as:

$$e_f(\tilde{\xi}, \tilde{\eta}_k) = F\left(\underset{\boldsymbol{x}}{\operatorname{argmin}} F(\boldsymbol{x}; \tilde{\eta}_k); \tilde{\xi}\right) - F\left(\underset{\boldsymbol{x}}{\operatorname{argmin}} F(\boldsymbol{x}; \tilde{\xi}); \tilde{\xi}\right)$$
$$= F\left(\boldsymbol{x}_k^*; \tilde{\xi}\right) - \min_{\boldsymbol{x}} F(\boldsymbol{x}; \tilde{\xi}) \ge 0.$$

### To evaluate $e_f(\tilde{\xi}, \tilde{\eta}_k)$ , we would need to:

- Evaluate the "true" objective function  $F(\mathbf{x}; \tilde{\xi})$ .
  - Can sometimes be done using a "simulator".
- Solve the original problem, i.e. (arg)  $\min F(\mathbf{x}; \hat{\boldsymbol{\xi}})$ .
  - ▶ Impossible ... Otherwise, we would not need scenarios.



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### To evaluate $e_f(\tilde{\xi}, \tilde{\eta}_k)$ , we would need to:

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Conditional sampling Property-matching methods "Optimal Discretization" Step-wise growing & cutting methods



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# Tests Using a Simulator

Assume that we have a "simulator" for evaluating  $F(\mathbf{x}; \tilde{\xi})$ , i.e. the true performance of a solution  $\mathbf{x}$ . This allows us to:

- Compare two solutions x<sub>1</sub><sup>\*</sup>, x<sub>2</sub><sup>\*</sup>.
- Compare two different scenario-generation methods.
- Test an out-of-sample stability of a given method:
  - 1. Generate a set of trees  $\tilde{\eta}_k$ , k = 1, ..., n.
  - 2. Solve problems using the trees  $\rightarrow$  solutions  $\boldsymbol{x}_{k}^{*}$ .
  - 3. Test whether  $F(\boldsymbol{x}_{k}^{*}; \tilde{\boldsymbol{\xi}}) \approx F(\boldsymbol{x}_{l}^{*}; \tilde{\boldsymbol{\xi}})$
  - The test is equivalent to  $e_f(\tilde{\xi}, \tilde{\eta}_k) \approx e_f(\tilde{\xi}, \tilde{\eta}_l)$ .
  - Without stability, we have a problem!



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Quality and how to measure it Stability tests

# Notes on the Stability Test

- $e_f(\tilde{\xi}, \tilde{\eta}_k) \approx 0$  implies  $e_f(\tilde{\xi}, \tilde{\eta}_k) \approx e_f(\tilde{\xi}, \tilde{\eta}_l)$  and stability.
- Stability test assumes that we get a different tree on each run of the scenario-generation method.
- Otherwise, we can run it with different tree sizes.

Another issue:

- Only the root variables can be moved from one tree to another, as the scenarios do not coincide.
- To evaluate F(x; ξ̃), we have to fix the root part of x and (re)solve the problem.
- Not such a big issue, as the root variables (decisions) are the only ones implemented.



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# Out-of-Sample Tests Without a Simulator

Instead of using a simulator, we can "cross test", i.e. test

$$\mathsf{F}ig(oldsymbol{x}^*_k; ilde{oldsymbol{\eta}}_lig)$$
 for  $l
eq k$ 

for all  $k = 1, \ldots, n$ .

- It is still an out-of-sample test, as we test the solutions on different trees than were used to find them.
- If we have to choose one of the solutions *x<sub>k</sub>*, we would choose the most stable one.



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## **In-Sample Stability**

Instead of the true performance, we look at the optimal objective value reported by the problem itself:

$$F(\boldsymbol{x}_{k}^{*}; \tilde{\boldsymbol{\eta}}_{k}) \approx F(\boldsymbol{x}_{l}^{*}; \tilde{\boldsymbol{\eta}}_{l}),$$

or, equivalently,

$$\min_{\boldsymbol{x}} F(\boldsymbol{x}; \tilde{\boldsymbol{\eta}}_k) \approx \min_{\boldsymbol{x}} F(\boldsymbol{x}; \tilde{\boldsymbol{\eta}}_l) \,.$$

- No direct connection to out-of-sample stability.
  - Can even have  $e_f(\tilde{\xi}, \tilde{\eta}) = 0$ , without in-sample stability.
- Without this, we can not trust the reported performance of the scenario-based solutions.



## What If We Do Not Have Stability?

What does it mean:

 $\blacktriangleright$  No stability  $\rightarrow$  decision depends on the choice of the tree.

What to do:

- Change/improve the scenario generation method.
- Increase the number of scenarios.
- Generate several trees, get the solutions and then "somehow" choose the best solution.

Example

Note: A proper theoretical treatment of stability can be found in Heitsch, Römisch and Strugarek (2006).



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# One-Period Case - Standard Sampling I.

#### Univariate random variable

- This is a standard random number generation.
- Methods exist for all possible distributions.

#### Independent multivariate random vector

- Generate one margin at a time, combine all against all
  - guaranteed independence
  - grows exponentially with the dimension
  - trees need often some "pruning" to be usable
- Generate one margin at a time, then join together, first with first, second with second...
  - independent only in the limit
  - size independent on the dimension



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## One-Period Case - Standard Sampling II.

#### General multivariate case

- Special methods for some distributions.
  - Ex.: normal distribution via Cholesky decomposition
- Use principal components to get "independent" variables.
  - Components are independent only for normal variables.
  - Generally, they are only uncorrelated.

### Bootstrapping / Sampling from historical data

- Does not need any distributional assumptions.
- Needs historical data.
- Are historical data a good description of the future?



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## Handling Multiple Periods

Generate one single-period subtree at a time. Start in the root, move to its children, and so on.

### Inter-temporal independence

Easy, as the distributions does not change.

Distribution depends on the history.

- Distribution of children of a node depends on the values on the path from the root to that node.
- The dependence is modeled using stochastic processes like ARMA, GARCH, ...
- Effects we might want to consider/model:
  - mean reversion
  - variance increase after a big jump



Conditional sampling

## Sampling Methods – Summary

#### Pros

- Easy to implement.
- Distribution converges to the true one.

### Cons

- Bad performance/stability for small trees.
  - This can be improved by using corrections or some special techniques, such as low-discrepancy sequences.
- Have to know the distribution to sample from.



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## Property-Matching Methods – Basic Info

- These methods construct the scenario trees in such a way that a given set of properties is matched.
- The properties are for ex. moments of the marginal distributions and covariances/correlations.
- Typically, the properties do not specify the distributions fully; the rest is left to the method.
  - Different methods produce very different results.
  - The issue is very significant for bigger trees, with many more degrees of freedom.



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## Example 1 - from Høyland and Wallace (2001)

- An optimization problem with values of the random variables and scenario probabilities as variables.
- The measured properties are expressed as function of these variables.
- The objective is to minimize a distance (usually L<sub>2</sub>) of these properties from their target values.
- Leads to highly non-linear, non-convex problems.

Example

- Works well for small trees, otherwise very slow.
- The optimization is often underspecified & no control what the solver does about the extra degrees of freedom.



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# Example 2 - from Høyland, Kaut, Wallace (2003)

- Developed as a fast approximation to the previous method, in the case of four marginal moments + correlations.
- Build around two transformations:
  - 1. Correcting correlations
    - Multiply the random vector by a Cholesky component
    - Changes also the marginal distributions (except normal)
  - 2. Correcting the marginal distributions
    - A cubic transformation of the margins, one margin at a time
    - Changes the correlation matrix
- The two transformations are repeated alternately.
- Starting point can be, for ex., a correlated normal vector.
- Works well for large trees (creates smooth distributions).
- Needs pre-specified probabilities (usually equiprobable).



Details

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# Property-Matching Methods – Summary

Pros

- Do not have to know/assume a distribution family, only to estimate values of the required properties.
- Can combine historical data with today's predictions.
- The marginal distributions can have very different shapes, so the vector does not follow any standard distribution.

### Cons

- ► No convergence to the true distribution.
- If we know the distribution, we can not utilize this information, i.e. we throw it away.



Can be hard to find which properties to use.

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Tutorial on Scenario Generation

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"Optimal Discretization"

## "Optimal Discretization" by G. Pflug I.

Starts with the approximation error  $e_f(\tilde{\xi}, \tilde{\eta}_k)$ :

$$e_{f}(\tilde{\xi}, \tilde{\eta}_{k}) = F\left(\underset{\boldsymbol{x}}{\operatorname{argmin}} F\left(\boldsymbol{x}; \tilde{\eta}_{k}\right); \tilde{\xi}\right) - F\left(\underset{\boldsymbol{x}}{\operatorname{argmin}} F\left(\boldsymbol{x}; \tilde{\xi}\right); \tilde{\xi}\right)$$
$$= F\left(\boldsymbol{x}_{k}^{*}; \tilde{\xi}\right) - \min_{\boldsymbol{x}} F\left(\boldsymbol{x}; \tilde{\xi}\right) \ge 0.$$

Pflug (2001) shows that, under certain Lipschitz conditions,

$$\operatorname{e}_{f}(\tilde{\xi}, \tilde{\eta}_{k}) \leq 2 \sup_{\boldsymbol{x}} \left| F(\boldsymbol{x}; \tilde{\eta}_{k}) - F(\boldsymbol{x}; \tilde{\xi}) \right| \leq 2 L \operatorname{d}(\tilde{\eta}_{k}, \tilde{\xi}),$$

where L is a Lipschitz constant of f(), with  $F(\mathbf{x}; \tilde{\mathbf{\xi}}) = \mathbb{E}^{\tilde{\mathbf{\xi}}} \left[ f(\mathbf{x}, \tilde{\mathbf{\xi}}) \right]$  and  $d(\tilde{\eta}_k, \tilde{\mathbf{\xi}})$  is a Wasserstein (transportation) distance of distribution functions of  $\tilde{\eta}_k$  and  $\tilde{\xi}$ .



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## "Optimal Discretization" by G. Pflug II.

The method then creates a scenario tree that minimizes the transportation distance  $d(\tilde{\eta}_k, \tilde{\xi})$ .

- Whole multi-period tree is generated at once.
- ► The tree is "optimal" in a clearly specified sense.
- The optimisation problem disappeared from the measure!
- Nothing is said about tightness of the bounds.



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## Step-Wise Growing & Cutting Methods

- Methods to transform a given scenario tree into a tree better suited for the given problem.
- Can have different starting points:
  - A big sampled tree then we need to reduce it.
  - One scenario only then we need to grow it.
  - A "fan" (collection of paths) need to make a tree out of it.
- Differ in the level of integration with the model.
  - Some work only with the distribution of the tree.
  - Some use the model to evaluate the quality.
  - Some are actually a part of the solution method.

These methods are useful if we have a data (or a simulation model that produces the "data") in a form that is *not suitable for the optimization model*.



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## Scenario Reduction by Dupačová et al

- Starts with discrete probability measure P (a scenario tree) often sampled from stochastic processes (time series).
- The goal is to find a discrete probability measure Q (a smaller tree) of given cardinality, that is closest to P in the sense of Fortet-Mourier type metric.
  - The metric is independent on the optimization problem.
- The evaluation of the distance leads to a linear transportation problem.
- Need heuristics for deciding which scenarios to remove from the scenario tree given by P.
  Details
- ► The results of their numerical example were:
  - ► 50% scenarios give 90% relative accuracy.
  - 2% scenarios give 50% relative accuracy.



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# Making Tree Out of a Fan by Heitsch and Römisch

- In practice, data are often available as sequences/paths.
   Examples: rainfall data each year is a scenario/path.
   : evolving a stochastic process.
- Put together, they form a fan, not a tree.
- Need to bind some nodes into, one to create a tree.
- Based on the same ideas as the scenario reduction, i.e. minimizes the *Fortet-Mourier* type metric.
- Two different method, backward and forward.
- ► The results of their numerical example were:
  - ▶ 15% nodes give 60% accuracy.
  - 6% nodes give 50% accuracy.

### Other methods are also available: clustering / "bucketing".



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## Model-Based Cutting and Growing Methods

Iterative methods, with a general structure:

### loop

improve the tree: cut and/or grow branches solve the problem on the new tree analyze the solution while solution/tree not good enough

- Can start with a single scenario, for ex. expected values.
- New scenarios added by (importance) sampling.
- Example: EVPI-based method by Dempster and Thomson.
  - EVPI = Expected value of perfect information.
  - Uses EVPI to decide where to add/delete scenarios.



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## Internal Sampling Methods

- Sampling of scenarios is a part of the solution procedure.
- The information where to add/delete scenarios is obtained from the model, for example from the *dual variables*.
  - Then it works only for linear stochastic programs!
- Scenario generation disappears from the modelling process, yet we still have to decide the number of periods etc.

### Examples:

Stochastic decomposition by Higle and Sen.

Importance sampling within Benders by Dantzig and Infanger.

Stochastic quasi-gradient method by Ermoliev, Gaivoronski.

This works for convex programs, not only LPs.



For Further Reading

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Quality and how to measure it Stability tests

### Scenario-Generation Methods

Conditional sampling Property-matching methods "Optimal Discretization" Step-wise growing & cutting methods



## Summary

- Scenario generation is an important, even if often overlooked, part of stochastic programming.
- A bad scenario-generation method can spoil the result of the whole optimization.
- There is an increasing choice of methods, but one has to test which one works best for a given problem.
- Open questions:
  - Is there a universally good scenario-generation method?
  - What is the optimal structure of a tree (deep vs. wide)?



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For Further Reading

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Michal Kaut (Molde University College)

Tutorial on Scenario Generation

Håholmen, June 10-12, 2006

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### Example: What Is the Best Method and/or Solution?

14000

13500 13000

12500

12000

11500

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In-sample stability of three different methods.

Shows the optimal objective values for different sizes of scenario trees.



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### Example: What Is the Best Method and/or Solution?

30000

25000

20000

10000

5000

Out-of-sample of three different methods.

Shows a level of infeasibility of the solutions for different sizes of scenario trees.



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### Example of the Optimization-Based Moment Matching



2 variables x, y + node probabilities pSpecifications:

- $\mathbb{E}[x], \mathbb{E}[y]; \mathbb{E}[x^2], \mathbb{E}[y^2]; \operatorname{Cov}(x, y)$
- Possibly other functions of x, y, p.

$$\begin{split} \min_{x,y,p} & \left(\sum_{i} p_{i} x_{i} - \mathbb{E}\left[x\right]\right)^{2} + \left(\sum_{i} p_{i} y_{i} - \mathbb{E}\left[y\right]\right)^{2} \\ & + \left(\sum_{i} p_{i} x_{i}^{2} - \mathbb{E}\left[x^{2}\right]\right)^{2} + \left(\sum_{i} p_{i} y_{i}^{2} - \mathbb{E}\left[y^{2}\right]\right)^{2} \\ & + \left(\sum_{i} p_{i} (x_{i} - \mathbb{E}\left[x\right])(y_{i} - \mathbb{E}\left[y\right]) - \operatorname{Cov}(x, y)\right)^{2} \\ \text{s.t.:} & \sum_{i} p_{i}^{i} = 1 \quad \text{and} \quad p_{i} \geq 0, \ i = 1, \dots, 3. \end{split}$$



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More Info on Transformation-Based Moment Matching Correction of the correlations

- The target correlation matrix is  $R_* = L_*L_*^T$ .
- The correlation matrix at step k is  $R_k = L_k L_k^T$ .
- Then  $Y = L_* L_k^{-1} X$  has correlation matrix  $R_*$ .

### The cubic transformation

- For each margin *i*:  $Y_i = a + bX_i + cX_i^2 + dX_i^3$
- ► To find the coefficients *a*, *b*, *c*, *d*, we have to:
  - express the moments of Y<sub>i</sub> as a function of a, b, c, d and the moments of X;
  - ▶ find the values of a, b, c, d that minimize the L<sub>2</sub> distance of the moments from their target values.
- This is a non-linear, non-convex optimization problem fortunately with only four variables.



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### Scenario-Reduction Heuristics I.

- Methods to remove k of the N scenarios.
- Then have to adjust probabilities of the rest of the tree.

#### **Backward reduction**

- ► Remove k<sub>1</sub> ≤ k scenarios, minimizing over all k<sub>i</sub> ≤ k and over all combinations of scenarios to be removed.
- If  $k_1 < k$ , repeat with  $k_2 \le k k_1$ , etc.

### Backward reduction of single scenarios

▶ Variant of the above, with  $k_i = 1$  (one scenario at a time).

### Forward selection

- Choosing the remaining N k scenarios.
- Selection is done recursively, one at a time.
- ► This method gets very slow for bigger trees P and Q: about 1000× slower for N = 3<sup>6</sup> = 729 and N - k = 600.



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### Scenario-Reduction Heuristics II.

Two additional heuristics were created Heitsch and Römisch, improving on the performance.

Simultaneous backward reduction

- The major difference is to include all deleted scenarios into each backward step simultaneously.
- Better results (smaller distance from P) than the original backward reduction, but slower.
- ▶ Running time *decreases* with the size of *Q*, for given *P*.

Fast forward selection

- An improvement of the forward method.
- This methods yields the best trees.
- Running times are comparable to the above, but the running time *increases* with the size of Q.

🖣 Go Back

- Start at the last stage, join some nodes into one.
- This joins all their predecessors as well.
- Move backwards until the first stage.





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Scenario Tree Modelling – Methods + Example Backward tree construction

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## Scenario Tree Modelling – Methods + Example Backward tree construction

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- Move backwards until the first stage.

## Forward tree construction

- Start at the first stage, join some nodes into one.
- Move forward until the last stage.

Comparison of the methods:

- Almost no difference in the speed.
- With equal settings, the forward method creates trees with (much) *less nodes and scenarios*.
  (Joining nodes in the last stage means deleting scenarios.)

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