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# A Multistage Stochastic Program for the Design and Management of Flexible Infrastructure Networks

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## Abstract

Throughout their lifetime, infrastructure network systems face unplanned events that impose pressures on their integrity, functionality, and ability to deliver value. Most of the existing infrastructure is designed to deal with the challenges imposed by uncertain external phenomena. Authors from different backgrounds have identified flexibility, changeability, and adaptability as key attributes that modern systems should have to face uncertain scenarios. Specifically, flexibility is an ability that allows a system to be *easily* adapted when necessary. The concept of flexibility is compelling, but it is not clear how to measure the value it may provide. Determining how much to pay to introduce flexibility is an essential aspect of designing flexible systems, but the dependence of this value on the future evolution of the system results in a complex decision process. The sequential nature of the process can be modeled using multistage stochastic programming. The model explicitly considers the flexibility built into the network components as a decision variable at the initial stage. The model is tested in a generic infrastructure network that must meet a stochastic demand. The results show the relationship between the value of flexibility and the life-cycle costs at the construction and operation stages.

*Keywords:* Flexibility, Multistage Stochastic Programming, Value of Flexibility, Infrastructure Networks

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# 1. Introduction

## 1.1. Background

Infrastructure networks, as any infrastructure system, are constantly exposed to ever-changing conditions. Changes in the demand, the supply sources (in the case of water and energy distribution systems), and regulations may impose large stresses on the system [1, 2, 3, 4]. This uncertainty can either challenge or boost the ability of the network to perform at required levels [5]. In the former case, networks usually rely on the robustness provided by over-dimensioned designs which can be largely inefficient, as in the case of sanitation systems [6]. In the latter case, even if the new conditions are favorable, the network may not have the tools to take advantage of the new opportunities [7]. To face these challenges, many authors have identified the need to develop flexible and adaptable systems, which have the potential to improve the sustainability and efficiency of the system under highly uncertain conditions [8, 9, 10, 11, 12].

Specifically, flexible systems are defined as systems with the ability to change as “easily” as possible [13, 14, 15, 4, 16]. This can be measured as the money or time investment required to modify the system. In the case of infrastructure networks, adaptations can be usually seen as the addition (or removal) of nodes and links or the expansion (or downgrade) of their capacity. Other changes, mostly managerial, may be possible (e.g. reversal of the flow direction). Flexibility is introduced by investing a number of resources during the design and construction phase to enable the option of deploying future adaptations at lower costs and shorter lead times. This investment is usually called the *value of flexibility* and is defined as the amount the system stakeholders’ are willing to pay to introduce flexibility into the system [7, 8]. It is assumed that the enabled adaptations are capped at a certain value that depends on the amount invested at the initial stages of the project [16]. This interpretation of flexibility is similar to the concept of shell capacity described by Angelus et al. [17].

## 1.2. Previous works and applications

While flexibility is not limited to capacity expansion, this type of problem is the most common and has been extensively studied in the manufacturing sector [18, 19, 20]. The first work comes from Manne [21], who modeled the optimal excess capacity of pipelines, highways, and steel plants subject to a random walk demand. Luss [18] further detailed the problem as determining the size, location, and timing of future adaptations while minimizing the discounted costs of the expansion

31 processes. This author also identified the modeling of the demand, the representation of the capacity  
32 as a continuous or discrete variable, the selection of the discount rate, and the presence of economies  
33 of scale as key elements of the problem formulation. Mathematical programming rapidly became  
34 one of the preferred methods to solve this type of problem, as shown by the work of Rajagopalan  
35 [22], who formulated a mathematical programming model to determine the optimal initial capacity  
36 and the technology acquisition decisions, for increasing demands. Later came the work of Ahmed  
37 and Sahinidis [23] who developed a multistage stochastic (MS) integer program to analyze a multi-  
38 period investment model for capacity expansion under uncertain demand and costs, and including  
39 the effect of economies of scale. Singh et al. [24] also developed an MS integer programming model  
40 for planning discrete capacity expansion of production facilities. Similarly, Huang and Ahmed [25]  
41 formulated a general MS capacity planning model with discrete capacity for the semiconductor  
42 industry.

43 The prevalence of stochastic and dynamic programming models to solve capacity expansion  
44 problems in the manufacturing sector led to the adoption of these techniques in other areas such  
45 as planning and design of infrastructure networks. For instance, in the context of transportation  
46 networks, Marín and Jaramillo [26] formulated a multi-period capacity expansion problem for rapid  
47 transit network design. Karoonsoontawong and Waller [27] developed a robust optimization model  
48 for the problem of continuous traffic network capacity expansion with dynamic traffic assignment  
49 and traffic signal optimization. Gao et al. [28] considered the case where a road network is expanded  
50 either by adding new links or by increasing the capacity of the existing links, integrated with the  
51 road maintenance problem using a mixed-integer, non-linear, bi-level optimization program, using  
52 multi-period decisions. In the area of water and sewage distribution systems, Mortazavi-Naeini  
53 et al. [9] developed a multi-objective optimization approach for the planning of urban water system  
54 expansions that considers the combined effect of operating rules and infrastructure conditions. Saif  
55 and Almansoori [29] developed a model for the expansion of water desalination and power supply  
56 infrastructure using a deterministic multi-period mixed-integer linear programming formulation.  
57 Similarly, Fraga et al. [10] used dynamic programming to develop an integrated framework for  
58 the optimization of water supply system expansions, considering short and long-term water supply  
59 sources. In the case of energy production and transmission networks, Loureiro et al. [30] used the  
60 concept of real options combined with a mixed-integer linear programming model for multistage  
61 expansion planning. Cardin et al. [31] combined decision rules and stochastic programming to model

62 flexibility in a nuclear infrastructure system, considering a random demand and including the social  
63 acceptance of nuclear power as a limitation to the system expansion capabilities. For networks in  
64 general, Taghavi and Huang [32] applied the concepts of spot market and contract capacity combined  
65 with an MS integer program to model a network with multiple sources of capacity.

66 In both manufacturing systems and infrastructure networks, the adaptation process requires  
67 large capital investments (in proportion with the total system size), which are sometimes irre-  
68 versible [33], and are susceptible to the negative consequences of large lead times. In both cases,  
69 there is a contradictory effect from economies of scale, which may favor both large initial designs  
70 and large future adaptations. However, infrastructure networks are subject to more strict gov-  
71 ernmental regulations, where failure to comply with minimum levels of performance can result in  
72 heavy societal costs. This poses an additional problem of strategically selecting the extent to which  
73 flexibility should be incorporated. Besides, infrastructure networks are usually planned for longer  
74 service horizons, which favors delayed deployments due to discounting [34]. Furthermore, the nature  
75 of stakeholders affects the management and adaptation strategies. While manufacturing systems  
76 are generally completely privately owned, infrastructure network ownership can range from com-  
77 pletely public to completely private, which may create conflicting interests. For instance, in energy  
78 infrastructure, maintaining a determined level of excess capacity may be valuable for society but  
79 not for profit maximization [35]. Finally, the frequency of adaptation is considerably different: in  
80 manufacturing systems is not uncommon to see changes every one or two years, while infrastructure  
81 networks may see changes in periods of five to ten years.

### 82 *1.3. Objectives and scope*

83 The works discussed in the previous section show the potential of (and the preference for) MS  
84 programming as a tool to model and solve complex sequential decision problems. Considering that  
85 the problem of designing and managing flexible infrastructure networks is in itself a sequence of  
86 decisions under uncertainty, this paper proposes a multistage stochastic program (MSP) to analyze  
87 the problem of flexibility. Operational and maintenance costs are explicitly considered, to take  
88 into account the relative importance of these costs in the systems modeled and the impact these  
89 costs may have on the preference of the model for flexible solutions. The model uses scenario  
90 trees generated by Monte-Carlo simulation and k-medoids clustering to simulate and discretize  
91 the random process. The novelty of the model is that it explicitly considers the flexibility range

92 introduced by design as a decision variable, which will restrict all the future planned adaptations.  
93 The proposed model results in an alternative methodology to real options as a tool to determine the  
94 *value of flexibility*. By modeling flexibility as a decision variable, the program decides how much  
95 should be paid at the initial stage to lower future expenses.

96 The article is organized as follows: 2 gives an overview of the concept of flexibility in infras-  
97 tructure systems and its numerical representation. A review of the theory behind two-stage and  
98 MSPs is presented in 3. 4 provides the formulation of the proposed MSP. 5 presents a methodology  
99 to solve the MSP using an approximate approach. Finally, ?? provide a numerical example with a  
100 generic network and a summary of the key results.

## 101 2. Designing for Flexibility

102 The concept of flexibility is considered to be not "academically mature" [14] due to the lack of a  
103 precise and universally accepted definition. In this study, flexibility will be understood as defined  
104 by [7, 15], and [16]. The authors define flexibility as the ability of a system to *easily* adapt any of  
105 its components (or subsystems). The effort necessary to complete an adaptation is measured as the  
106 number of required resources, which are usually represented as a monetary quantity. Furthermore,  
107 any adaptation will be limited to a maximum value given by the system's context and the resources  
108 invested to make the system flexible. These additional costs may be incurred at the initial stage  
109 of the project to introduce the option to adapt some of the system components. These expenses  
110 may come from research and development activities or by installing physical elements that will  
111 facilitate future adaptations. For instance, the floating platforms used in offshore wind farms could  
112 be designed to be expanded or be built larger-than-required to facilitate future adaptations to the  
113 turbine sizes.

114 The problem of determining how much should be invested to have flexibility in the system is  
115 usually known as measuring the *value of flexibility*. This is a complex problem because capturing the  
116 value of having the option to modify the system under certain circumstances is not a straightforward  
117 process [8]. Different approaches have been developed based on different assumptions and modeling  
118 frameworks. For instance, the Real Options Analysis (ROA) method was developed by adapting the  
119 concept of *options* in financial markets to physical assets [36, 37]. Under this approach, the value  
120 of flexibility is measured as the pricing of an option that provides the right but not the obligation  
121 to modify the system in some predefined way. In a different approach, Cardin et al. [7] defined the

122 value of flexibility as the difference between the expected net present value (ENPV) of a flexible  
123 system and an inflexible system subjected to the same conditions. Similarly, Špačková and Straub  
124 [15] defined it as the additional investment that should be made to have a flexible system compared  
125 with the inflexible alternative, using Markov Decision Processes (MDP) to model the sequential  
126 decision process. Following these works, the value of flexibility will be understood in this paper  
127 as the maximum value that should be paid at the start of the system life-cycle to minimize the  
128 discounted costs of future adaptations and maximize the received utility.

129 In the area of chemical processes, the concept of Flexibility Analysis (FA) has been proposed to  
130 optimize the design and operation of chemical plants under uncertainty [38, 39, 23, 40]. The main  
131 objective of this approach is to determine the optimal design and control variables that allow feasible  
132 operation for the whole range of uncertain parameters. If feasible operation is achieved, then the  
133 process is considered flexible enough. To guarantee feasibility, FA uses the worst-case approach [40]  
134 as in the case of robust optimization. In fact, FA and robust optimization share many concepts  
135 and methods, even if historically they evolved separately. One key difference, however, is the use of  
136 recourse variables (the control variables) to modify the plant's response to particular realizations of  
137 the uncertain parameters. While recourse variables are traditionally not used in robust optimization,  
138 they are a key concept in stochastic optimization. By combining concepts from these optimization  
139 approaches, FA can be used to determine the optimal design characteristics of flexible chemical  
140 plants.

141 The formulation of the flexibility concept and the optimization models proposed in FA may  
142 suggest that the approach can be extended to other engineering systems. Indeed, the design and  
143 management of flexible infrastructure networks can be properly modeled using the representation  
144 of design, state, and control variables from the FA approach. The recourse options provided via  
145 control variables can represent adaptation decisions instead. In both cases, flexibility exists to  
146 face the uncertainty in external phenomena. Despite these similarities, the concept of flexibility in  
147 infrastructure systems (and networks) is more closely related to the concept of Real Options [36, 37],  
148 while the definition of flexibility in FA is more similar to the concept of robustness in infrastructure  
149 systems (as defined in [13]). The problem of how much should be paid today to have the option to  
150 modify the system in the future is a very important notion in flexibility for infrastructure systems  
151 that does not exist in FA. Furthermore, the changes implemented using control variables in chemical  
152 processes are usually reversible, while modifying infrastructure systems involves a sequential decision

153 process that results in incremental modifications. The sequential nature of the decision process  
 154 requires a modeling approach that considers the temporal interdependence of the decisions (such  
 155 as dynamic or stochastic programming) for which the tools developed in FA are insufficient. For  
 156 these reasons and despite the conceptual similarities, the FA approach is not used in this paper and  
 157 rather an MS programming model is proposed.

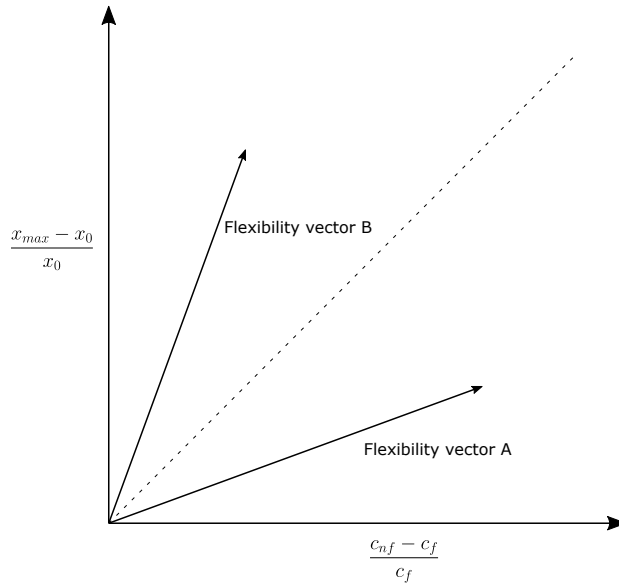
### 158 2.1. Numerical representation of flexibility

159 To formulate and solve the problem of the value of flexibility, it is useful to have a numerical  
 160 representation of flexibility. Unfortunately, the lack of consensus in the conceptual definition is  
 161 also present in the formal description. Various authors have proposed an array of indices with  
 162 different levels of complexity [38, 13, 41, 42] but none has been universally adopted. This study  
 163 will measure flexibility using the *flexibility vector* defined by Torres-Rincón et al. [16], shown in  
 164 Equation 1. This formulation explicitly represents two characteristics usually associated with the  
 165 concept flexibility: the presence of the option to change, and a measurement of the effort required to  
 166 complete the change. The flexibility vector for the design or operation variable  $i$  has two dimensions:  
 167 the first dimension measures the effort necessary to complete an adaptation as the ratio between  
 168 the unitary cost of modifying the component without flexibility (without being specifically designed  
 169 to be adapted) and the unitary cost of performing an adaptation when flexibility was introduced  
 170  $c_{nf,i}/c_{f,i}$ ; the second dimension measures the size of the available adaptation space as the ratio  
 171 between the maximum value the design or operation property can take divided by its initial value  
 172  $x_{max,i}/x_{0,i}$ . Therefore, a system can increase its flexibility by increasing the number of states that  
 173 can reach through low-cost adaptations, or by reducing the cost of such adaptations.

$$\mathbf{fv}_{i,t} = \left[ \frac{c_{nf,i} - c_{f,i}}{c_{f,i}}, \frac{x_{max,t,i} - x_{0,i}}{x_{0,i}} \right] \quad (1)$$

174 For instance, Figure 1 shows two flexibility vectors of the same magnitude. Vector A, how-  
 175 ever, has a larger cost component (horizontal axis), while vector B has a larger adaptation space  
 176 component (vertical axis). Clearly, the expected behavior of both designs under the same external  
 177 conditions will be different. The vectorial representation of flexibility allows capturing the complex  
 178 nature of the property.





**Fig. 1.** Flexibility vector representation

179 *2.2. Managing flexibility through policies*

180 The elements of flexibility described previously are deeply interconnected with the physical  
 181 characteristics of the system. A system is specifically designed and built to be flexible, which  
 182 affects its morphology. Therefore, future management process to decide the optimal timing and  
 183 magnitude of adaptations will be constrained by the limitations of the design [13, 41, 7, 31, 4, 16].  
 184 The management process is also conditioned by external factors and the system’s current state,  
 185 but also on particular preferences of the stakeholders, technical limitations, user requirements, and  
 186 regulatory frameworks. For instance, risk-averse stakeholders may prefer to build large systems from  
 187 the beginning with enough flexibility to perform small adaptations, while stakeholders with a higher  
 188 risk tolerance may favor smaller initial systems with high flexibility to deploy large adaptations.  
 189 These complex interactions between external elements and individual preferences can be modeled  
 190 in the form of *policies*.

191 Policies are functions that map a set of states to decisions [31, 43]. Depending on the modeling  
 192 framework, policies can be deterministic or stochastic with variable degrees of complexity. For  
 193 many applications, however, a simplified framework can be formulated using “*if-then*” conditionals  
 194 that instruct when to trigger an adaptation process [44]. Under this formulation, the conditional

195 threshold and the size of interventions become the main parameters to be defined. These elements  
196 can be used to construct more complex policies. For instance, a more complex policy can be  
197 constructed from the if-then conditional by defining the magnitude of the adaptation as the optimal  
198 change that minimizes the expected present value of the associated costs and maximizes the expected  
199 utility, while constraining the desired performance to remain at certain levels.

200 Generally, flexibility management requires not one but a complete sequence of decisions. The  
201 sequence starts with an initial decision to define the design characteristics of the system, i.e., the  
202 initial dimensions and the flexibility (maximum adaptation range and adaptation costs). Once  
203 the system is fully commissioned and starts operation, a monitoring process is required to verify  
204 the adaptation conditions defined by the policy. The successful implementation of any policy is  
205 conditioned on an inspection and monitoring program. When the conditions are met, a decision is  
206 made concerning the magnitude of the adaptation. The complexity of this problem lies in that every  
207 decision made will affect the future state of the system and, in consequence, the input for the policy  
208 in the future. Furthermore, the future state will also depend on uncertain external conditions that  
209 may not be stationary (changes in traffic, demand, climate change, etc.) [12]. Thus, the problem of  
210 managing flexibility is a classic example of sequential decision problems.

211 In summary, designing and managing flexible systems requires at least the following tasks (for  
212 one flexible component):

- 213 1. determine the optimal initial design  $\mathbf{x}_0$ ,
- 214 2. determine the optimal initial flexibility level  $\mathbf{f}_0$ ,
- 215 3. define the policy  $\pi$  to represent the management decisions,
- 216 4. following  $\pi$ , determine the optimal timing  $\tau_1, \tau_2, \dots$ , and size  $y_{\tau_1}, y_{\tau_2}, \dots$  of future adaptations.

217 The model presented in this paper addresses the first two items. Figure 2 presents a diagram that  
218 synthesizes this design and management process.

### 219 *2.3. Sequential decision-making*

220 Typical decision-making models require an agent and an environment. At time  $t$ , the agent  
221 observes the state of the environment  $s_t$  and selects an action  $a_t$  according to the policy  $\pi$ . Then,  
222 the environment produces a reward  $r_t$  for the agent and evolves to a new state  $s_{t+1}$  following a  
223 probabilist model that depends on the sequence of previous states  $s_{1:t}$  and actions  $a_{1:t}$  [45]. The

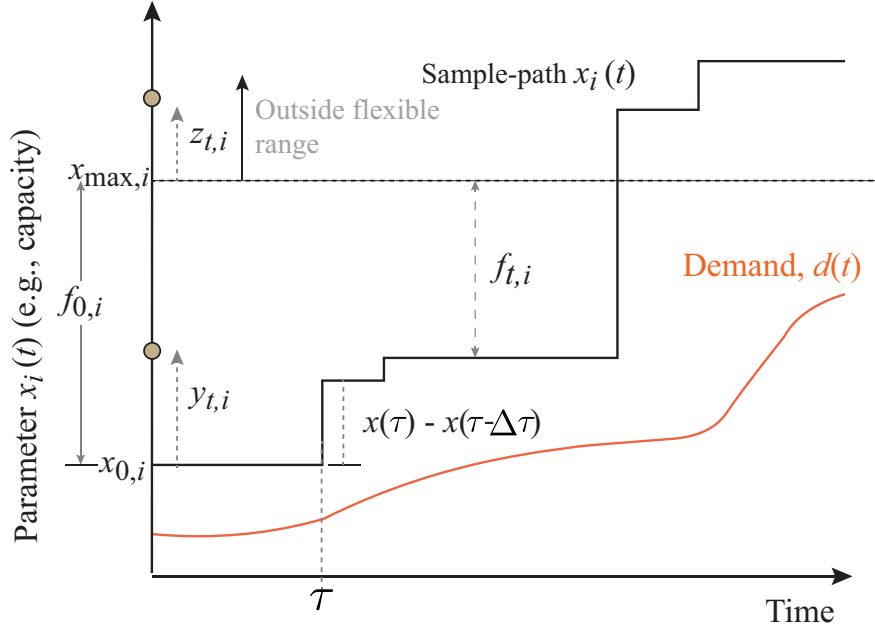


Fig. 2. Description of the main elements for flexible designs

224 agent observes this new state and selects another action  $a_{t+1}$ . If the new state only depends  
 225 on the previous state and action, then the decision model is referred to as a Markov Decision  
 226 Process (MDP). While the basic version assumes that the probabilistic model is known and the  
 227 environment is fully observable, these conditions are not a requirement. For instance, Partially  
 228 Observable Markov Decision Processes (POMDPs) are a generalized version of MDPs.

229 Solving a sequential decision problem is not a unique problem; each model may have many  
 230 different elements that need to be determined, which requires different methods. For instance, a  
 231 key problem is finding the optimal policy, i.e., the optimal function that selects an action  $a_t$  for  
 232 each pair of action and state history  $a_{1:t-1}, s_{1:t-1}$ . Problems of optimal policy are usually solved  
 233 using methods such as dynamic programming (DP), approximate dynamic programming (APD),  
 234 reinforcement learning, genetic algorithms, and Monte Carlo tree searches. A different problem  
 235 is finding the optimal initial decisions that optimize a certain performance measurement over the  
 236 system lifetime, i.e., the optimal design that minimizes discounted adaptation costs. In this case,  
 237 the optimal initial decisions are determined considering future sequences of decisions that may result  
 238 from a particular decision rule and a probability model, even if the optimal sequence of decisions

239 is not determined. Decision problems focused on finding a robust, optimal initial decision can be  
 240 solved using MS programming [46, 47, 48].

241 The problem of flexibility and the value of flexibility as presented before is better suited to be  
 242 solved using MS programming. The next section presents an overview of the theory behind MSPs  
 243 and 4 presents the proposed MS model for the problem of flexibility.

### 244 3. Stochastic Programming

#### 245 3.1. Two-stage program with fixed recourse

246 The simplest stochastic programming model is the linear two-stages model with recourse shown  
 247 in Equation 2 [48], where the objective is to minimize the costs at the initial stage  $t = 0$  and at the  
 248 recourse stage  $t = 1$ :

$$\begin{aligned}
 \min_{\mathbf{x}_0} f &= \underbrace{\mathbf{c}^T \mathbf{x}_0}_{\text{Initial stage costs}} + \underbrace{\mathbb{E}_{\boldsymbol{\xi}}[\min \mathbf{q}(\omega)^T \mathbf{x}_1(\omega)]}_{\text{Recourse costs}} \\
 \text{s.t. } \mathbf{A}\mathbf{x}_0 &= \mathbf{b} \\
 \mathbf{H}(\omega)\mathbf{x}_0 + \mathbf{J}\mathbf{x}_1(\omega) &= \mathbf{h}(\omega) \\
 \mathbf{x}_0 \geq 0, \mathbf{x}_1 &\geq 0
 \end{aligned} \tag{2}$$

249 At the initial stage, the decision  $\mathbf{x}_0 \in \mathbb{R}^{n_1}$  is made considering that the first stage data is  
 250 known: matrix  $\mathbf{A} \in \mathbb{R}^{m_1 \times n_1}$  and vector  $\mathbf{b} \in \mathbb{R}^{m_1}$ . At the second stage, a random event  $\omega \in \Omega$  is  
 251 realized ( $\Omega$  represents the set of all random outcomes) and the second stage information is revealed:  
 252 technology matrix  $\mathbf{H}(\omega) \in \mathbb{R}^{m_2 \times n_1}$ , recourse cost vector  $\mathbf{q}(\omega) \in \mathbb{R}^{n_2}$ , and right-hand side vector  
 253  $\mathbf{h}(\omega) \in \mathbb{R}^{m_2}$ . Then, the second stage decision  $\mathbf{x}_1(\omega) \in \mathbb{R}^{n_2}$ , the *recourse decision*, is made. This  
 254 model is classified as with fixed recourse because the recourse matrix  $\mathbf{J} \in \mathbb{R}^{m_2 \times n_2}$  is assumed  
 255 deterministic. This assumption implies that the effect of the recourse decision  $\mathbf{x}_1$  in the constraints  
 256 is known, which greatly simplifies the solution of the problem and still can be used to model a wide  
 257 range of real life situations.

258 Each element in the random matrix and vectors  $\mathbf{H}(\omega)$ ,  $\mathbf{q}(\omega)$ , and  $\mathbf{h}(\omega)$  is a random variable.  
 259 Therefore, the random vector  $\boldsymbol{\xi} = (\mathbf{q}(\omega), \mathbf{h}(\omega), \text{vec}(\mathbf{H}(\omega)))$  with support  $\Xi \subset \mathbb{R}^d$  can be constructed  
 260 to represent all the data that depends on the random event  $\omega$ . By taking the expectation with  
 261 respect to  $\boldsymbol{\xi}$ , the estimation of the second stage costs is considering all possible realizations of  $\omega$  (at  
 262 least those with non-zero probability).

263 A key characteristic of stochastic programs (two-stages or multistage) is that the recourse de-  
 264 cisions  $\mathbf{x}_1$  will be different for each realization of the random event  $\omega$ . Therefore, if the random  
 265 parameter distribution is discretized into  $r$  intervals, there will be  $r$  different  $\mathbf{x}_1$  solutions, which is  
 266 not very useful from a planning perspective. The true value of stochastic programs lies in the ini-  
 267 tial stage solutions  $\mathbf{x}_0$  because they are unique for all trajectories of the random parameter. These  
 268 decisions are being selected to guarantee that the expected value of future costs (which depend  
 269 on  $\boldsymbol{\xi}$  and  $\mathbf{x}_1$ ) will be minimal. The next section presents how this model can be extended to the  
 270 multistage case.

### 271 3.2. Multistage stochastic programs

272 Multistage stochastic programming is a modeling framework that generalizes the two-stage  
 273 problem to a sequence of recourse decisions. In the two-stage problem, the realization of the  
 274 uncertain parameter becomes known at the second stage and the decision-maker has the option to  
 275 make a second decision  $\mathbf{x}_1$  -the recourse- to adjust the initial decision  $\mathbf{x}_0$ . When the approach is  
 276 extended to the multistage case, every recourse decision  $\mathbf{x}_t$  will be selected based on the expected  
 277 value of this decision for stage  $t + 1$  assuming that every future decision will be optimal [48]. This  
 278 results in a particular sequence of recourse decisions for every sequence of uncertain parameters.

279 The general MS programming model can be formulated as follows [47]:

$$\begin{aligned} \min_{\mathbf{x}_1 \in \mathcal{X}_1} \quad & f_1(\mathbf{x}_1) + \mathbb{E} \left[ \inf_{\mathbf{x}_2 \in \mathcal{X}_2(\mathbf{x}_1, \boldsymbol{\xi}_2)} f_2(\mathbf{x}_2, \boldsymbol{\xi}_2) + \mathbb{E}[\dots \right. \\ & \left. + \mathbb{E} \left[ \inf_{\mathbf{x}_T \in \mathcal{X}_T(\mathbf{x}_{T-1}, \boldsymbol{\xi}_T)} f_T(\mathbf{x}_T, \boldsymbol{\xi}_T) \right] \dots \right] \end{aligned} \quad (3)$$

280 where  $\mathbf{x}_t \in \mathbb{R}^{n_t}$  is the vector of decisions variables at time  $t$ ;  $\boldsymbol{\xi}_t \in \mathbb{R}^{M_t}$  is the vector of uncertain  
 281 parameters at time  $t$  (with  $M_t$  as large as  $n_t + m_t + n_t \times m_t$ ); functions  $f_t(\mathbf{x}_t, \boldsymbol{\xi}_t)$  define the cost of  
 282 making the decision  $\mathbf{x}_t$ ; and  $\mathcal{X}_t$  represent the set of constraints that define the feasibility regions.

283 By using an expectation functional in the recourse functions, it is being assumed that the  
 284 decision-maker is risk-neutral. Risk-averse attitudes can be modeled by replacing the expectation  
 285 functional with risk functionals that consider both the mean and the variance of the random out-  
 286 come in the optimization process. Functionals such as mean-variance, semi-deviations, weighted  
 287 mean deviations from quantiles, and average value at risk can be used to generate solutions with  
 288 limited risk [47]. Nonetheless, for the case of infrastructure networks where the performance is con-  
 289 sidered long-term and the structural integrity is not being subject to optimization, the expectation

290 functional can be used as long as the number of scenarios considered is large enough for the Law  
291 of Large Numbers to apply. Other requirements defined by the decision-maker, e.g. performance  
292 levels, can be specified either as hard constraints in the feasibility set  $\mathcal{X}_t$  or the deviations can be  
293 penalized in the cost function.

294 In an MSP there may be four uncertain elements: future costs, right-hand side vector, technol-  
295 ogy matrix, and recourse matrix. The right-hand side vector is usually associated with demand, the  
296 technology matrix with the initial decision response, and the recourse matrix with the recourse de-  
297 cisions response. For instance, the technology matrix could represent the productivity of the initial  
298 conditions while the recourse matrix could represent the productivity of the recourse decisions, and  
299 both affect the system's ability to serve the random demand given by the right-hand side vector.  
300 Clearly, the decision of which elements are considered random in the model depends on the type of  
301 system and the modeler's assumptions.

302 The decision on how to model the random parameters depends entirely on the type of problem.  
303 Historical data, econometric projections, experts' opinions, all can be used to define the probability  
304 distributions of the elements selected to be random. The scenario generation techniques discussed  
305 in the following section are used to transform these probability distributions and the filtration  
306 structure of the information into discrete approximations in the form of scenario trees that can be  
307 used to solve numerically the MSP.

308 An important property of MSPs is that the information available is represented as  $\sigma$ -algebras  
309  $\mathcal{F}_t$ . As the stages move forward, the information available increases, which is modeled as a sequence  
310 of increasing  $\sigma$ -algebras:  $\mathcal{F}_t \subseteq \mathcal{F}_{t+1}$ . This growing sequence of  $\sigma$ -algebras is known as a *filtration*.  
311 This is an important property of the problem because it implies that decisions at each stage  $x_t$  can  
312 only consider the information available up to that stage [49]. This requirement can be explicitly or  
313 implicitly modeled in the constraint set and it is known as *non-anticipativity constraints*.

### 314 3.3. Challenges in stochastic programming

315 The MS programming approach, while useful to capture the presence of uncertainty in planning  
316 problems, faces limitations due to its computational complexity. The first limitation is defined by  
317 the representation of the uncertain parameters in the model. Regardless of whether the distribution  
318 of the random processes is known or if only sample paths are available, this information has to be  
319 transformed somehow to be entered as an input to the model. Scenario trees are the usual approach

320 to represent the uncertain elements in MSP and constructing them implies the finite discretization  
321 of the original distributions (if they are continuous in the first place).

322 To properly represent the original distribution a large number of points are required. Further-  
323 more, the nested structure of scenario trees results in exponential growth of the number of scenarios  
324 with the number of stages. These two issues (many points and exponential growth) render the prob-  
325 lem intractable if a detailed representation of the underlying distribution is desired in a model with  
326 many stages. For this reason, methods for the generation and reduction of scenario trees constitute  
327 a very active area of research. Høyland and Wallace [50] developed an approach based on mini-  
328 mizing a distance measure (e.g. squared norm) between a predefined statistical property and the  
329 statistical property from the approximation. This approach is known as moment matching and has  
330 been further expanded in various works (e.g. [51]). However, as shown in [50], matching some mo-  
331 ments of the distributions is not enough to guarantee that the solutions of the stochastic program  
332 will be similar. For this reason, Heitsch and Römisch [52] developed scenario generation heuristics  
333 based on the concept of stability. Stability is a property in stochastic programs that guarantees  
334 that the optimal value does not change excessively by changing the scenario tree if both come from  
335 the same distribution. The approaches developed by Heitsch and Römisch [52] recursively reduce  
336 and bundle scenarios using the concept of filtration distance. The more recent approach developed  
337 by Pflug and Pichler [53], based on the concept of nested distance, allows generating the structure  
338 of the tree dynamically to meet a prescribed precision.

339 The second limitation is associated with the solution of the optimization problem. The nested  
340 structure found in MSPs severely complicates the problem and special algorithms are sometimes  
341 required to provide a solution. Two general approaches are usually recognized in the literature  
342 [54, 55, 56]: Primal and Dual decomposition. In the primal decomposition approach, the problem  
343 is divided into a master problem for the current stage and sub-problems for the previous stages.  
344 During each iteration, cuts are generated to linearly approximate the recourse function and generate  
345 a candidate solution  $\mathbf{x}^*$  [48]. Examples of primal decomposition algorithms can be found in the  
346 works of Birge [57], Ruszczyński [58], and Ruszczyński [59]. In the dual decomposition approach,  
347 non-anticipativity constraints are relaxed and moved to the Lagrangian. The division between a  
348 master problem and many sub-problems also exists in this approach, but here the sub-problems  
349 are connected with scenarios instead of stages. As in the case of primal decomposition, most of the  
350 advances came during the late 80s and early 90s with the Progressive Hedging Algorithm [60] and

351 the Diagonal Quadratic Approximation [61]. Most recent efforts have focused on extending these  
 352 approaches to mixed-integer problems, as in the Branch and Price approach from Lulli and Sen  
 353 [62].

354 Nonetheless, not all the MSP required special algorithms to be solved. Alternative approaches  
 355 exist to exploit particular structures of the problem. For instance, if Block-Separability Recourse  
 356 (BSR) exists, the MSP can be analyzed as a two-stage problem with aggregate-level decisions being  
 357 made at the first stage and planning-level decisions happening during the second stage. Commercial  
 358 solvers are also capable of handling MSPs with linear constraints and non-linear objectives [63] while  
 359 state-of-the-art solvers can handle problems in the deterministic equivalent formulation [56].

## 360 4. Multistage Stochastic Programming Model for Flexibility

### 361 4.1. Problem description

362 An important challenge faced by infrastructure network systems consists of managing changes  
 363 in demand such as traffic, consumption, or population growth efficiently. This can be accomplished  
 364 with sporadic adaptations in size, capacity, or any other performance parameter to maintain min-  
 365 imum safety and operational standards. Decisions on the timing and sizes of these interventions  
 366 should be carefully made to maintain an acceptable level of performance while keeping the costs  
 367 minimal. In this section, an MSP has been adapted to model this problem.

368 Consider a network represented as a directed graph  $G(E, V)$ , where  $E$  is the set of edges and  
 369  $V$  a set of nodes, such that every edge  $e_{uv} \in E$  connects nodes  $u$  and  $v$  with  $u, v \in V$ . Each edge  
 370 is associated with a flow  $w_t(u, v)$  occurring at time  $t$ . This flow can represent traffic, electricity,  
 371 water, information, etc., moving through typical infrastructure network systems such as highways,  
 372 power distribution networks, water supply and sewage distribution networks, and telecommunica-  
 373 tion networks. Simplifying the notation, each edge  $e$  can be characterized by a vector of design and  
 374 operational variables  $\mathbf{x}_{t,e} \in \mathbb{R}^{n_e}$  that may change over time (e.g., number of lanes in a highway or  
 375 capacity in a power transmission network), where  $n_e$  represents the number of variables considered  
 376 for edge  $e$ . These potential changes may occur as a result of some external random phenomena  
 377 (e.g., change in traffic demand or flow), described by event  $\omega \in \Omega$ , and are represented by the  
 378 variables  $\mathbf{y}_{t,e} \in \mathbb{R}^{n_e}$ , in the case of flexible adaptations, and  $\mathbf{z}_{t,e} \in \mathbb{R}^{n_e}$  for unplanned adaptations.

379 An additional element is the flexibility built into each design or operational variable, which  
 380 is represented in the model as  $\mathbf{f}_{0,e} \in \mathbb{R}^{n_e}$  (a decision variable), the maximum range of change



381 allowed by design for  $\mathbf{x}_{t,e}$ . This is not the flexibility vector  $\mathbf{fv}$  presented in Equation 1, but the  
382 difference between  $x_{max}$  and  $x_0$ . For simplicity,  $\mathbf{f}_{0,e}$  will be regarded as the flexibility from now on.  
383 The flexibility decisions are made at the initial stage, together with the decision concerning initial  
384 design and operation properties  $\mathbf{x}_{0,e}$ , and their purpose is to restrict the flexible adaptations  $\mathbf{y}_{t,e}$   
385 that can occur in the future. These modeling decisions allow introducing the problem of balancing  
386 three approaches: investing at the initial stage to reduce future adaptation costs, investing at  
387 the initial stage to have robust/unchangeable systems, and not investing and risking larger future  
388 adaptation costs. This is, deciding the optimal values of  $\mathbf{x}_{0,e}$ ,  $\mathbf{f}_{0,e}$ ,  $\mathbf{y}_{t,e}$ , and  $\mathbf{z}_{t,e}$ . It is expected that  
389 most solutions will involve a combination of the three strategies.

#### 390 4.2. Definition of costs

391 Each decision variable of the model has a cost function associated. These cost functions can  
392 represent costs related with activities of design, construction, adaptation, operation, and mainte-  
393 nance of the network edges. The model considers the initial stage costs (design and construction) as  
394 known, while the costs associated with future activities (adaptation, operation, and maintenance)  
395 can be affected by uncertainty. This distinction is represented in the following cost functions: for  
396 the initial stage,  $a_e$  is the cost function of building edge  $e$  with the initial design parameters  $\mathbf{x}_{0,e}$ ,  
397 and  $b_e$  is the cost function of adding features to network edge  $e$  that facilitate future changes,  
398 i.e., the cost of adding flexibility to the system. For example,  $b_e$  can represent the additional  
399 construction costs for a larger foundation in a building to facilitate future expansions. For the  
400 recourse stages,  $c_e(\mathbf{y}_{t,e}, \omega)$  is the cost function of adapting the network edge parameters by  $\mathbf{y}_{t,e}$   
401 units within the flexible range  $\mathbf{f}_{0,e}$  (i.e., the initial design value of variable  $i$  plus the sum of all the  
402 flexible adaptations over the lifetime must be less or equal than the initial value plus the flexibil-  
403 ity  $x_{0,e}(i) + \sum_{t=1}^T y_{t,e}(i) \leq x_{0,e}(i) + f_{0,e}(i)$ ), and  $d_e(\mathbf{z}_{t,e}, \omega)$  is the cost function of performing an  
404 adaptation  $\mathbf{z}_{t,e}$  outside the flexible range. This option is included in the model to represent the  
405 fact that any infrastructure network can be modified if enough resources are invested; however, this  
406 does not mean that the alternative will be efficient. Additional costs related with operation are the  
407 flow cost  $q(w_e, \omega)$ , the operation and maintenance (O&M) cost  $g_e(\mathbf{x}_{t,e}(i), \omega)$ , and the function of  
408 revenue received from exploiting the network  $h_e(\omega)$ .

409 The parameters of these cost functions depend on, first, the type of function used for the  
410 representation and, second, the procedure performed to obtain the data. For many applications,

411 a linear or convex function is enough to represent the required behavior. However, to represent  
412 specific conditions, e.g. economies of scale [7], concave functions may be needed. The values of  
413 these parameters can be obtained from autoregressive models, reports in the literature, experts'  
414 opinions, industry surveys, and sensitivity analyses. If the model considers random costs, then the  
415 cost function parameters become random variables and additional parameters for their distributions  
416 must be defined (using historical data, available literature, surveys, etc.).

417 In the model proposed, all the cost functions can be represented using convex functions. If a  
418 typical linear cost representation is used, then the only cost parameter is the unitary cost coefficient.  
419 In this case, the only requirement is that the unitary costs of functions  $d_e$  (unplanned adaptations)  
420 must be larger than the unitary costs of functions  $c_e$  (planned adaptations); otherwise, the model  
421 will never assign value to the flexible option. If a different convex function is used, then it must be  
422 guaranteed that  $d_e(x) > c_e(x) \forall x > 0$ . This does not mean that flexibility will always be preferred  
423 due to the additional cost be of introducing flexibility at the initial stage. However, if the condition  
424 is not met, then flexibility will never be a viable option from a cost standpoint.

#### 425 *4.3. MSP problem formulation*

426 The elements described in the previous sections are combined in the following objective function  
427 for an MSP to analyze flexible infrastructure networks:

$$\begin{aligned}
& \min_{\mathbf{x}_0, \mathbf{f}_0} \underbrace{\sum_{e \in E} \sum_{i=1}^{n_e} a_e(\mathbf{x}_{0,e}(i))}_{\text{Initial design costs}} + \underbrace{\sum_{e \in E} \sum_{i=1}^{n_e} b_e(\mathbf{f}_{0,e}(i))}_{\text{Flexibility introd. cost}} \\
& + \mathbb{E}_{\xi_1} \left[ \min \gamma_1 \left( \underbrace{\sum_{e \in E} \sum_{i=1}^{n_e} c_e(\mathbf{y}_{1,e}(i), \omega)}_{\text{Flexible adaptations cost}} + \underbrace{\sum_{e \in E} \sum_{i=1}^{n_e} d_e(\mathbf{z}_{1,e}(i), \omega)}_{\text{Unplanned adaptations cost}} + \underbrace{\sum_{e \in E} q(w_{1,e}, \omega)}_{\text{Flow cost}} \right. \right. \\
& \left. \left. + \underbrace{\sum_{e \in E} \sum_{i=1}^{n_e} g_e(\mathbf{x}_{1,e}(i), \omega)}_{\text{O\&M cost}} \pm \underbrace{h(\omega)}_{\text{Exploitation cost/revenue}} \right) + \dots \right. \\
& \left. + \mathbb{E}_{\xi_T} \left[ \min \gamma_T \left( \sum_{e \in E} \sum_{i=1}^{n_e} c_e(\mathbf{y}_{T,e}(i), \omega) + \sum_{e \in E} \sum_{i=1}^{n_e} d_e(\mathbf{z}_{T,e}(i), \omega) + \sum_{e \in E} q(w_{T,e}, \omega) \right. \right. \right. \\
& \left. \left. \left. + \sum_{e \in E} \sum_{i=1}^{n_e} g_e(\mathbf{x}_{T,e}(i), \omega) \pm h(\omega) \right) \right] \dots \right] \tag{4}
\end{aligned}$$

428 where  $i$  indexes the design and operational parameters being considered for each edge  $e$ ,  $n_e$  is  
429 the number of design and operational parameters, and  $\gamma_t$  is the discount factor. To represent the  
430 limitations and special conditions associated with the management of flexibility and the optimal  
431 flow distribution inside the network, the following constraints are formulated:

432 First, the constraints for flow conservation between converging and diverging links at a node  $k$   
433 are:

$$\sum_v w_{(k,v)} - \sum_u w_{(u,k)} = \phi_k(\omega) \quad \forall u, v, k \in V, \tag{5}$$

434 where  $\phi_k = 0$  if  $k$  is a transshipment node and  $\phi_k \neq 0$  if  $k$  is either a supply or a demand node.

435 Second, the constraints for the minimum and maximum flow that can move through each link  
436  $e$  are:

$$\ell_{lower,t,e} \leq w_{t,e} \leq \ell_{upper,t,e} \quad t = 1 \dots T, \forall e \in E \tag{6}$$

437 where the lower and upper limits  $\ell_{lower}, \ell_{upper}$  are part of the design and operational variables  
438 vector  $\mathbf{x}_{t,e}$  and may have a flexibility value associated (can be adapted).

439 Third, the constraints that control the trigger of an adaptation process:

$$V(\mathbf{x}_{t,e}, \xi_t) \geq \pi_{t,e} \quad t = 1 \dots T, \forall e \in E \tag{7}$$

440 where the performance function  $V$  provides a quality measure of the design and operation  
 441 variables  $\mathbf{x}_{t,e}$  in comparison with the pressure caused by the random parameters  $\boldsymbol{\xi}_t$ . This set of  
 442 constraints establishes that the performance measure must be larger than a certain value  $\pi_{t,e}$  given  
 443 by the management policy. In this way, the constraints defines the criteria to make a change. For  
 444 example, it can define the maximum ratio flow/capacity in an edge before it has to be expanded.

445 Fourth, the constraints for the maximum planned adaptation in a design or operation variable  
 446 in an edge are:

$$\sum_{j=1}^t \mathbf{y}_{j,e}(i) \leq \mathbf{f}_{0,e}(i) \quad t = 1, \dots, T, \quad i = 1, \dots, n_e, \quad \forall e \in E \quad (8)$$

447 These constraints establish that the sum of the total planned changes for a design/operation variable  
 448  $i$  in an edge  $e$  must be, at most, the flexibility built for that variable  $i$  and edge  $e$ .

449 Fifth, the constraints to update the state variables of an edge in accordance with the available  
 450 actions are:

$$\mathbf{x}_{t,e}(i) = \mathbf{x}_{t-1,e}(i) + \mathbf{y}_{t-1,e}(i) + \mathbf{z}_{t-1,e}(i) \quad t = 1, \dots, T, \quad i = 1, \dots, n_e, \quad \forall e \in E \quad (9)$$

451 Other constraints can be added depending on the nature of the network, or to properly character-  
 452 ize the adaptations (e.g. non-negativity constraints restrict adaptations to expansions; integrality  
 453 changes the nature of the adaptations from modular to continuous). There are non-anticipativity  
 454 constraints implicitly formulated in the other constraints to restrict the knowledge available to make  
 455 a decision at each stage; this is, at each time  $t$ , the decisions can only depend on the information  
 456 available up to  $t$ .

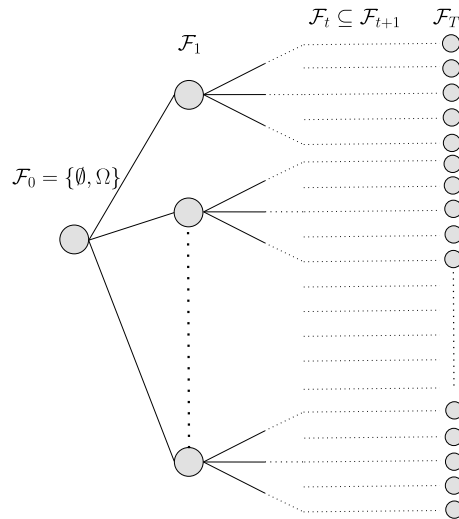
457 The decision stages  $t$  are selected considering the frequency of the decision process. This fre-  
 458 quency may not coincide with the frequency of the random processes, in which case one decision  
 459 stage may encompass many random process periods. For instance, it is not expected for an infras-  
 460 tructure network to be expanded every year, even if the demand is reported every month. In such  
 461 a case, the decision stage  $t$  can consider the average, the maximum, or a quantile of the demand  
 462 periods clustered in  $t$ . It is also not required for the decision stages  $t_1, t_2, \dots$  to be equal in size.  
 463 Considerations regarding the life-cycle of the network and the reliability of the uncertain data may  
 464 result in a higher frequency of decisions during the first years of the network. It must also be con-  
 465 sidered that increasing the frequency of the decision stages also increases the size of the problem.

466 In brief, it is a modeling decision that depends on the purpose of the model and the experience of  
 467 the modeler.

## 468 5. Approximate Solution of MSPs

### 469 5.1. Criteria for approximating the solution

470 Solving a multistage stochastic program using the original distribution of the uncertain param-  
 471 eters  $\xi_t$  may not be feasible in many real applications because the set of possible paths (realizations  
 472 of the demand) is infinite. For this reason, several methods have been developed to approximate  
 473 the distribution of the random phenomena [52, 49, 64]. Overall, the available methods focus on:  
 474 minimizing some measure of the distance between the original and the approximated distribution  
 475 (e.g. Wasserstein distance) [52, 65], matching moments between the distributions [50], and generat-  
 476 ing samples (e.g. Monte-Carlo sampling [66]). As a result, the original distribution becomes a set of  
 477 scenarios (each with an associated probability), usually organized in a tree structure. This scenario  
 478 tree represents the increasing finite filtrations of available information, as shown in Figure 3.



**Fig. 3.** Scenario tree representation of increasing finite filtrations

479 The accuracy of the stochastic program solution highly depends on the quality of the resulting  
 480 discretization [67]. However, it is important to keep in mind that the main objective is to optimize  
 481 the quality of the solution obtained by the stochastic program and not necessarily to produce an

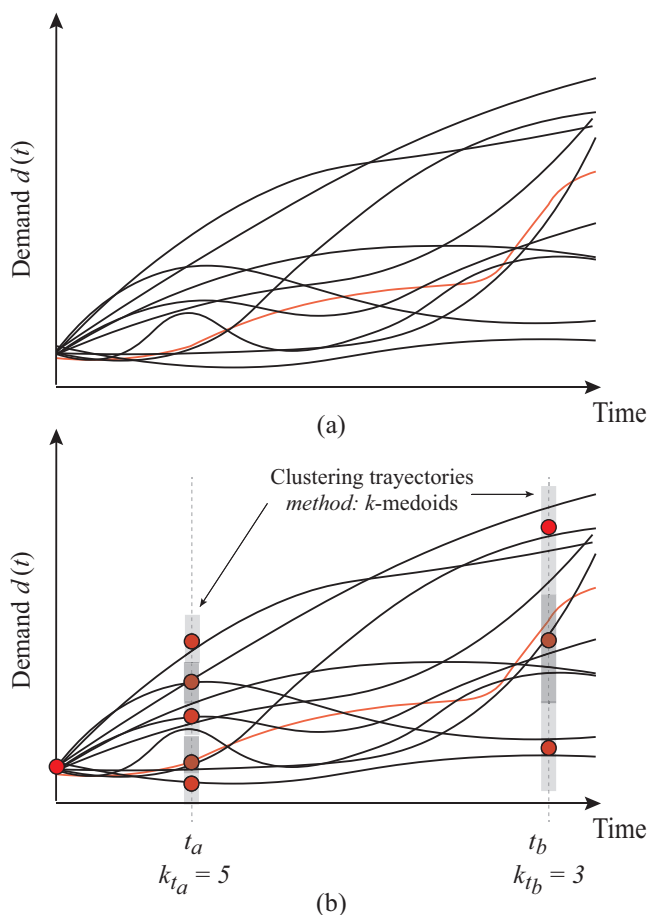
482 optimal discretization of the original distribution. This can be achieved by having stability and  
483 low bias in the solution [68]. Stability means that the variation in the optimal value is minimal  
484 among different scenario trees (obtained from the same distribution). Low bias refers to a small  
485 gap between the real (unobtainable) and the approximated solution. The most direct approach to  
486 achieve both stability and low bias is to simulate a large number of scenarios [69, 68]. A trial and  
487 error procedure is usually necessary to achieve these objectives with the smaller scenario tree as  
488 possible.

### 489 5.2. Discretization method by clustering

490 As explained before, it is generally not possible to solve an MSP using the real distribution  
491 of  $\xi_t$ ; instead, an approximation is required. Typical approximate distributions are represented  
492 in the form of scenario trees. In this paper, the discretization process is performed by combining  
493 Monte-Carlo sampling and a k-medoids clustering algorithm (see Figure 4).

494 The methodology requires listing the properties of the random process to be simulated, which  
495 can include values such as the mean and the standard deviation, or additional shape parameters.  
496 Then, the time mission is divided in a finite set of time steps (stages)  $t = 1, \dots, T$ , and a large  
497 number  $N$  of random trajectories are generated (see Figure 4(a)). At the first time stage  $t = 1$ ,  
498 the coefficient  $k_1$  is defined to represent the number of clusters in which the trajectories will be  
499 aggregated; this coefficient is known as the *branching factor*. Then, the trajectories are combined  
500 into  $k_1$  clusters using a k-medoids clustering algorithm. At the next time stage, the trajectories  
501 grouped inside each cluster are further divided into  $k_2$  clusters using the same algorithm. This  
502 process is repeated until the end of the time mission when a total of  $K = \prod_{t=1}^T k_t$  clusters are  
503 generated. This process results in a symmetric scenario tree.

504 This method requires a large number of trajectories per cluster to avoid clustering single tra-  
505 jectories. Considering that the number of scenarios grows exponentially with the number of stages,  
506 the number of required trajectories may be difficult to generate for large scale applications. While  
507 it works well for problems with a number of scenario paths of order  $10^5$  to be clustered in trees  
508 with a number of scenarios of order  $10^3$ , problems of larger scale may require more complex ap-  
509 proaches. For instance, a larger number of clusters can be used at the initial stages to obtain a  
510 finer discretization due to the importance of the prediction at these early stages (Figure 4(b)).  
511 Fortunately, in most cases, flexibility problems in infrastructure networks usually involve a small



**Fig. 4.** (a) realization of system path trajectories; (b) clustering of sample paths at different stages.

512 number of variables and stages due to the limited number of characteristics that can be adapted  
 513 and the low frequency of changes.

514 *5.3. Approximated flexibility MSP model*

515 The approximation of the distribution of  $\xi_t$  using a scenario tree can be combined with the  
 516 original flexibility MS approach ((4)) to produce an approximated MSP that can be solved with  
 517 numerical solvers. By replacing the probability model with an approximate, simpler, model with  
 518 finite support [65], the original filtration becomes a finite filtration with a tree structure (scenario  
 519 tree). This approximation leads to the formulation of an equivalent deterministic program, as shown  
 520 in Equation 10:

$$\begin{aligned}
\min_{\mathbf{x}_0, \mathbf{f}_0} & \sum_{e \in E} \sum_{i=1}^{n_e} a_e(\mathbf{x}_{0,e}(i)) + \sum_{e \in E} \sum_{i=1}^{n_e} b_e(\mathbf{f}_{0,e}(i)) \\
& + \underbrace{\sum_{k=1}^s p_k}_{\text{Scenario probability}} \left[ \gamma_1 \left( \sum_{e \in E} \sum_{i=1}^{n_e} c_{e,k}(\mathbf{y}_{1,e,k}(i)) + \sum_{e \in E} \sum_{i=1}^{n_e} d_{e,k}(\mathbf{z}_{1,e,k}(i)) + \sum_{e \in E} q_k(w_{1,k}) \right. \right. \\
& \left. \left. + \sum_{e \in E} \sum_{i=1}^{n_e} g_{e,k}(\mathbf{x}_{1,e,k}(i)) \pm h_{1,k} \right) + \dots \right. \\
& \left. + \gamma_T \left( \sum_{e \in E} \sum_{i=1}^{n_e} c_{e,k}(\mathbf{y}_{T,e,k}(i)) + \sum_{e \in E} \sum_{i=1}^{n_e} d_{e,k}(\mathbf{z}_{T,e,k}(i)) + \sum_{e \in E} q_k(w_{T,k}) \right. \right. \\
& \left. \left. + \sum_{e \in E} \sum_{i=1}^{n_e} g_{e,k}(\mathbf{x}_{T,e,k}(i)) \pm h_{T,k} \right) \right] \tag{10}
\end{aligned}$$

521 where  $s$  indicates the number of scenarios and  $p_k$  is the individual probability of each scenario.  
522 Scenarios are understood as a complete path from the root node to a leaf node in the scenario tree.  
523 This formulation of the objective function clearly shows that a particular solution is obtained for  
524 each scenario  $k$  except for the initial stage variables ( $\mathbf{x}_0$  and  $\mathbf{f}_0$ ) which are the same for all scenarios.

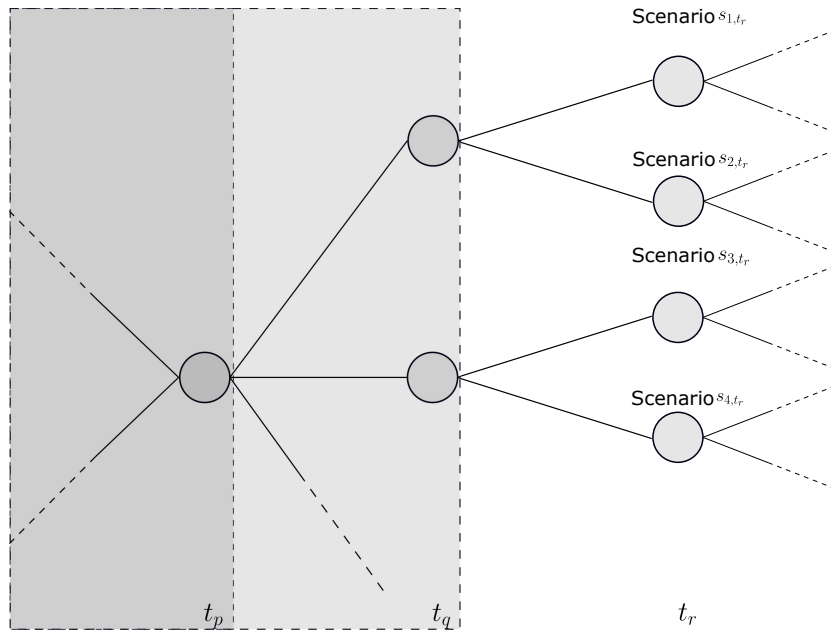
525 Formulating the MSP in this form requires to explicitly develop the non-anticipativity con-  
526 straints. The objective of these constraints is to ensure that scenarios with the same history up to  
527 stage  $t$  are indistinguishable [47].

$$\begin{aligned}
\mathbf{x}_{t,e,j}(i) &= \mathbf{x}_{t,e,k}(i) \\
\mathbf{y}_{t,e,j}(i) &= \mathbf{y}_{t,e,k}(i) \\
\mathbf{z}_{t,e,j}(i) &= \mathbf{z}_{t,e,k}(i) \quad \forall j, k \text{ for which } \boldsymbol{\xi}_{t,j} = \boldsymbol{\xi}_{t,k}, \quad t = 1, \dots, T, \quad i = 1, \dots, n_e, \quad \forall e \in E
\end{aligned} \tag{11}$$

528 To illustrate the non-anticipativity conditions, Figure 5 shows a fragment of a scenario tree. The  
529 figure shows that Scenario  $s_{1,t_r}$  and Scenario  $s_{2,t_r}$  are identical up to stage  $t_q$ , same as Scenario  
530  $s_{3,t_r}$  and Scenario  $s_{4,t_r}$ . Furthermore, the four scenarios are indistinguishable up to stage  $t_p$ . The  
531 restrictions in Equation 11 ensure that the decision variables comply with the non-anticipativity  
532 conditions given by the scenario tree of the random process.

533 The procedures described in Sections 5.1-5.3 to formulate and solve the proposed MSP are  
534 summarized in the chart presented in Figure 6.



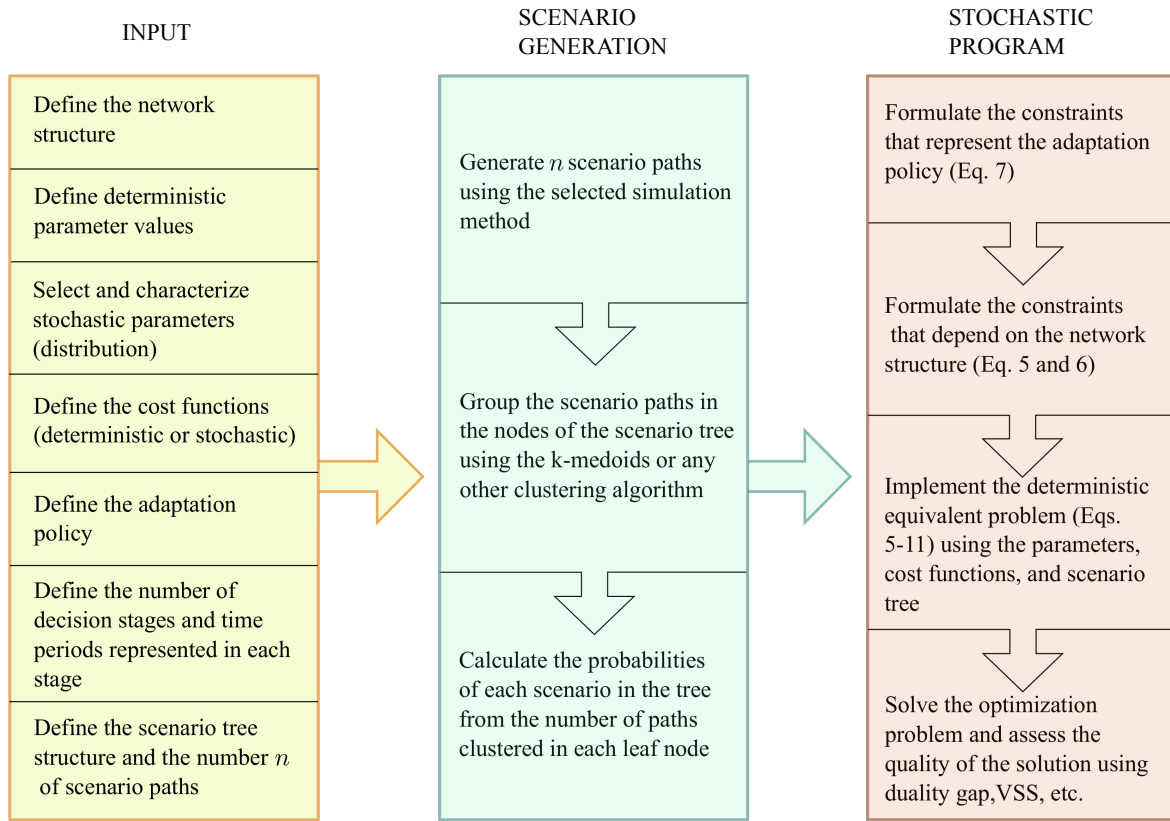


**Fig. 5.** Non-anticipativity conditions in scenario tree

535 *5.4. Model scalability*

536 The scalability of the proposed model can be analyzed for two elements: the scenario tree  
 537 generation algorithm and the solution method. First, the scenario generation algorithm is based on  
 538 the general approach described by Dupačová et al. [63] where a set of scenario paths are generated  
 539 according to a probabilistic model (based on, for instance, historical data series), a scenario tree  
 540 structure is predefined according to some heuristic (e.g. detailed branching for early stages and  
 541 coarse branching for later stages), and a clustering algorithm is applied to the scenario paths based  
 542 on some dissimilarity measure. The scenario path generation process, even for the multivariate  
 543 case, scales linearly in the worst case, and it is never regarded in the literature as a worrisome  
 544 source of computational complexity. The clustering algorithms, however, do not scale as well due  
 545 to the required comparisons between all the data points (distance or dissimilarity measures).

546 The k-medoid algorithms used in this paper are the Partitioning Around Medoids (PAM) and  
 547 the Clustering LARge Applications (CLARA) implementations in Matlab<sup>®</sup>. The CLARA algorithm  
 548 is used to cluster the first 2-3 stages of the scenario tree where the number of data points is large  
 549 ( $> 5000$ ). This algorithm is of order  $O(k^3)$  [70] and can be used for large data sets to be bundled in



**Fig. 6.** General procedure to formulate and solve proposed MSP model

550 a small number of clusters. The subsequent stages require clustering progressively smaller number  
 551 of points in an also small number of clusters, which can be done using the PAM algorithm of order  
 552  $O(k(n - k)^2)$ . While these clustering algorithms work well for a wide range of data set sizes and a  
 553 limited number of branching factors, the structure of the scenario tree requires that the algorithms  
 554 have to be executed an increasing number of times at each stage. This is, the number of calls for  
 555 the clustering algorithms grows exponentially with the number of stages. Therefore, the scalability  
 556 of the scenario generation procedure depends on both the scalability of the clustering algorithms  
 557 and the size of the scenario tree.

558 The second element that affects the scalability of the model is the solution method. As explained  
 559 in Section 3.3, solving an MSP is challenging due to the considerable number of variables, the  
 560 interdependence between them, and possible non-linear constraints. While special methods have

561 been developed to solve MSPs, in some cases commercial solvers are enough to obtain a solution  
 562 in reasonable times for problems with hundreds of thousands of variables. One of these cases is  
 563 when the problem has a linear (or non-linear) objective and linear constraints [63]. By introducing  
 564 the scenario tree representation to formulate the deterministic equivalent problem, the result is a  
 565 large scale linear (or non-linear) optimization problem that can be solved efficiently by commercial  
 566 solvers. The model presented in Section 5.3 has linear constraints and the cost functions can be  
 567 properly represented as linear or quadratic functions for many applications. Therefore, commercial  
 568 solvers can be used to solve the proposed model, as is shown in the example in Section 6.

569 Nonetheless, the exponential growth in the number of variables as the number of stages increases  
 570 poses a significant limitation to the frequency of the decision process. This limitation can be  
 571 circumvented as the nature of infrastructure systems makes monthly or even annual adaptation  
 572 plans unrealistic due to the time and resources required to complete an adaptation. The decision  
 573 stages for infrastructure adaptation problems can encompass years and, in consequence, it is possible  
 574 to model the complete or a considerable portion of the system’s lifetime with a limited number of  
 575 stages.

576 In addition to the linearity of the constraints and the control to the scenario tree explosion by  
 577 limiting the number of stages, the proposed model has two additional properties that reduce its  
 578 computational complexity. The first property is the diagonal structure in the constraint matrices.  
 579 Limiting the dependence of the decision variables to their immediate predecessor by adding state  
 580 variables results in sparse matrices that are much faster to solve [46]. The second property is  
 581 block-separable recourse. This property allows transforming an MSP into a two-stage problem by  
 582 separating the aggregate level decision variables from the planning level variables. The aggregate  
 583 level decisions can represent capacity expansion decisions while the planning level decisions can  
 584 refer to the use of this capacity [48]. If the aggregate level decisions do not depend on the planning  
 585 level decisions, then the former can be moved to the first stage while the latter are placed on the  
 586 second stage. Specifically, block-separable recourse exists if i) at stage  $t$  the cost functions can be  
 587 written as:

$$f_t(\mathbf{u}_t) + g_t(\mathbf{v}_t) \tag{12}$$

588 where  $\mathbf{u}_t$  represents the aggregated level decisions,  $\mathbf{v}_t$  the planning level decisions, and  $f_t$  and  
 589  $g_t$  are the respective cost functions. And ii) if the constraints can be written as:

$$\begin{pmatrix} T_t & 0 \\ S_t & 0 \end{pmatrix} \begin{bmatrix} \mathbf{u}_{t-1} \\ \mathbf{v}_{t-1} \end{bmatrix} + \begin{pmatrix} W_t & 0 \\ 0 & D_t \end{pmatrix} \begin{bmatrix} \mathbf{u}_t \\ \mathbf{v}_t \end{bmatrix} = \begin{bmatrix} \mathbf{a}_t \\ \mathbf{b}_t \end{bmatrix} \quad (13)$$

590 where  $T_t$  and  $S_t$  are submatrices of the technology matrix,  $W_t$  and  $D_t$  are submatrices of the  
 591 recourse matrix, and  $\mathbf{a}_t$  and  $\mathbf{b}_t$  are subvectors of the right-hand side vector. This equation clearly  
 592 shows that both current aggregate and current planning level decisions depend only on previous  
 593 aggregate level decisions.

594 The model proposed in Equations 4-11 is block-separable for the following reasons: i) the cost  
 595 functions are clearly segregated between the aggregate level variables ( $\mathbf{x}_t$ ,  $\mathbf{y}_t$ ,  $\mathbf{z}_t$ , and  $\mathbf{f}_0$ ) and the  
 596 planning variables  $\mathbf{w}_t$ ; ii) the constraints in Equations 5-9 and 11 are not enforcing any dependence  
 597 between the set of aggregate decisions  $\mathbf{x}_t$ ,  $\mathbf{y}_t$ ,  $\mathbf{z}_t$ , and  $\mathbf{f}_0$  and the decisions  $\mathbf{w}_{t-1}$ . Constraints 6 and  
 598 7 do generate a dependence between  $\mathbf{w}_t$  and  $\mathbf{x}_{t-1}$  but this relationship is included in the definition  
 599 of block-separability.

600 In summary, the proposed model has advantageous characteristics in its structure that can be  
 601 exploited to vastly reduce its computational complexity and allow the use of commercial solvers  
 602 to find a solution. The main bottleneck happens in the scenario tree generation procedure due to  
 603 the combinatorial nature of the process. Despite these advantages, the number of variables in the  
 604 problem still grow exponentially with the number of stages, and even if the MSP can be transformed  
 605 into a large scale linear problem and a simple binary tree structure is used, having more than  $\sim 22$   
 606 stages implies hundreds of millions of variables.

## 607 **6. Numerical Example**

### 608 *6.1. Case description*

609 This section presents an example of modeling flexibility in network design and operation using  
 610 the proposed MSP. The purpose of this example is threefold: i) to show how the model can be  
 611 used to make decisions when managing flexible networks; ii) to study how the presence of flexibility  
 612 affects the cost performance of the network; and iii) to identify the elements in the model that have  
 613 the highest impact in the assessment of the value of flexibility.

614 The network used in the example is shown in Figure 7; it is a generic network that may describe  
 615 telecommunication, energy, water distribution, or a transportation network. This example only  
 616 considers one element in the random parameters vector  $\boldsymbol{\xi}_t = \delta_t$  to represent the demand that enters

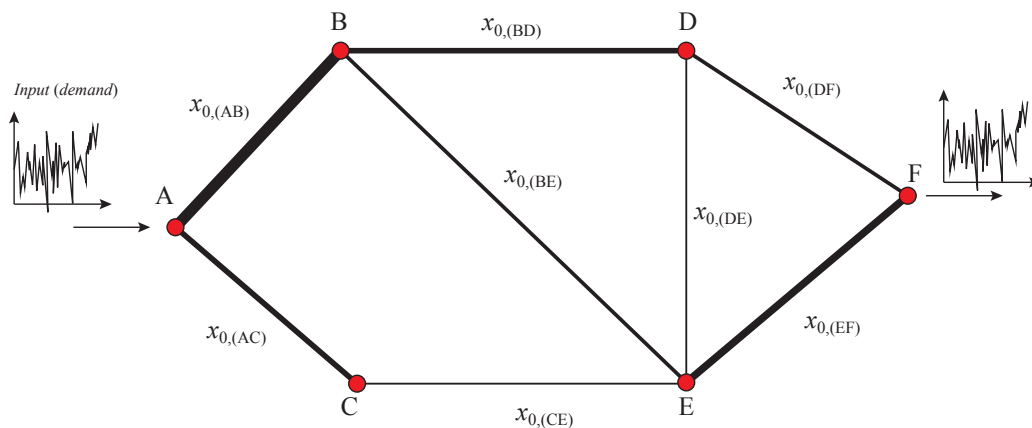
617 the network through node  $A$  and propagates throughout the network until it reaches node  $F$ , where  
 618 it exits. This demand is modeled as a stochastic process defined by:

$$\delta(t) = \beta_1 t + e^{\beta_2 t} \beta_3 t \sin(\beta_4 t) + B(t) \quad (14)$$

619 where  $\beta_1, \beta_2, \beta_3, \beta_4$  are normally distributed random variables and  $B(t)$  is a Wiener process. Table  
 620 1 shows the values of the parameters used in the example. Figure 8 shows five realizations of this  
 621 process.

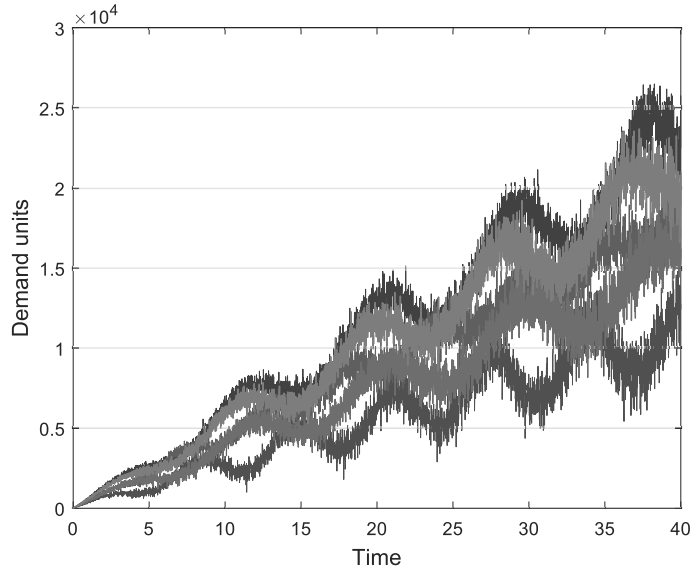
**Table 1.** Random demand process parameters

Parameter	Distribution( $\mu, \sigma^2$ )
$\beta_1$	$\mathcal{N}(450, 1.26 \times 10^4)$
$\beta_2$	$\mathcal{N}(-0.02, 2.5 \times 10^{-5})$
$\beta_3$	$\mathcal{N}(100, 625)$
$\beta_4$	$\mathcal{N}(0.9, 5.06 \times 10^{-2})$



**Fig. 7.** Network used in the numerical example.

622 The design and operation variables vector  $\mathbf{x}_{t,e}$  of each link in the network only contains the link  
 623 capacity  $x_{t,e}$ . The initial capacity is notated as  $x_{0,e}$ , and together with the flexibility range  $f_{0,e}$   
 624 define the initial stage decisions. The maximum capacity that can be reached by flexibility for each  
 625 link at any time is given by  $x_{max,e} = x_{0,e} + f_{0,e}$ . However, the system can be modified beyond



**Fig. 8.** Realizations of the stochastic process

626 that value but at a larger cost. This may happen, for instance, due to larger times required to  
 627 modify the system, larger material and labor costs that result from last-minute contracts, and the  
 628 related disturbances and damages caused by the unexpected partial or total cease of operation. In  
 629 the example, only capacity expansions are considered.

630 The time mission of the network is  $T = 40$  years starting from the date of commissioning. To  
 631 reduce the size of the problem, it is assumed that adaptations can only occur at specific times:  
 632  $[6, 12, 18, 24, 32, 40]$  (except for the sensitivity analysis in Section 7.1.2). This limitation allows  
 633 downsizing the scenario tree, which highly impacts the computational performance. The reduction  
 634 can be justified by the fact that infrastructure networks, and in general infrastructure systems,  
 635 cannot be changed frequently in most of their dimensions without incurring high costs.

636 The model uses two families of cost functions. The initial design cost functions  $a_e$ , flexible  
 637 adaptation cost functions  $c_e$ , and the unplanned adaptation cost functions  $d_e$  (see Equation 10) are  
 638 assumed linear of the form  $a_e = \alpha_0 \mathbf{x}_{0,e}$ ,  $c_e = \alpha_{fa} \mathbf{y}_{t,e}$ , and  $d_e = \alpha_{ia} \mathbf{z}_{t,e}$ , equal for all the edges.  
 639 The linear cost assumption reduces the comparison to a straightforward relationship between the  
 640 cost coefficients. Quadratic functions are used to represent the costs of introducing flexibility of the  
 641 form  $b_e = \alpha_f f_{0,e}^2$ . This non-linear increasing function is used to consider the effect of dis-economies

642 of scale that may exist in systems that cannot be expanded indefinitely without restrictions, such  
 643 as most of infrastructure networks.

644 Coefficient  $\alpha_0$  is equal to 5 cost units per capacity unit. Coefficients  $\alpha_{fa}$  and  $\alpha_{ia}$  vary for the  
 645 analyses shown in Section 7.2. Operation and maintenance costs (O&M)  $g_e$  is assumed equal to  
 646 2% of  $\alpha_0$  per unit of capacity installed, except for the last analysis. Flow costs  $q_e$  are function of  
 647 O&M costs  $g_e$  as shown in Table 2.

**Table 2.** Flow costs summary

Link	Flow Cost
A-B	$0.05g_e$
A-C	$1.2q_{AB}$
B-D	$1.1q_{AB}$
B-E	$q_{AB}$
C-E	$1.2q_{AB}$
D-E	$1.3q_{AB}$
D-F	$1.1q_{AB}$
E-F	$1.2q_{AB}$

648 The flow costs vary between links to represent an existing minimal cost route and increase the  
 649 stability of the solution by avoiding a random allocation of initial capacity and flexibility.

### 650 6.2. Discretization of the demand space

651 The first task is the discretization of the demand space using the sampling and clustering algo-  
 652 rithm presented in Section 5.2. This requires defining first the scenario tree branching factors which  
 653 vary between  $[4\ 4\ 2\ 2\ 2\ 2]$  (256 scenarios) and  $[4\ 4\ 4\ 4\ 2\ 2]$  (1024 scenarios). Then, the algorithm  
 654 generates between 15000 and 25000 demand trajectories according to Equation 14 depending on the  
 655 total number of scenarios. The clustering algorithm processes these inputs to generate a scenario  
 656 tree whose nodes contain the demand values at the decision stages  $[6, 12, 18, 24, 32, 40]$  years, with  
 657 an associated probability that depends on the number of trajectories clustered in each node.

### 6.3. MSP solution

To obtain the optimal network initial conditions,  $x_{0,e}^*$  and  $f_{0,e}^*$  for every edge  $e$  in the network, it is necessary to solve the multistage stochastic problem described by Equation 10, subject to the restrictions presented in Equations 5 to 11. The model assumes that every time a flexible adaptation  $y_{t,e}$  occurs, the flexibility built into the system at the initial stage  $f_{0,e}$  is reduced until its depletion. Once this point is reached only unplanned adaptations  $z_{t,(u,v)}$  can be deployed. Finally, adaptations (i.e., increments incapacity) can only occur at  $t \in \{0, 6, 12, 18, 24, 32, 40\}$ .

The evolution of the network capacity is controlled by a policy  $\pi(\xi_t, x_{t,e})$  based on a safety criteria that establishes that the capacity of every edge at time  $t$  should be such that  $x_{t,e} \geq SF w_{t,e}$ , with  $w_{t,e}$  the flow moving through link  $e$ , and  $SF$  some safety factor. This formulation keeps the constraints in Equation 7 linear. Additional flow conservation constraints are formulated for each network node according to the topology shown in Figure 7.

The numerical results were obtained using the CPLEX 12.8 API for Matlab® 2017b and the YALMIP toolbox as algebraic interpreter [71] with an Intel®Core™ i5-5200 2.20GHz processor. An average run for 1000 scenarios takes approximately 100 seconds of processing time, where 95% of the time is spent in the scenario tree generation algorithm and less than 5% in solving the optimization program.

The solver used (CPLEX) automatically selects the barrier optimizer due to the large size and sparsity of the problem. This algorithm stops iterating when the primal and dual solution are complementary, i.e., when a sum of products between the primal and dual solutions is smaller than a predefined tolerance. The tolerance of the complementary used in this numerical example is defined as  $1^{-8}$ .

## 7. Network Design for Flexibility: Results

Solving the MSP defined by Equations 5 to 11 a results in an optimal (minimal) value of the total present costs  $C_{total}^*$ , an optimal value of the initial capacity  $x_{0,e}^*$  for each link  $e$ , an optimal value of the flexibility  $f_{0,e}^*$  for each link  $e$ , and optimal values each variable  $y_{t,e,k}^*$  and  $z_{t,e,k}^*$ , that represent the evolution process of each network link, for every stage  $t$  and scenario  $k$ . Figure 9 shows three realizations of the demand process and the respective evolution of the whole network capacity.



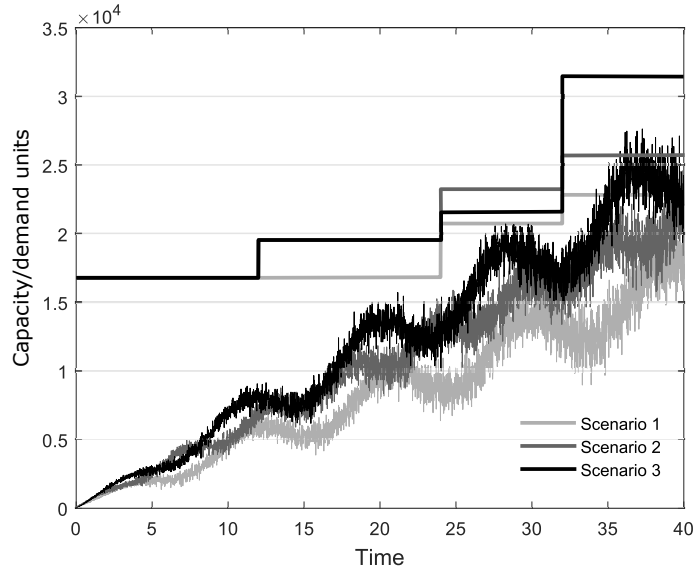


Fig. 9. Network capacity evolution for three demand scenarios

687 This figure illustrates one of the main properties of MSPs: The optimal solution for the initial  
688 capacity, i.e. the initial stage decision, is the same for all scenarios while the recourse decisions  
689 that expand the system are particular for each scenario. By averaging the optimal costs of all the  
690 system's future responses, the model makes an initial decision that is optimal in average for all  
691 scenarios.

692 Considering that the solutions of the recourse decisions  $y_{t,e,k}^*$  and  $z_{t,e,k}^*$  are generated for each  
693 scenario, they are not suited for the comparisons intended in the forthcoming analyses. Only the  
694 initial solutions  $x_{0,e}^*$  and  $f_{0,e}^*$  are the same for all scenarios. For this reason, only these solutions,  
695 together with the optimal costs  $C_{total}^*$ , will be considered in the analysis of results.

### 696 7.1. Numerical stability of the model

#### 697 7.1.1. Stability verification of the demand tree generation

698 Stability in the generation of the demand tree is essential for the accuracy of the model. If  
699 the program is not stable, the solution can vary considerably between scenario trees. To verify  
700 the stability of the solution, three scenario tree structures were generated using different branching  
701 factors. These factors determine how many nodes grow from each node at each time stage and,

ultimately, the number of scenarios. Furthermore, the demand values in the nodes of the scenario tree vary due to the Monte-Carlo generation procedure. To address these sources of variability, the MSP was solved in batches of increasing size (from 2 solutions up to 40 solutions) and the resulting optimal costs were averaged for each batch. Figure 10 presents the coefficient of variation,  $CV$ , of the optimal costs for each batch size, and for three sets of branching factors (scenario tree structures).

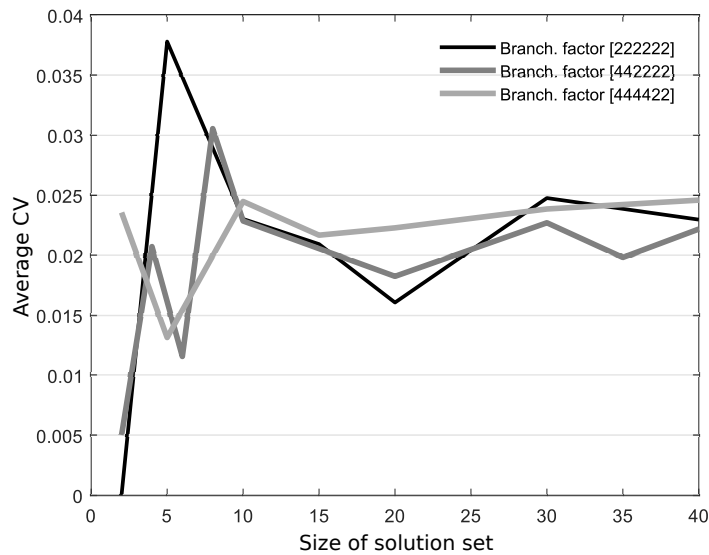


Fig. 10. Solution variability as function of number of scenarios and runs

The scenario tree structures compared in Figure 10 were selected starting by the smallest possible symmetrical tree [2 2 2 2 2]. Additional nodes were increasingly added to the initial stages to improve the quality of the short-term predictions. The largest scenario tree considered, [4 4 4 4 2 2], showed similar behavior with larger trees but with considerably lower computational times.

Figure 10 shows that there is variability due to the number of solutions being considered and due to the instability in the solution. As the size of the batch increases, the first source decreases and only instability remains. It is observed that the optimal costs are relatively stable with a  $CV = 2.5\%$ . It is also observed that a larger number of scenarios reduces the number of solutions required to reach a stable  $CV$  (branching factor [4 4 4 4 2 2]). This result is expected as a larger number of scenarios represent better the underlying distribution, achieving higher stability as a

**Table 3.** Sensitivity analysis results

Decision stages	Optimal value	$f_{0,AB}^*$	$x_{0,AB}^*$	Processing time(s)
4	361619	2546	14787	45
5	340954	2657	13341	62
6	334664	2614	12798	85
7	339480	2661	12894	95
8	329768	2793	11175	92
9	341655	2664	12618	90
10	341035	2693	12961	110

718 result. Generally, only the optimal costs are compared in stability analyses and not the optimal  
719 solutions due to the typical flat objective functions found in MSPs [72].

#### 720 7.1.2. Planning horizon discretization into decision stages

721 The results from the previous section assumed that the planning horizon is divided into 6 decision  
722 stages. This section presents a sensitivity analysis to determine how this modeling decision affects  
723 the MSP results.

724 To this end, the planning horizon is divided into 4, 5, . . . , 10 decision stages, and the resulting  
725 MSP is solved. In the cases when the planning horizon is not a multiple of the number of stages, the  
726 initial stages encompass fewer years than later stages, but the purpose is to cover the entirety of the  
727 planning horizon as uniformly as possible. The scenario trees are designed to have the same number  
728 of scenarios ( $2^{10}$ ) which requires using variable branching factors. Therefore, the discretization of  
729 the probability space for the intermediate stages will not be equal for all cases, with a difference of  
730 a factor of 2 at most in the number of scenario tree nodes for similar time instants. For instance,  
731 for 4 decision stages, there are 64 nodes representing year 20, while for 5 stages there are 32 nodes  
732 at year 16. Table 3 shows the optimal value, the optimal flexibility solution  $f_{0,AB}^*$  for link  $AB$ ,  
733 the optimal initial capacity solution  $x_{0,AB}^*$ , and the processing time obtained for each number of  
734 decision stages.

735 The results in Table 3 show that when the number of stages that divide the planning horizon is  
736 5 or larger, only the processing times are affected. For 4 decision stages, the model solutions seem

737 to be significantly different, beyond what could be explained by the random variation present in the  
738 solutions for the remaining number of stages. This tendency was found in multiple executions. This  
739 difference could be explained by the relationship between the frequency of the required adaptations  
740 and the frequency of the decision stages. As shown in Figure 9, the time between adaptations can  
741 vary between 8 and 12 years on average, with longer times during the first half of the planning hori-  
742 zon. This means that during the system’s lifetime only 3 or 4 adaptations are expected. Therefore,  
743 when the planning horizon has 4 decision stages or fewer, it can be expected that an adaptation  
744 will take place at every stage and that the magnitude of these adaptations (and the initial capacity)  
745 will be larger to accommodate the changes in the demand during such long time periods.

746 In summary, the discretization of the planning horizon into decision stages can affect the solution  
747 when there is insufficient opportunity to use the recourse to respond to the changes in the external  
748 conditions.

#### 749 7.1.3. *Out-of-sample behavior of the model*

750 The verification of the out-of-sample behavior consists in solving the optimization program with  
751 a particular tree and using the optimal solution, i.e.,  $x_{0,e}^*$  and  $f_{0,e}^*$ , as the initial solution for MSPs  
752 with different scenario trees of the same size and generated from the same stochastic process. Figure  
753 11 compares the optimal costs obtained in the baseline program (horizontal line), with the optimal  
754 costs found in 10 out-of-sample programs. This figure shows that 70% of the out-of-sample costs  
755 have a difference of 1.2% or less with the base case, while the remaining 30% has, at most, a  
756 difference of 3.3%. The results from the stability analysis and the out-of-sample analysis suggest  
757 that even if there is some instability because the scenario tree is not infinite, it is under control  
758 and the program exhibits both *in* and *out* sample stability, which is a requirement for low bias and  
759 general stability.

#### 760 7.1.4. *Value of the stochastic solution*

761 A second key element in the analysis of MSPs is the value of the stochastic solution (VSS).  
762 This metric compares how much is gained by solving the stochastic program instead of solving a  
763 deterministic program where the scenario tree is replaced with the expected value of the random  
764 process. To calculate the VSS, first, the expected value problem is solved and the optimal solution  
765 is used as the initial solution for an MSP. The optimal costs obtained for this new program are

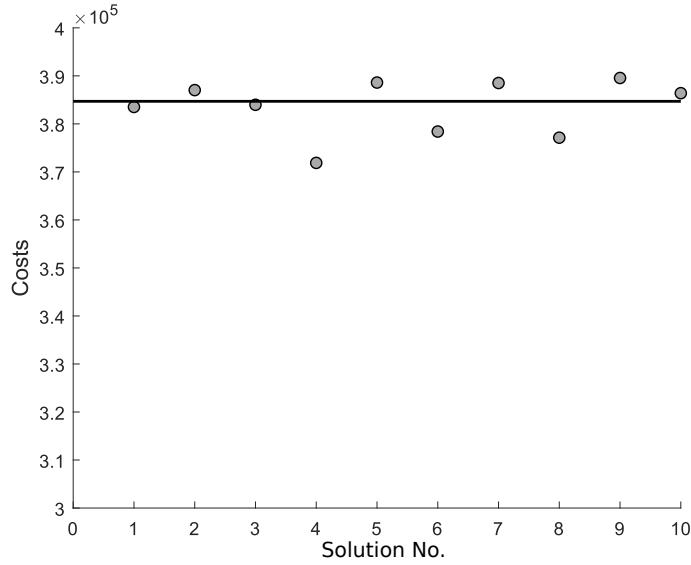


Fig. 11. Out-of-sample solution comparison

766 known as the *expected value* solution (EV). The VSS is obtained as the difference between the  
 767 original MSP optimal costs and the EV.

768 Using the scenario tree structure regarded as the most stable from the analysis in Section 7.1.1,  
 769 [4 4 4 4 2 2], generating 50 scenario trees and averaging the VSS, it was obtained a value that is  
 770 16% of the average optimal costs. This result is not negligible and suggests that the VSS is large  
 771 enough to justify solving a stochastic program instead of the much simpler expected value problem.

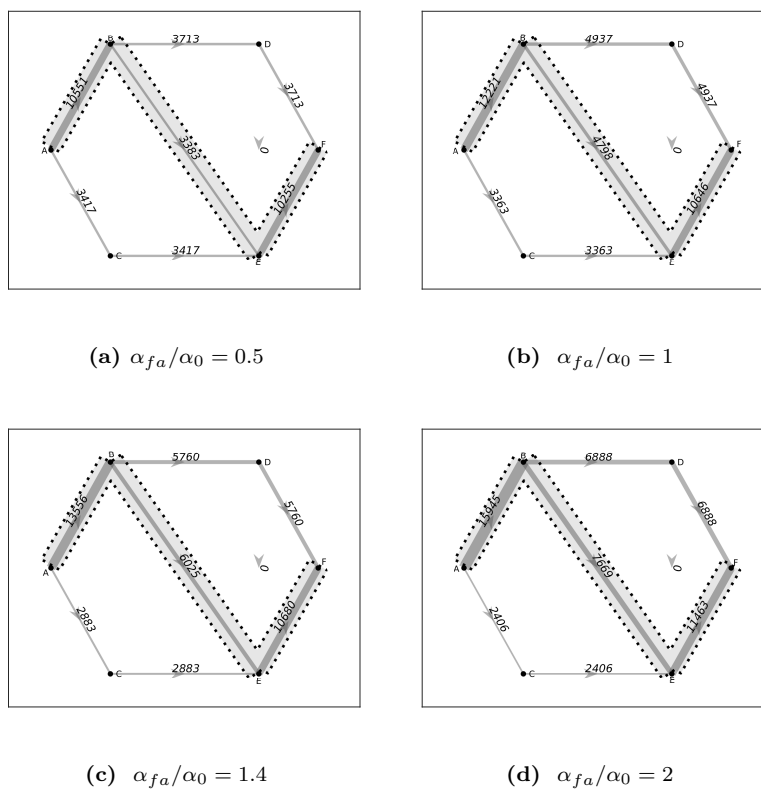
772 *7.2. The value of flexibility*

773 The third element of the analysis focuses on the effects of the cost functions on the value of  
 774 flexibility. Different relationships between  $\alpha_0$ ,  $\alpha_{fa}$ , and  $\alpha_{ia}$  are considered to determine the effect  
 775 on: i) the optimal initial capacity  $x_{0,e}^*$ , ii) the optimal flexibility  $f_{0,e}^*$ , and iii) the optimal costs.

776 Figures 12 and 13 show, respectively, the evolution of the optimal solution for the capacity  $\mathbf{x}_{0,e}^*$   
 777 and the flexibility  $\mathbf{f}_{0,e}^*$  in each link for different ratios  $\alpha_{fa}/\alpha_0$ . The critical route is highlighted  
 778 with the dotted lines and light shadow. As expected, the larger the cost of future adaptations  $\alpha_{fa}$   
 779 compared with the cost of building the required capacity from the beginning  $\alpha_0$ , the less flexibility  
 780 is introduced, and the system relies more on the initial capacity to serve the demand. This means

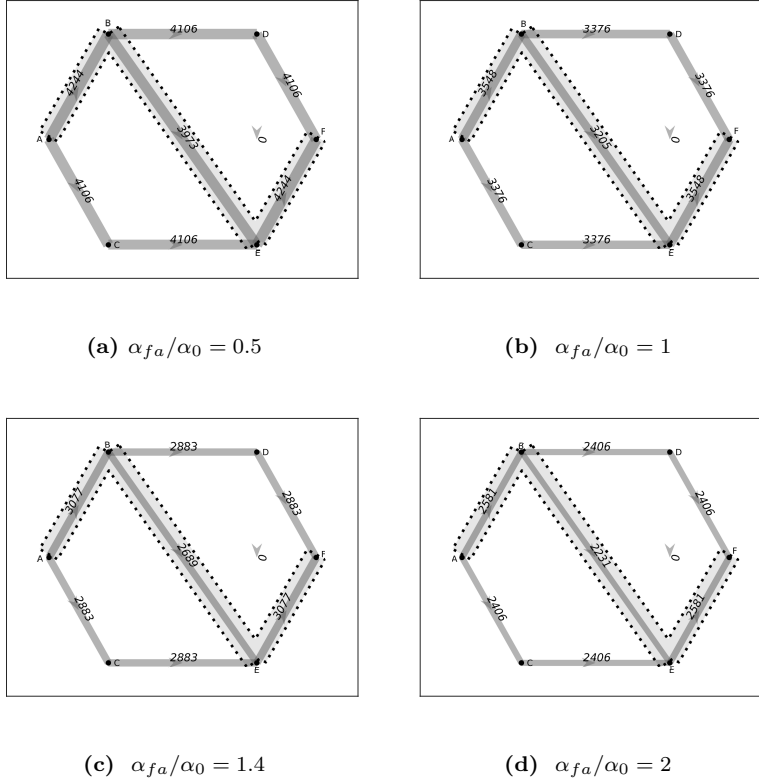
781 that reducing  $\alpha_0$  or increasing  $\alpha_{fa}$  decreases the value associated with flexibility, and the system  
 782 manager is willing to pay less to have it in the network.

783 It is interesting to observe in Figures 12 and 13 that the optimal solution for the initial capacity  
 784  $\mathbf{x}_{0,e}^*$  results in larger values for the links in the minimum cost route, while the optimal solution for  
 785 flexibility  $\mathbf{f}_{0,e}^*$  is similar for all the links in the network, excluding DE. This suggests that the short  
 786 and medium-term demand is mostly met by the minimum cost route until a point where it is less  
 787 expensive to use the flexibility built in other links to expand them and reroute part of the demand.  
 788 Besides, the quadratic cost function used for the introduction of flexibility discourages the approach  
 789 of adding too much flexibility into one link.



**Fig. 12.** Initial capacity evolution for different ratios  $\alpha_{fa}/\alpha_0$

790 Figure 14 compares the optimal costs obtained for different ratios  $\alpha_{fa}/\alpha_0$ . The figure includes  
 791 in the comparison the flexibility vectors  $\mathbf{fv}$  (see Equation 1) for each link of the network. The  
 792 horizontal component of the vector  $\mathbf{fv}$  depends on the ratio between planned and unplanned adap-



**Fig. 13.** Initial flexibility for different ratios  $\alpha_{fa}/\alpha_0$

793 tations, while the vertical component depends on the ratio between the flexibility  $\mathbf{f}_{0,e}$  and the initial  
 794 design/operation conditions  $\mathbf{x}_{0,e}$ . It is first observed the increment in optimal costs by increasing  
 795 the ratio  $\alpha_{fa}/\alpha_0$ ; expectedly, increasing the flexible adaptation costs increases the overall costs. As  
 796 shown in Figures 12 and 13, the model reacts by the decreasing the flexibility  $\mathbf{f}_{0,e}$  and increasing  
 797 the initial capacity  $\mathbf{x}_{0,e}$ ; nonetheless, the model cannot completely offset the increments in costs  
 798 because flexibility is still a cost-efficient strategy. This behavior is replicated in the flexibility vec-  
 799 tors, whose vertical component decreases as  $\alpha_{fa}/\alpha_0$  increases (the horizontal component decreases  
 800 by definition).

801 It is interesting to observe that the decrement is not uniform for all links. For  $\alpha_{fa}/\alpha_0 = 0.5$ ,  
 802 the vectors are divided into two groups (vector for link  $DE$  has a zero vertical component): i)  
 803 links  $AB, EF$ , which are part of the critical route, and ii) the remaining. Links  $AB, EF$  are key  
 804 for the entrance and exit of the demand to the network, and the model privileges initial capacity,

805 which results in  $\mathbf{fv}$  with a lower vertical component. Because the demand is free to flow through all  
 806 the remaining links, the program can assign more flexibility. As  $\alpha_{fa}/\alpha_0$  increase to 1 and 1.4, the  
 807 vertical component of the  $\mathbf{fv}$  keeps decreasing non-uniformly, resulting now in three distinct groups:  
 808 i) key input and output links of the critical route  $AB, EF$ , with the lowest vertical component; ii)  
 809 internal transit links  $BD, BE, EF$  whose vertical component keeps decreasing as flexibility becomes  
 810 less attractive and it is replaced by adding more initial capacity; and iii) the less used links  $AC, AE$ ,  
 811 which start transporting flow later on the network life-cycle and can keep relying on flexibility.  
 812 This tendency is clearly observed when  $\alpha_{fa}/\alpha_0 = 2$  and the vertical component of  $\mathbf{fv}$  decreases  
 813 considerably for all links except  $AC, AE$ .

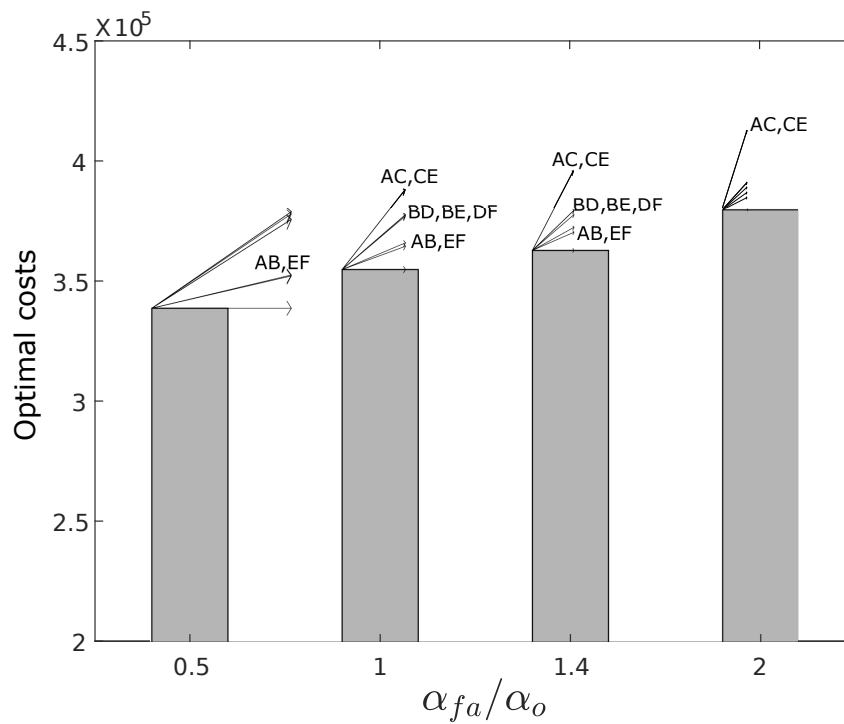


Fig. 14. Optimal costs and flexibility vectors  $\mathbf{fv}$  for different ratios  $\alpha_{fa}/\alpha_0$



814 *7.3. Effect of the discount rate*

815 A similar analysis was conducted to examine the effect of the discount rate on the optimal  
816 values  $x_{0,e}^*$  and  $f_{0,e}^*$ . Figure 15 compares the capacity and flexibility of link  $AB$  (other links follow  
817 a similar tendency) for three discount rates:  $dr = \{3\%, 5\%, 8\%\}$  as a function of  $\alpha_{fa}/\alpha_0$ . While the  
818 values of flexibility are mostly unaffected by the change in the discount rate  $dr$ , the initial capacity  
819 presents a clear decreasing tendency with an increment in the rate. In this case, larger discount  
820 rates make future adaptations (inside or beyond the flexible range) more attractive in the medium  
821 and long-term.

822 The decision of adding flexibility depends both on the cost of adding flexibility, which is incurred  
823 at the initial stage and it is not affected by the discount rate, and the costs of performing adap-  
824 tations, which are discounted. Increasing the discount rate reduces the present value of all future  
825 cost making both planned and unplanned adaptations more attractive, or at least moves forward  
826 the time stage where they are the optimal option. As a result, the short and medium-term demand  
827 is served using planned adaptations (flexibility) and long-term demand is served with unplanned  
828 adaptations, in detriment of the initial capacity. Therefore, it is expected that for typical ranges of  
829 the discount rate ( $\sim 3 - 10\%$ ) flexibility will be considered valuable. However, it could be argued  
830 that for unrealistically large discount rates the model would rely entirely on unplanned adaptations,  
831 except for the initial demand, abandoning completely the option of flexibility.

832 *7.4. Costs of adaptation beyond the flexible range*

833 In this analysis, the effect of the cost of unplanned adaptations  $\alpha_{ia}$  is determined by using  
834 different ratios  $\alpha_{fa}/\alpha_{ia}$  and  $\alpha_0/\alpha_{ia}$  to solve the MSP. Figure 16 shows a similar tendency as Figure  
835 15, with the optimal initial capacity and flexibility decreasing as the cost of unplanned adaptations  
836  $\alpha_{ia}$  decreases, and the initial capacity being affected by the increasing discount rate, which further  
837 bolsters the cost-effectiveness of unplanned adaptations. However, in this case, a reversing tendency  
838 is detected for the 8% discount rate. Upon closer inspection, it is revealed that there is a point  
839 where the short-term demand must be met before unplanned adaptation can take place. At this  
840 point it does not matter how much further  $\alpha_{ia}$  can be reduced; there is a minimum demand that  
841 must be met.

842 For lower discount rates it was cost-effective to use more flexibility to meet this short-term  
843 demand; however, for large discount rates, the initial cost of flexibility plus the adaptation cost

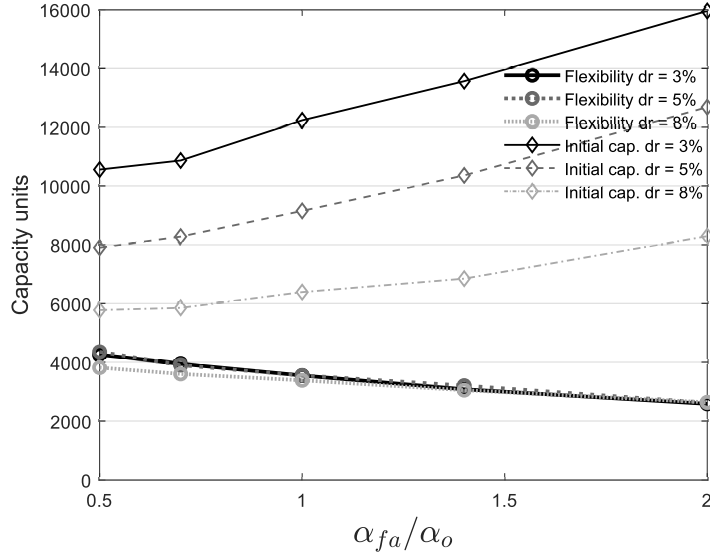


Fig. 15. Installed capacity and flexibility in link AB as function of ratio  $\alpha_{fa}/\alpha_o$  and discount rate

844 is not as cost-effective as just relying on the initial capacity for the short-term and unplanned  
 845 adaptations for the medium and long-term. This could explain the monotonic decreasing tendency  
 846 for flexibility while the initial capacity behaves asymptotically. This means that reducing the cost  
 847 of unplanned adaptations can only reduce the dependence on initial capacity up to the point where  
 848 there is enough capacity to attend the short-term demand that could not be served in any other  
 849 way. This point is dictated by the initial demand and its growth during the first decision period.

850 A final analysis was conducted to examine the effect of the unitary O&M costs on the optimal  
 851 initial capacity and flexibility. By increasing the unitary O&M costs from 2% of  $\alpha_o$  to 10% of  $\alpha_o$ ,  
 852 the optimal costs increase approximately 20%. The optimal initial capacity in all links is reduced by  
 853 approximately 12% which is compensated by a similar increment in the optimal installed flexibility.  
 854 If the O&M costs are further increased to 16% of  $\alpha_o$ , the optimal initial capacity decreases another  
 855 9% with a similar increment in the optimal flexibility. Increasing the O&M costs discourage large  
 856 system configurations in the short and medium-term, which makes flexibility more valuable.

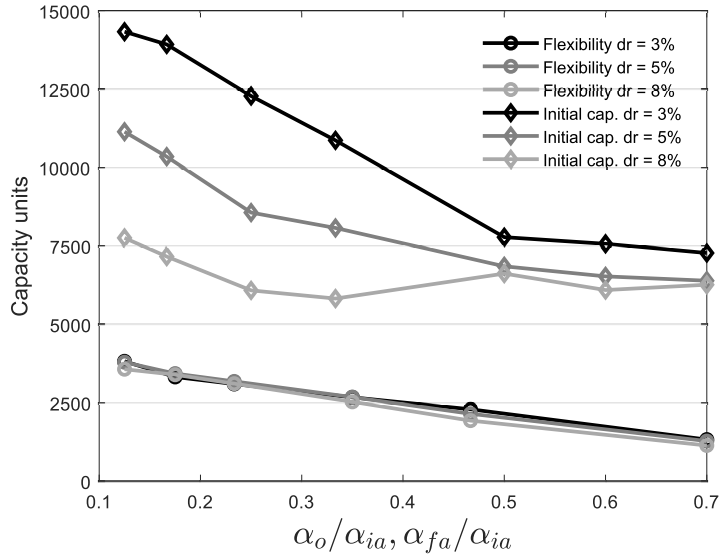


Fig. 16. Installed capacity and flexibility in link AB as function of ratios  $\alpha_{fa}/\alpha_{ia}$ ,  $\alpha_o/\alpha_{ia}$  and discount rate

857 **8. Summary and Conclusions**

858 This paper presented a multistage stochastic programming model for the design and management  
 859 of flexible infrastructure networks. The model considers the initial design characteristics of each  
 860 network link for different design elements as an initial decision that can be modified in future  
 861 stages by implementing planned and unplanned adaptations to face random external conditions.  
 862 By modeling the flexibility built at the initial stage as a decision variable that has an associate cost  
 863 and that limits future planned adaptations, the program can determine the optimal configuration  
 864 that minimizes costs. This formulation also provides an indirect measure of the value of flexibility  
 865 by finding the optimal *amount* of flexibility that is cost-effective to introduce.

866 An approximate solution method was implemented using Monte-Carlo simulation and k-medoids  
 867 clustering to generate the discrete representation of the stochastic process (scenario tree). The de-  
 868 terministic equivalent program was formulated and tested for a generic network with one input and  
 869 one output node for a stochastic demand. The numerical solution showed stability for reasonably  
 870 sized scenario trees and a not negligible VSS of around 16%. Furthermore, the results showed how  
 871 the value of flexibility is affected by the discount rate and the ratios between all the costs involved,  
 872 not just the cost of deploying planned adaptations. If the ratios  $\alpha_{fa}/\alpha_0$ , and  $\alpha_{ia}/\alpha_0$  are too large,

873 the system will prefer to meet the short and medium-term demand with the initial capacity, lowering  
874 the value of flexibility. As these ratios increase, the adaptations are further pushed into the future,  
875 especially for low discount rates. In the case where the ratio  $\alpha_{fa}/\alpha_{ia}$  is large, unplanned adapta-  
876 tions become cost-effective, also decreasing the value of flexibility. In contrast, for a given  $\alpha_{fa}$ , as  
877 the ratio  $\alpha_{ia}/\alpha_0$  grows, flexibility becomes more desirable. These examples show how the value of  
878 flexibility constantly evolves due to complex decisions that happen at different time instants.

879 The proposed model and the procedure implemented in the numerical example assumed that  
880 all decision and state variables are continuous. A mixed-integer formulation may require specific  
881 algorithms (e.g. primal decomposition) to find a solution efficiently. Furthermore, all cost functions  
882 were assumed convex, which is a reasonable assumption for most applications, but if concave func-  
883 tions are required, the solution procedure may not efficient nor may guarantee to find a solution.  
884 The scenario generation procedure can be extended to the multivariate case (for independent vari-  
885 ables) but the combinatorial nature of the problem restricts the number of decision stages than can  
886 be modeled. The formulation and solution of the MSP is also restricted by the exponential scala-  
887 bility. The expectation functional used in the model (Equation 4) enforces a risk-neutral approach  
888 that may not be appropriate for some applications. Further works should consider a formulation of  
889 the model with risk-averse functionals.

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## 894 List of symbols and abbreviations

- 895  $a_e$  Cost function of building edge  $e$  with intial parameters  $\mathbf{x}_{0,e}$
- 896  $\alpha_0$  Unitary cost of building initial design  $\mathbf{x}_{0,e}$
- 897  $\alpha_{fa}$  Unitary cost of performing flexible adaptation  $\mathbf{y}_{t,e}$
- 898  $\alpha_{ia}$  Unitary cost of performing unplanned adaptation  $\mathbf{z}_{t,e}$
- 899  $b_e$  Cost function of adding  $\mathbf{f}_{0,e}$  flexibility to edge  $e$
- 900  $c_e$  Cost function of changing edge  $e$  by  $\mathbf{y}_{t,e}$

901 **CV** Coefficient of variation  
902  $d_e$  Cost function of changing edge  $e$  by  $\mathbf{z}_{t,e}$   
903  $\gamma_t$  Discount factor at time  $t$   
904  $G$  Directed graph  
905  $dr$  Discount rate  
906  $e$  Edge/link in directed graph  $G$   
907  $\mathbf{f}_{0,e}$  Flexibility range of design/operation parameters for edge  $e$   
908  $w_{t,e}$  Flow through edge  $e$  at time  $t$   
909  $\mathbf{fv}$  Flexibility vector  
910  $g_e$  Operation and maintenance cost function for edge  $e$   
911  $h(\boldsymbol{\xi}_t)$  Revenue function  
912 **MDP** Markov decision process  
913 **MS** multistage stochastic  
914 **MSP** multistage stochastic program  
915 **O&M** Operation and Maintenance  
916  $p_k$  Probability of scenario  $k$   
917  $\pi$  Policy function  
918  $q_e$  Flow cost function for edge  $e$   
919  $\boldsymbol{\xi}_t$  Vector of random, external parameters at time  $t$   
920 **ROA** real options analysis  
921 **VSS** Value of stochastic solution  
922  $\mathbf{x}_{t,e}$  Vector of design/operation parameters at time  $t$  for edge  $e$   
923  $\mathbf{x}_{0,e}$  Vector of initial design/operation parameters for edge  $e$   
924  $\mathbf{y}_{t,e}$  Vector of flexible adaptations at time  $t$  for edge  $e$   
925  $\mathbf{z}_{t,e}$  Vector of unplanned adaptations at time  $t$  for edge  $e$

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