Multistage stochastic optimization of a hydrogen supply chain

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Cermics, École des Ponts ParisTech & Persee



- Hydrogen displays promising features for decarbonization industry, transportation and building sectors
- Transition towards a hydrogen economy requires hydrogen costs to come down, through optimal choices of infrastructure design and operation
- The optimal choices of design and operation rely on multistage stochastic optimization

Problem statement for the management of a hydrogen supply chain

Solving the problem by decomposition method

Numerical results

Optimizing the stock capacity

Future works and extensions

Problem statement for the management of a hydrogen supply chain

Problem statement

• Schiever company: diesel trucks → hydrogen trucks



The objective is to minimize the operation cost of this supply chain by making decisions every hour during one week

Special characteristics of the problem



• A nonlinear electricity consumption for the electrolyser

• An energy mix to power the supply chain



Decision	Description
E ^{PPA} _h	Electricity from PPA contract (kWh)
E_{h+1}^{G}	Electricity from the grid (kWh)
$\overset{\mathrm{E}}{h}$	Load at which the electrolyser is functioning $(\%)$
M_h^{E}	Turn the electrolyser to cold, idle or start mode
$H_h^{\rightarrow D}$	Quantity of hydrogen extracted from the
	storage (kg) to satisfy demand

Uncertainty	Description
E_{h+1}^{PV}	Renewable (PV) electricity (kWh) during $[h, h + 1]$
D_{h+1}	Demand of hydrogen (kg) during $[h, h + 1[$

Optimization problem formulation

$$\underset{h \in \mathbb{H}}{\underset{h \in \mathbb{H}}{\underset{h \in \mathbb{H}}{\underset{h \in \mathbb{H}}{\overset{p \neq a}{\underset{h \in \mathbb{H}}{\underset{h \in \mathbb{H}}{\underset{h$$

subject to

- nonanticipativity constraints
- operational constraints
- renewable energy constraints
- a coupling constraint between the energy mix

and the hydrogen equipments

$$\underbrace{\mathsf{E}_{h}^{\mathrm{PPA}} + \mathsf{E}_{h+1}^{\mathrm{G}} + \mathsf{E}_{h+1}^{\mathrm{PV}}}_{\text{electricity supply}} = \underbrace{g(\mathsf{M}_{h}^{\mathrm{E}}, \mathsf{M}_{h}^{\mathrm{E}}, \mathsf{I}_{h}^{\mathrm{E}})}_{\text{electricity consumption}}$$

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Renewable energy constraints of the problem

· Constraint on energy from the grid

Electricity from the grid is less than p percent of the total electricity

$$\frac{\sum_{h \in \mathbb{H}} \mathbf{E}_{h+1}^{G}}{\sum_{h \in \mathbb{H}} \mathbf{E}_{h}^{PPA} + \mathbf{E}_{h+1}^{G} + \mathbf{E}_{h+1}^{PV}} \leq p$$
$$\iff \sum_{h \in \mathbb{H}} \left((1-p) \mathbf{E}_{h+1}^{G} - p(\mathbf{E}_{h}^{PPA} + \mathbf{E}_{h+1}^{PV}) \right) \leq 0$$

reformulated as a cost function

$$\mathcal{K}\left((\mathbf{E}_{h}^{\text{PPA}}, \mathbf{E}_{h+1}^{\text{G}}, \mathbf{E}_{h+1}^{\text{PV}})_{h \in \mathbb{H}}\right) = \alpha \max\left(0, \sum_{h \in \mathbb{H}}\left((1-p)\mathbf{E}_{h+1}^{\text{G}} - p(\mathbf{E}_{h}^{\text{PPA}} + \mathbf{E}_{h+1}^{\text{PV}})\right)\right)$$

• Constraint on PPA contract

Electricity from the PPA contract is bounded

$$\sum_{h \in \mathbb{H}} \mathbf{E}_{h}^{\mathrm{PPA}} \leq \overline{E}^{\mathrm{PPA}}$$

To solve the problem by dynamic programming,

we introduce the mode of electrolyser and three stock variables

State variable	Description
$M_h^{ m E}$	mode of the electrolyser ({ <i>start</i> , <i>idle</i> , <i>cold</i> })
S _h	quantity of hydrogen in the storage (kg)
Q_h	"cumul of electricity"
P _h	remaining stock of available PPA (kWh)

State dynamics for the Schieve case

Letting $X_h = (M_h^{\text{E}}, S_h, P_h, Q_h)$ be the four dimensional state, we have a state dynamics $\mathbf{X}_{h+1} = f(\mathbf{X}_h, \mathbf{I}_h^{\text{E}}, \mathbf{M}_h^{\text{e}^{\frown}}, \mathbf{H}_h^{\text{d}^{\text{D}}}, \mathbf{E}_h^{\text{PPA}}, \mathbf{E}_{h+1}^{\text{G}}, \mathbf{E}_{h+1}^{\text{PV}}, \mathbf{D}_{h+1})$ with

$$\mathbf{M}_{h+1}^{\mathrm{E}} = \mathbf{M}_{h}^{\mathrm{E}^{\sim}} \qquad (\text{Mode of the electrolyser})$$
$$\mathbf{S}_{h+1} = \mathbf{S}_{h} + \underbrace{\mathbf{I}_{h}^{\mathrm{E}} \mu(\mathbf{M}_{h}^{\mathrm{E}}, \mathbf{M}_{h}^{\mathrm{E}^{\sim}})\overline{m^{\mathrm{E}}}}_{\mathbf{H}_{2} \text{ produced}} - \underbrace{\mathbf{H}_{h}^{\rightarrow \mathrm{D}}}_{\mathbf{H}_{2} \text{ extracted}} \qquad (\text{Stock of hydrogen})$$

$$\begin{split} \mathbf{P}_{h+1} &= \mathbf{P}_{h} - \mathbf{E}_{h}^{\text{PPA}} & (\text{Stock of PPA}) \\ \mathbf{Q}_{h+1} &= \mathbf{Q}_{h} + \rho \mathbf{E}_{h+1}^{\text{G}} - (1-\rho) (\mathbf{E}_{h}^{\text{PPA}} + \mathbf{E}_{h+1}^{\text{PV}}) & (\text{Cumul of electricity}) \end{split}$$

Thanks to the state Q_h , the cost $K((\mathbf{E}_h^{\text{PPA}}, \mathbf{E}_{h+1}^{\text{G}}, \mathbf{E}_{h+1}^{\text{PV}})_{h \in \mathbb{H}})$ can be written as $J(\mathbf{Q}_T) = \alpha \max(0, \mathbf{Q}_T)$ A difficult numerical problem:

- one week horizon with hourly decisions (168 time steps)
- four dimensional state
 - using Stochastic Dynamic Programming, we discretize the states
 - the stock of PPA (P) and of the "cumul of electricity" (Q) take large values and require a fine discretization which is numerically demanding
- two random variables
- five decisions at each hour

Solving the problem by decomposition method

A decomposition approach



A decomposition approach

$$\operatorname{val}(\mathcal{P}) = \min_{\left(\mathbf{E}_{h}^{\operatorname{PPA}}, \mathbf{E}_{h+1}^{\operatorname{G}}, \mathbf{M}_{h}^{\operatorname{E}^{\circ}}, \mathbf{I}_{h}^{\operatorname{E}}, \mathbf{H}_{h}^{\operatorname{PD}}\right)_{h \in \mathbb{H}}} \mathbb{E}_{\left(\mathbf{D}_{h+1}, \mathbf{E}_{h+1}^{\operatorname{PV}}\right)_{h \in \mathbb{H}}} \left[\underbrace{\sum_{h \in \mathbb{H}} c^{ppa} \mathbf{E}_{h}^{\operatorname{PPA}} + c_{h}^{g} \mathbf{E}_{h+1}^{\operatorname{G}} + \mathcal{K}\left(\left(\mathbf{E}_{h}^{\operatorname{PPA}}, \mathbf{E}_{h+1}^{\operatorname{G}}, \mathbf{E}_{h+1}^{\operatorname{PV}}\right)_{h \in \mathbb{H}}\right)}_{\text{electricity cost}} + \underbrace{\sum_{h \in \mathbb{H}} c^{d} \left(\mathbf{D}_{h+1} - \mathbf{H}_{h}^{\operatorname{PD}}\right)_{+}}_{\text{demand dissatisfaction cost}}\right]$$

subject to nonanticipativity constraints, operational constraints, electricity constraints and the following coupling constraint

$$\underbrace{\mathbf{E}_{h}^{\text{PPA}} + \mathbf{E}_{h+1}^{\text{G}} + \mathbf{E}_{h+1}^{\text{PV}}}_{\text{electricity supply}} = \underbrace{g(\mathbf{M}_{h}^{\text{E}}^{\frown}, \mathbf{M}_{h}^{\text{E}}, \mathbf{I}_{h}^{\text{E}})}_{\text{electricity consumption}}$$

Decoupling the operational and electricity problems

Dualize the coupling constraints with Lagrange multipliers: $\lambda = \{\lambda_h\}_{h \in \mathbb{H}}$

• electrolyser/compressor/storage operational (O) problem

$$\phi^{O}(\lambda) = \min_{(\mathsf{M}_{h}^{\mathbb{E}^{\sim}}, \mathsf{I}_{h}^{\mathbb{E}}, \mathsf{H}_{h}^{\rightarrow D})_{h \in \mathbb{H}}} \mathbb{E}_{(\mathsf{D}_{h+1})_{h \in \mathbb{H}}} \left[\sum_{h \in \mathbb{H}} c^{d} (\mathsf{D}_{h+1} - \mathsf{H}_{h}^{\rightarrow D})_{+} - \sum_{h \in \mathbb{H}} \lambda_{h} (g(\mathsf{M}_{h}^{\mathbb{E}^{\sim}}, \mathsf{M}_{h}^{\mathbb{E}}, \mathsf{I}_{h}^{\mathbb{E}})) \right]$$

s.t. (undetailed) operational constraints

• electricity (E) allocation problem

$$\begin{split} \phi^{E}(\lambda) &= \min_{(\mathbf{E}_{h}^{\text{PPA}}, \mathbf{E}_{h+1}^{\text{G}})_{h \in \mathbb{H}}} \mathbb{E}_{(\mathbf{E}_{h+1}^{\text{PV}})_{h \in \mathbb{H}}} \left[\sum_{h \in \mathbb{H}} c^{\rho p_{a}} \mathbf{E}_{h}^{\text{PPA}} + c_{h}^{g} \mathbf{E}_{h+1}^{\text{G}} \right. \\ &+ \mathcal{K} \left((\mathbf{E}_{h}^{\text{PPA}}, \mathbf{E}_{h+1}^{\text{G}}, \mathbf{E}_{h+1}^{\text{PV}})_{h \in \mathbb{H}} \right) \\ &+ \sum_{h \in \mathbb{H}} \lambda_{h} (\mathbf{E}_{h}^{\text{PPA}} + \mathbf{E}_{h+1}^{\text{G}} + \mathbf{E}_{h+1}^{\text{PV}}) \right] \end{split}$$

s.t. electricity constraints

Decoupling the operational and electricity allocation problems

- For a fixed deterministic multiplier $\lambda = \{\lambda_h\}_{h \in \mathbb{H}}$, independently:
 - compute $\phi^{O}(\lambda)$ (operational problem) by Stochastic Dynamic Programming (SDP) $\phi^{O}(\lambda) = V_{0}^{O,\lambda}(S_{0}, M_{0}^{E})$ given by induction $V_{b}^{O,\lambda} = B^{O,\lambda}(V_{bal}^{O,\lambda})$
 - compute $\phi^{E}(\lambda)$ (electricity allocation problem) by Stochastic Dual Dynamic Programming (SDDP) $\phi^{E}(\lambda) = V_{0}^{E,\lambda}(P_{0}, Q_{0})$ given by induction $V_{h}^{E,\lambda} = B^{E,\lambda}(V_{h+1}^{E,\lambda})$
- Update the multiplier λ by a gradient based optimization algorithm to maximize the dual function $\phi^{O}(\lambda) + \phi^{E}(\lambda)$

$$\phi^{O}(\lambda) + \phi^{E}(\lambda) \leq \underbrace{\max_{\lambda'} \phi^{O}(\lambda') + \phi^{E}(\lambda')}_{\text{dual problem}} \leq \underbrace{\operatorname{val}(\mathcal{P})}_{\text{primal problem}}$$

Policy design

For a fixed multiplier $\lambda = \{\lambda_h\}_{h \in \mathbb{H}}$

• we obtain a feasible policy $\pi^{\lambda} = \{\pi_{h}^{\lambda}\}_{h \in \mathbb{H}}$ for the problem (\mathcal{P}) by

$$\begin{split} \widetilde{\pi_{h}^{\lambda}} & \left(S_{h}, M_{h}^{\mathrm{E}}, P_{h}, Q_{h}\right) = \underset{\left(\mathbf{E}_{h}^{\mathrm{PPA}}, \mathbf{M_{h}^{\mathrm{E}}}^{\wedge}, \mathbf{E}_{h}^{\mathrm{E}}, \mathbf{H}_{h}^{\mathrm{D}}\right)}{\mathrm{arg\,min}} \mathbb{E}_{\left(\mathbf{D}_{h+1}, \mathbf{E}_{h+1}^{\mathrm{PV}}\right)} \left[\underset{\mathbf{E}_{h+1}^{\mathrm{G}}}{\min} \ L_{h} \left(\mathbf{E}_{h}^{\mathrm{PPA}}, \mathbf{E}_{h+1}^{\mathrm{G}}, \mathbf{E}_{h+1}^{\mathrm{PV}}, \mathbf{H}_{h}^{\mathrm{D}}\right) \\ & + \underbrace{V_{h+1}^{O, \lambda}(\mathbf{S}_{h+1}, \mathbf{M}_{h+1}^{\mathrm{E}}) + V_{h+1}^{E, \lambda}(\mathbf{P}_{h+1}, \mathbf{Q}_{h+1})}_{\mathbf{Q}_{h+1}} \right] \end{split}$$

surrogate additive value function

under nonanticipativity constraints, operational constraints, renewable energy constraints and the coupling constraint

• we have $\operatorname{val}(\mathcal{P}) \leq \operatorname{val}(\mathcal{P}_{\pi^{\lambda}})$,

where $\operatorname{val}(\mathfrak{P}_{\pi^{\lambda}})$ denotes the cost when applying the policy π^{λ}

PV and demand data

The independent random variables $(D_{h+1}, E_{h+1}^{PV})_{h \in \mathbb{H}}$ are given by

Table 1: Probability distribution of D_{h+1}

Outcome	$0.8 \mu_{h+1}^{d}$	$0.9 \mu_{h+1}^d$	μ_{h+1}^d	$1.1 \mu_{h+1}^{d}$	$1.2\mu_{h+1}^{d}$
Probability	$\frac{1}{5}$	$\frac{1}{5}$	$\frac{1}{5}$	$\frac{1}{5}$	$\frac{1}{5}$

Table 2: Probability distribution of E_{h+1}^{PV}

Outcome	$0.8\mu_{h+1}^{pv}$	$0.9\mu_{h+1}^{pv}$	μ_{h+1}^{pv}	$1.1 \mu_{h+1}^{pv}$	$1.2\mu_{h+1}^{pv}$
Probability	$\frac{1}{5}$	$\frac{1}{5}$	$\frac{1}{5}$	$\frac{1}{5}$	$\frac{1}{5}$

where $(\mu_{h+1}^d, \mu_{h+1}^{e^{PV}})_{h \in \mathbb{H}}$ are deterministic and given in the following figure



Monte-Carlo evaluation of a policy

 Let (d, e^{PV}) = (d_{h+1}, e^{PV}_{h+1})_{h∈ℍ} be a sample of hydrogen demand and PV production

We simulate a policy as follows: $\begin{aligned} x_0 &\rightsquigarrow \pi_0^{\lambda}(x_0) \rightsquigarrow (d_1, e_1^{\text{PV}}) \rightsquigarrow x_1 = f(x_0, \pi_0^{\lambda}(x_0), (d_1, e_1^{\text{PV}})) \rightsquigarrow \pi_1^{\lambda}(x_1) \rightsquigarrow \\ (d_2, e_2^{\text{PV}}) \rightsquigarrow x_2 = f(x_1, \pi_1^{\lambda}(x_1), (d_2, e_2^{\text{PV}})) \dots \rightsquigarrow (d_{h+1}, e_{h+1}^{\text{PV}}) \rightsquigarrow x_h = \\ f(x_{h-1}, \pi_h^{\lambda}(x_{h-1}), (d_{h+1}, e_{h+1}^{\text{PV}})) \end{aligned}$

Let {(d, e^{PV})_i}_{i∈[1,N]} be a set of noise trajectories, we use the approximation

$$\operatorname{val}(\mathfrak{P}_{\pi^{\lambda}}) \approx \frac{1}{N} \sum_{i=1}^{N} \operatorname{val}(\mathfrak{P}_{\pi^{\lambda}}^{i})$$

where val $(\mathcal{P}_{\pi\lambda}^{i})$ is the cost of the simulation for the noise trajectory $(d, e^{\mathrm{PV}})_{i}$

Numerical results

Maximizing the dual function



maximization of the dual function with decomposition algorithm

Evolution of the hydrogen stock over time



Electricity consumption over time



Figure 1: Time evolution of the electricity consumption for the three different scenarios

Optimizing the stock capacity

The stock design problem can be written as

$$\min_{i \in \mathbb{I}} \min_{(\mathbf{U}_{h})_{h \in \mathbb{H}} \in Y_{i}} \mathbb{E}_{(\mathbf{D}_{h+1}, \mathbf{E}_{h+1}^{\mathrm{PV}})_{h \in \mathbb{H}}} \left[\sum_{h \in \mathbb{H}} \mathcal{L}_{h} \left(\mathbf{E}_{h}^{\mathrm{PPA}}, \mathbf{E}_{h+1}^{\mathrm{G}}, \mathbf{E}_{h+1}^{\mathrm{PV}}, \mathbf{H}_{h}^{\rightarrow \mathrm{D}} \right) \right. \\ \left. + \mathcal{K} \left(\left(\mathbf{E}_{h}^{\mathrm{PPA}}, \mathbf{E}_{h+1}^{\mathrm{G}}, \mathbf{E}_{h+1}^{\mathrm{PV}} \right)_{h \in \mathbb{H}} \right) \right] + c_{i}$$

where \mathbb{I} is the set of designs, $\mathbf{U}_h = (\mathbf{E}_h^{\text{PPA}}, \mathbf{E}_{h+1}^{\text{G}}, \mathbf{M}_h^{\text{E}}, \mathbf{I}_h^{\text{E}}, \mathbf{H}_h^{\text{-}\text{D}})$, Y_i is the set of nonanticipativity constraints, operational constraints (that depends on *i*), renewable energy constraints and the coupling constraints between the energy mix and the hydrogen equipments and c_i is the cost of the design *i*.

We consider the following optimization problem

$$\min_{i\in\mathbb{I}}\max_{\lambda\in\mathbb{R}^{T}}\phi^{E}(\lambda)+\phi^{O}_{i}(\lambda)+\boldsymbol{c}_{i},$$

where

- $\phi^E(\lambda)$ is the electricity allocation problem that does not dependant on *i*
- $\phi_i^O(\lambda)$ is the operational problem that depends on *i*

The computation of $\phi_i^O(\lambda)$ is faster than the computation of $\phi^E(\lambda)$, which is the key ingredient used in the following algorithm to solve the minmax optimization problem

Solving the minmax problem

- 1. set $\mathbb{J} \leftarrow \mathbb{I}$, choose an initial design $i \in \mathbb{J}$, set $\mathbb{J} \leftarrow \mathbb{J} \setminus \{i\}$, choose an initial multiplier $\lambda^0 \in \mathbb{R}^T$
- 2. maximize the dual function $\phi^E + \phi^O_i + c_i$ associated to the design problem *i*. The multiplier obtained at the end of the optimization is denoted by λ^*
- 3. store the oriented pair $(i, \phi^E(\lambda^*) + \phi^O_i(\lambda^*) + c_i)$ in the list \mathbb{O}
- 4. for all $i' \in \mathbb{J}$, if $\phi_i^O(\lambda^*) + c_i < \phi_{i'}^O(\lambda^*) + c_{i'}$, it follows that $\max_{\lambda \in \mathbb{R}^T} \phi^E(\lambda) + \phi_i^O(\lambda) + c_i < \max_{\lambda \in \mathbb{R}^T} \phi^E(\lambda) + \phi_{i'}^O(\lambda) + c_{i'} \text{ and therefore}$ that the design i' is not optimal, set $\mathbb{J} \leftarrow \mathbb{J} \setminus \{i'\}$
- 5. if $\mathbb{J} \neq \{\emptyset\}$, choose $i \in \mathbb{J}$, set $\mathbb{J} \leftarrow \mathbb{J} \setminus \{i\}$, set $\lambda^0 \leftarrow \lambda^*$ and goto2
- 6. if $\mathbb{J} = \{\emptyset\}$, search for the best design in the list \mathbb{O}

In one numerical experiment with six different stock capacity, this algorithm entered step 2 only once, the other five designs were removed at step 4, which gives promising perspectives

Future works and extensions

- We modeled a hydrogen supply chain with three sources of energy
- We solved the optimal management of the Schiever supply chain with decomposition method involving two subproblems:
 - an operational problem solved by SDP
 - an electricity allocation problem solved by SDDP
- We proposed a simple algorithm to optimize the capacity of the hydrogen storage
- The next step will be to consider the design of the hydrogen equipments (storage and electrolyser) and the PPA contracts

Any questions ?

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