Prospective Modeling and Climate Change: Energy & Water issues. ETSAP & TTI.5 Autumn School 2023

combinatorial optimization for water management

Sophia-Antipolis, 13 november 2023

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water management ?

a commodity to collect, treat, distribute, value

ex: design and operate wastewater networks under normal or extreme conditions

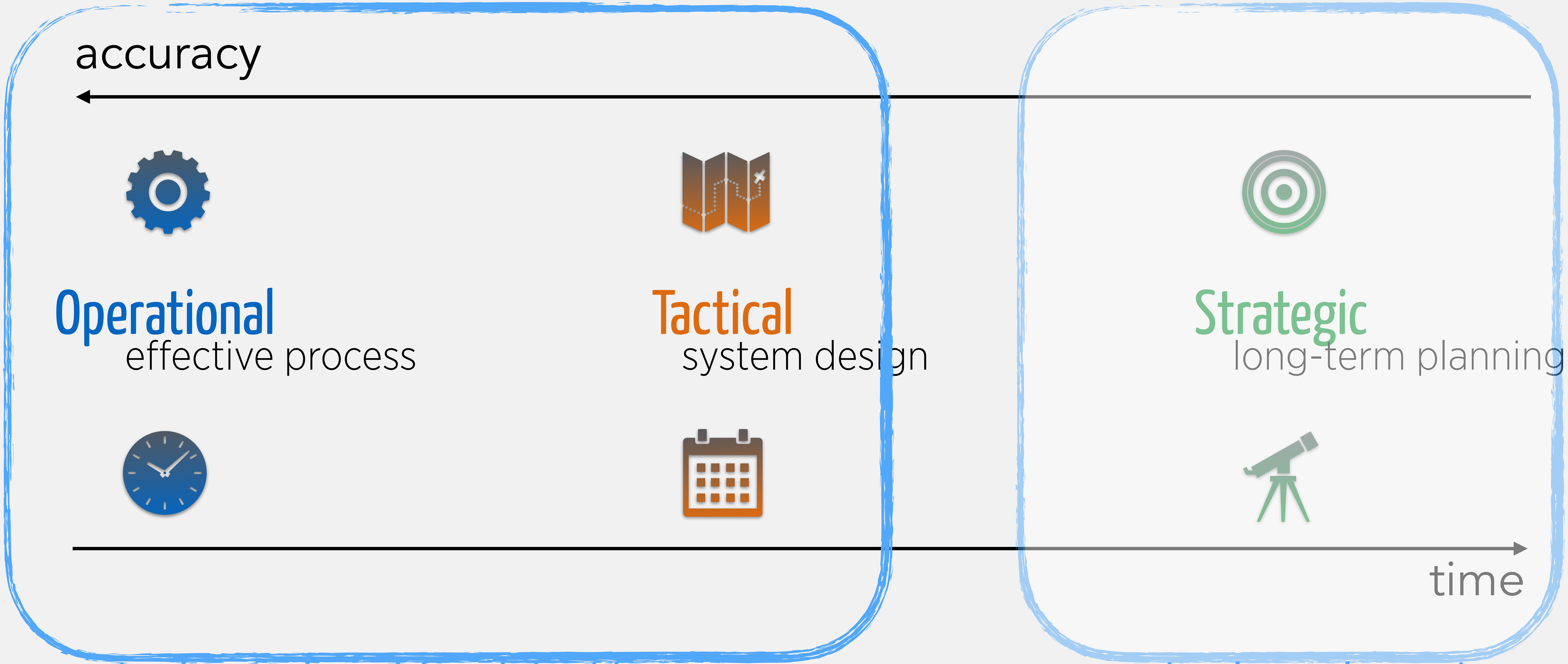
a resource with limited availability to mobilize in processes

ex: withdraw water for cooling or cleaning while preserving water source quality

a biotope to preserve or a natural hazard to deal with

ex: adapt landscape to flood resilience

decision & management



operational research: models and algorithms

prospective: data and scenarios

during the next hour

overview of prescriptive tools in decision support

focus on mathematical optimization and discrete decision

selected applications in water management

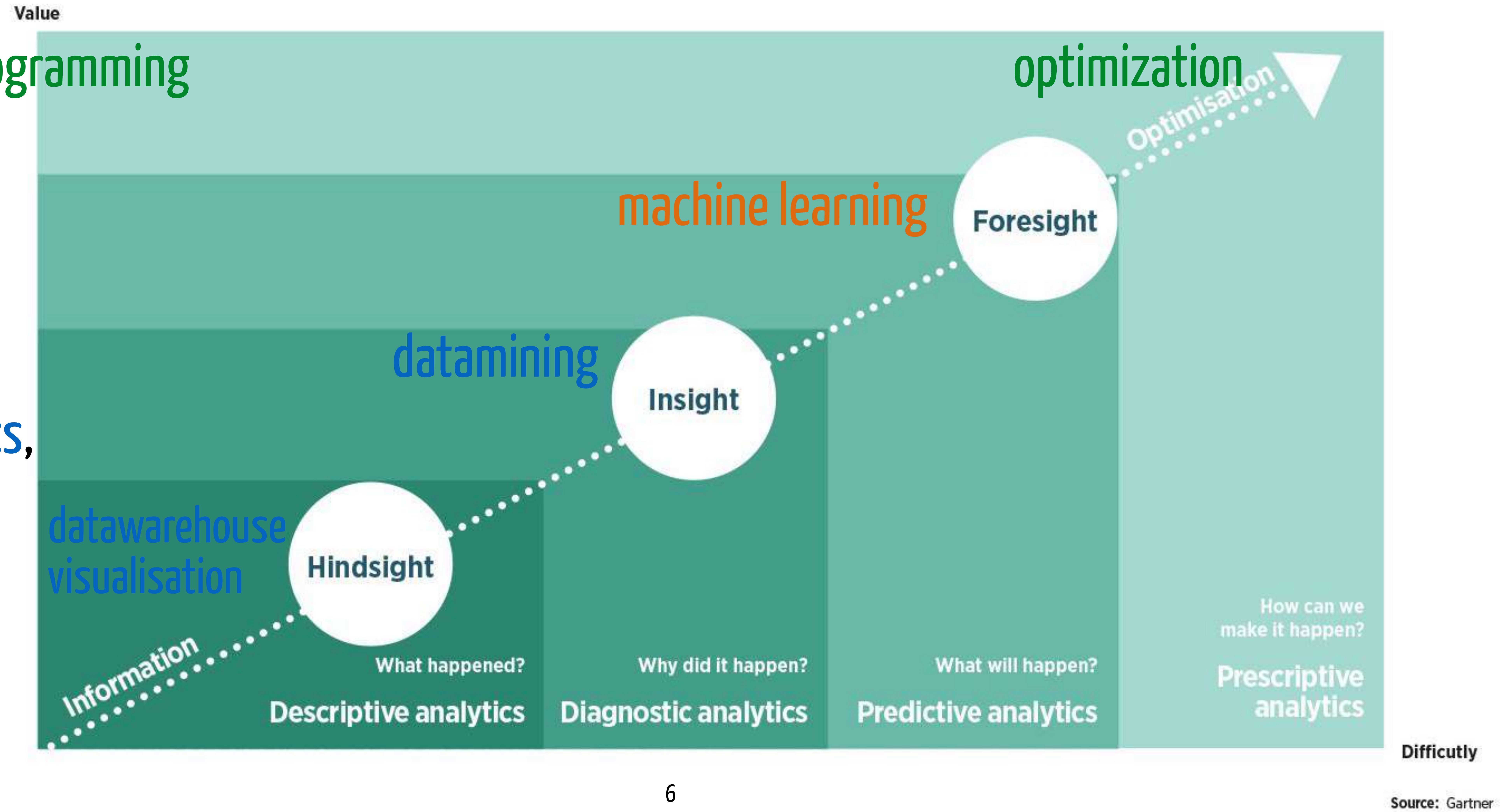
prescriptive tools in decision support

decision support

from WWII:
mathematical programming

in the 2010s:
AI, deep learning

in the 2000s:
business analytics,
big data



decision = optimization

Decision Making

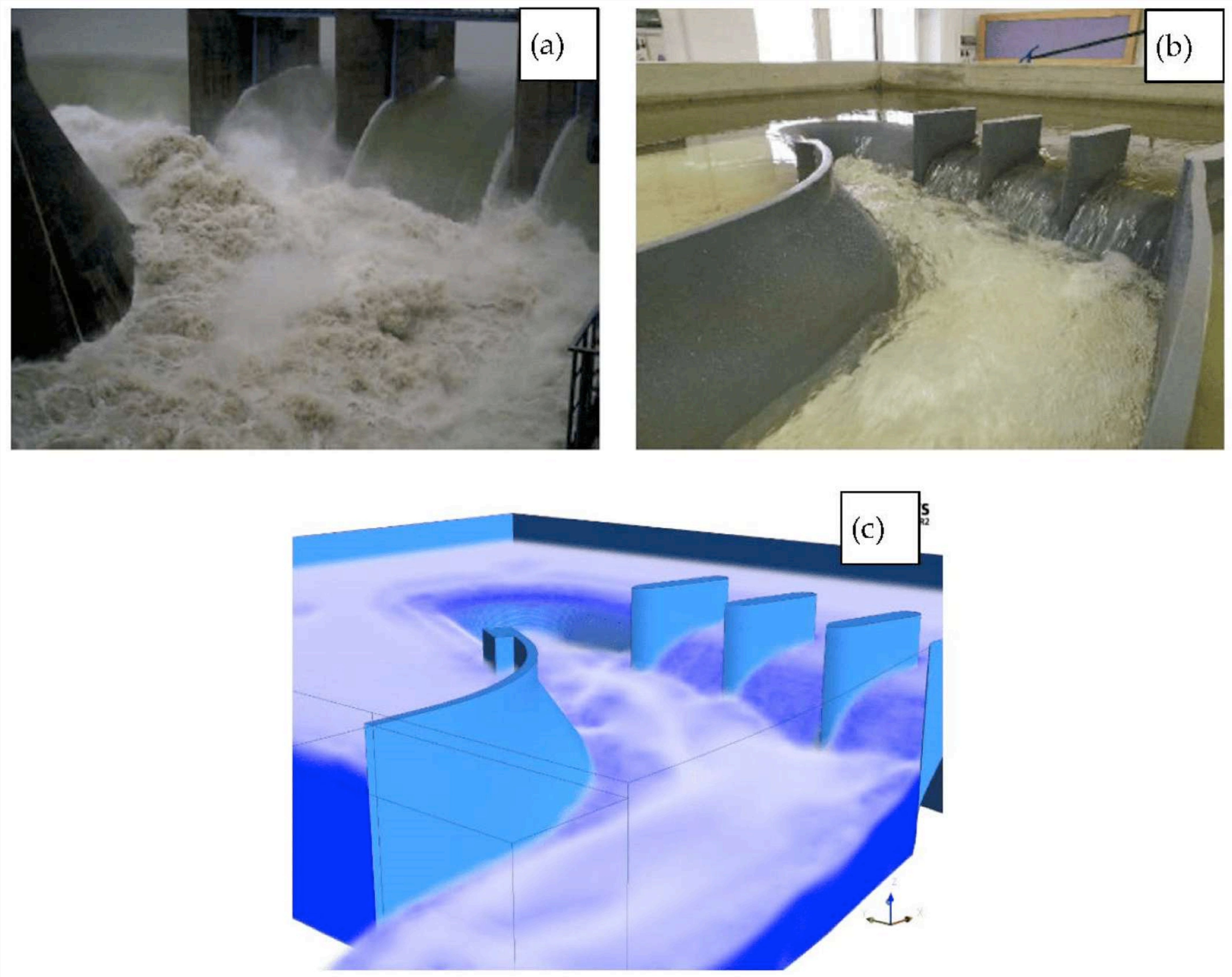
identify possible alternatives, attach a quantitative score,
search an alternative with the highest score

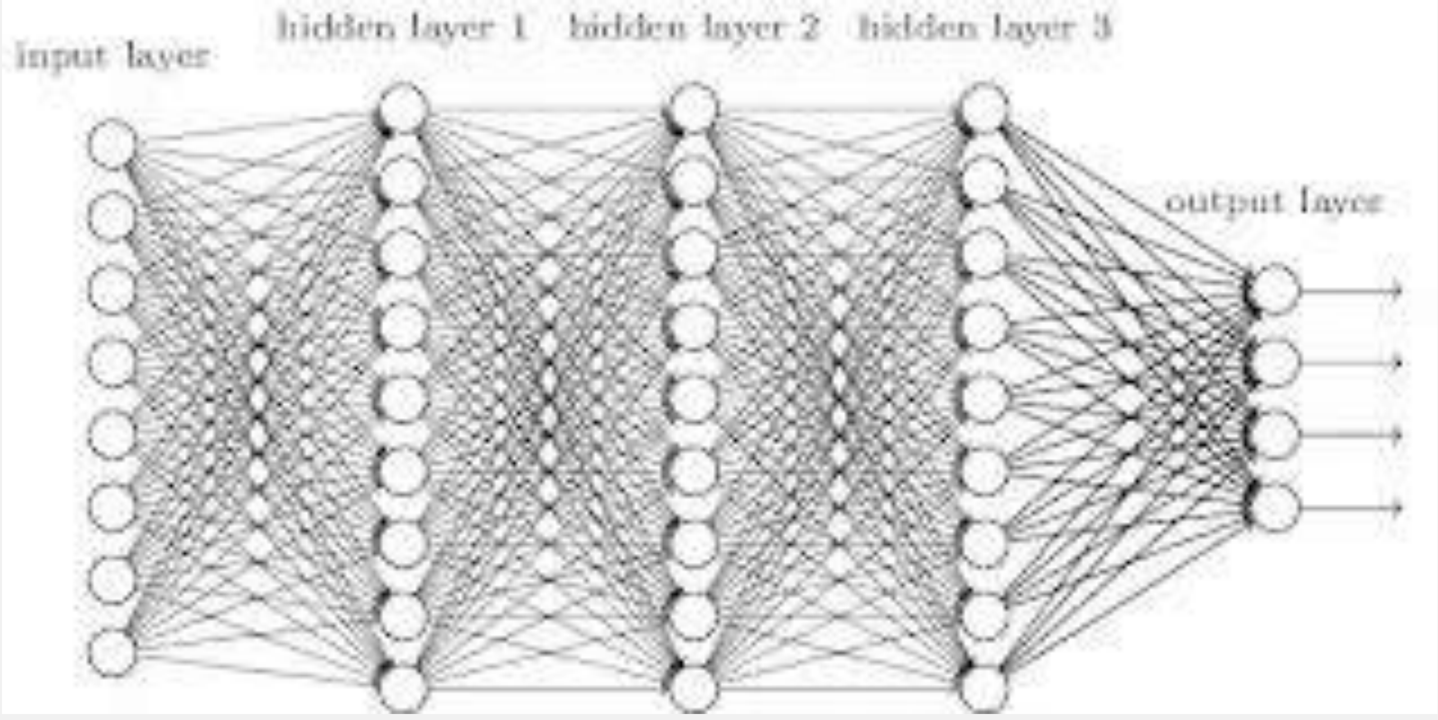
Optimization

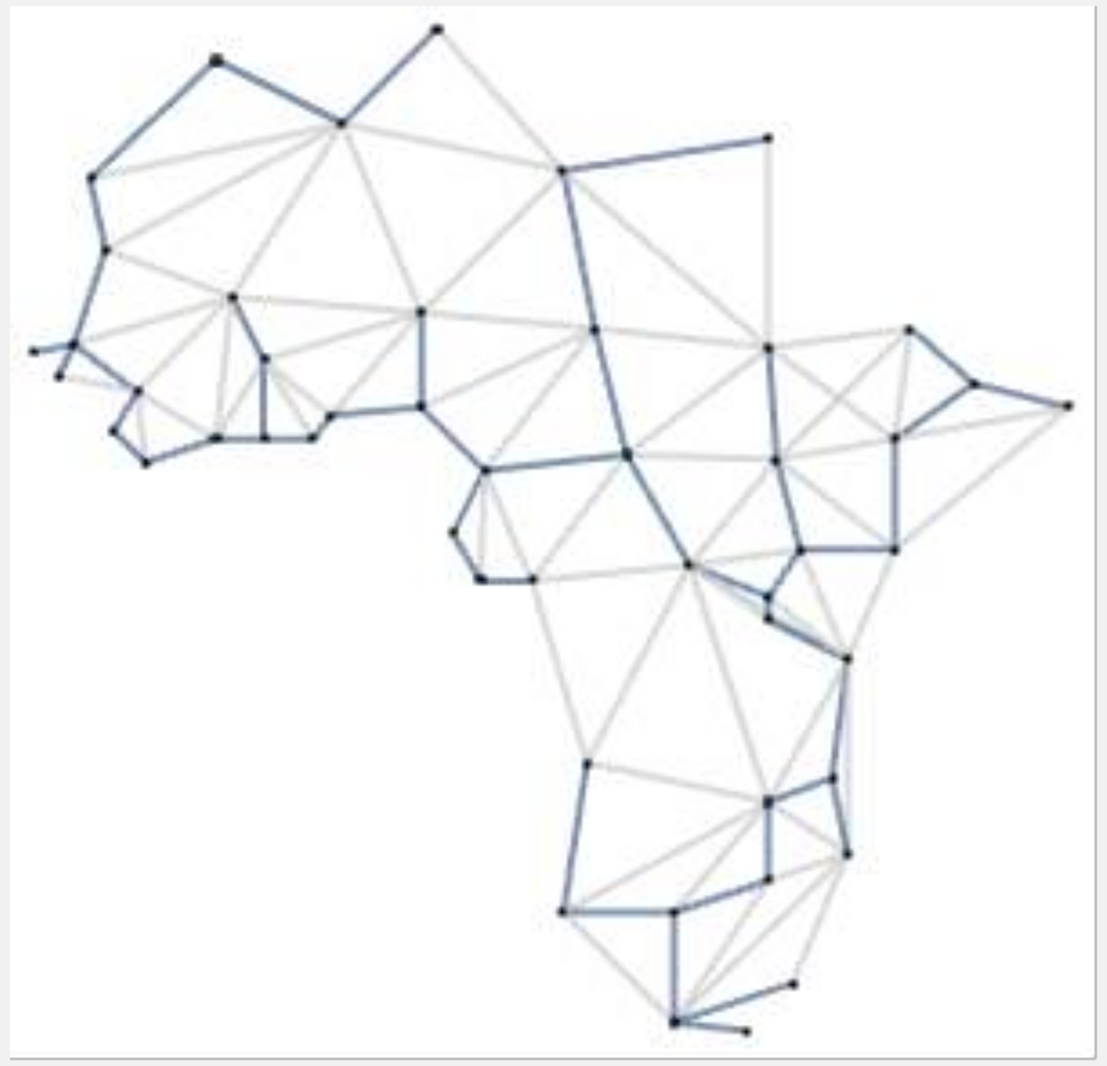
model : describe the feasible solutions
objective: a mapping from solutions to scores
optimize : compute a feasible solution of maximum score

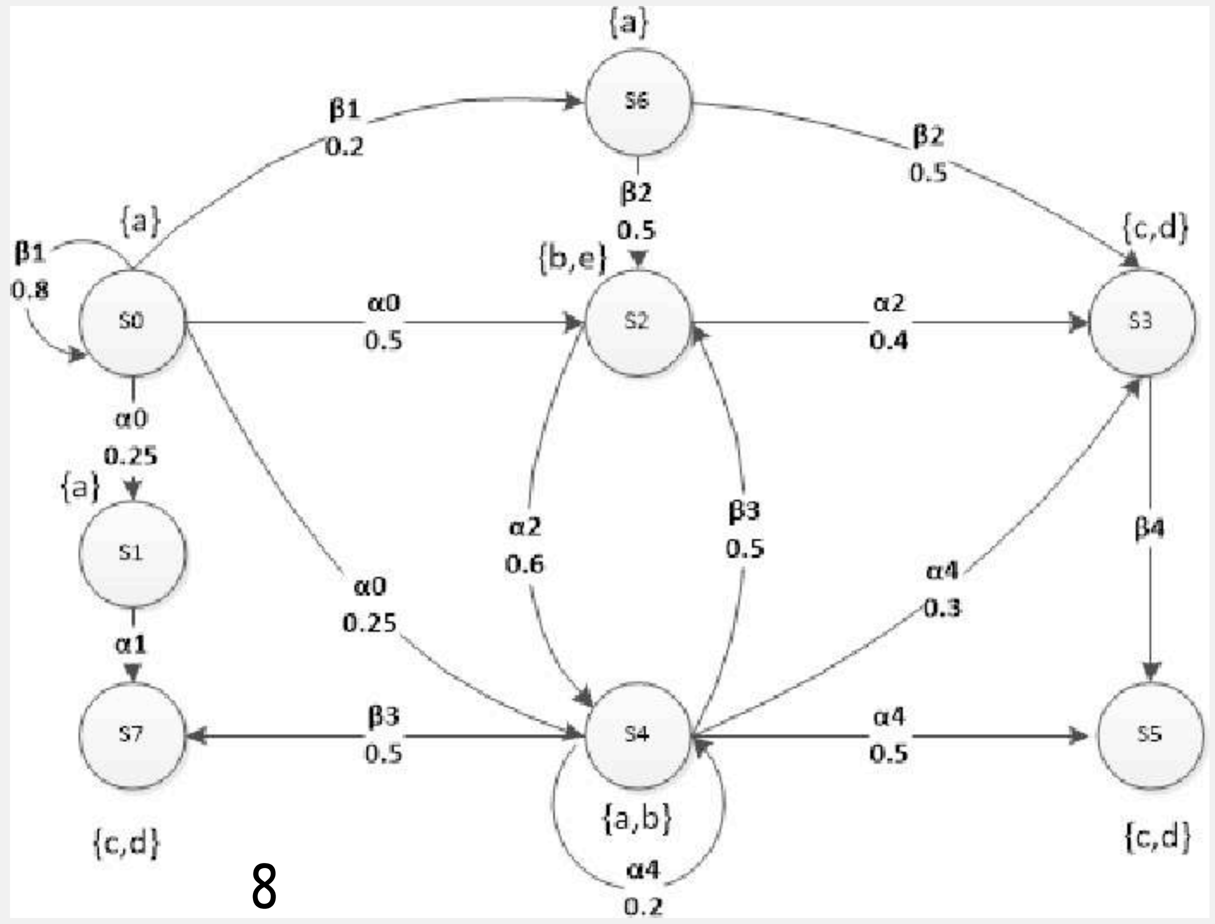
physical and virtual/numerical models

simulators: *imperative* "how"









models

$$\min \sum_{k=1}^{K} \sum_{j=1}^{n} d_{jk}$$

$$s.t.\; d_{jk} \geq \sum_{i=1}^{p} (m_j^i - y_k^i)^2 - \bar{d}_{jk}(1 - x_{jk}) \quad \forall j,k$$

$$\sum_{k=1}^{K} x_{jk} = 1 \quad \forall j$$

$$x_{jk} \in \{0,1\}, y_k^i \in \mathbb{R}, d_{jk} \geq 0$$

$$\frac{\Delta;\Gamma,\alpha}{\Delta;\Gamma,\alpha_1 \mid \Delta;\Gamma,\alpha_2}\ (\alpha\text{-}\Gamma) \qquad \frac{\Delta;\Gamma,\beta}{\Delta;\Gamma,\top \mid \Delta;\Gamma,\beta_1,\beta_2}\ (\beta\text{-}\Gamma)$$

$$\frac{\Delta;\Gamma,\neg\neg A}{\Delta;\Gamma,A}\ (\neg\neg\text{-}\Gamma) \qquad \frac{\Delta;\Gamma,A,\neg A}{\Delta;\Gamma,\top}\ (\top\text{-}\Gamma)$$

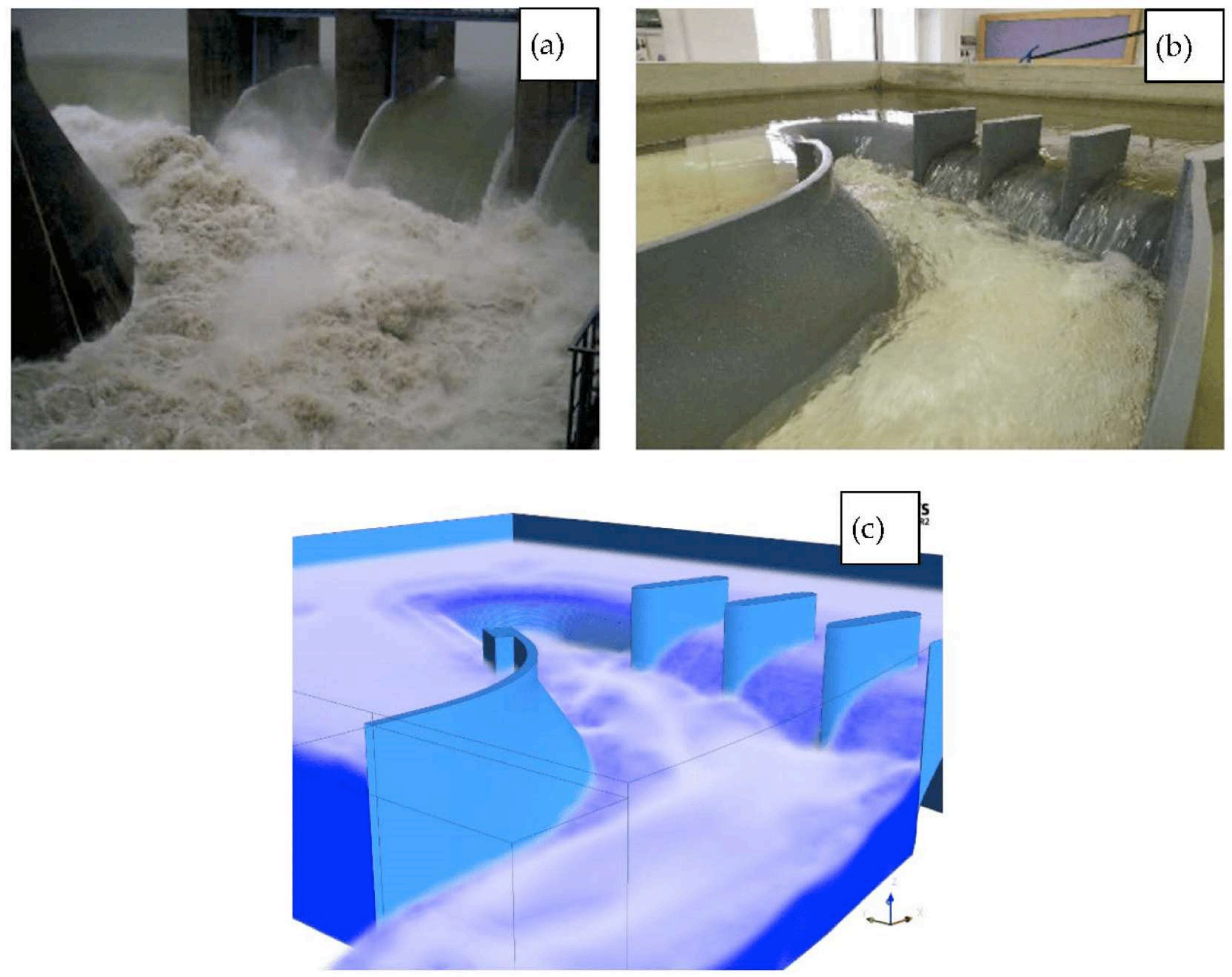
$$\frac{\Delta,\alpha;\Gamma}{\Delta,\alpha_1,\alpha_2;\Gamma}\ (\alpha\text{-}\Delta) \qquad \frac{\Delta,\beta;\Gamma}{\Delta,\beta_1;\Gamma \mid \Delta,\beta_2;\Gamma}\ (\beta\text{-}\Delta)$$

$$\frac{\Delta,A,\neg A;\Gamma}{\Delta,\blacksquare;\Gamma}\ (\blacksquare) \qquad \frac{\Delta,A;\Gamma,A}{\Delta,A;\Gamma,\top}\ (\top\text{-intr})$$

conceptual models

formulation: *declarative* "what"

models



$$\min \sum_{k=1}^{K} \sum_{j=1}^{n} d_{jk}$$

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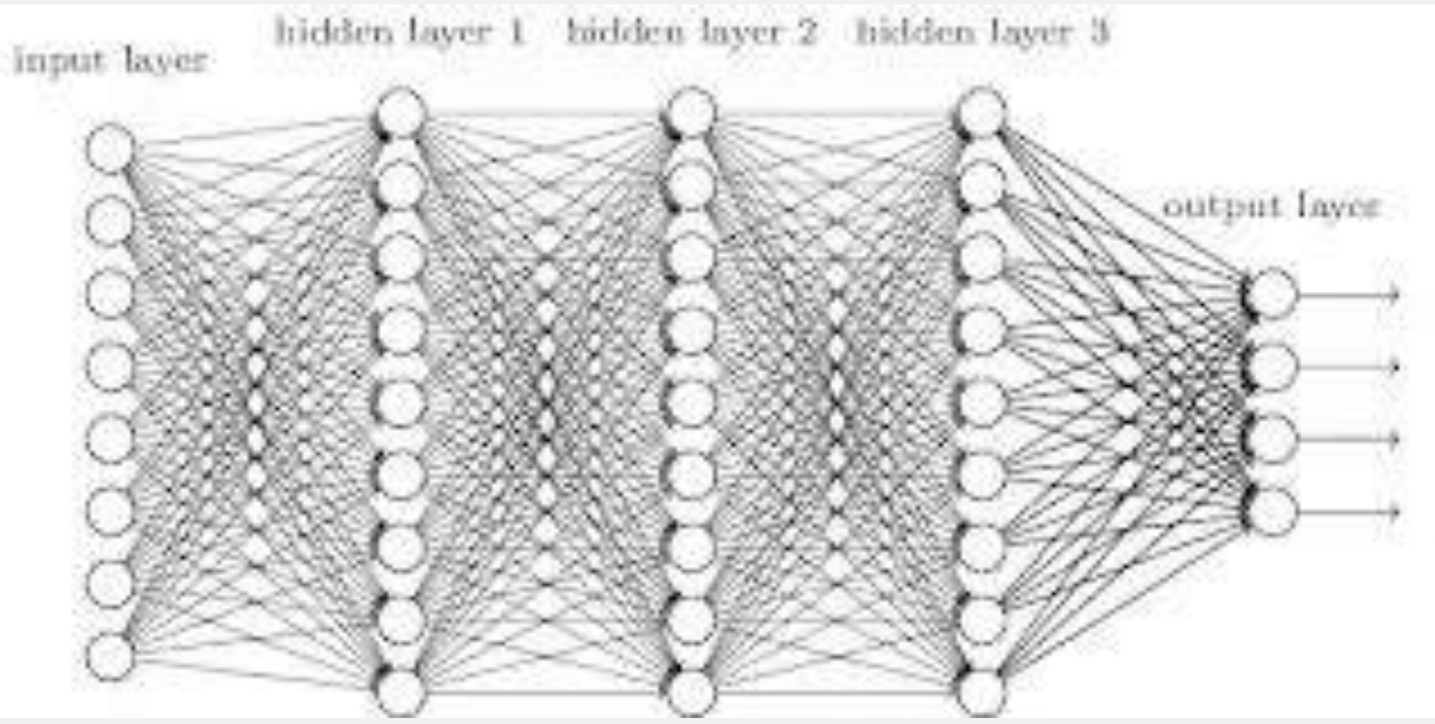
$$\sum_{k=1}^{K} x_{jk} = 1 \quad \forall j$$

$$x_{jk} \in \{0,1\}, y_k^i \in \mathbb{R}, d_{jk} \geq 0$$

built by experts
or automatically from data
(machine learning)

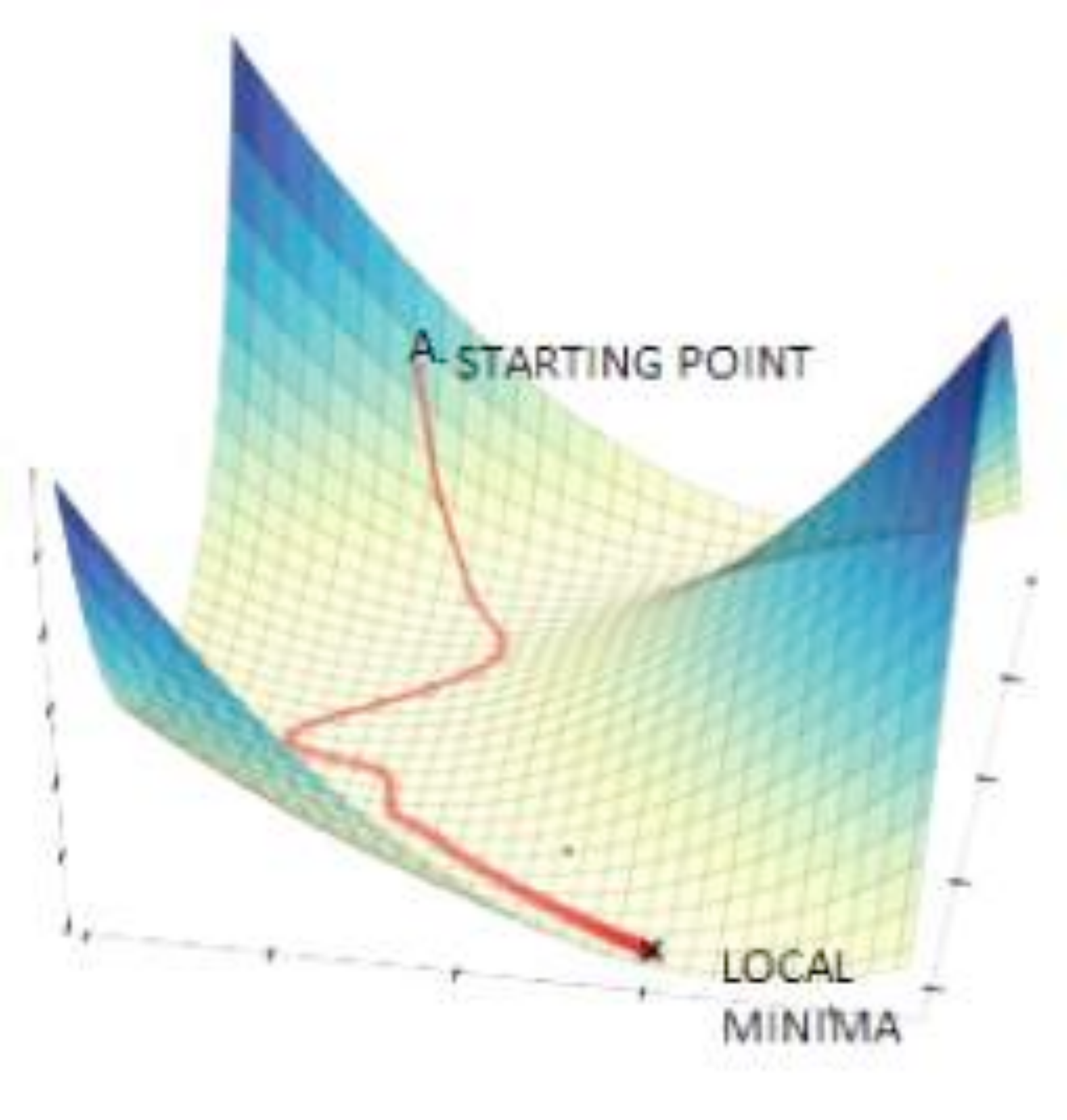
35	-50	73787	28083	1439	2240	2746	3687	5293	2740
48	101	758353	383745	201999	62107	36293	130536	57243	25354
57	-5	2E+06	129350	61236	17084	11488	62462	49960	33932
53	-8	1E+06	354328	37102	88881	45307	99603	44790	29749
66	73	2E+06	176766	59352	26157	15054	33669	33782	31750
69	130	635191	122446	90107	65072	36230	53019	62938	59307
61	-2	161098	12119	1963	809	1277	3186	3266	2518
69	17	492796	120998	63697	68242	10769	88403	73756	22676
69	-59	82048	116131	47317	26197	41642	28866	32551	41810
38	-14	757165	186196	3242	3841	18854	43021	46799	11928
48	72	667513	141854	75050	16234	45926	34496	74875	31839
34	121	165360	42119	3158	6256	7270	19462	10984	8148
30	-52	737665	84275	2235	38748	21705	28343	80927	24735
48	69	577024	179555	25937	21604	43790	44432	69203	25586
43	44	234964	80944	7991	32568	11828	63682	41013	18147
40	144	671467	133227	7142	14300	23373	65591	47860	16501
40	25	33290	14729	10980	10407	14316	37112	60378	36306
44	-138	1E+06	268122	67285	36996	10083	80826	90350	26345
53	25	756442	97387	59785	32241	16122	53157	44602	14331
66	124	87109	7200	4987	2817	2130	11413	9422	4922
53	43	802937	83858	3229	7895	27104	17791	18901	12191
51	35	157687	283941	27259	47930	15132	38238	31599	10121
50	119	613031	758257	246386	132015	26636	83848	94542	56127



optimize (black-box)

numerical methods:

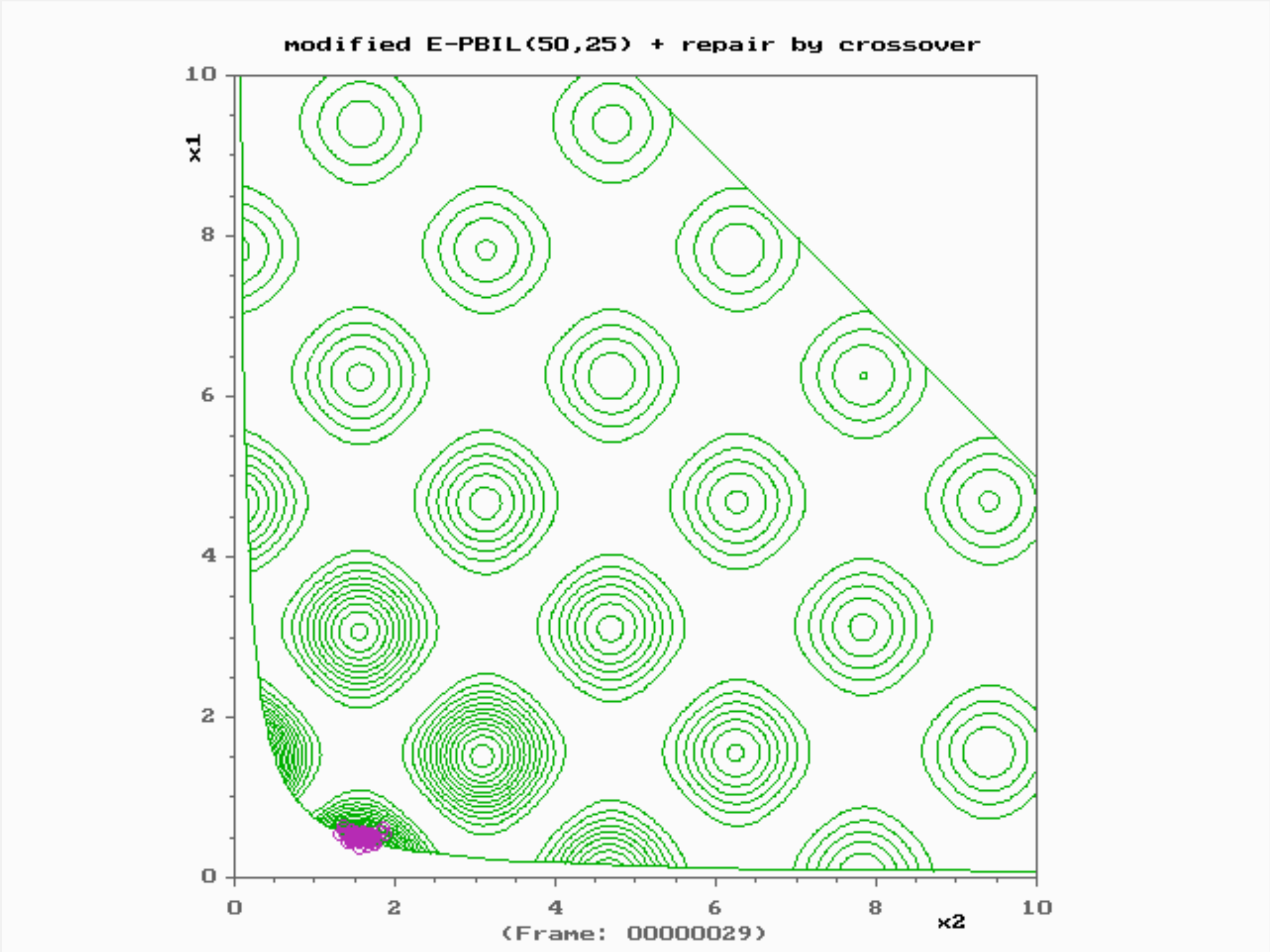
1. select a candidate decision
2. simulate/evaluate feasibility and score
3. stop or iterate

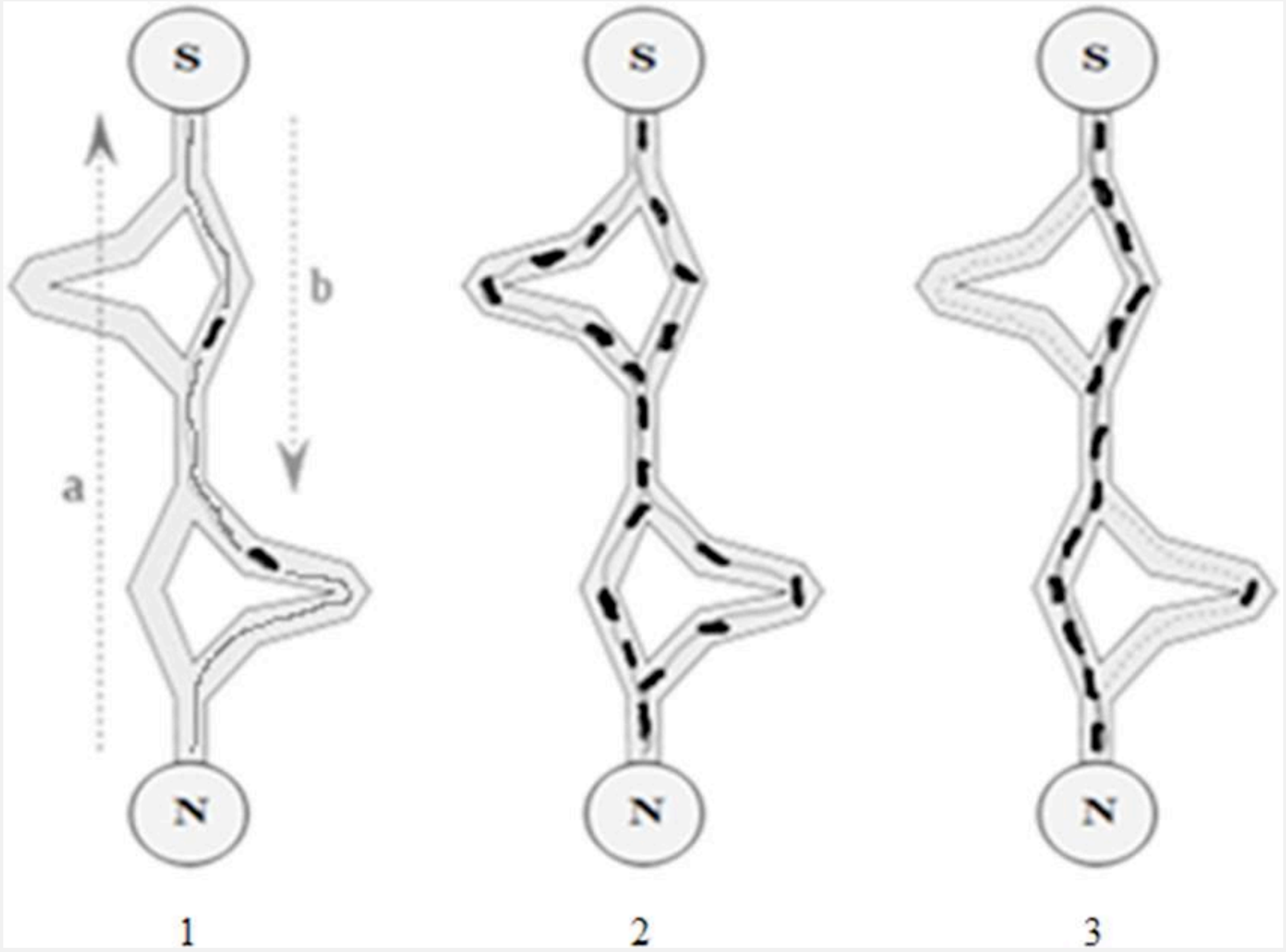


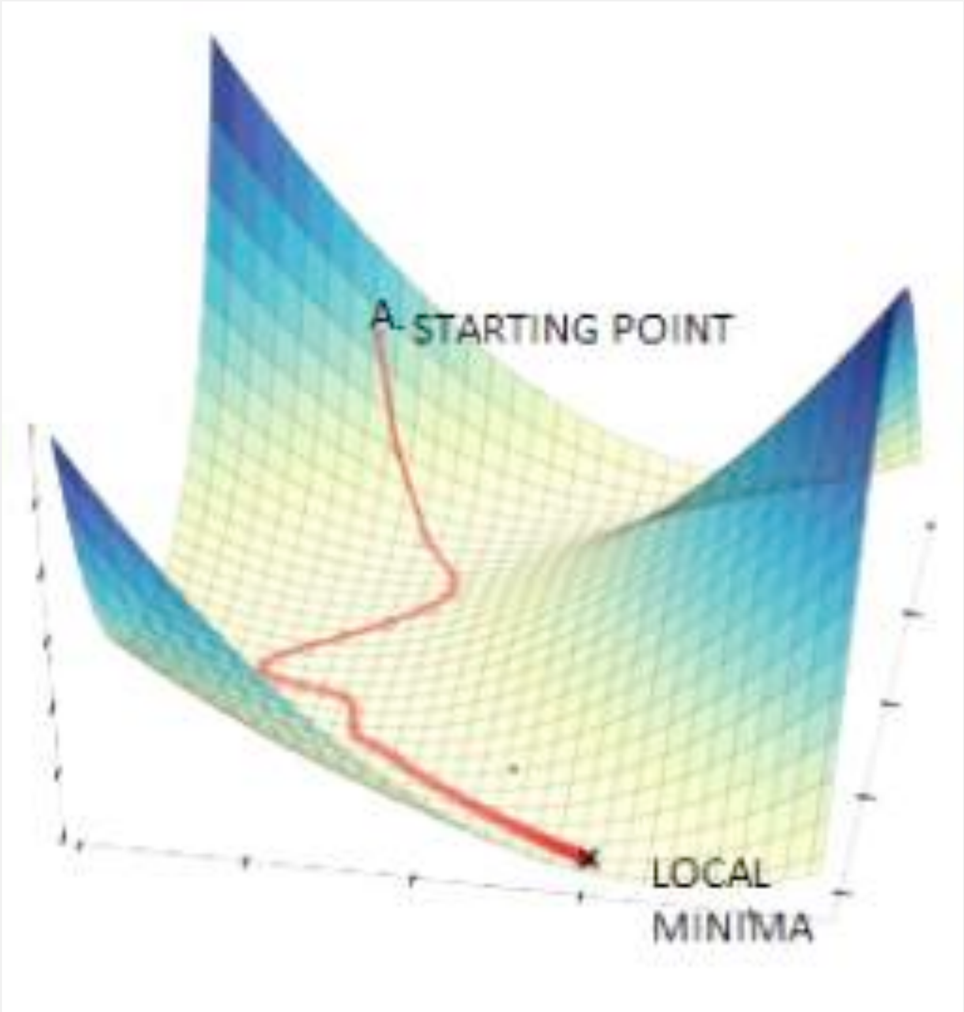
search: which candidates to evaluate ?

- partial, exhaustive, exhaustive but implicit
- random or directed by the proximity, the scores or highest-order information

optimize (black-box)







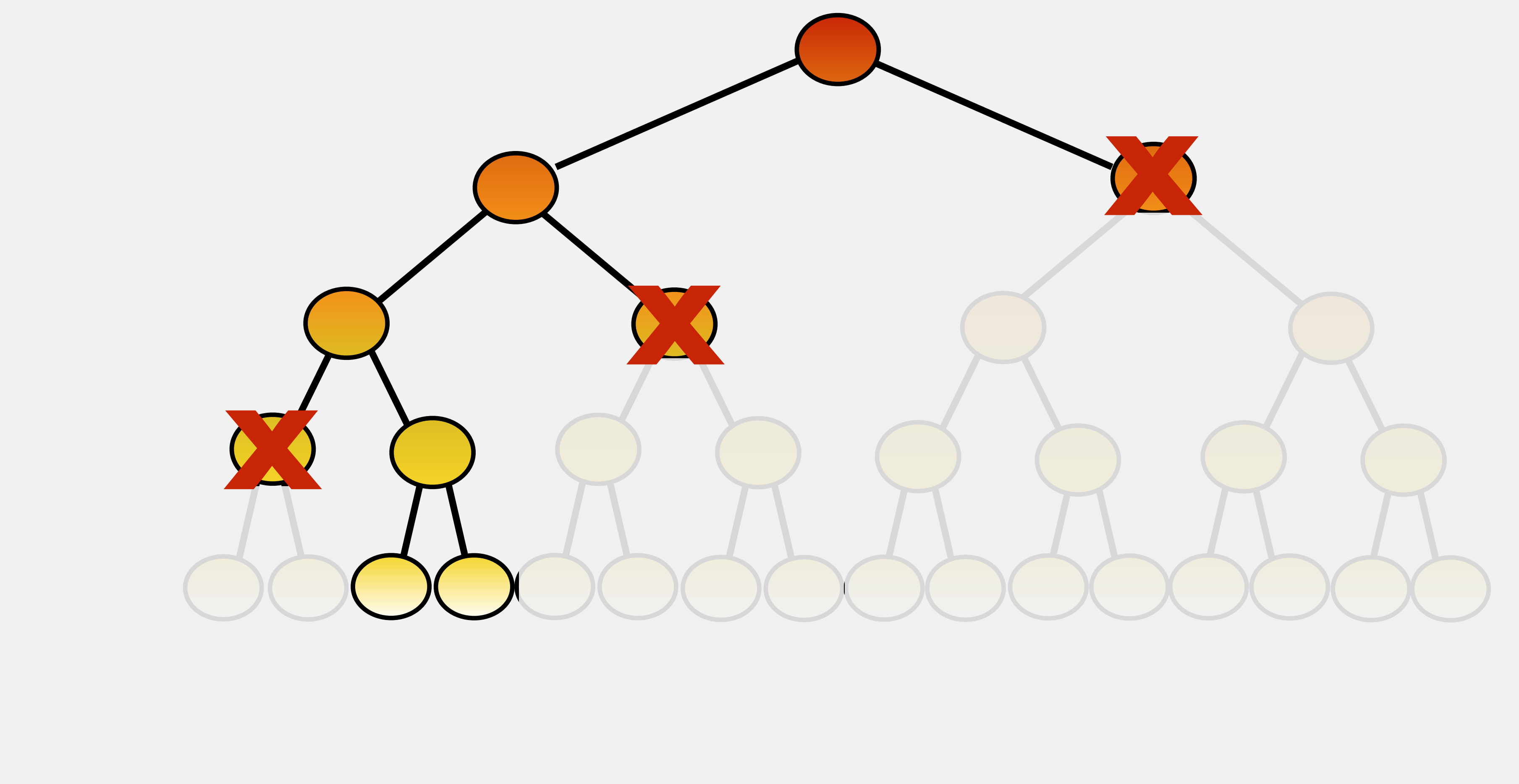
examples:

- local search: move to a neighbour candidate, the best one or in an improving direction (may converge to a global optimum, e.g. gradient descent in convex optimization, simplex algorithm in linear programming)
- metaheuristics (evolutionary, swarm): combine candidates, use collective memory

optimize (relaxation)

divide-and-conquer:

1. separate the search space (and refine the model)
2. estimate feasibility and best score in a simpler relaxed model
3. backtrack if not better, record if full solution, or iterate



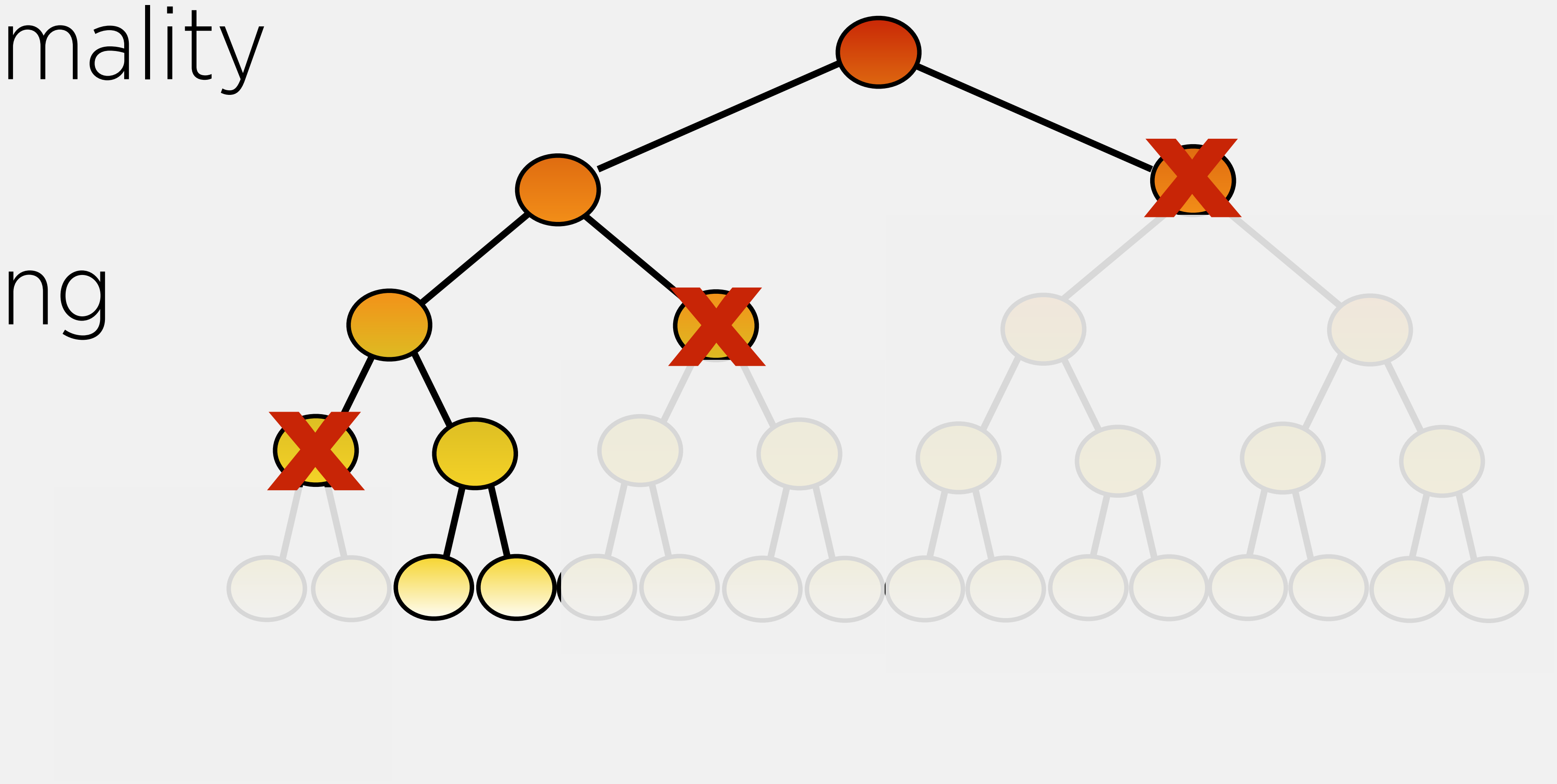
bounding the maximal score:

- certificate of optimality: gap between relaxations (UB) and full solutions (LB)
- rely on tight but simple relaxations

optimize (relaxation)

examples:

- greedy algorithm: no backtrack, no certificate of optimality
- graph algorithms, dynamic programming
- backtracking methods in logic/constraint programming
- branch-and-bound in combinatorial optimization



accuracy & approximation

Decision Making

Mathematical Optimization

$$\min_{x \in \mathbb{R}^n} f(x) \,:\, g_i(x) = 0 \;\forall i = 1,\ldots,m$$

concrete problem → abstract model

abstract model → (solve) → optimal solution

optimal solution → practical decision

solve a model not a problem

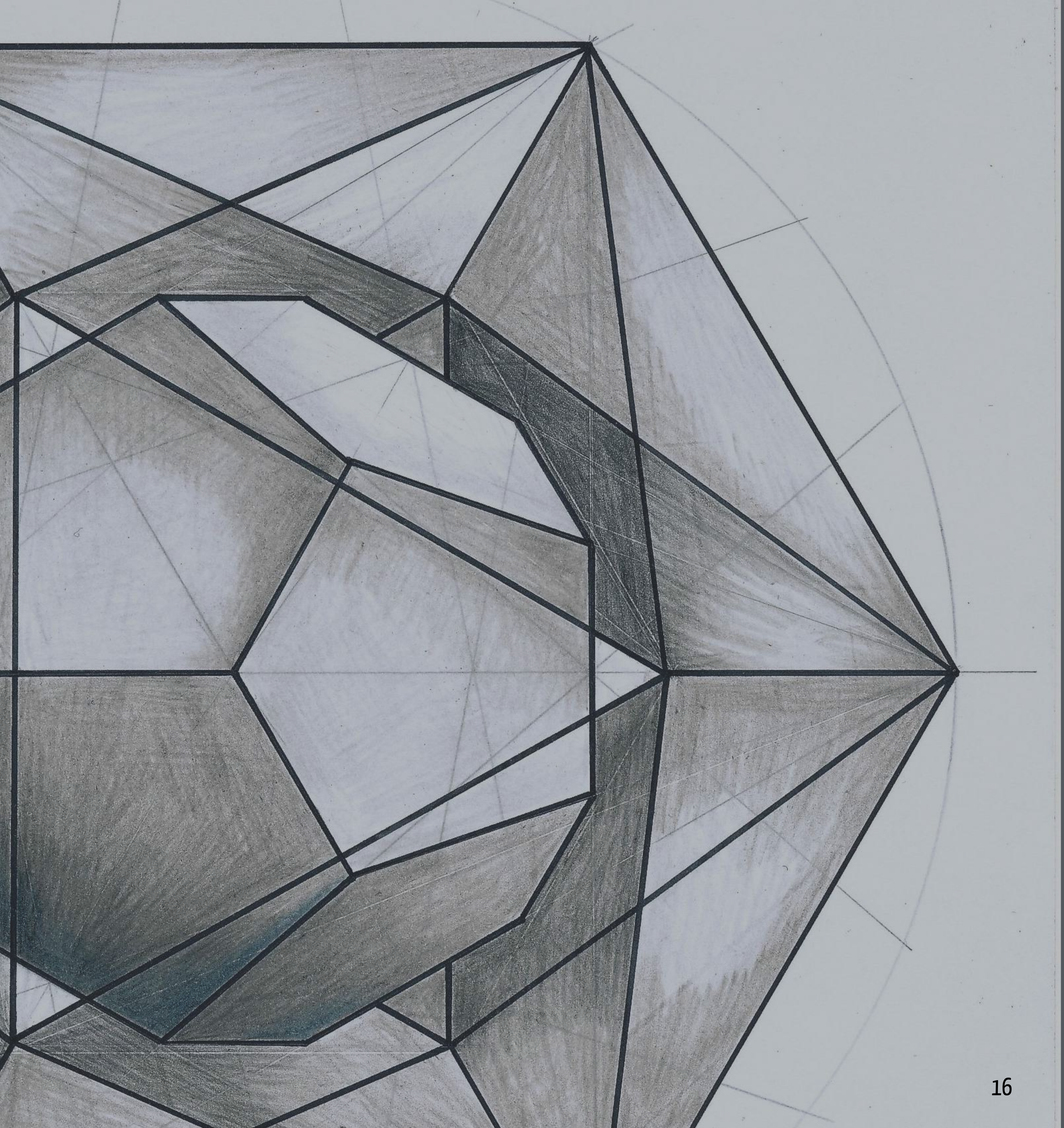
solving

solve a model not a problem

- imprecise (truncated) and uncertain (forecast) data
- approximate dynamics and simplified (soften) constraints
- conceptual objective

solve ?

- solution may be infeasible or feasible with a tolerance gap
- solution may be sub-optimal or optimal with a tolerance gap
- solution may not be provably optimal, neither globally nor locally
- theoretic complexity and convergence give no practical guarantees



mathematical optimization

mathematical program

$$\min f(x) : g(x) \leq 0,\ x \in \mathbb{Z}^p \times \mathbb{R}^{n-p}$$

$f : \mathbb{R}^n \mapsto \mathbb{R}$ objective

$g : \mathbb{R}^n \times \mathbb{R}^m \mapsto \mathbb{R}^m$ constraints

$x \in \mathbb{R}^n$ variables / solution

mathematical program

$$\min f(x) : g(x) \leq 0,\ x \in \mathbb{Z}^p \times \mathbb{R}^{n-p}$$

well-solved classes:

f, g linear $p = 0$	linear programming
f convex, $g \equiv 0, p = 0$	unconstrained optimization
f, g smooth convex $p = 0$	convex programming
f, g linear $p > 1$	mixed integer linear programming

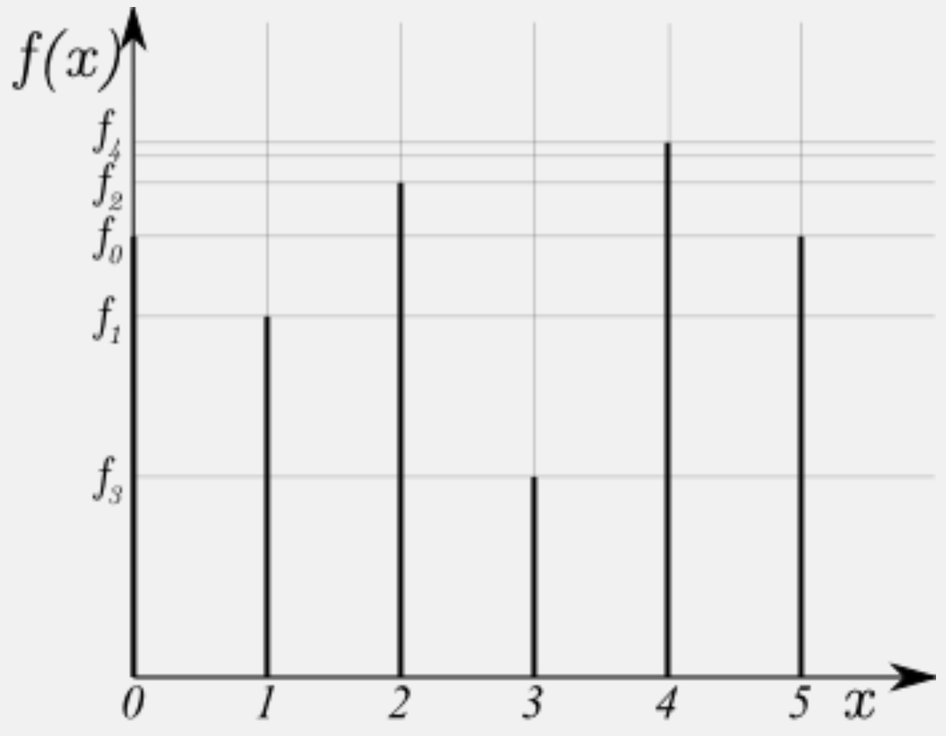
Mixed Integer Linear Program

covers discrete decisions: off/on status $x \in \{0,1\}$, operation level $l \in \{0,1,\ldots,N\}$

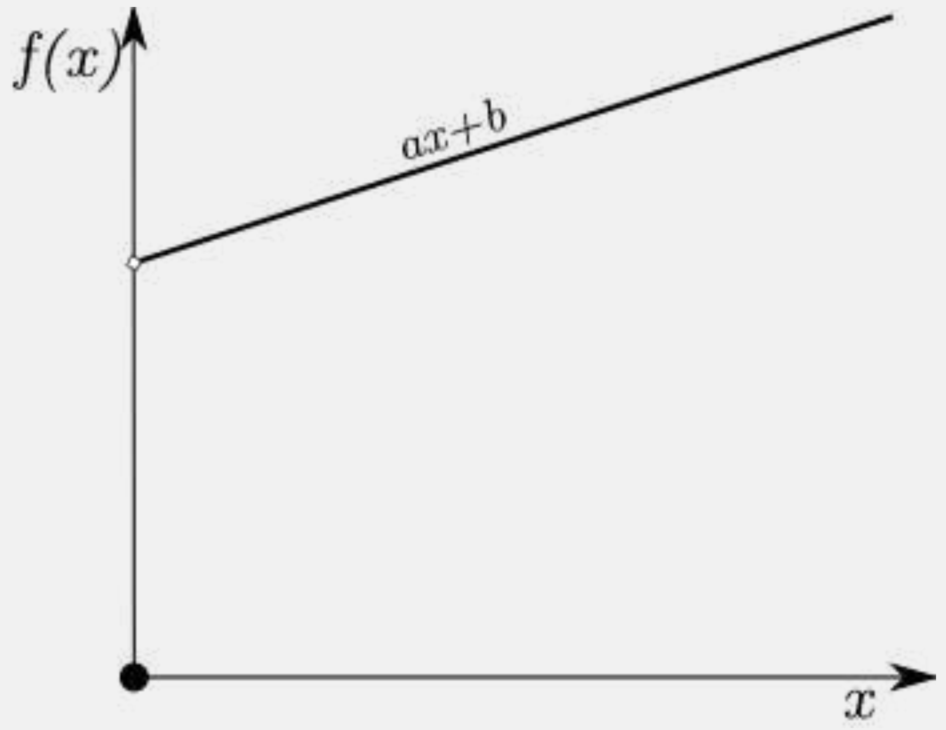
covers logical relations: $l \leq N(1-x)$ level is 0 if status is on: $x = 1 \implies l = 0$

covers nonlinear relations: $l = \sum_{i=0}^{N} i x_i,\ y = \sum_{i=0}^{N} f_i x_i,\ 1 = \sum_{i=0}^{N} x_i,\ x_i \in \{0,1\}\,\forall i \in \{0,\ldots,N\}$

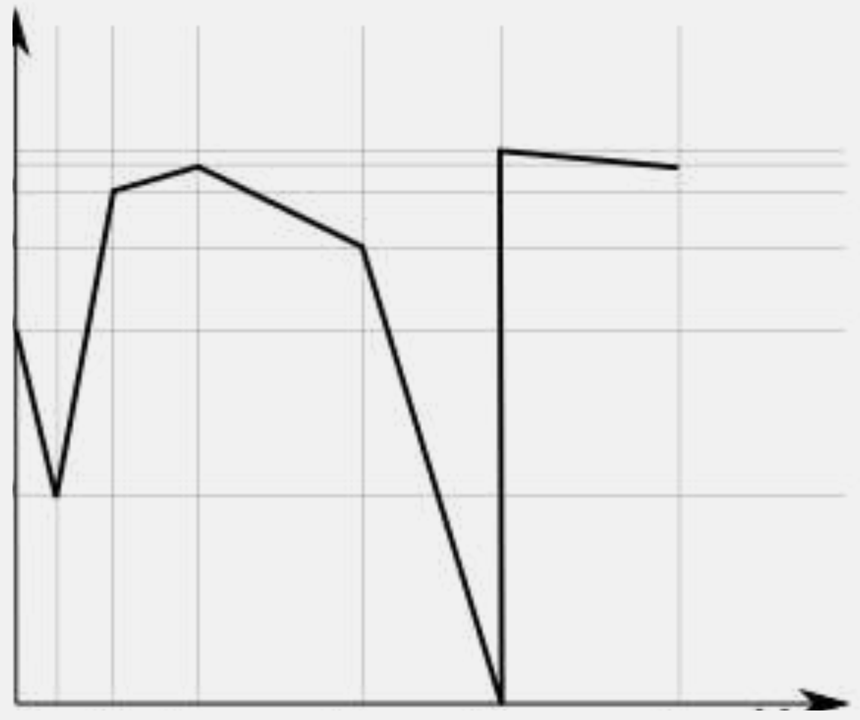
$y = f(l)$ a discrete function



discrete



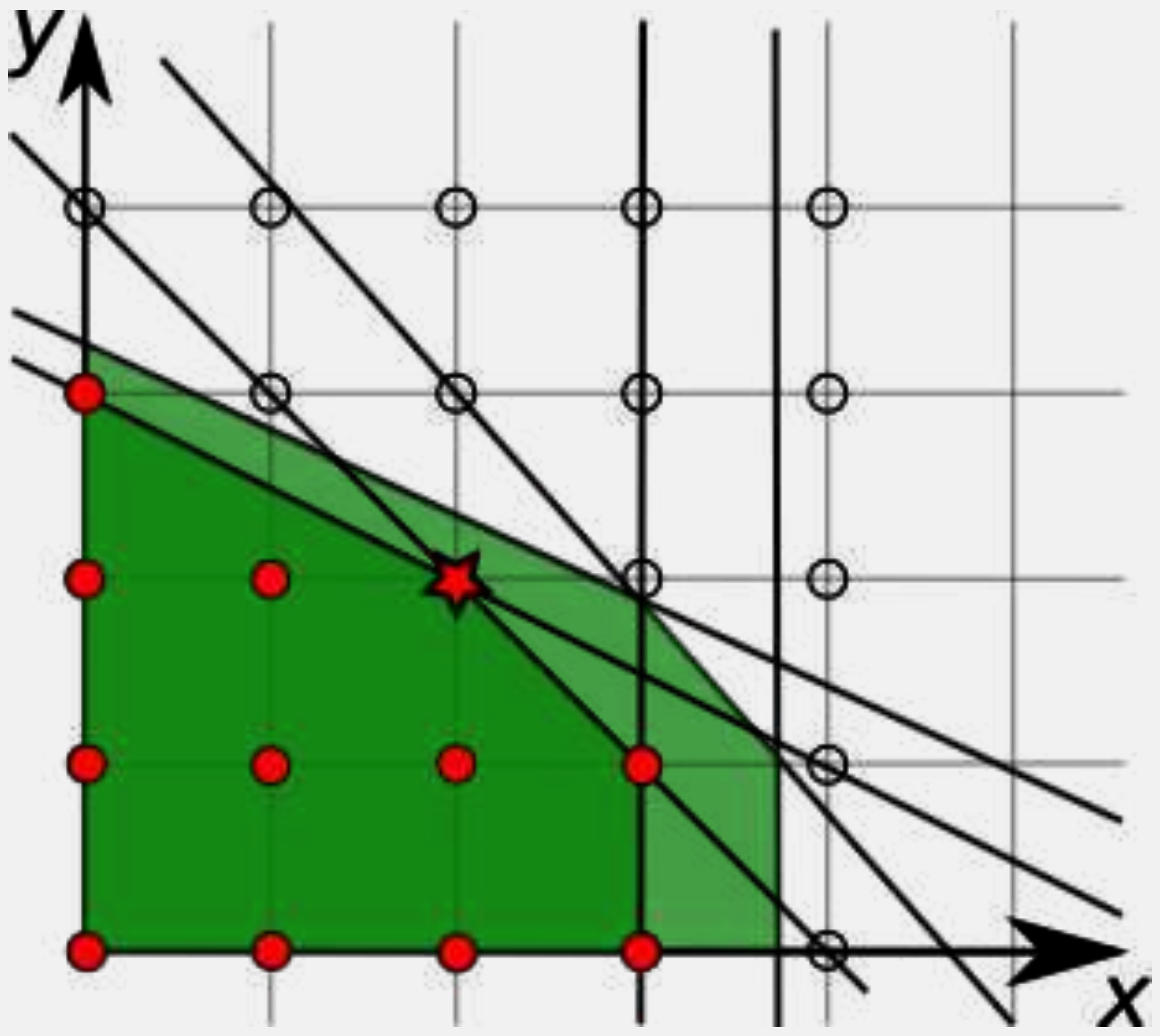
setup

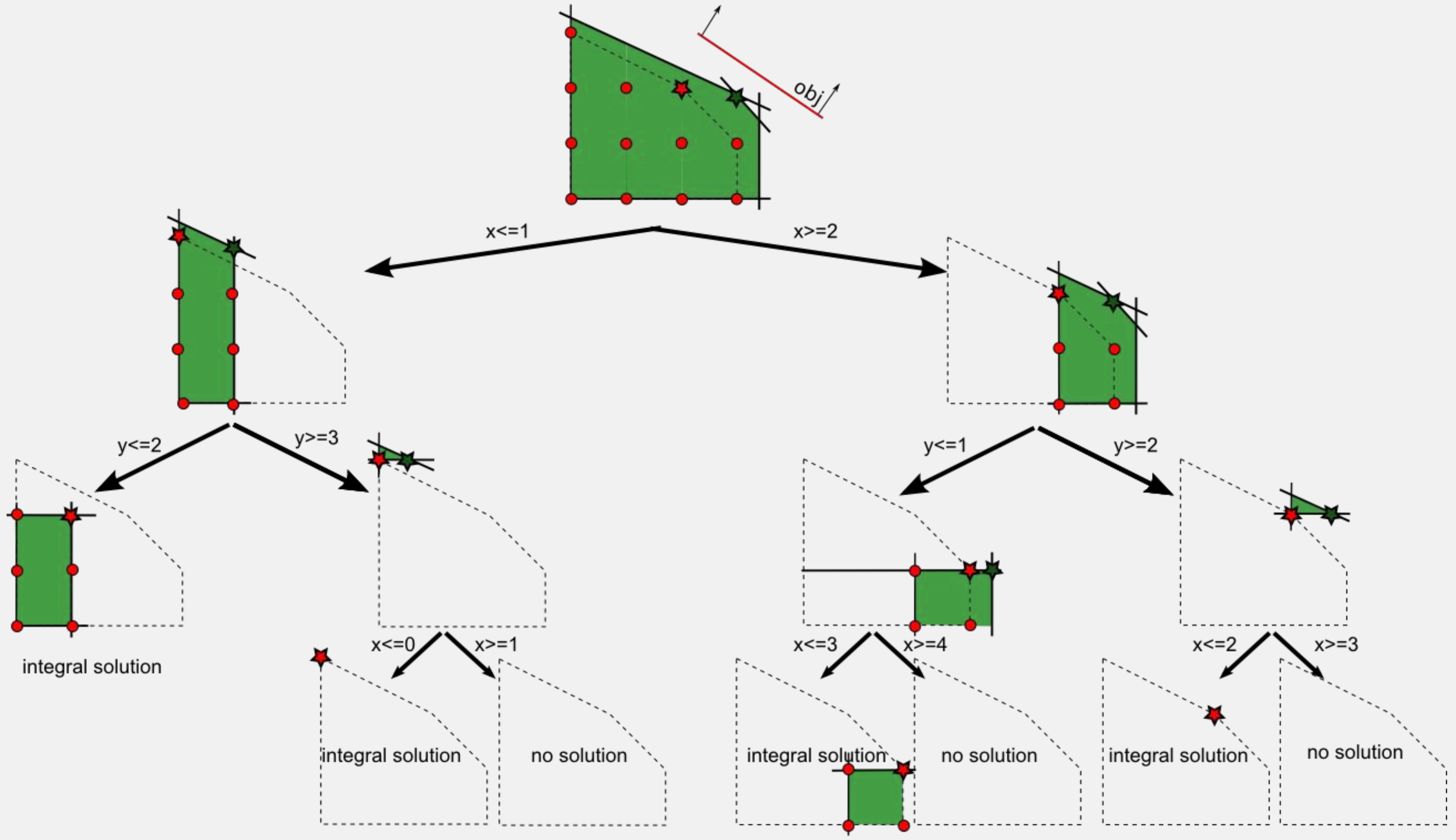

piecewise linear

MILP algorithms

cutting-plane algorithm
branch-and-bound
branch-and-cut

- based on the LP relaxation
- evaluate, refine, iterate
- separate (on discrete variables), estimate, backtrack/iterate
- refine then estimate





MILP perks

declarative
equations, not algorithms

performance
sophisticated solvers

versatile
covers logic & nonlinear

optimality
primal-dual bounds

flexible
general-purpose format & solvers

large-scale
decomposition methods

MILP perks*

declarative
equations, not algorithms
*good model ?

performance
sophisticated solvers
*still NP-hard: scale to some extent
(or consider LP)

versatile
covers logic & nonlinear
*approximation
(or consider MINLP)

optimality
primal-dual bounds

large-scale
decomposition methods
*algorithmic challenge

flexible
general-purpose format & solvers
*generic ≠ best

water optimization

water is

a commodity, a resource, an environment

drinking water
wastewater
rain, ice, surface water, ground water
fresh, brackish, saline water
irrigation water
source of hydropower (river, tide, wave)
vector of pumped-storage hydroelectricity
steam to generate heat and energy
water for cooling or cleaning
water for processing (fracking, diluting, drilling)
storms, floods, droughts, mudflows, tsunamis
subject to thermal, chemical pollution
related to climate change, climate variability
wetlands, rain forests, oceans, coasts and rivers

to process

extract,
supply,
treat,
produce,
irrigate,
desalinate,
purify,
drain,
heat,
blend,
store,
pump,
flow,
preserve,
measure,
prevent,
control

in small/large systems

urban networks
sewers
desalination plants
farms
power systems
hydropower plants
thermal plants
industries
municipalities
pumps, turbines
aquifers
drainage basins
ecosystems
world

water optimization

Operational

organize the process

select elements to operate
assign operation level
allocate resources
schedule operations
position elements

Tactical

design the system

select elements to dimension, maintain
assign dimension, equipment
plan resources and times

often discrete decisions
nonlinear physical dynamics
minimize an economic/social/ecological cost

study cases

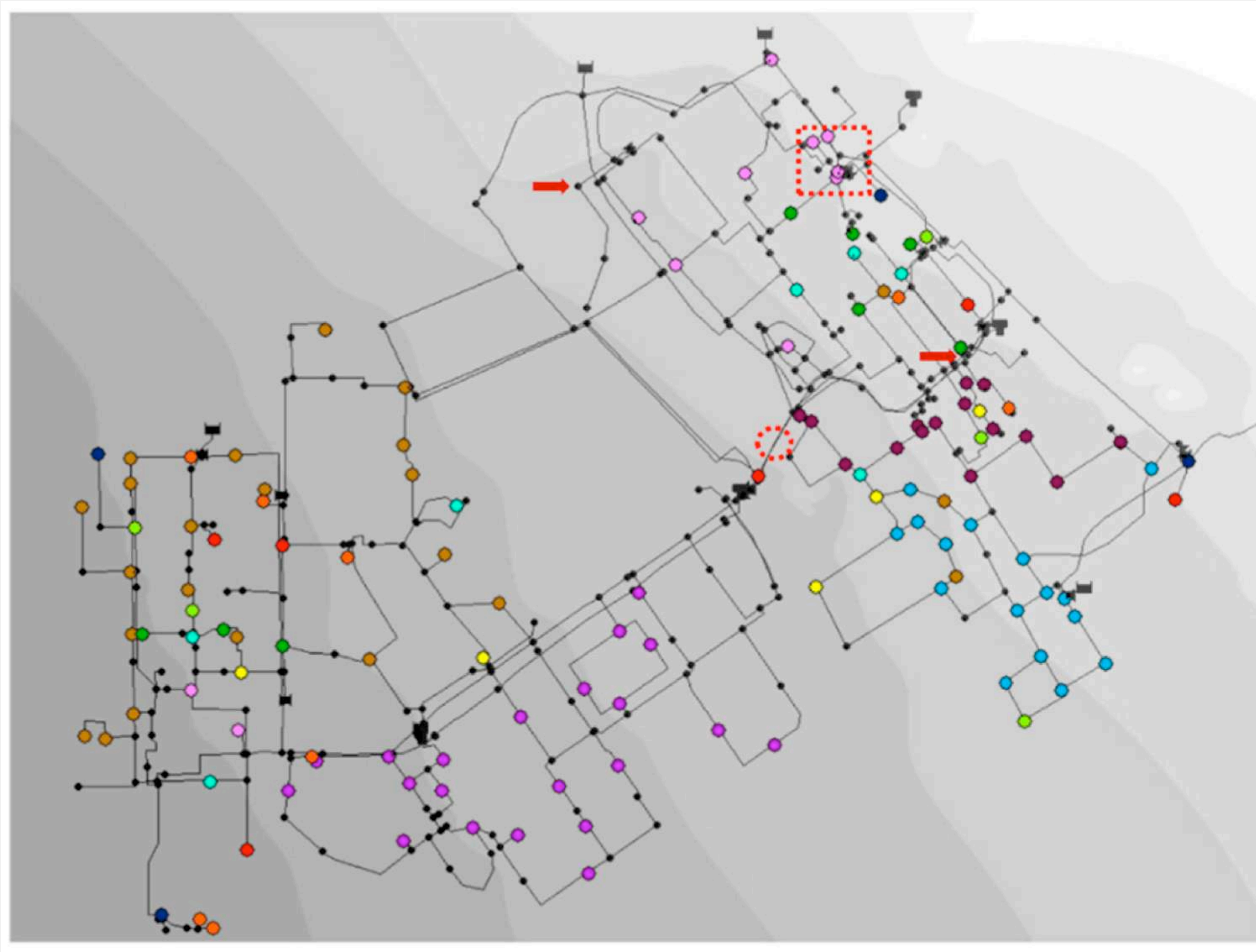
urban water networks

groundwater abstraction

hydroelectricity production

Urban networks

ex1: pipe sizing



select the size of the pipes in a gravity-fed network
to satisfy the demand at each delivery node
while minimizing the installation costs

finite catalog of pipes: size ↗ capacity ↗ cost ↗

ex1: pipe sizing

assign a size k to each pipe a: $x_{ak} = 1$ (otherwise $x_{ak} = 0$)

hydraulic equilibrium between flows q and heads h, v in the selected network

$$\min_{x,q,h} \sum_a \sum_k c_{ak} x_{ak}$$

$$\text{s.t.} \; x_{ak} = 0 \implies q_{ak} = v_{ak} = 0 \qquad \forall a \in A, k \in K$$

$$\sum_k x_{ak} = 1, h_i - h_j = \sum_k v_{ak} \qquad \forall a = (i,j) \in A$$

$$(q_{AK}, h_S) \in NAP(D_S, H_R, \phi_{AK(x)}).$$

bilevel program or
simulation-based genetic algorithm

convex MINLP or approximate MILP
+ branch-and-bound

ex1: pipe sizing

convex MINLP reformulation

$$\min_{x,q,h} \sum_a \sum_k c_{ak} x_{ak}$$

$$s.t. x_{ak} = 0 \implies q_{ak} = v_{ak} = 0 \qquad \forall a \in A, k \in K$$

$$\sum_k x_{ak} = 1, h_i - h_j = \sum_k v_{ak} \qquad \forall a = (i,j) \in A$$

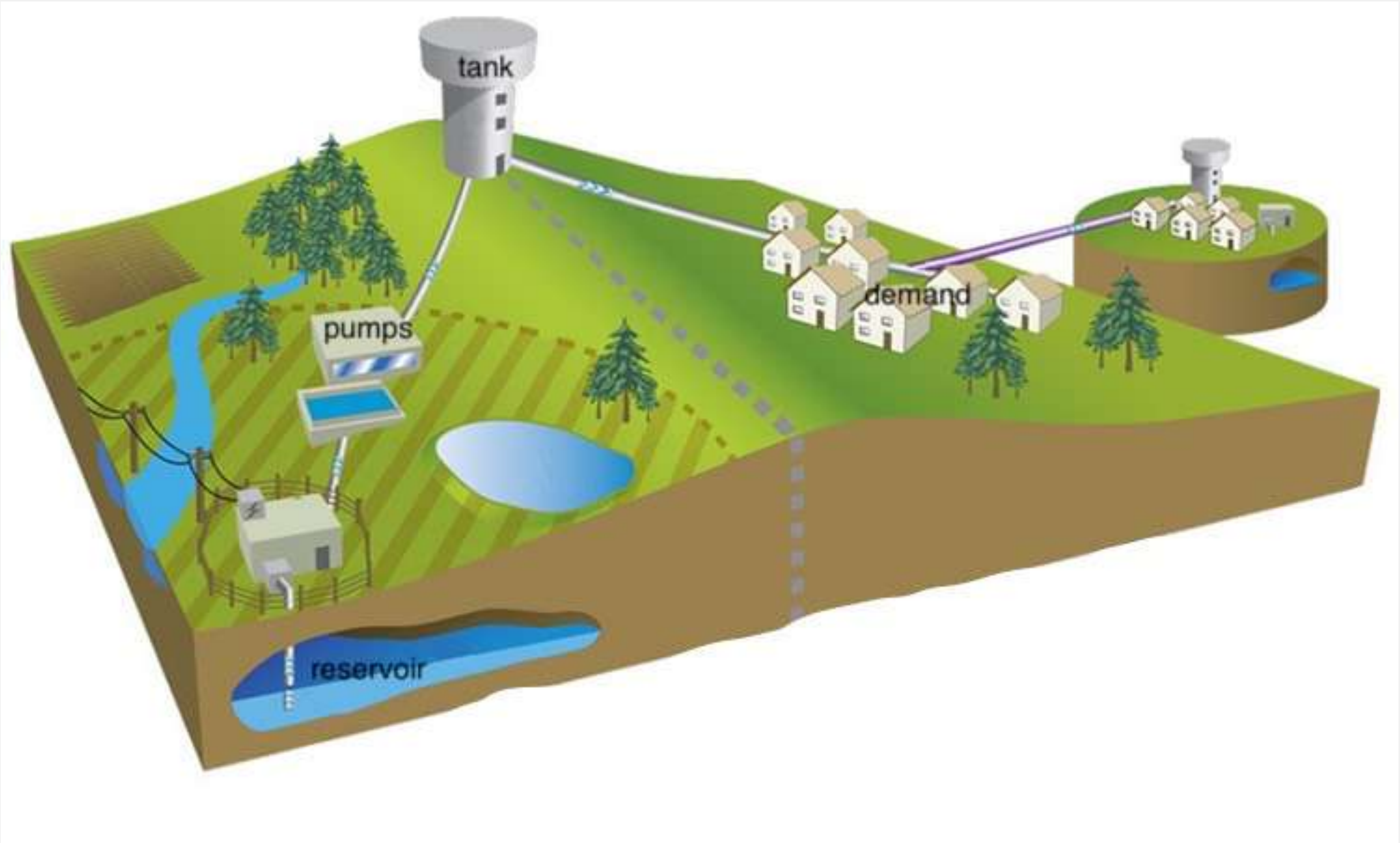
$$\sum_{ak} E_{as} q_{ak} = D_s \qquad \forall s \in S$$

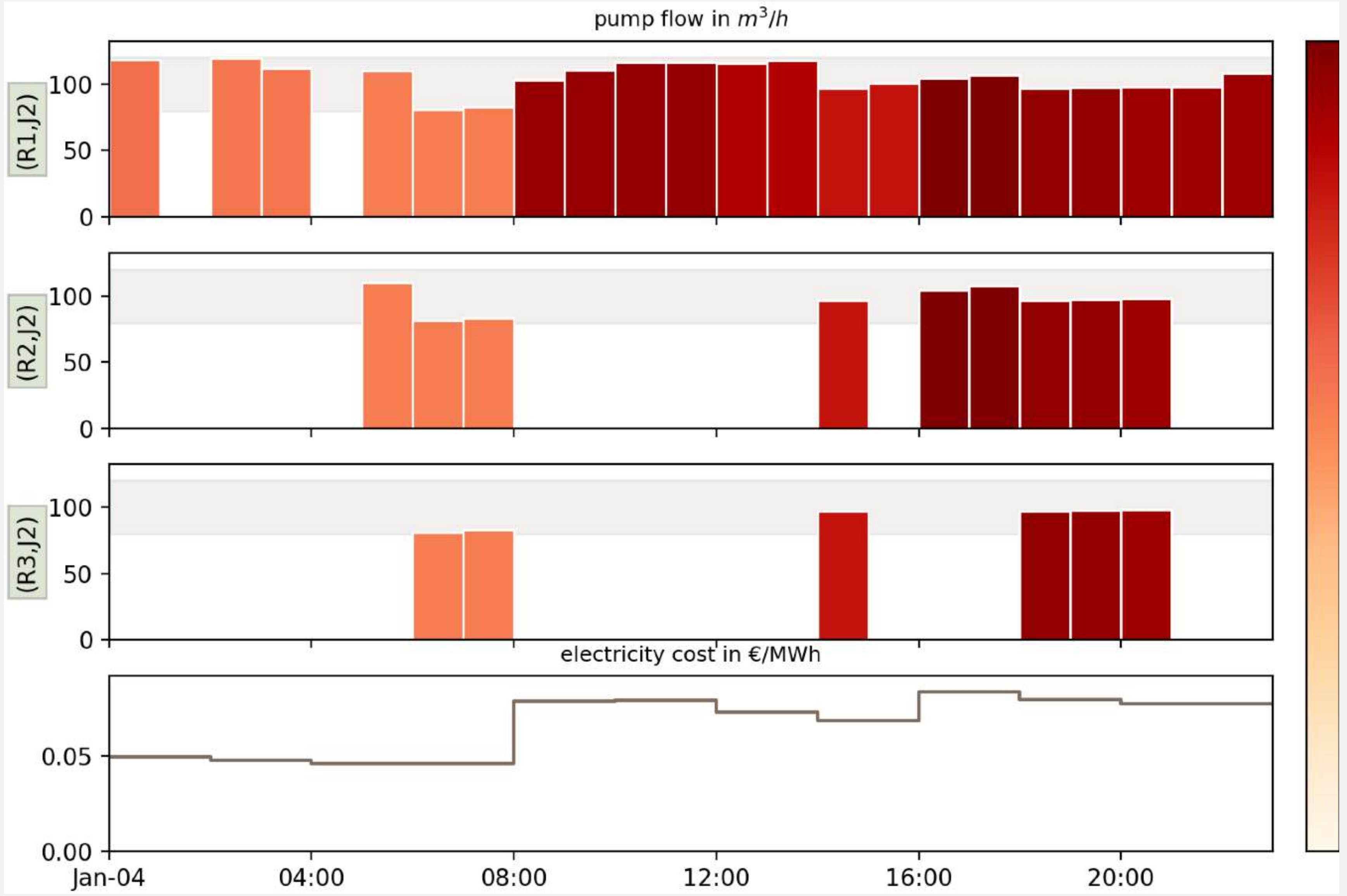
$$\sum_{ak} \left(f_{ak}(q_{ak}) + f^*_{ak}(v_{ak}) \right) + H_R^\top q_R + D_S^\top h_S \leq 0 \qquad (SD)$$

[Demassey. Strong duality reformulation for bilevel optimization over nonlinear flow networks. 2023]

ex2: pump scheduling
(load shifting in pressurized networks)

schedule pumps and valves in a pressurized network on a time horizon
to satisfy the varying demand at each delivery node
and the capacity of the water tanks
while minimizing the electricity bill





ex2: pump scheduling

activate pump/valve a at time t: $x_{at} = 1$ (otherwise $x_{at} = 0$)

hydraulic equilibrium between flows q and heads h, v in the active network

limit the water tank level H

$$
\begin{aligned}
&\min \sum_a \sum_t c^0_{at} x_{at} + c^1_{at} q_{at} \\
&s.t. (q_{At}, h_{St}) \in NAP(D_{St}, H_{Rt}, \phi_{A(x_t)}) && \forall t \in T \\
&\quad x_{at} = 0 \implies q_{at} = 0 && \forall a \in A, t \in T \\
&\quad H_{R(t+1)} = H_{Rt} + s_R^\top q_{Rt} && \forall t \in T \\
&\quad \underline{H}_{Rt} \leq H_{Rt} \leq \overline{H}_{Rt} && \forall t \in T.
\end{aligned}
$$

additional complexity: temporal inter-dependency

[Demassey Strong duality reformulation for bilevel optimization over nonlinear flow networks. 2023]

water network optimization

(drinking, waste, irrigation)

decisions

dimension
renovation
extension
sectorization
scheduling operations
scheduling maintenance
place equipments and controllers
calibrate hydraulic models

concerns

demand: standard, worst-case, emerg
network topology
energy consumption
leakage, over-pressure
flow conservation
pressure-flow relation
chlorine consumption
water quality, treatment
storage capacity
resilience to failures or storms
sewer overflow

[Bello, et al. Solving Management Problems in Water Distribution Networks: A Survey of Approaches and Mathematical Models. Water 2019]

[Mala-Jetmarova, Sultanova, Savic. Lost in Optimisation of Water Distribution Systems? A Literature Review of System Design. Water 2018]

Groundwater

credit: nasa.gov

ex3: sustainable abstraction

place pumps and plan pumping
to prevent aquifer depletion (then land subsidence or seawater intrusion)
and quality degradation (temperature, salinity)
while maximizing the abstraction value

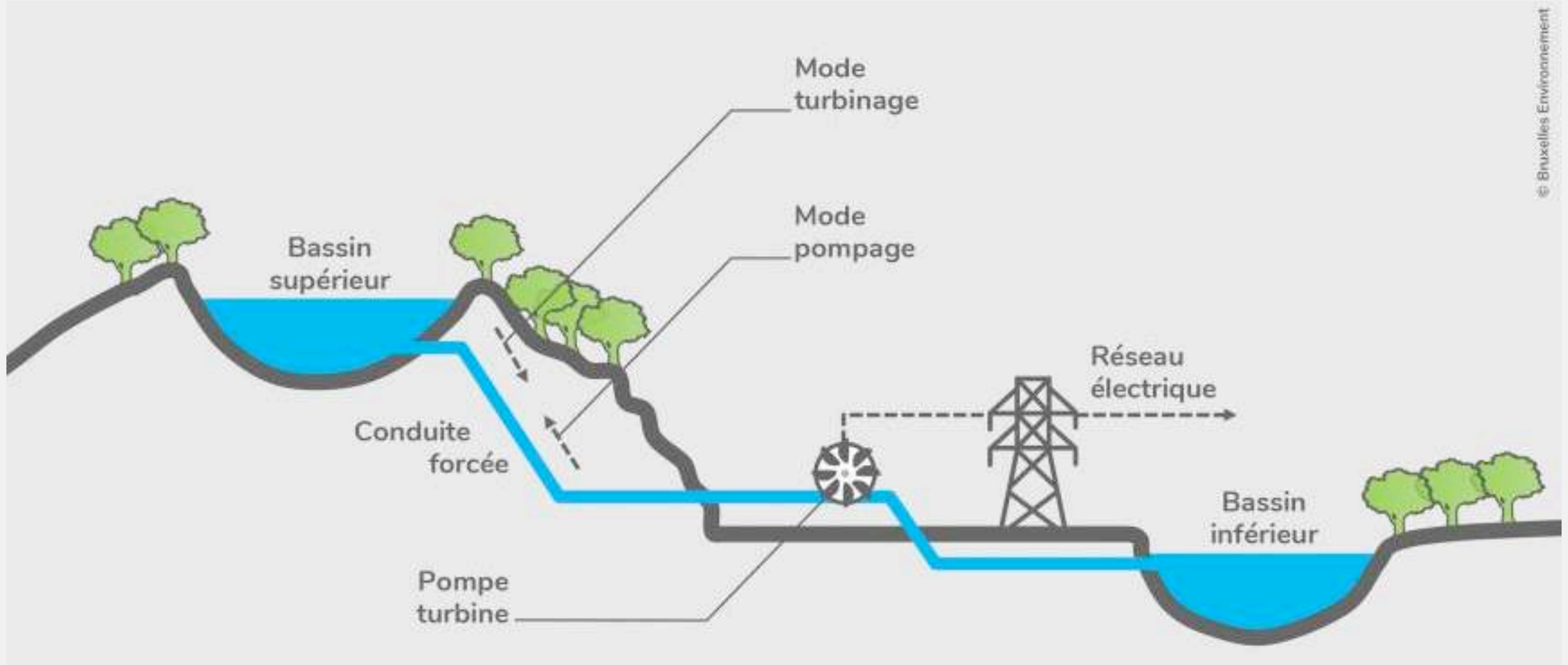
strong uncertainties (aquifer recharge rate), approximate dynamics(quality) and sustainability models

[Hassan et al. Mapping the optimization of groundwater abstraction research: A bibliometric review in the context of South Asian region. Heliyon 2023]

Hydropower

ex4: hydro unit commitment

schedule pumps and turbine
to ensure flow conservation
and maintain reservoir level in their limits
w.r.t strategic constraints (load balance, ramp, irrigation)
while maximizing the power production value



(lagrangian) subproblem of day-to-day unit commitment encompassing national power systems

ex4: hydro unit commitment

flow q_{it}, volume v_{it}, power production/consumption p_{it} in plant i at time t

nonlinear flow-power relation ϕ (turbine), disjunctive flow domains

volume conservation and limits in reservoirs

$$\max \sum_{i \in I} \sum_{t \in T} \lambda_{it} p_{it} \quad (1)$$

$$p_{it} = \Phi(q_{it}, v_{it}) \quad \forall t, \forall i \quad (2)$$

$$v_{it} = v_{i(t-1)} + I_{it} + \Delta T\Big(-q_{it} + \sum_{r \in I_i^+} q_{r(t-1)} - \sum_{r \in I_i^-} q_{r(t-1)}\Big) \quad \forall t, \forall i \quad (3)$$

$$q_{it} \in \{Q_i^-\} \cup \{0\} \cup [\underline{Q}_i, \overline{Q}_i] \quad \forall t, \forall i \quad (4)$$

$$\underline{V}_i \le v_{it} \le \overline{V}_i \quad \forall t, \forall i \quad (5)$$

[Taktak & d'Ambrosio. An overview on mathematical programming approaches for the deterministic unit commitment problem in hydro valleys. Energy Sys 2017]

conclusion

- huge diversity of water systems & processes
- management involves decision involves optimization, e.g. maximize sustainability
- mathematical optimization as a low-tech solution (except computation and data acquisition) to get as much out of existing investments
- uncertain forecasts, intricated systems, nonlinear dynamics, fuzzy objectives: trade-off between accurate models and efficient algorithms

and next

- modelling sustainability accurately
- short/long-term model coupling: time-scale reconciliation to shed light on the plausibility of prospective pathways