

ORF522 – Linear and Nonlinear Optimization

22. Data-driven algorithms

Ed forum

- Updated proof of spacial branch and bound convergence to clarify last step.
- Although on slide 15 we assume that lower bound L is non-decreasing, what if after a new refinement and a new relaxation process at step $k+1$, our new lower bound $L^{k+1} \leq L^k$? Does this happen in applications? If it happens, do we keep the new one (L^{k+1}) or do we keep the "better" one (L^k).

$$L = \min_i \{L_i\} \quad \rightarrow \quad L_i \geq L^{k-1}$$

Today's lecture

[Machine Learning for Combinatorial Optimization: a Methodological Tour d'Horizon, Bengio, Lodi, Prouvost]

[The Voice of Optimization, Bertsimas and Stellato]

[Online Mixed-Integer Optimization in Milliseconds, Bertsimas and Stellato]

[On learning and branching: a survey, Lodi and Zarpellon]

Data-driven algorithms (research topics)

- Machine learning
- Learning heuristics in branch and bound algorithms
- Learning strategies for parametric optimization
 - Strategies definition
 - Learning and sampling the strategies
 - Examples

Methods for nonconvex optimization

Convex optimization algorithms: global and typically fast

Nonconvex optimization algorithms: must give up one, global or fast

- **Local methods: fast but not global**
Need not find a global (or even feasible) solution.
They cannot certify global optimality because KKT conditions are not sufficient.
- **Global methods: global but often slow**
They find a global solution and certify it.

Data to the rescue!

Nonconvex optimization is hard

Many algorithmic
choices inside solvers

Lots of data available
from experience



**Can we use machine learning to
build better algorithms?**

Similar problems

- In practice, we solve many **similar problems with varying data**
- Most solvers do not exploit it
- We will consider families of similar problems



Machine learning

Imitation learning

Machine Learning



- Discover patterns
- Understand structure

Minimize expected loss

$$\underset{w}{\text{minimize}} \quad \mathbf{E}_{X,Y \in \mathcal{P}} \ell(Y, f_w(X))$$

f_w : model
 w : parameters

Imitation learning

Machine Learning



- Discover patterns
- Understand structure

Minimize expected loss

$$\underset{w}{\text{minimize}} \quad \mathbf{E}_{X,Y \in \mathcal{P}} \ell(Y, f_w(X))$$

f_w : model
 w : parameters



(we do not know \mathcal{P})

Training data

$$\mathcal{D}_{\text{train}} = \{(x_i, y_i)\}_{i=1}^N$$

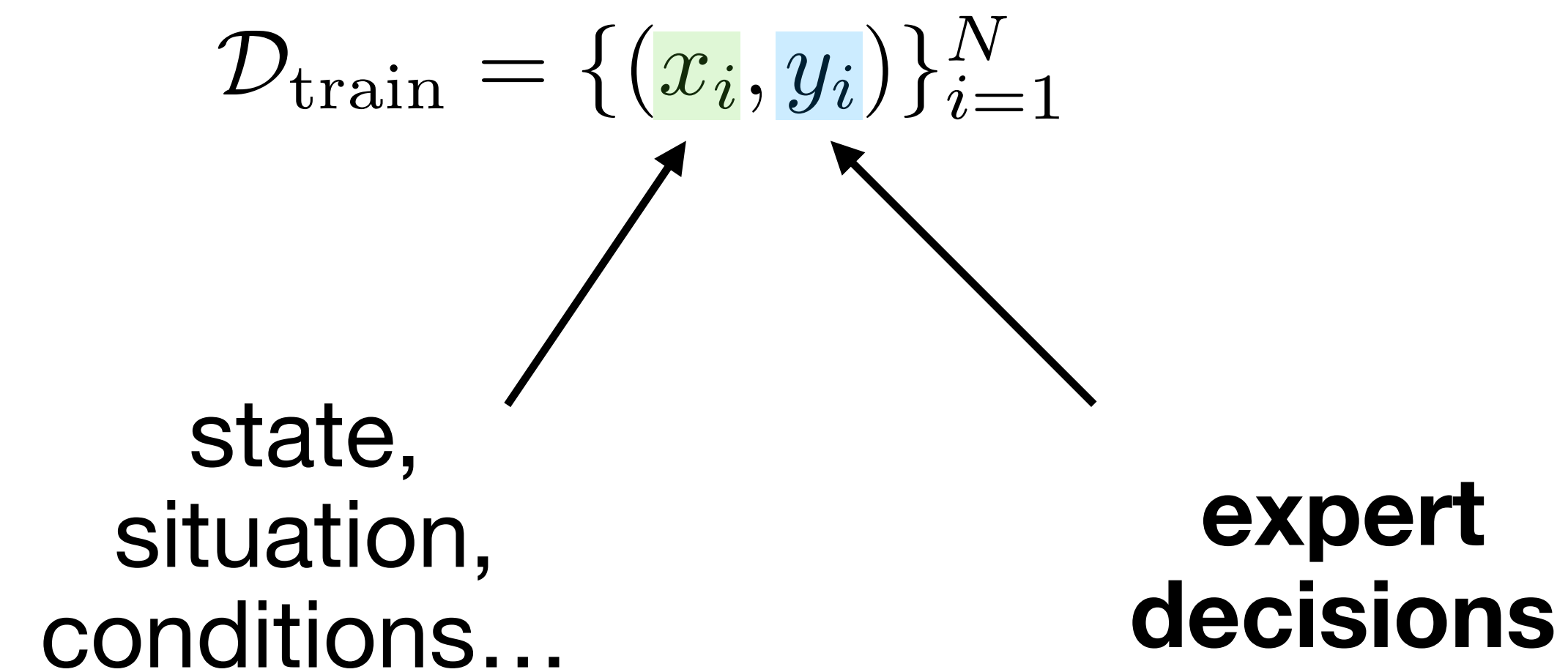


Empirical probability

$$\underset{w}{\text{minimize}} \quad \sum_{i=1}^N \ell(y_i, f_w(x_i))$$

Learning algorithmic decisions

Learning from demonstrations

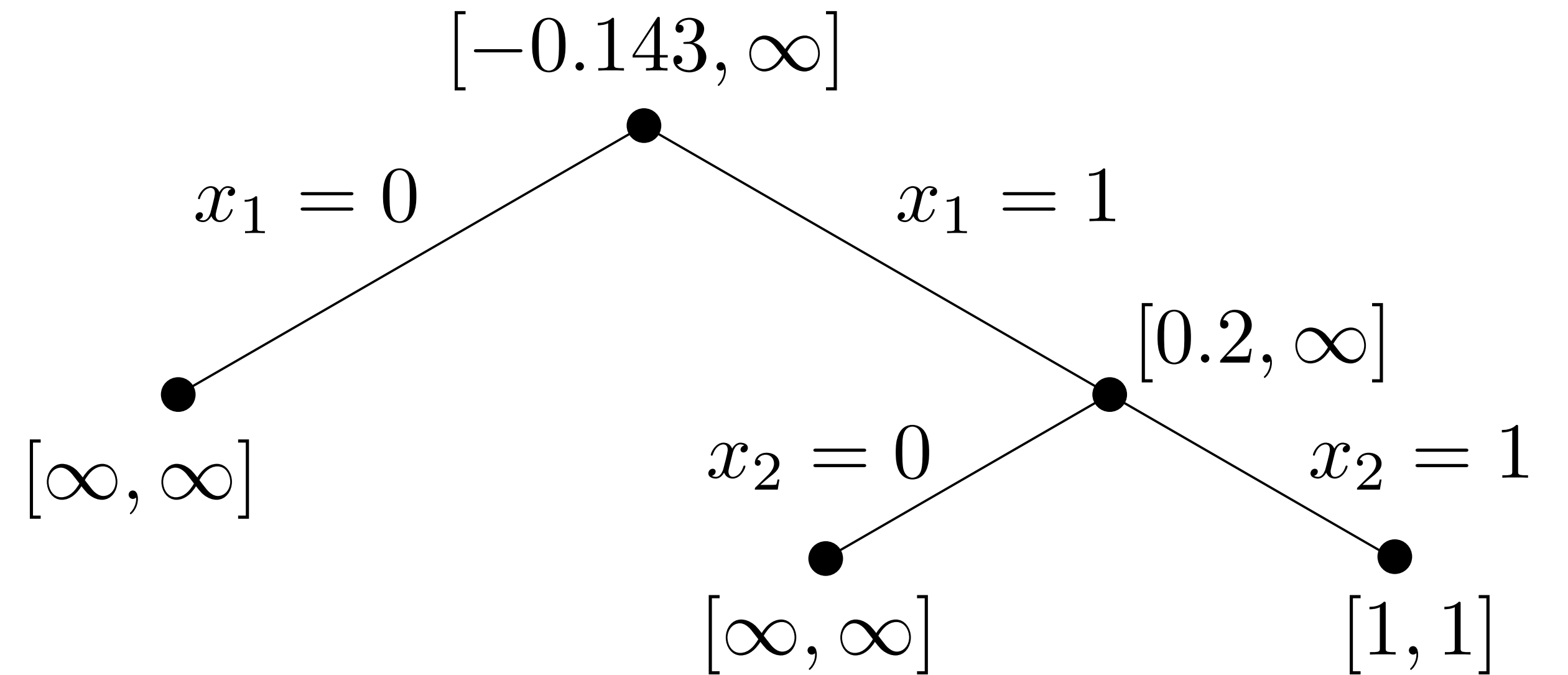


Goal: mimic expert decisions as closely as possible

Learning heuristics in branch and bound algorithms

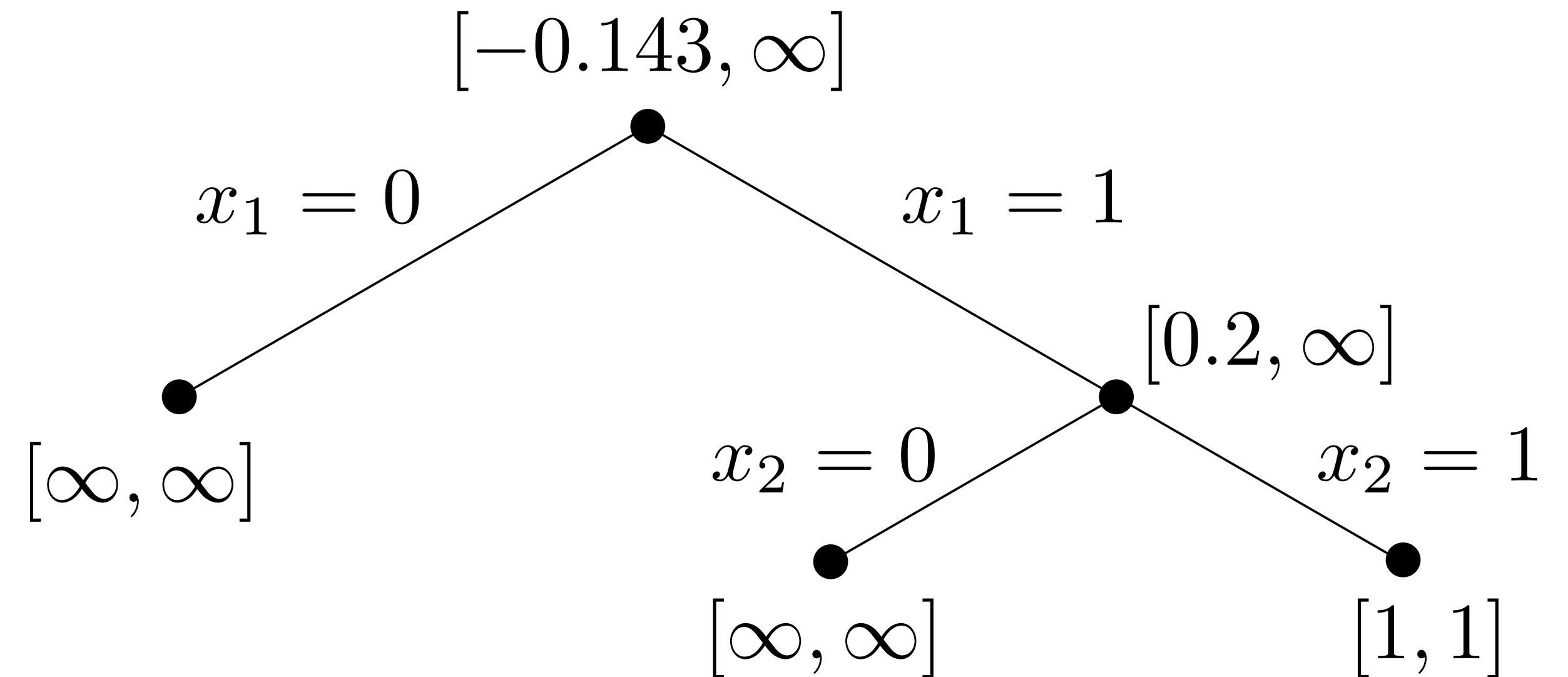
Branch and bound for integer optimization

minimize $c^T x$
subject to $Ax \leq b$
 $x \in \{0, 1\}^n$



Branch and bound for integer optimization

$$\begin{array}{ll}\text{minimize} & c^T x \\ \text{subject to} & Ax \leq b \\ & x \in \{0, 1\}^n\end{array}$$



1. **Branch:** pick node i and index k
form subproblems for $x_k = 0$ and $x_k = 1$

2. **Bound:**

- Compute **lower** and **upper bounds**
- Update global lower bounds on $f(x^*)$

$$L = \min_i \{L_i\}, \quad U = \min_i \{U_i\}$$

3. If $U - L \leq \epsilon$, **break**

Branch and bound decisions

Node selection: which node i ?

- best-first: node with smallest lower bound
- depth-first: node with greatest depth

Branch and bound decisions

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Variable selection: which fractional variable k ?

- “least ambivalent”: $x_k^* \approx 0$ or 1
- “most ambivalent”: $|x_k^* - 1/2|$ is minimum

Branch and bound decisions

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Heuristic selection: which upper bound algorithm? when?

- Rounding
- Randomization
- Neighborhood search

$$x_k = 0.6 \leftarrow$$

$$L_i > 0$$

Branch and bound decisions

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**Can we learn better
heuristics
from data?**

Heuristic selection: which upper bound algorithm? when?

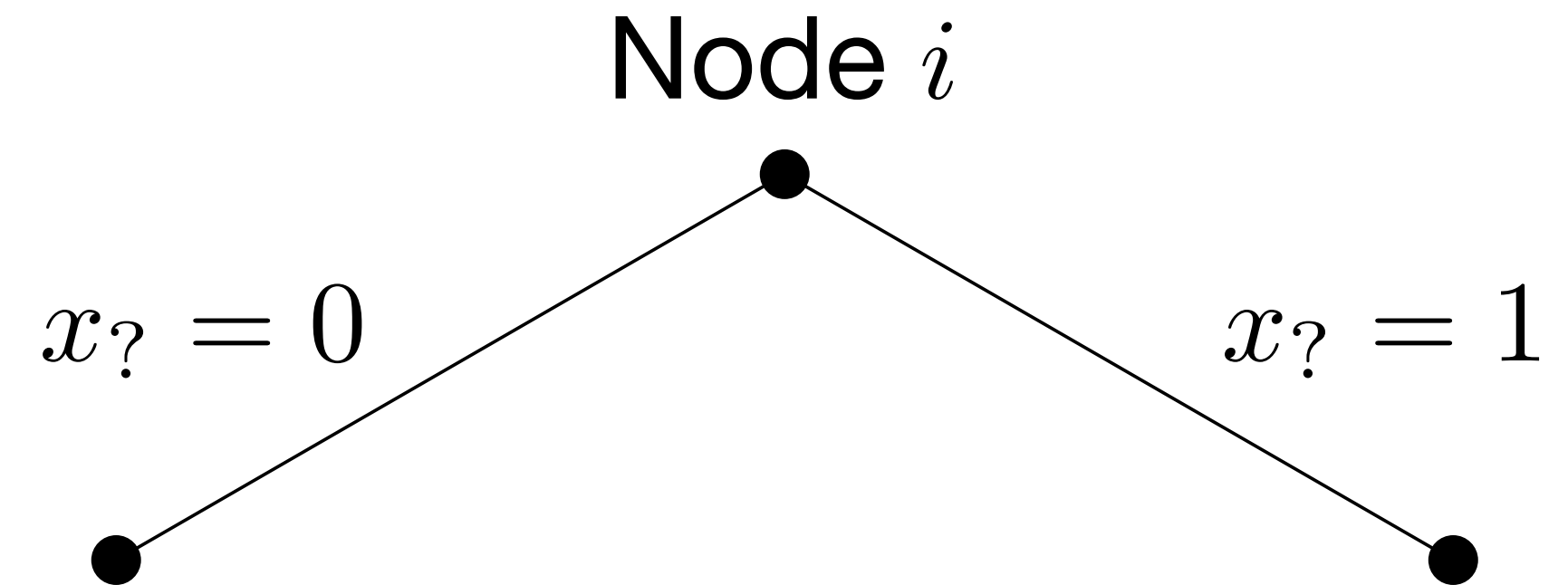
- Rounding
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Variable selection and strong branching

Relaxed problem at node i

integer fixed components \longrightarrow

$$\begin{array}{ll} \text{minimize} & c^T x \\ \text{subject to} & Ax \leq b \\ & x_{\mathcal{I}} = \bar{x} \\ & 0 \leq x \leq 1 \end{array}$$

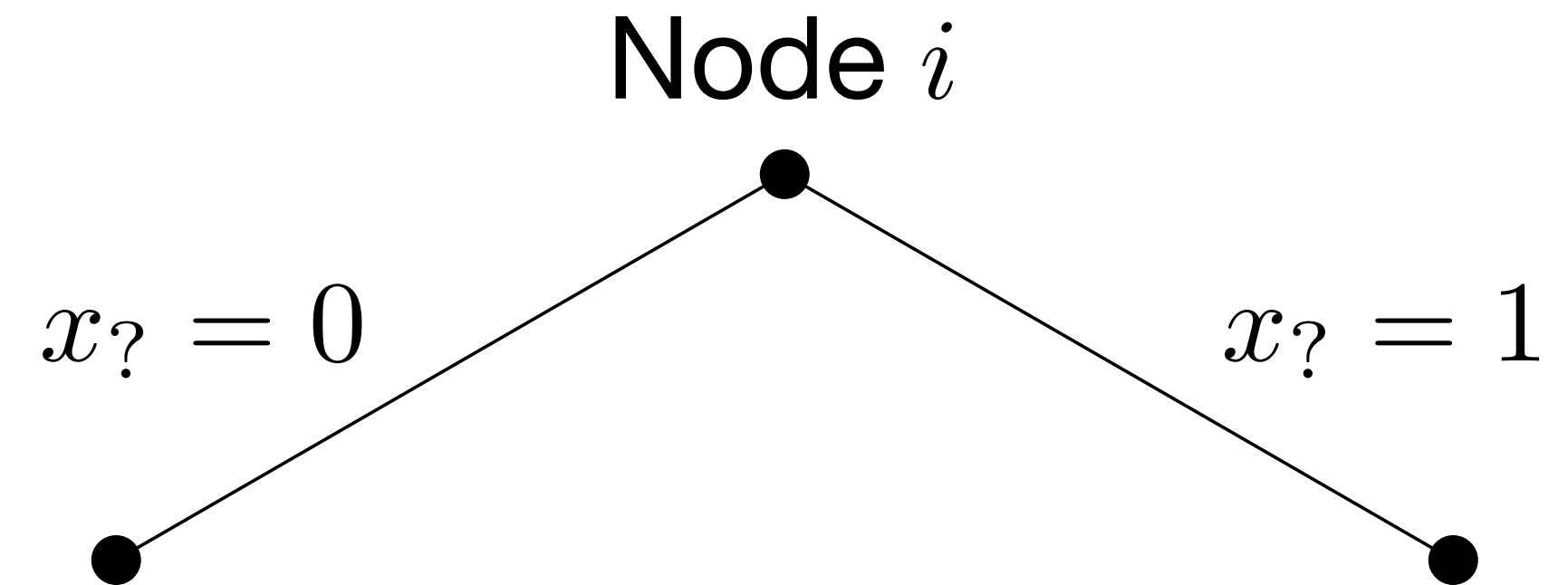


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Potential branching variables

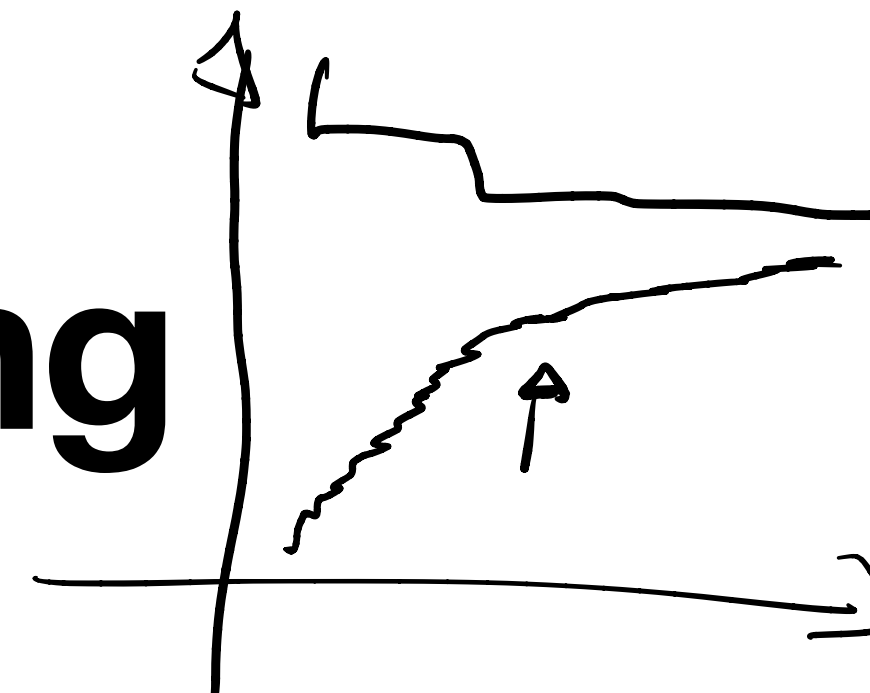
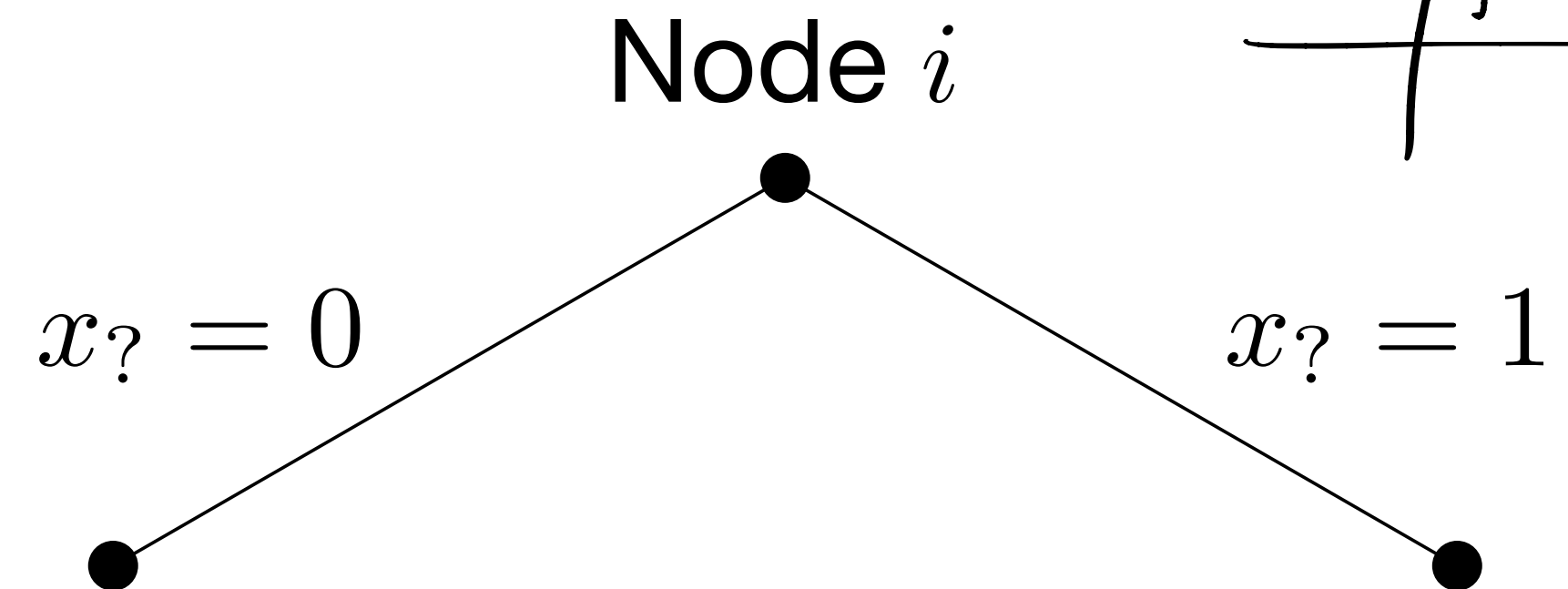
Fractional x_k , $k \in \mathcal{F} = \{1, \dots, n\} \setminus \mathcal{I}$

Variable selection and strong branching

Relaxed problem at node i

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integer fixed
components



Potential branching variables

Fractional x_k , $k \in \mathcal{F} = \{1, \dots, n\} \setminus \mathcal{I}$

$$\underline{2|\mathcal{F}|} \leq R$$

Strong branching

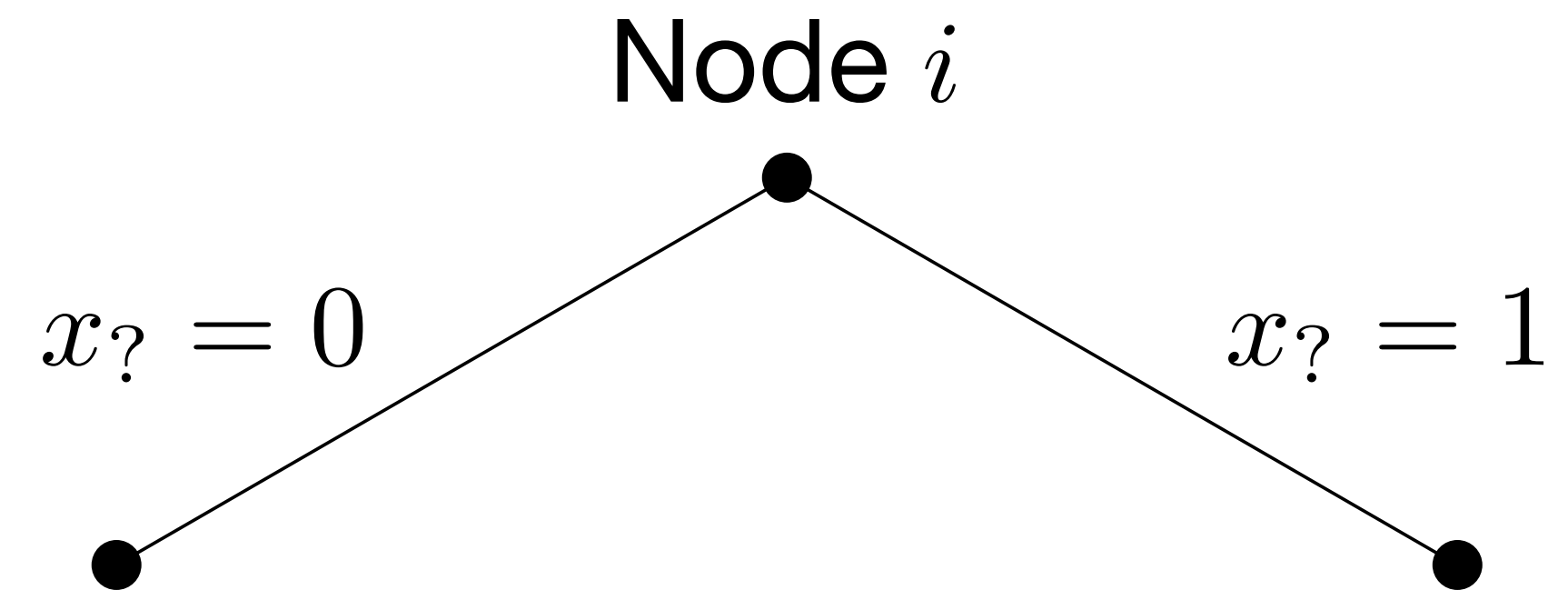
- Split all potential candidates k
- For each one, solve relaxed problems for $x_k = 0$ and $x_k = 1$
- Pick k with highest “score”:
the left and right lower bound increase the most

Variable selection and strong branching

Relaxed problem at node i

integer fixed components \longrightarrow

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Potential branching variables

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Strong branching

- Split all potential candidates k
- For each one, solve relaxed problems for $x_k = 0$ and $x_k = 1$
- Pick k with highest “score”:
the left and right lower bound increase the most

Too expensive!

Learning strong branching

Node features

$$\theta_i$$



Strong branching scores

$$(f_w(\theta_i))_k = s_k, \quad k \in \mathcal{F}$$



Best variable

$$k^* = \operatorname{argmax}_k s_k$$

Learning strong branching

Node features

θ_i



Strong branching scores

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Best variable

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Feature types

- **Static (problem instance):**
 - objective function coefficients,
 - constraint coefficients stats.,
 - constraint degrees (# of variables), etc.
- **Dynamic (incumbent, current LP relaxation, etc.):**
 - χ^* ~~incumbent~~ distance to rounding,
 - constraint degrees (# of variables), etc.

Learning strong branching

Node features

θ_i



Strong branching scores

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Multiclass classifier

- Linear function (SVM^{rank})
- Decision tree
- Neural network

Learning strong branching results

MIPLIB Examples with node limit 10,000

Solved by all methods				Not solved by at least one method			
	S/T	Nodes	Time (s)	S/T	Cl. Gap	Nodes	Time (s)
Most ambivalent	9/44	2,532	6.03	6/44	0.50	9,274	233.19
Strong	9/44	692	14.48	12/44	0.73	7,184	629.87
Learned	9/44	1,194	2.73	10/44	0.62	8,073	162.87

Learning strong branching results

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↑
nodes
reduction

Learning strong branching results

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nodes reduction

faster than strong branching

Learning strong branching results

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nodes reduction

faster than strong branching

Extensions

- What if we learn the 2-step strong branching (doubly-strong branching)?
- Can we learn while we solve the problem?

Many more directions in branch and bound

Optimal node selection

[Learning to Search in Branch-and-Bound Algorithms, He et al]

Upper bound heuristic selection

[Learning to Run Heuristics in Tree Search, Khalil et al]

Many more directions in branch and bound

Optimal node selection

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Upper bound heuristic selection

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What if we do not have expert demonstrations?

[Machine Learning for Combinatorial Optimization: a Methodological Tour d'Horizon, Bengio, Lodi, Prouvost]

Reinforcement learning

`ecole.ai`: OpenAI gym-like environment for Reinforcement Learning and Combinatorial Optimization

Learning for parametric optimization

Parametric optimization

Limitations

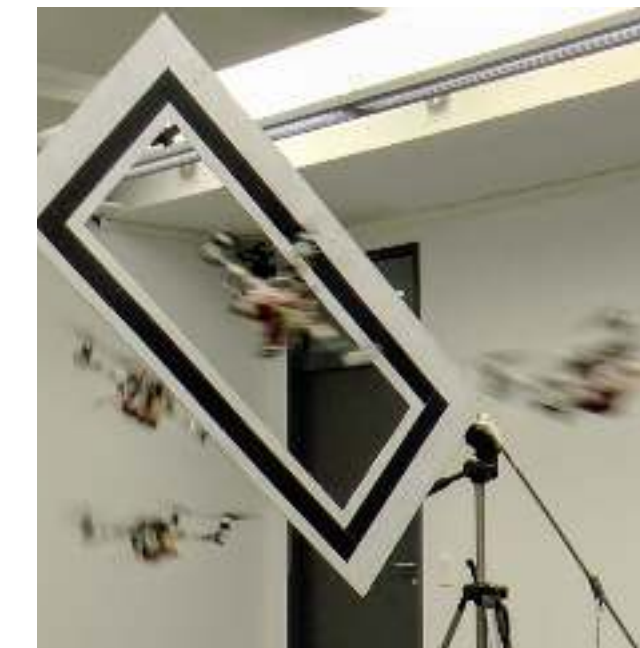
$$\begin{array}{ll} \text{minimize} & f(x, \theta) \\ \text{subject to} & g(x, \theta) \leq 0 \end{array}$$



Real-time optimization

Fast real-time requirements

Low-cost computing platforms



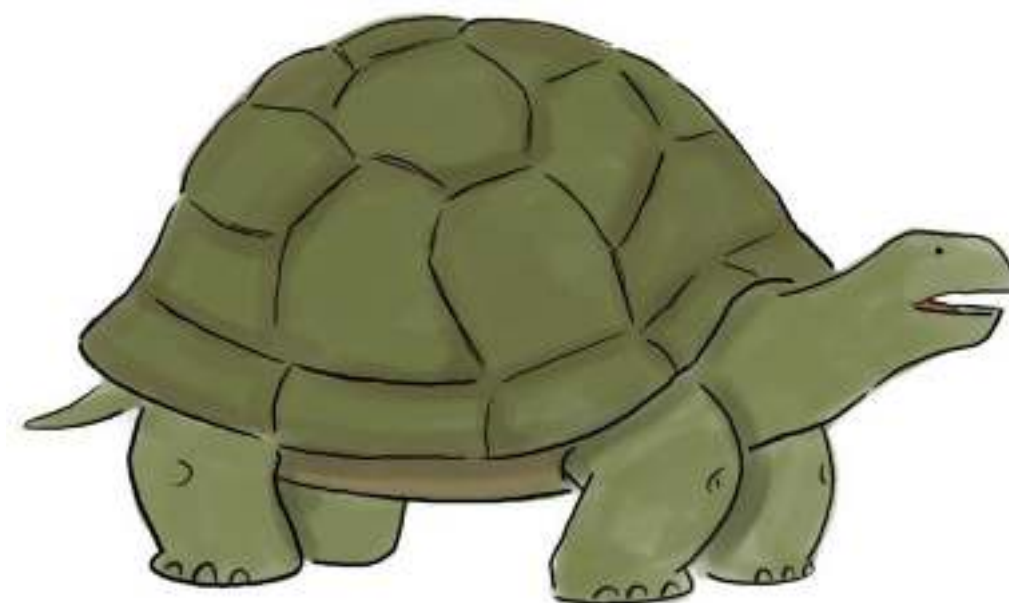
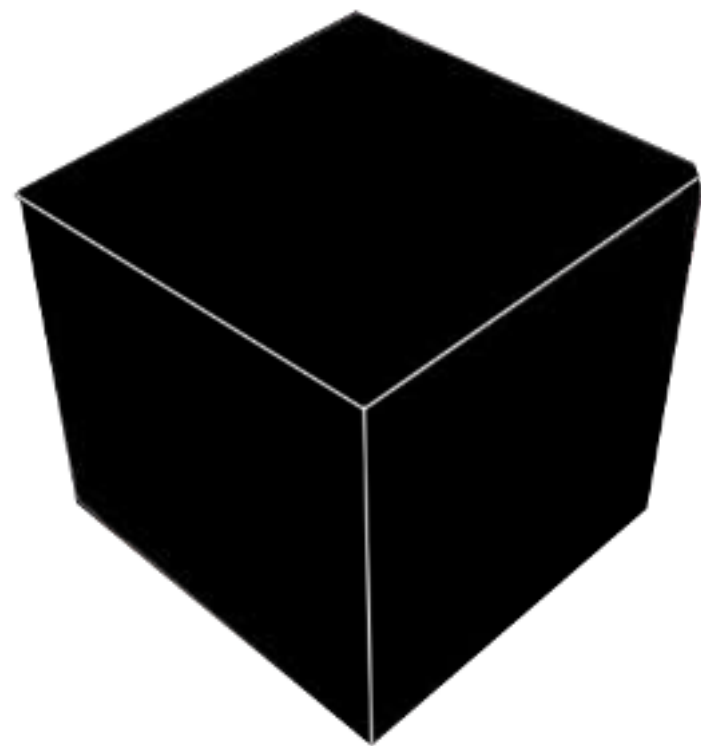
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Parametric optimization

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Real-time optimization

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+

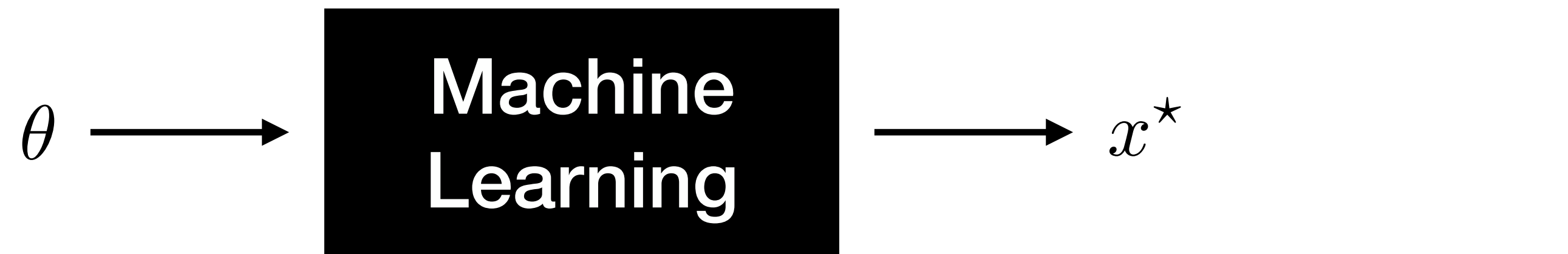


End to end learning



[Smith (1999)]
[Bello et al (2017)]
[Vinyals et al (2017)]

End to end learning



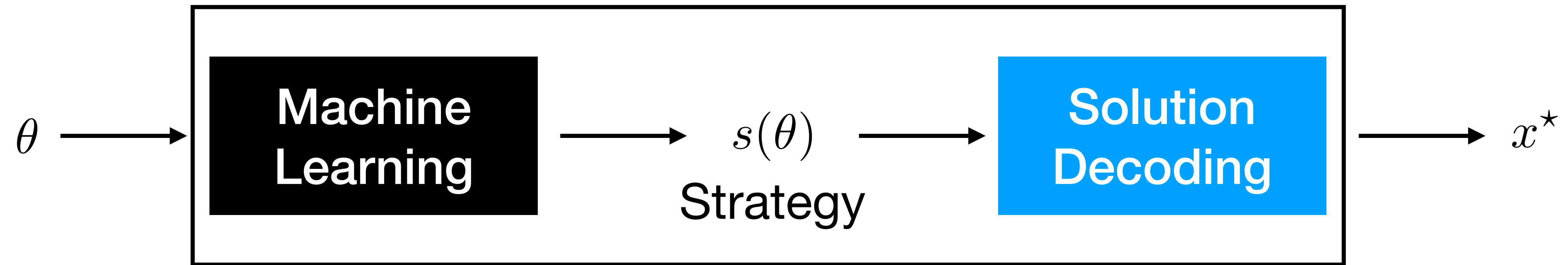
[Smith (1999)]
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Very small problems

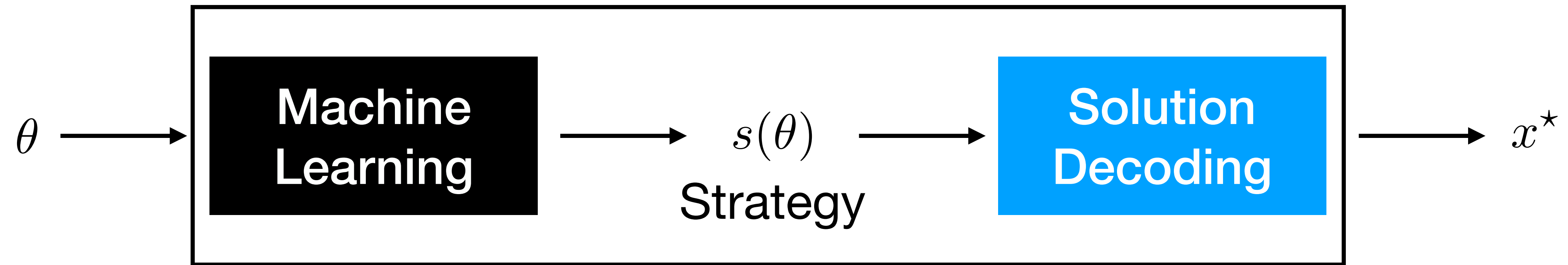
Imprecise

Needs lots of “babysitting”

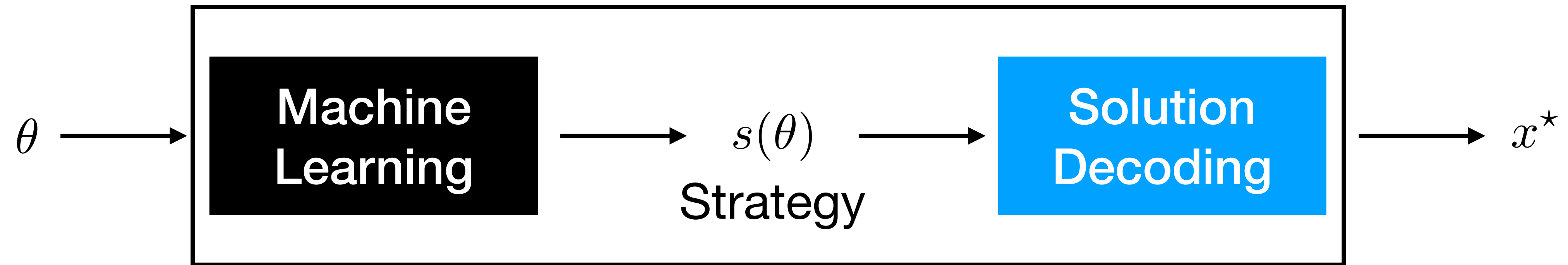
Machine learning optimizer



Machine learning optimizer

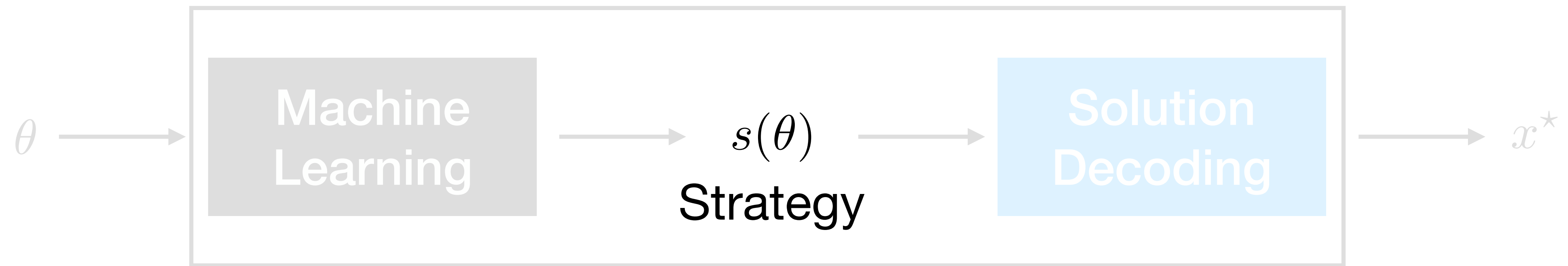


Machine learning optimizer



Strategies in optimization

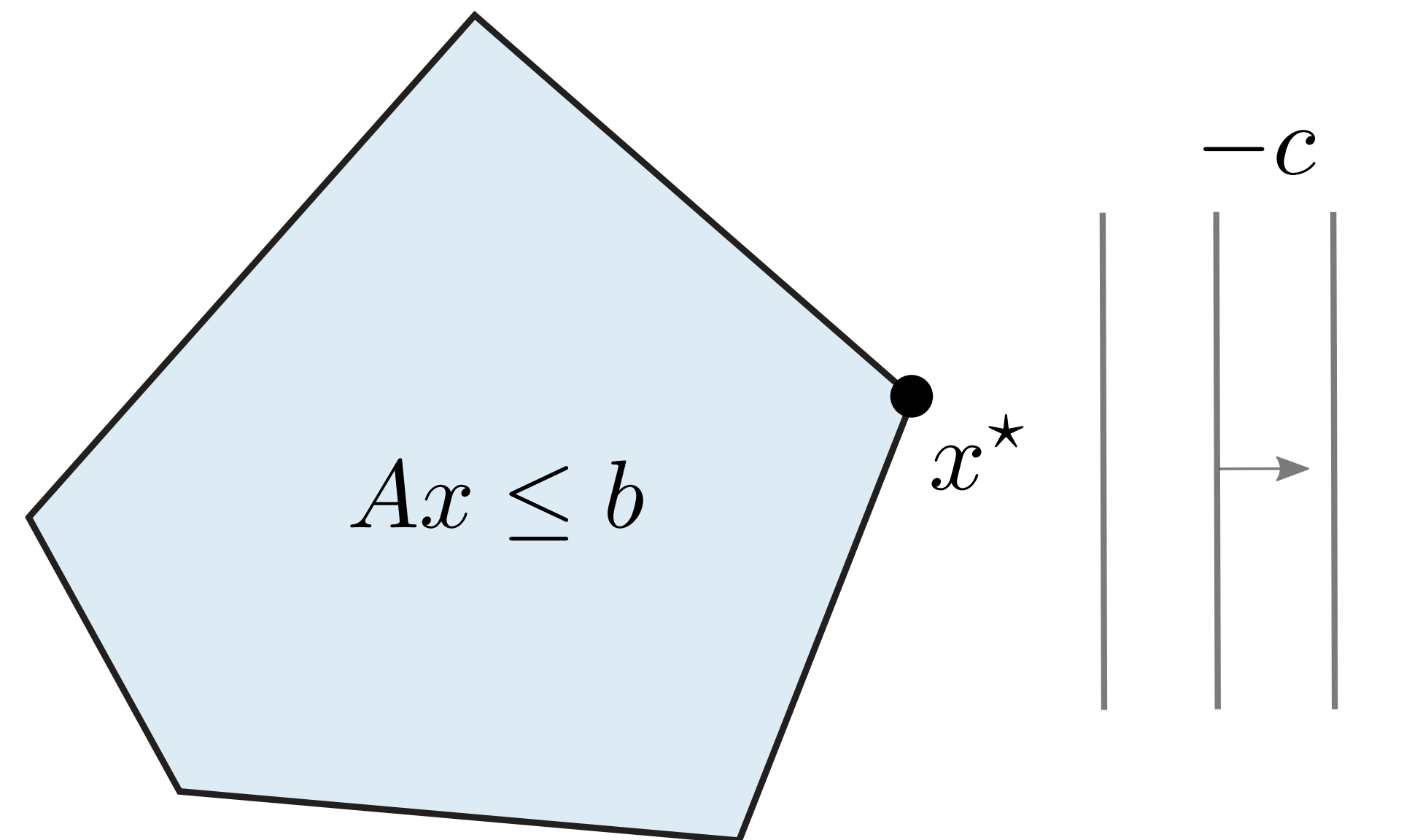
What is a strategy?



The complete information we need to efficiently compute the optimal solution

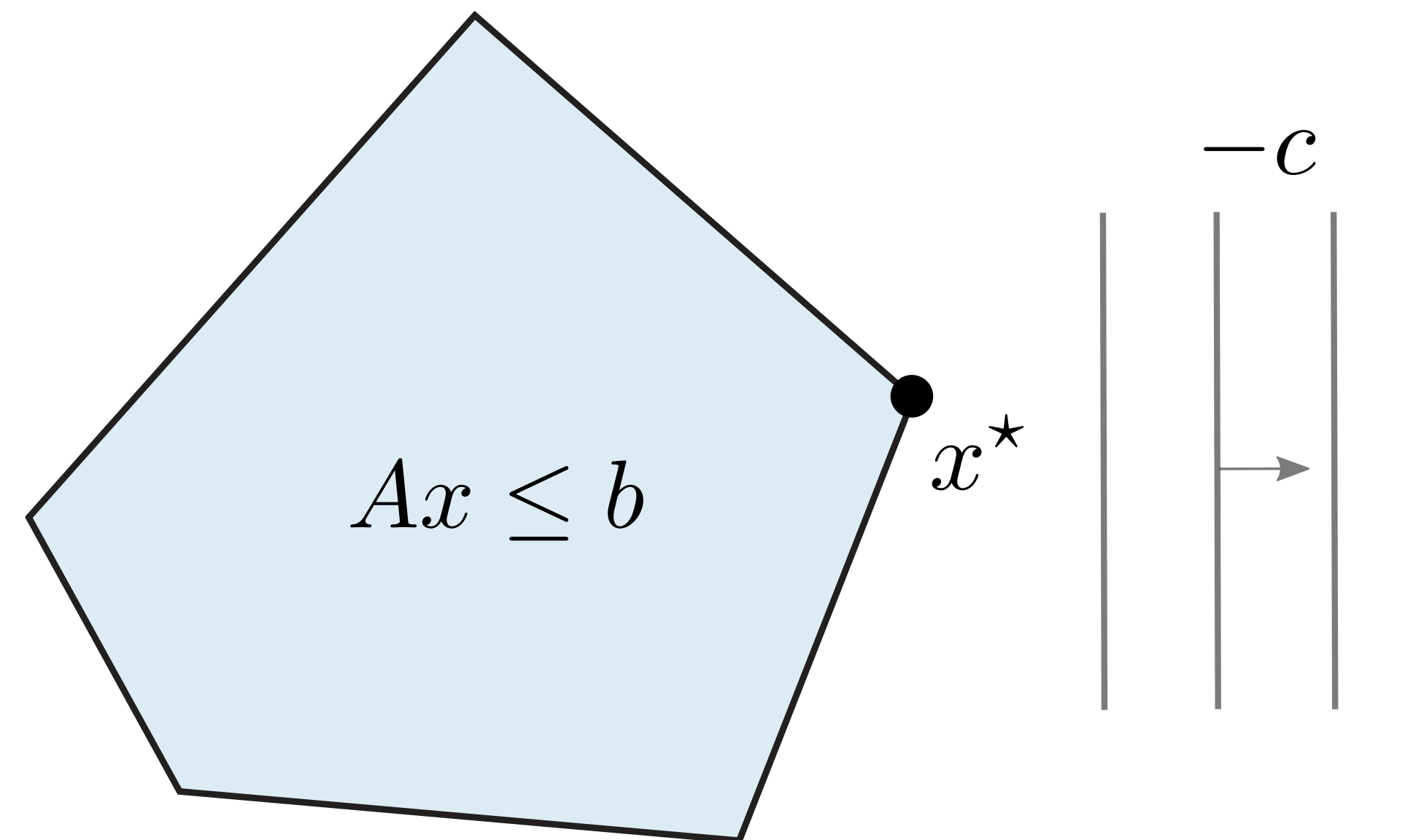
Parametric linear optimization

$$\begin{array}{ll}\text{minimize} & c(\theta)^T x \\ \text{subject to} & A(\theta)x \leq b(\theta)\end{array}$$



Parametric linear optimization

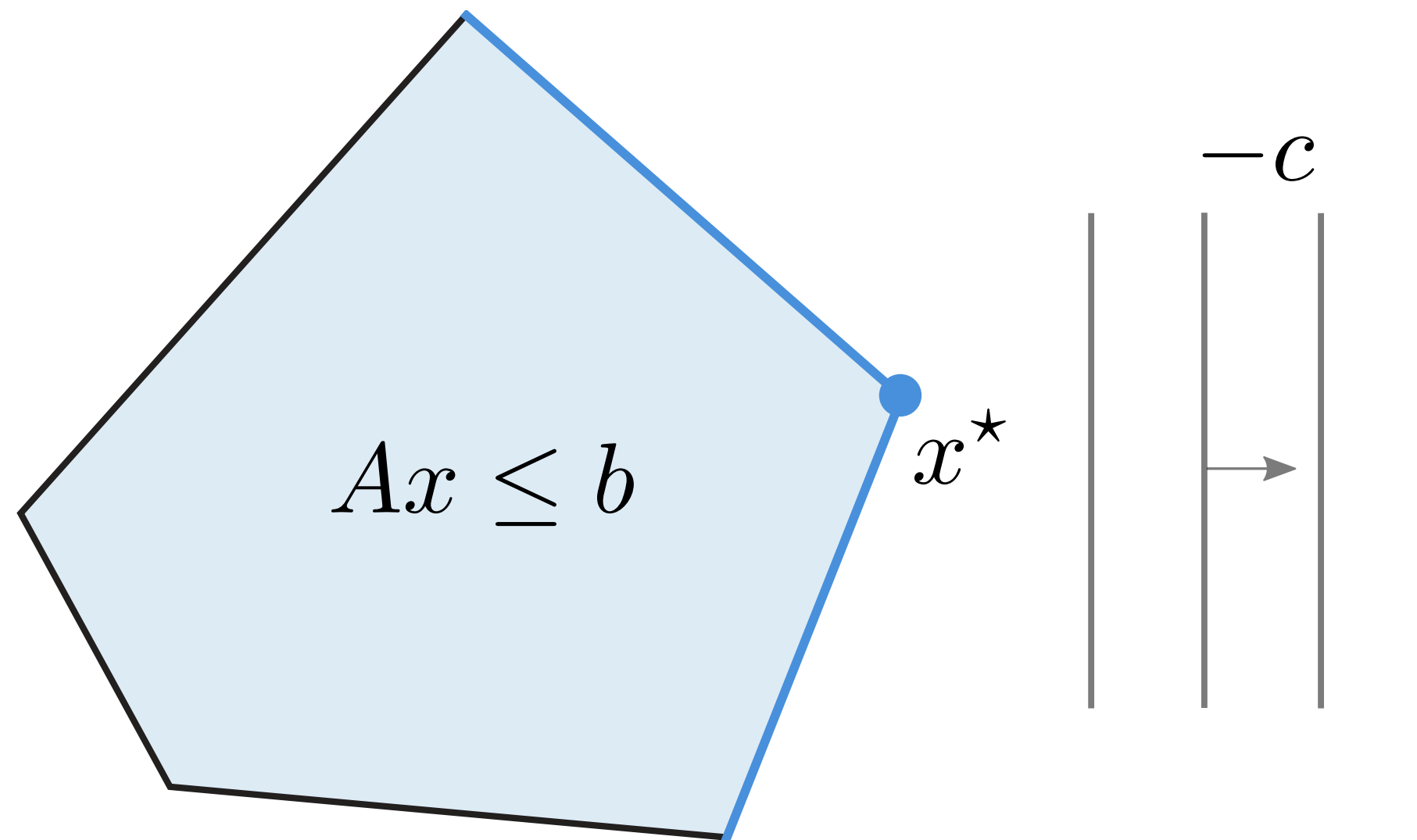
$$\begin{array}{ll}\text{minimize} & c(\theta)^T x \\ \text{subject to} & A(\theta)x \leq b(\theta)\end{array}$$



How can we define a strategy?

Tight constraints in linear optimization

$$\mathcal{T}(\theta) = \{i \mid A_i(\theta)x^* = b_i(\theta)\}$$



$|\mathcal{T}(\theta)| = \# \text{ variables}$

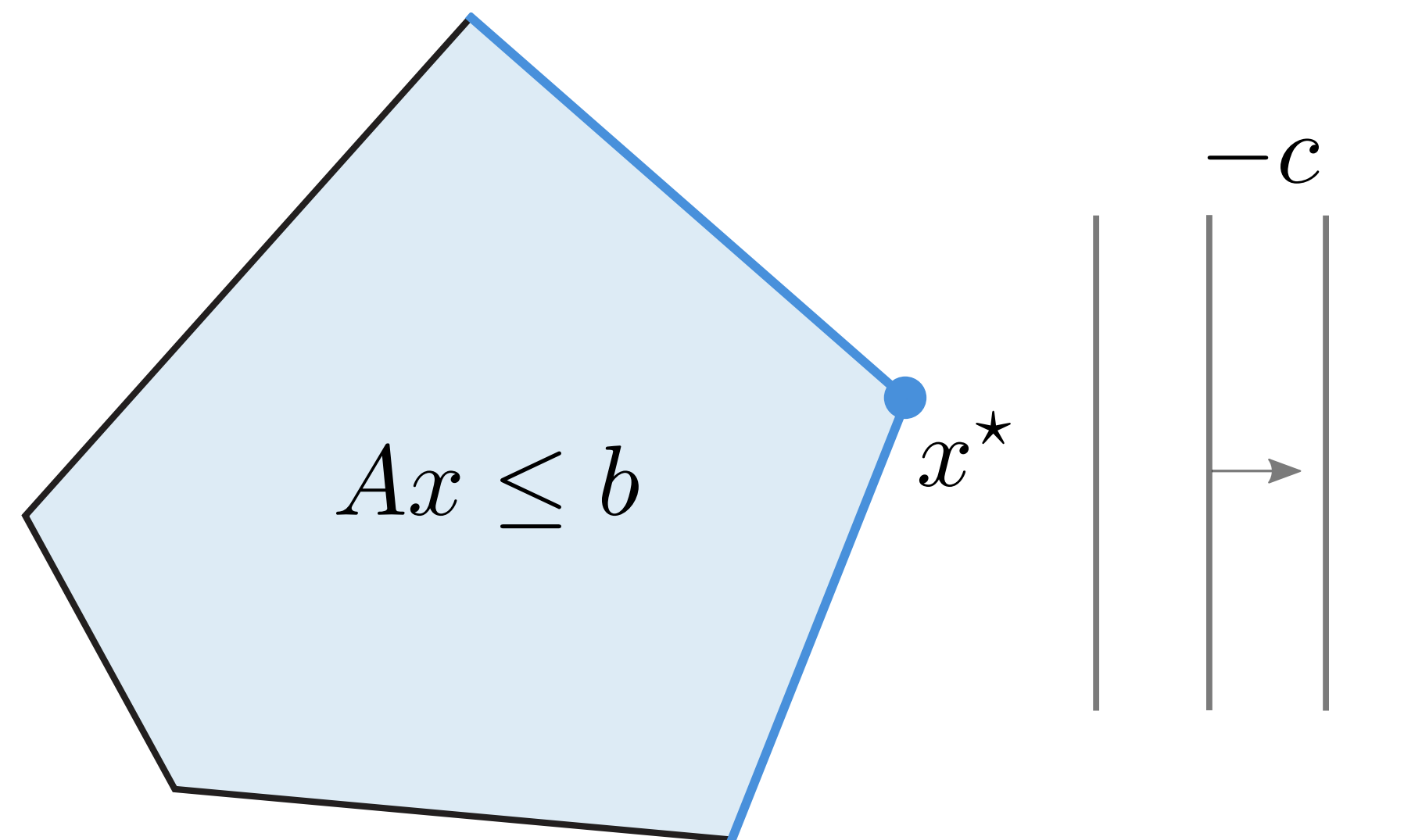
$|\mathcal{T}(\theta)| \ll \# \text{ constraints}$

if non-degenerate

in general

Tight constraints in linear optimization

$$\mathcal{T}(\theta) = \{i \mid A_i(\theta)x^* = b_i(\theta)\}$$



**Strategies for
linear optimization**

$$s(\theta) = \mathcal{T}(\theta)$$

$$|\mathcal{T}(\theta)| = \# \text{ variables}$$

$$|\mathcal{T}(\theta)| \ll \# \text{ constraints}$$

if non-degenerate
in general

Computing the solution from the strategy



$$\begin{array}{ll} \text{minimize} & c(\theta)^T x \\ \text{subject to} & A(\theta)x \leq b(\theta) \end{array}$$

Computing the solution from the strategy



Convex optimization

$$\begin{array}{ll} \text{minimize} & c(\theta)^T x \\ \text{subject to} & A(\theta)x \leq b(\theta) \end{array} \xrightarrow{s(\theta)} \begin{array}{ll} \text{minimize} & c(\theta)^T x \\ \text{subject to} & A_i(\theta)x = b_i(\theta), \quad \forall i \in \mathcal{T}(\theta) \end{array}$$

Computing the solution from the strategy



Convex optimization

$$\begin{array}{ccc} \text{minimize} & c(\theta)^T x & \\ \text{subject to} & A(\theta)x \leq b(\theta) & \end{array} \xrightarrow{s(\theta)} \begin{array}{ccc} \text{minimize} & c(\theta)^T x & \\ \text{subject to} & A_i(\theta)x = b_i(\theta), \quad \forall i \in \mathcal{T}(\theta) & \end{array}$$

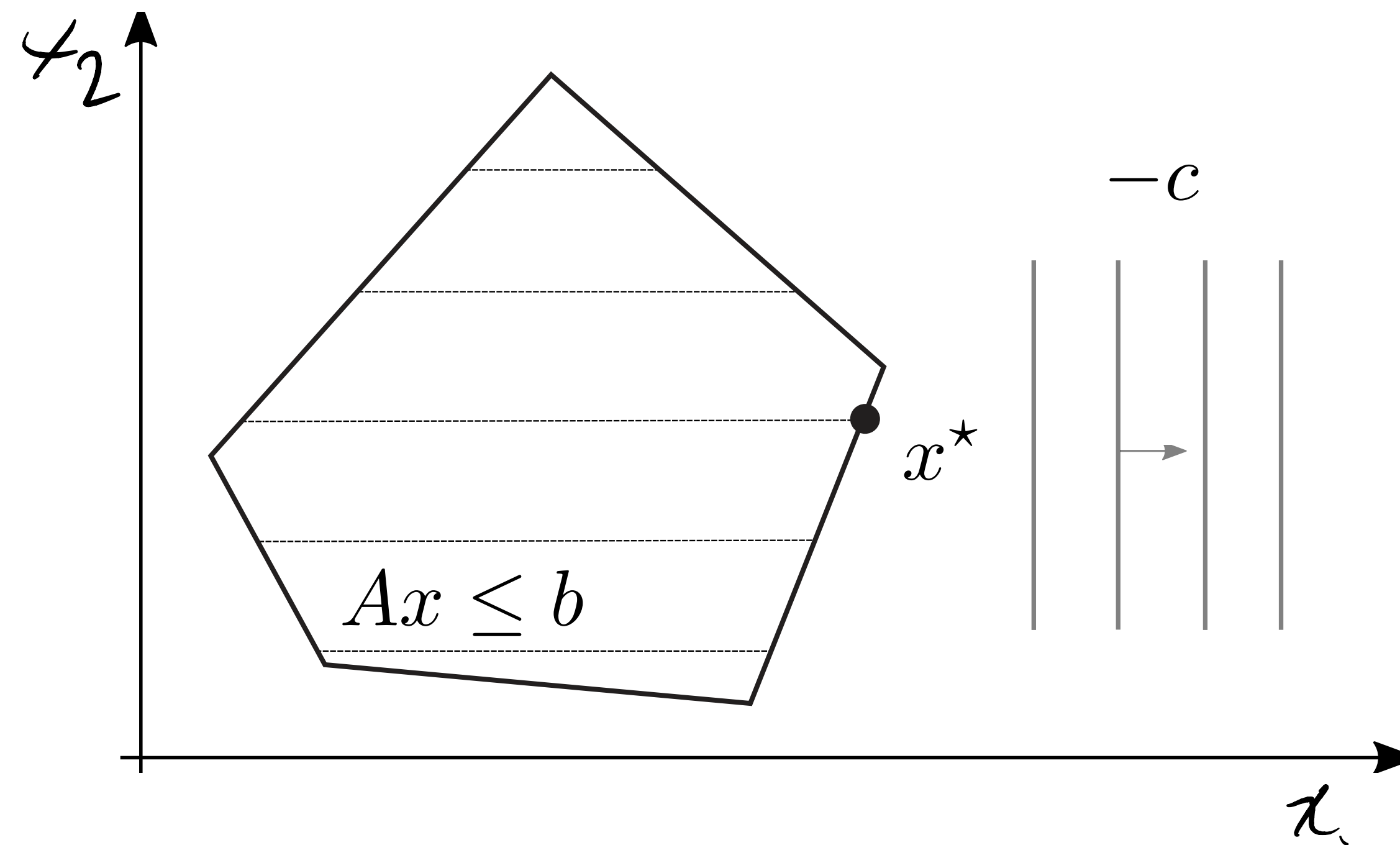
$$\begin{array}{l} Ax = b \\ A^T y = -c \end{array} \Rightarrow \begin{bmatrix} 0 & A_z^T \\ A_z & 0 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} b \\ -c \end{bmatrix}$$

KKT Linear system



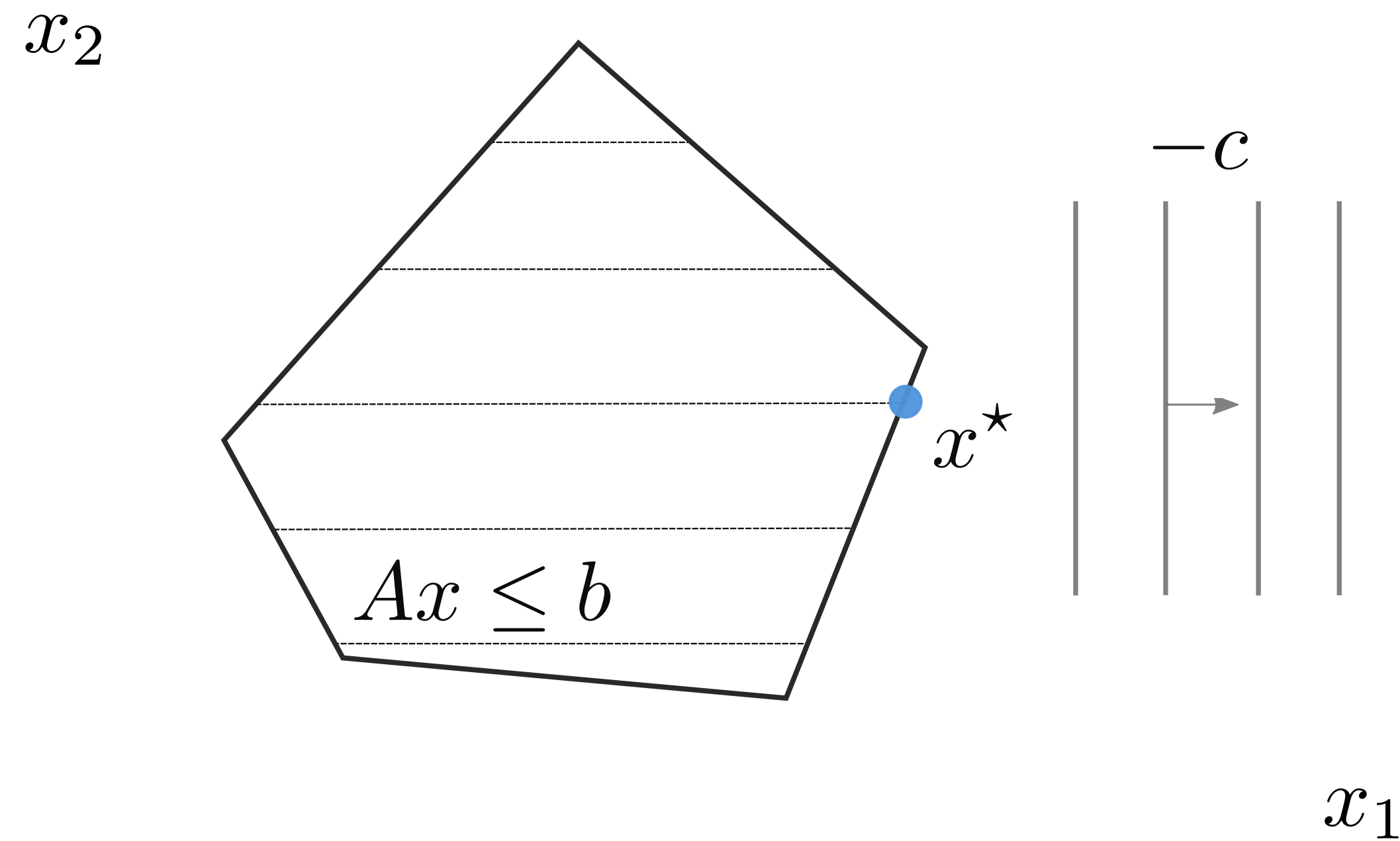
Parametric mixed-integer linear optimization

$$\begin{array}{ll}\text{minimize} & c(\theta)^T x \\ \text{subject to} & A(\theta)x \leq b(\theta) \\ & x_{\mathcal{I}} \in \mathbf{Z}^d \quad \text{integers}\end{array}$$



How can we define a strategy?

Tight constraints are not enough

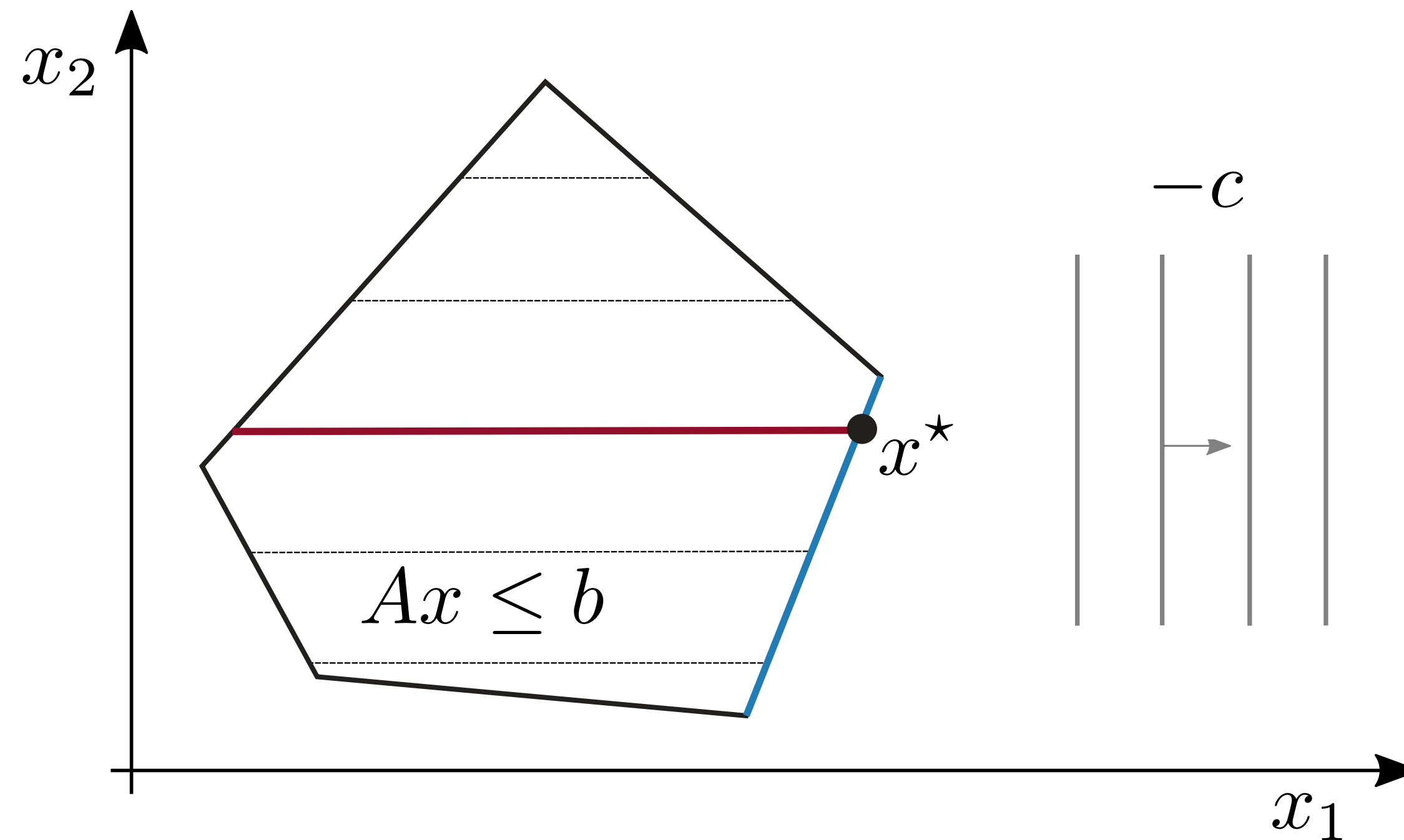


Strategies for mixed-integer optimization

$$s(\theta) = (\mathcal{T}(\theta), x_{\mathcal{I}}^*(\theta))$$

Tight constraints

Integer variables



Computing the solution from the strategy



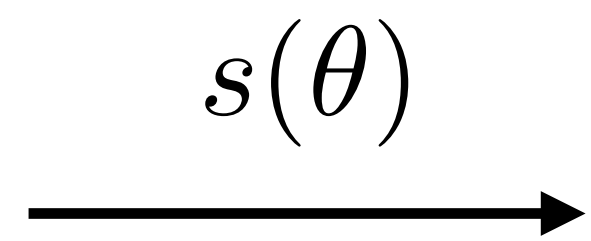
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Computing the solution from the strategy



Convex optimization

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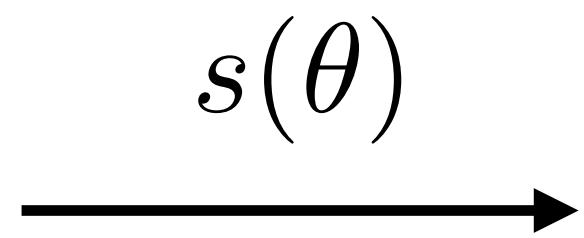
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Computing the solution from the strategy



Convex optimization

minimize $c(\theta)^T x$
subject to $A(\theta)x \leq b(\theta)$
 $x_{\mathcal{I}} \in \mathbf{Z}^d$



minimize $c(\theta)^T x$
subject to $A_i(\theta)x = b_i(\theta), \quad \forall i \in \mathcal{T}(\theta)$
 $x_{\mathcal{I}} = x_{\mathcal{I}}^\star(\theta)$

**KKT Linear
system**

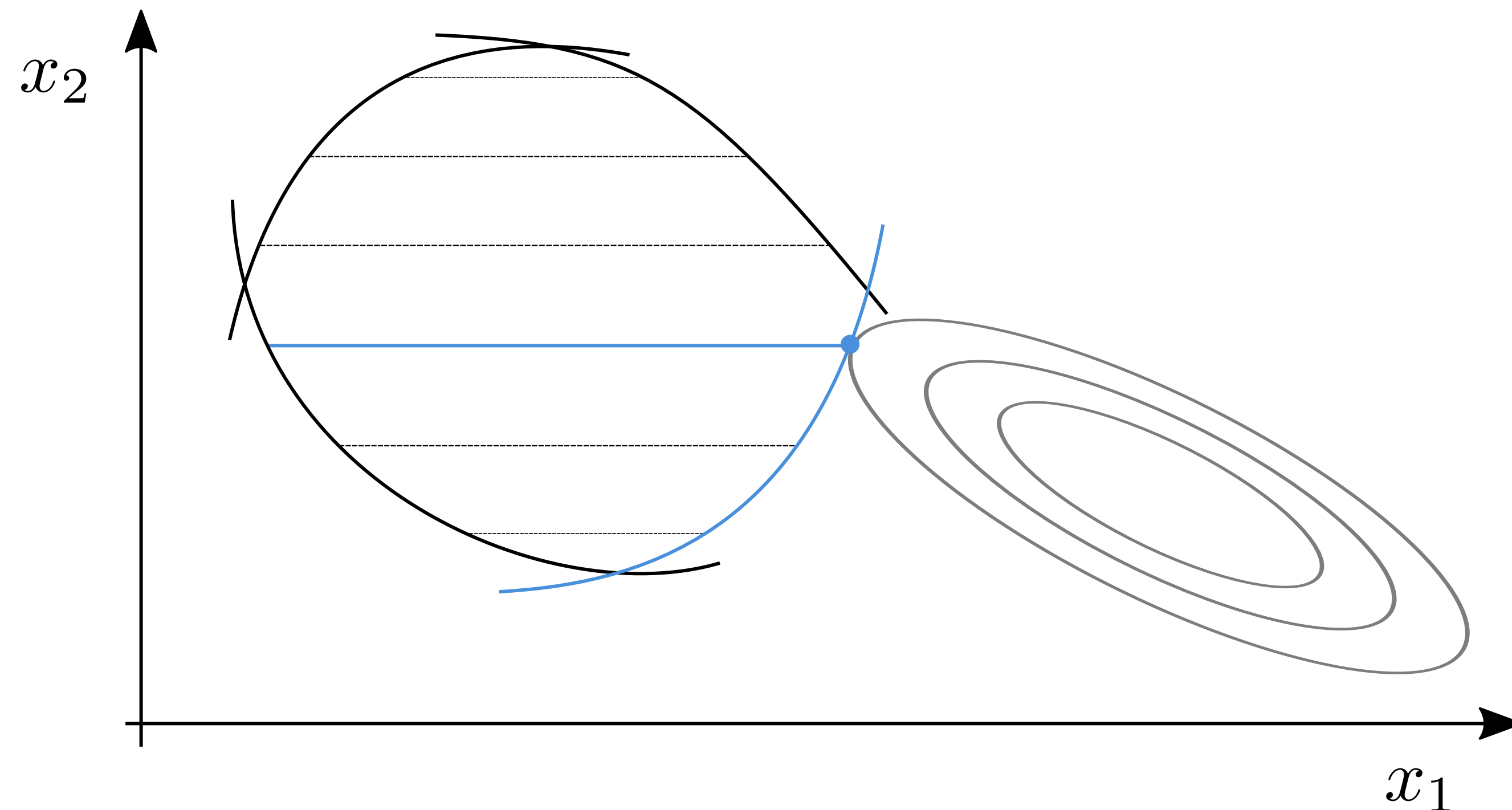


Mixed-integer convex optimization

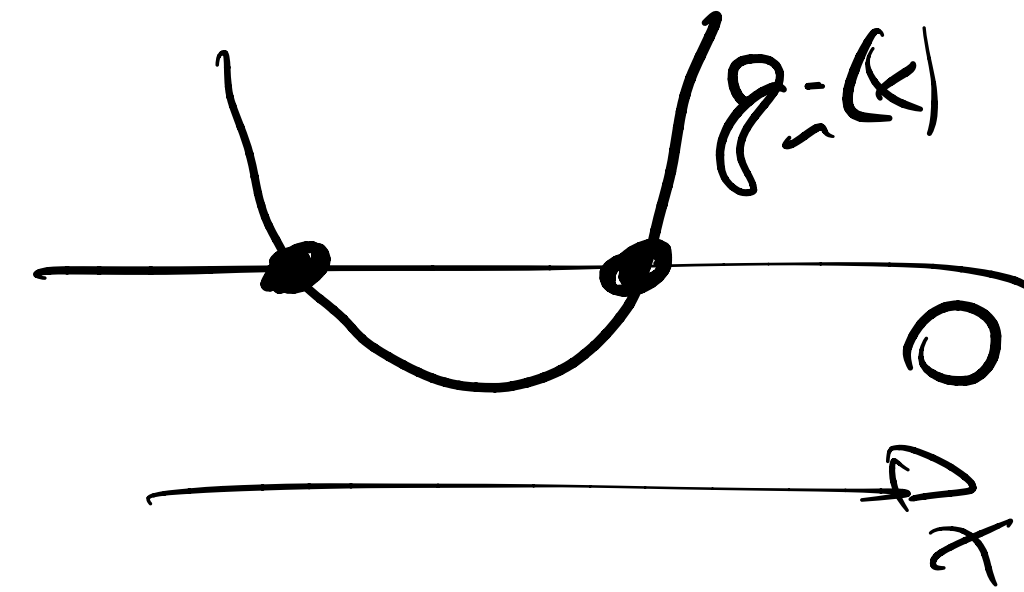
$$\begin{array}{ll}\text{minimize} & f(x, \theta) \\ \text{subject to} & g(x, \theta) \leq 0 \\ & x_{\mathcal{I}} \in \mathbf{Z}^d\end{array}$$

**Same strategy
definition**

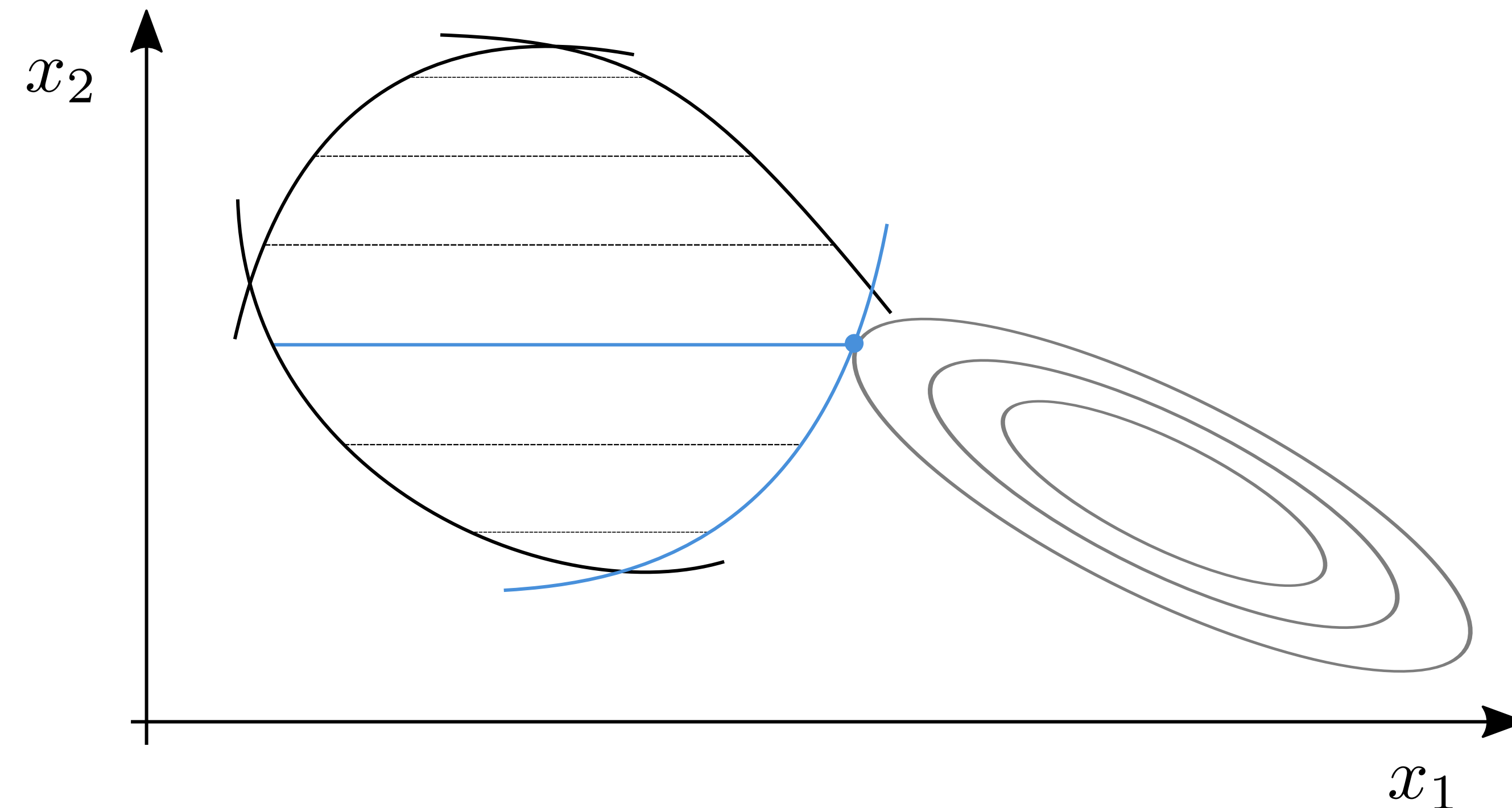
$$s(\theta) = (\mathcal{T}(\theta), x_{\mathcal{I}}^*(\theta))$$



Mixed-integer convex optimization



$$\begin{aligned} &\text{minimize} && f(x, \theta) \\ &\text{subject to} && g(x, \theta) \leq 0 \\ &&& \mathbf{x}_I \in \mathbf{Z}^d \end{aligned}$$



**Same strategy
definition**

$$s(\theta) = (\mathcal{T}(\theta), x_I^*(\theta))$$

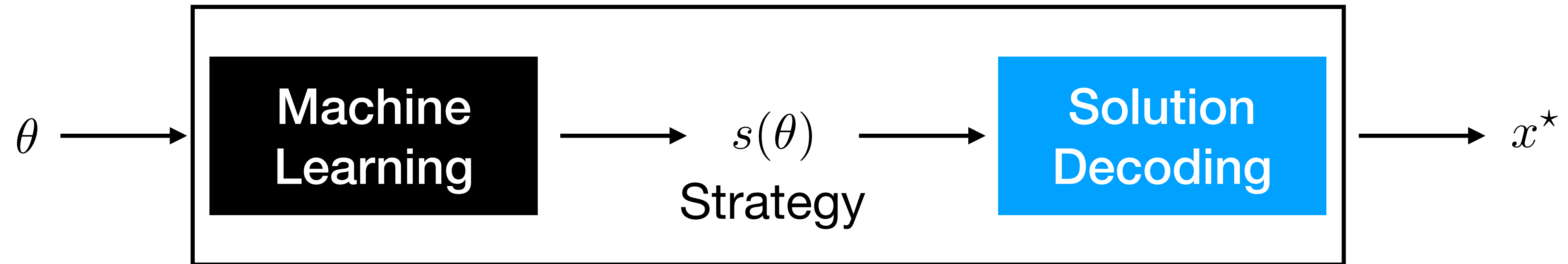


**How can we recover
the solution?**

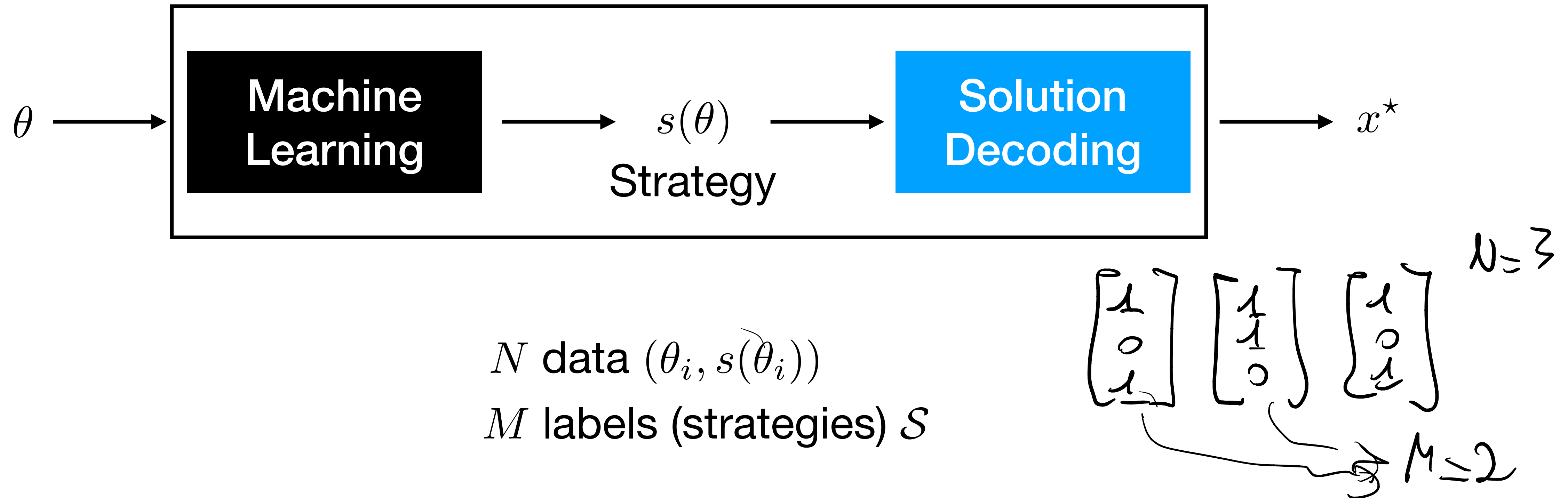
$$\begin{aligned} &\min f(x, \theta) \\ &\text{st. } g(x, \theta) \leq 0 \quad \forall \theta \in \mathcal{T} \\ &\quad \mathbf{x}_I = \mathbf{x}_I^* \end{aligned}$$

Learning the strategies

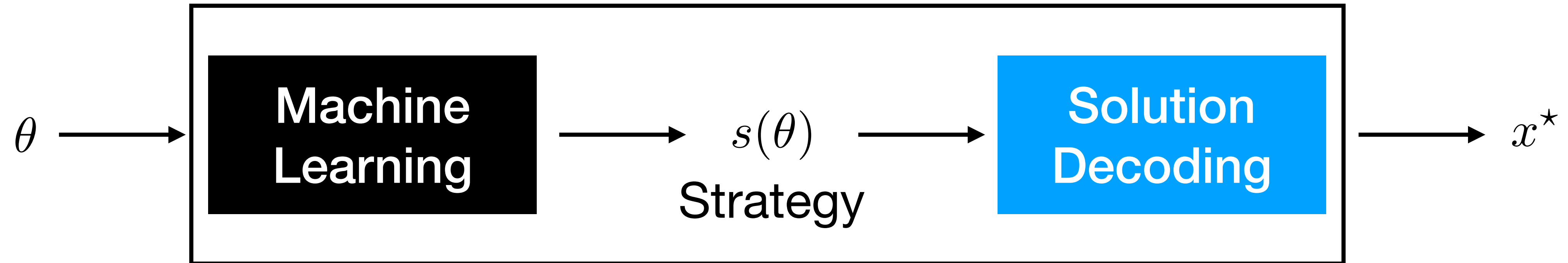
Predicting the strategies



Predicting the strategies



Predicting the strategies



N data $(\theta_i, s(\theta_i))$

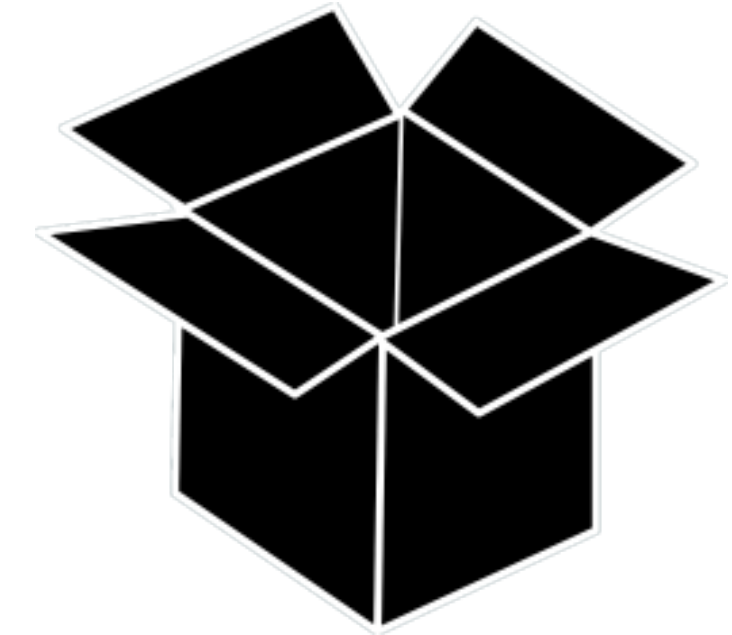
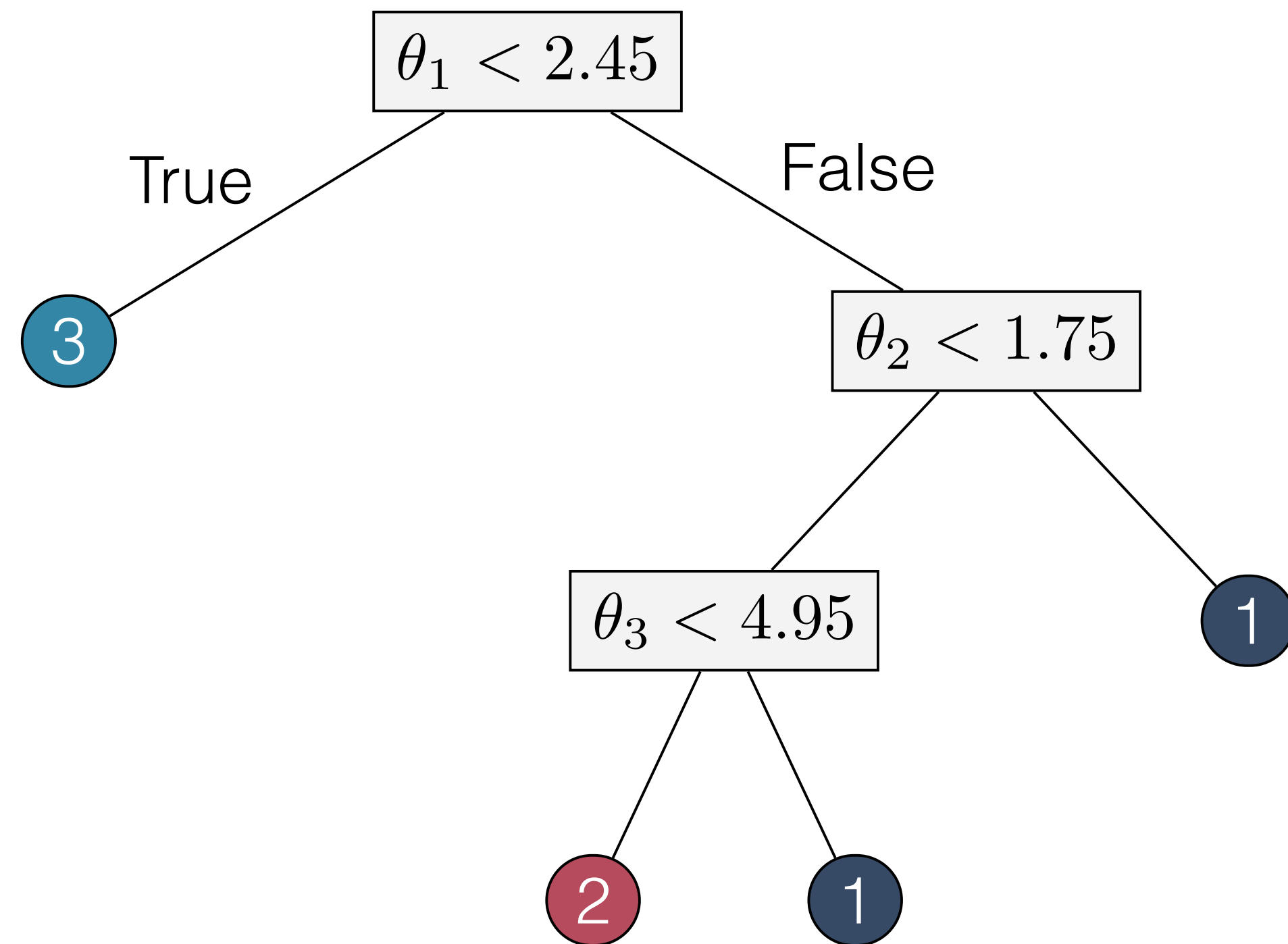
M labels (strategies) \mathcal{S}

Multiclass classification



Interpretable classifier

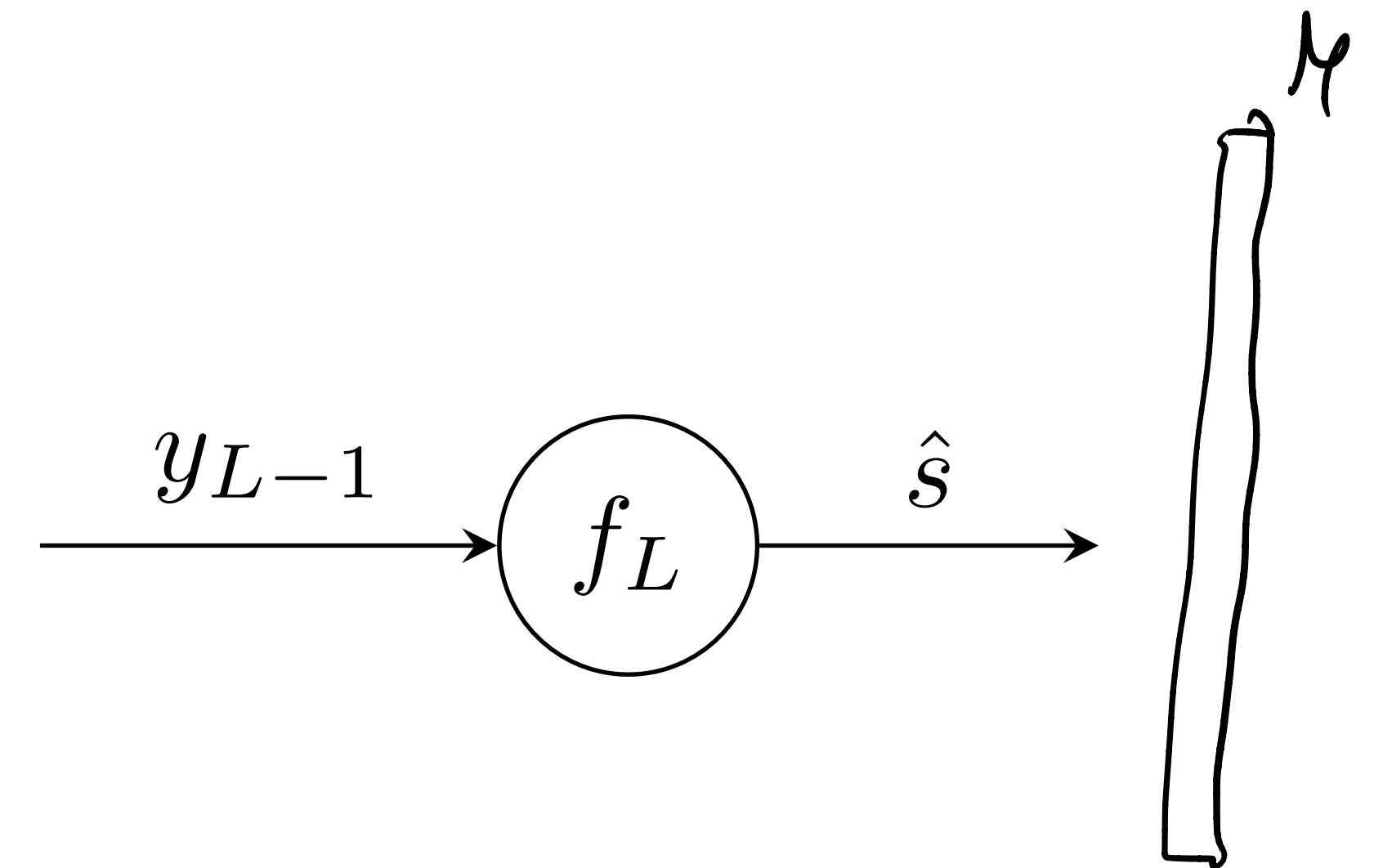
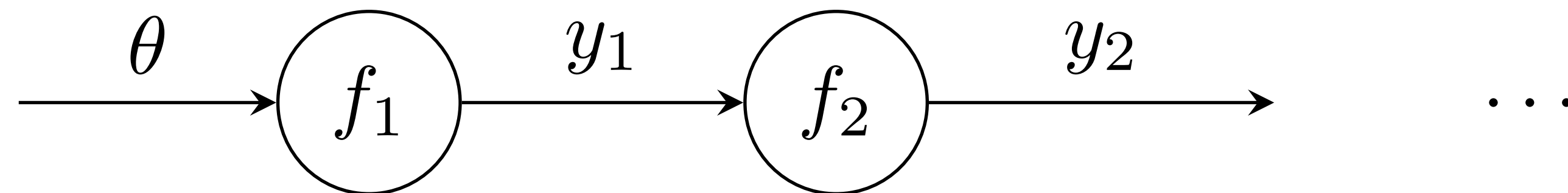
Decision Trees



Features

- Easy to understand
- It works for small problems

Neural network classifiers



Single layer

$$y_l = f(y_{l-1}) = (W_l y_{l-1} + b_l)_+ \quad \text{ReLU}$$

Output layer (softmax)

$$\hat{s} = f(y_L) = \sigma(y_L), \quad \text{with} \quad (\sigma(x))_i = \frac{e^{x_i}}{\sum_{j=1}^M e^{x_j}}$$

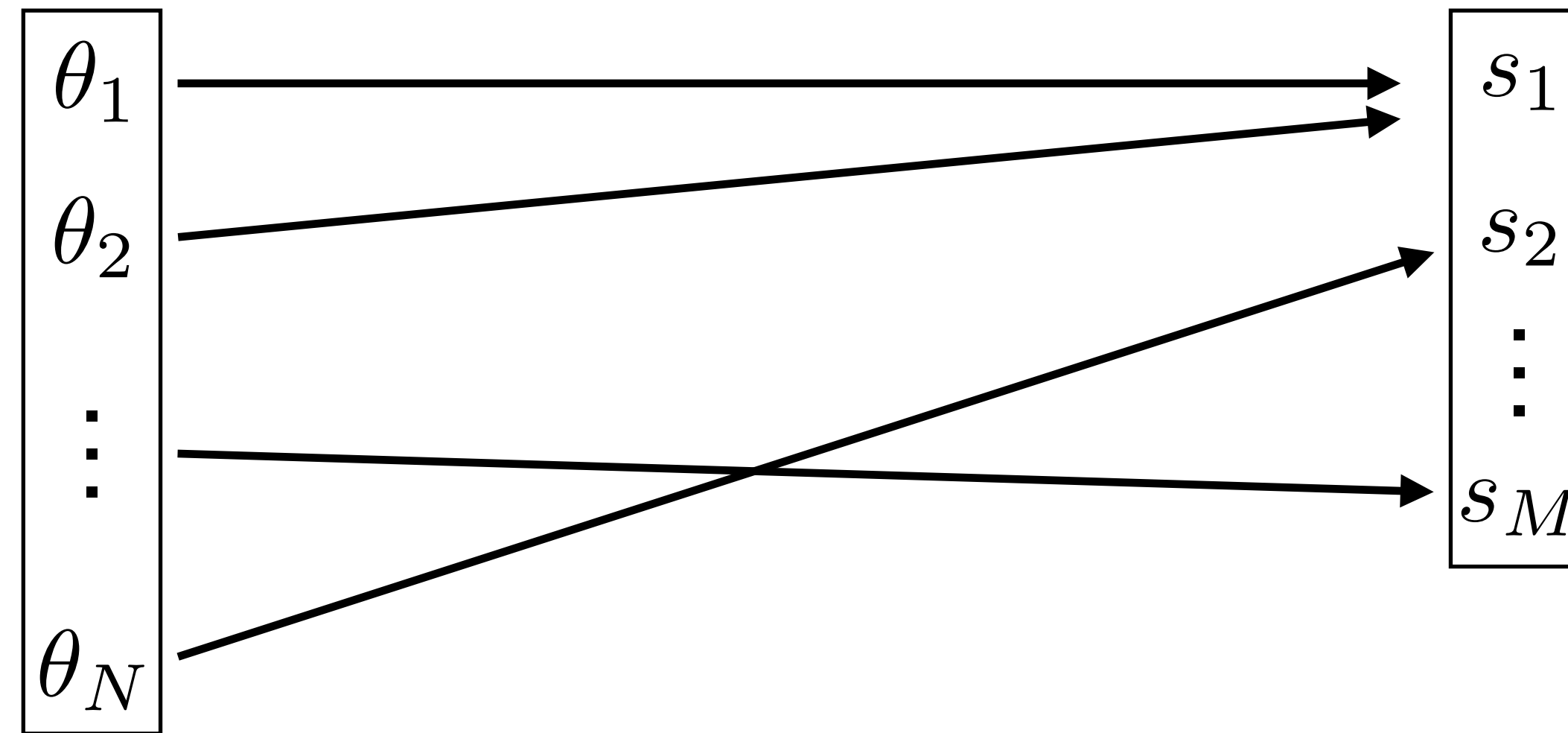
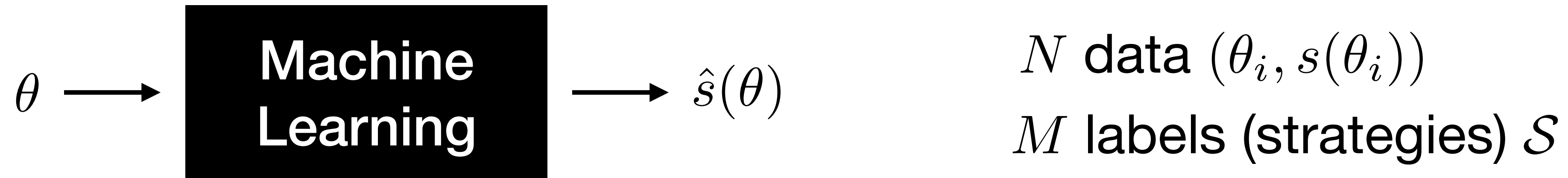
Features

- Hard to understand
- It works for large problems

Sampling the strategies

Have we seen enough data?

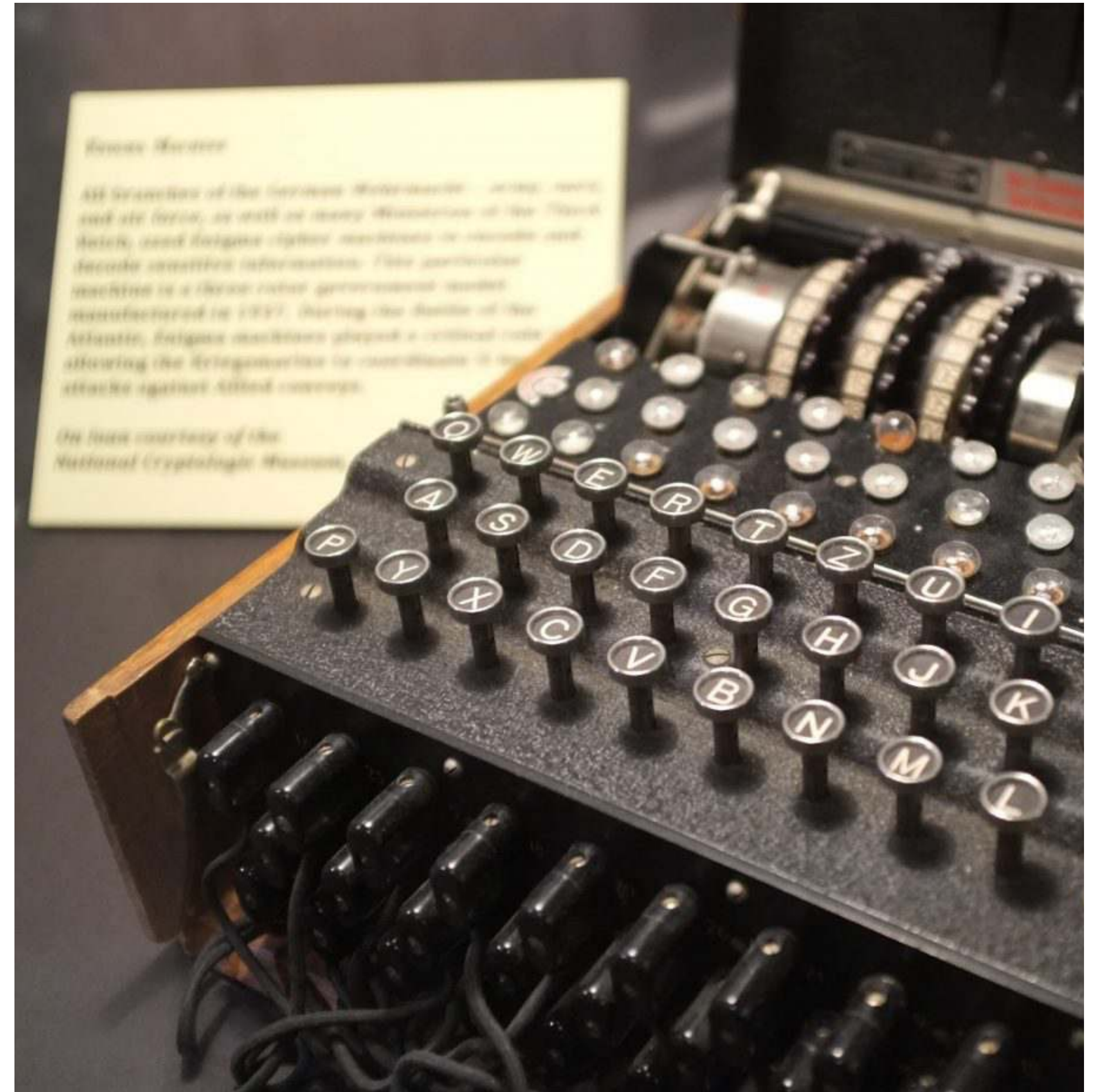
Multiclass classification



What happens with θ_{N+1} ?

Alan Turing

Already worked on this...



Good-Turing estimator

$$GT = \frac{N_1}{N} \approx \mathbf{P}(s(\theta_{N+1}) \notin \mathcal{S}(\Theta_N))$$

Probability of
unseen strategies

Good-Turing estimator

$$GT = \frac{N_1}{N} \approx \mathbf{P}(s(\theta_{N+1}) \notin \mathcal{S}(\Theta_N))$$

samples

Probability of
unseen strategies

Good-Turing estimator

strategies
appeared once

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samples

Probability of
unseen strategies

Concentration bound (confidence β)

$$\mathbf{P}(s(\theta_{N+1}) \notin \mathcal{S}(\Theta_N)) \leq GT + C \sqrt{(1/N) \ln(3/\beta)}$$

Good-Turing estimator

strategies
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Probability of
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$$\mathbf{P}(s(\theta_{N+1}) \notin \mathcal{S}(\Theta_N)) \leq GT + C \sqrt{(1/N) \ln(3/\beta)}$$

Example

$$\begin{aligned} N &= 15 \\ M &= 5 \end{aligned}$$



s_1 6 times
 s_2 3 times
 s_3 1 time
 s_4 3 times
 s_5 2 times



$$GT = 1/15$$

Good-Turing estimator

strategies
appeared once

$$GT = \frac{N_1}{N} \approx \mathbf{P}(s(\theta_{N+1}) \notin \mathcal{S}(\Theta_N))$$

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Probability of
unseen strategies

Concentration bound (confidence β)

$$\mathbf{P}(s(\theta_{N+1}) \notin \mathcal{S}(\Theta_N)) \leq GT + C \sqrt{(1/N) \ln(3/\beta)}$$

Sample until

$$\leq \epsilon$$

Example

$$N = 15$$
$$M = 5$$



s_1 6 times
 s_2 3 times
 s_3 1 time
 s_4 3 times
 s_5 2 times



$$GT = 1/15$$

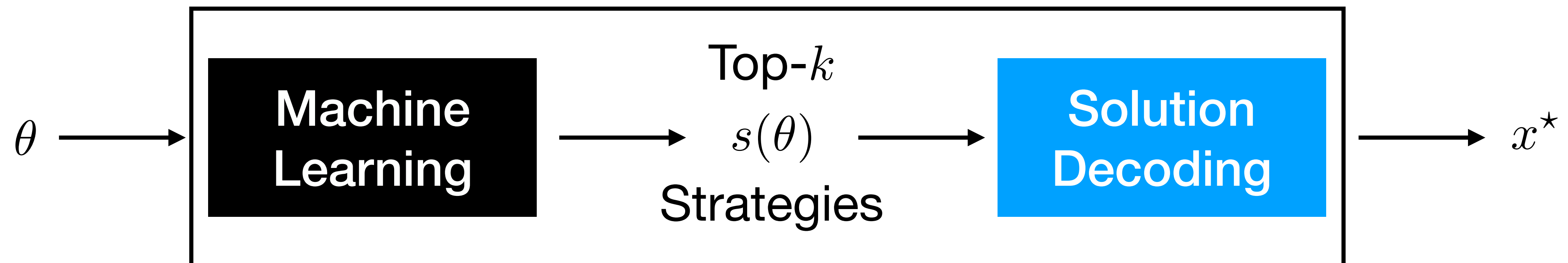
MLOPT: Machine Learning Optimizer

github.com/bstellato/mlopt

Offline learning



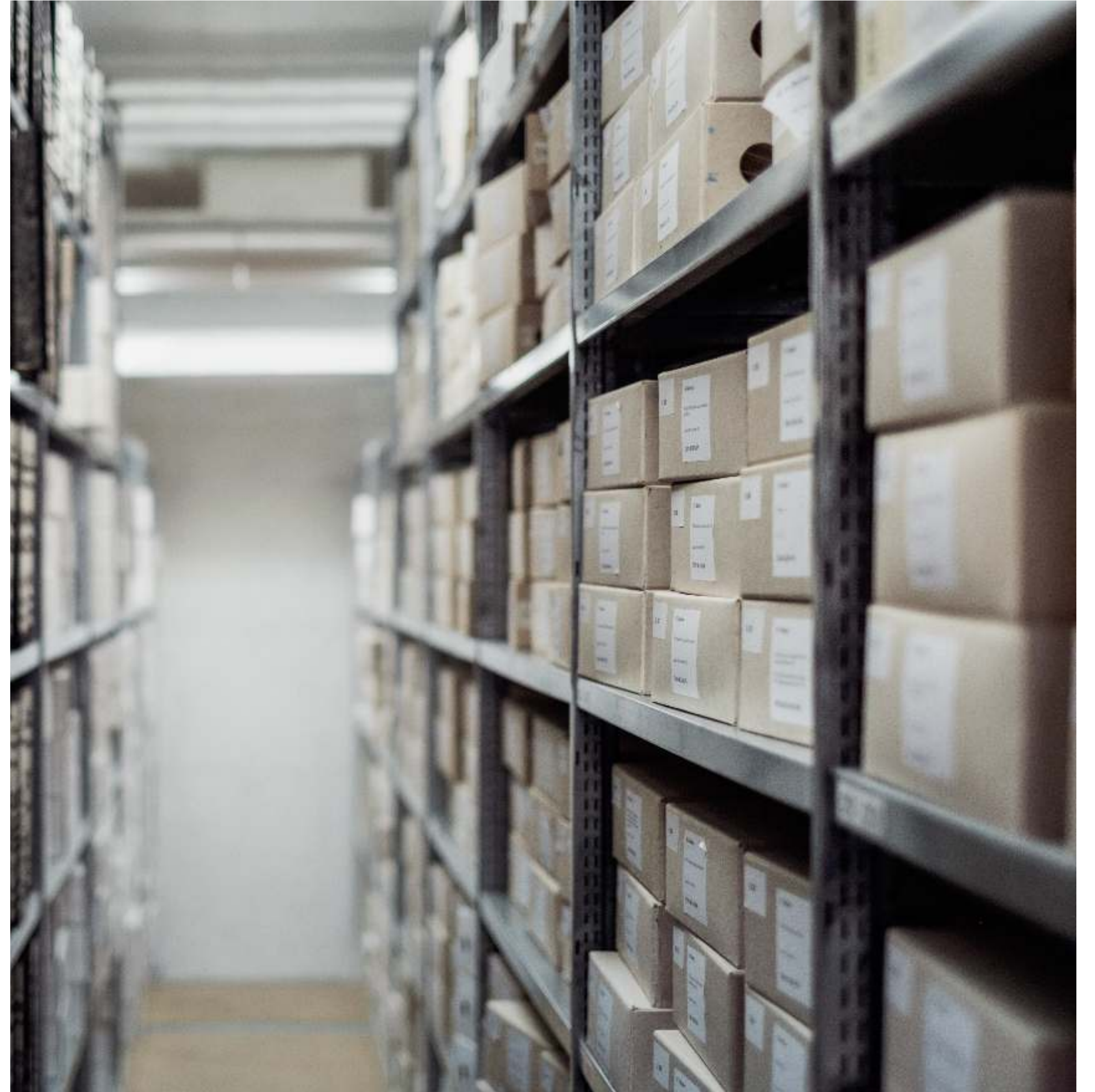
Fast online predictions



Examples

Inventory management

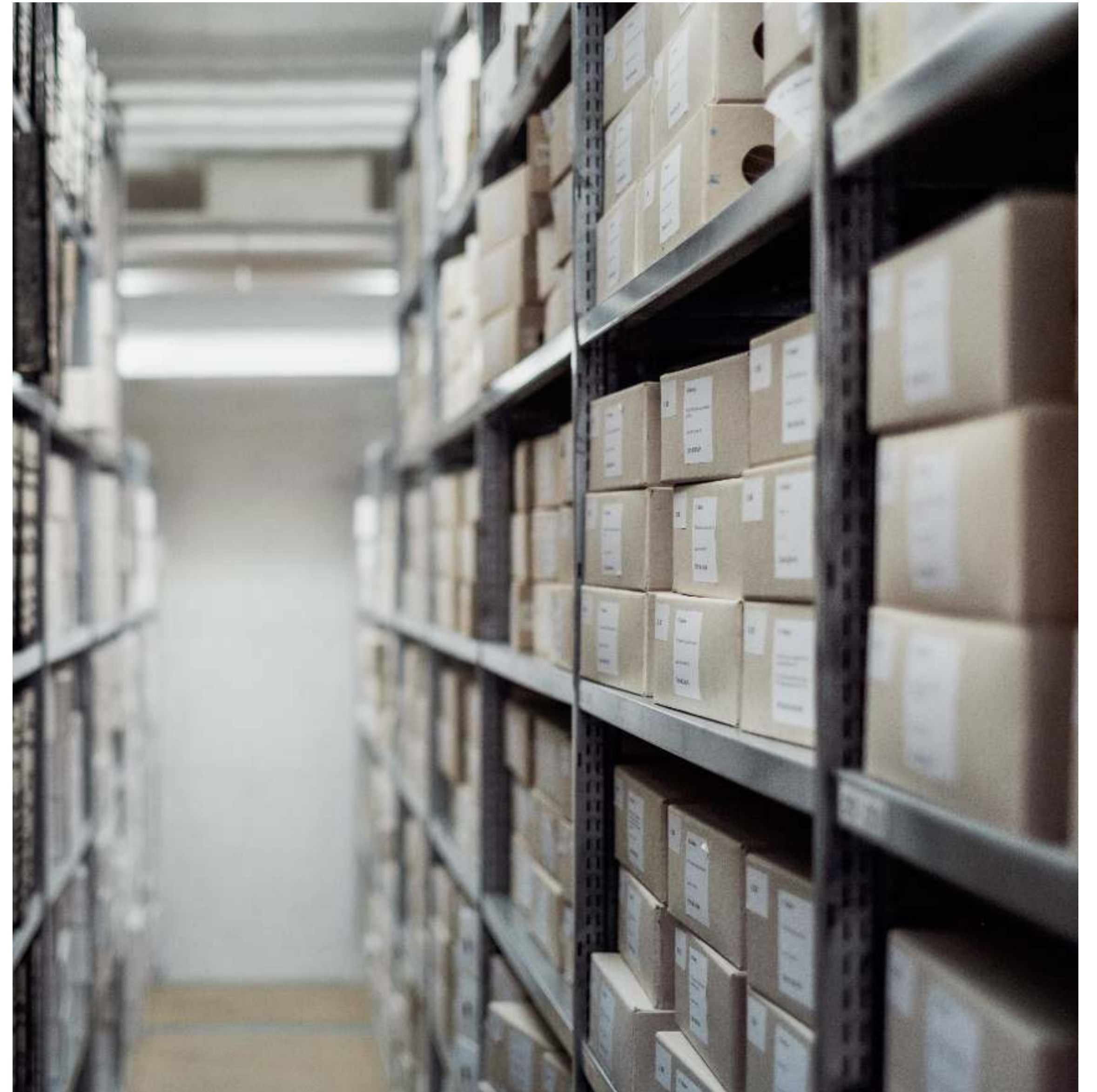
minimize $\sum_{t=0}^{T-1} h(x_t) + o(u_t)$
subject to $x_{t+1} = x_t + u_t - d_t$
 $x_0 = x_{\text{init}}$
 $0 \leq u_t \leq M$



Inventory management

minimize $\sum_{t=0}^{T-1} h(x_t) + o(u_t)$
subject to $x_{t+1} = x_t + u_t - d_t$
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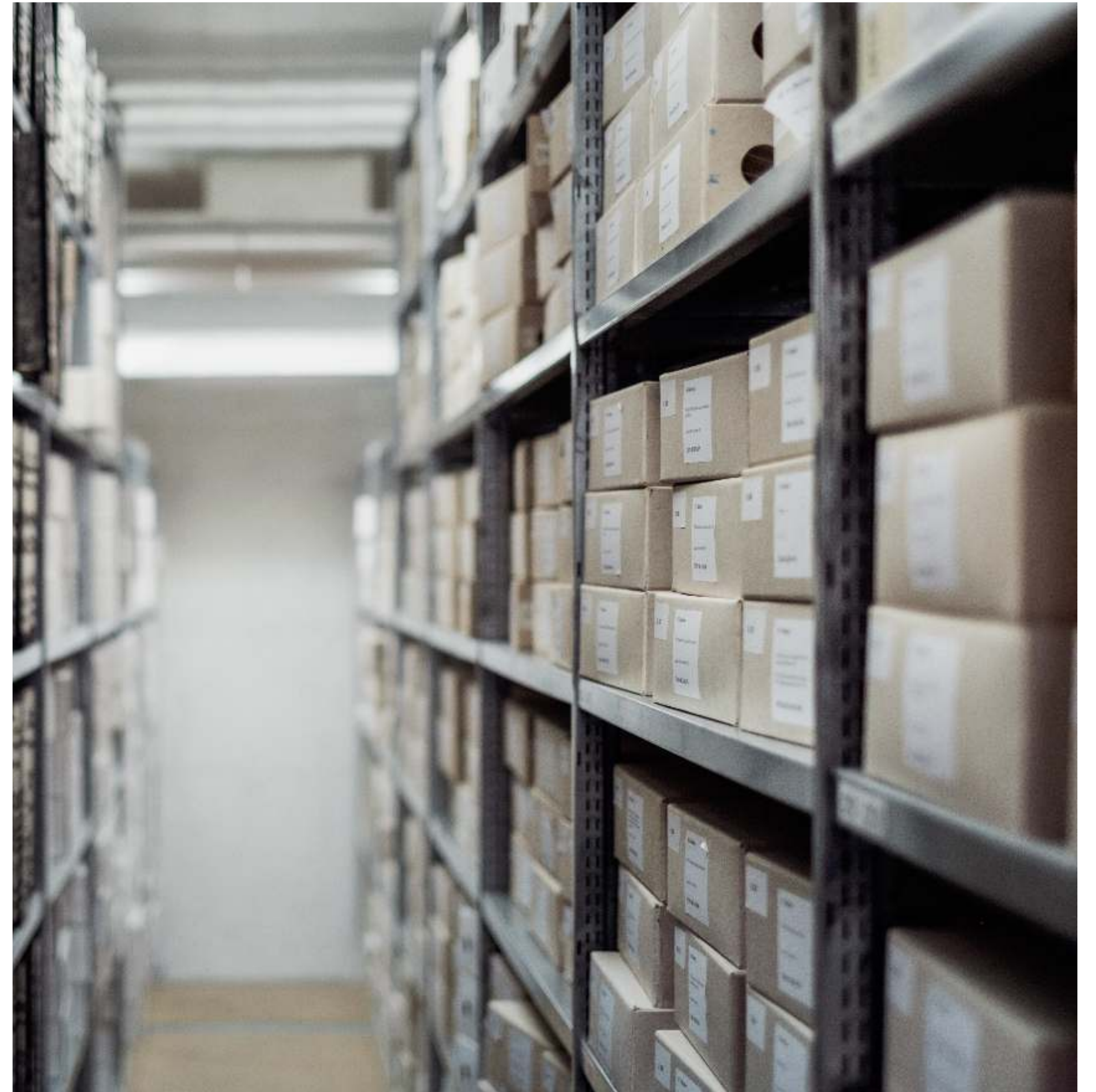
inventory \nearrow
 \uparrow order
 \uparrow demand



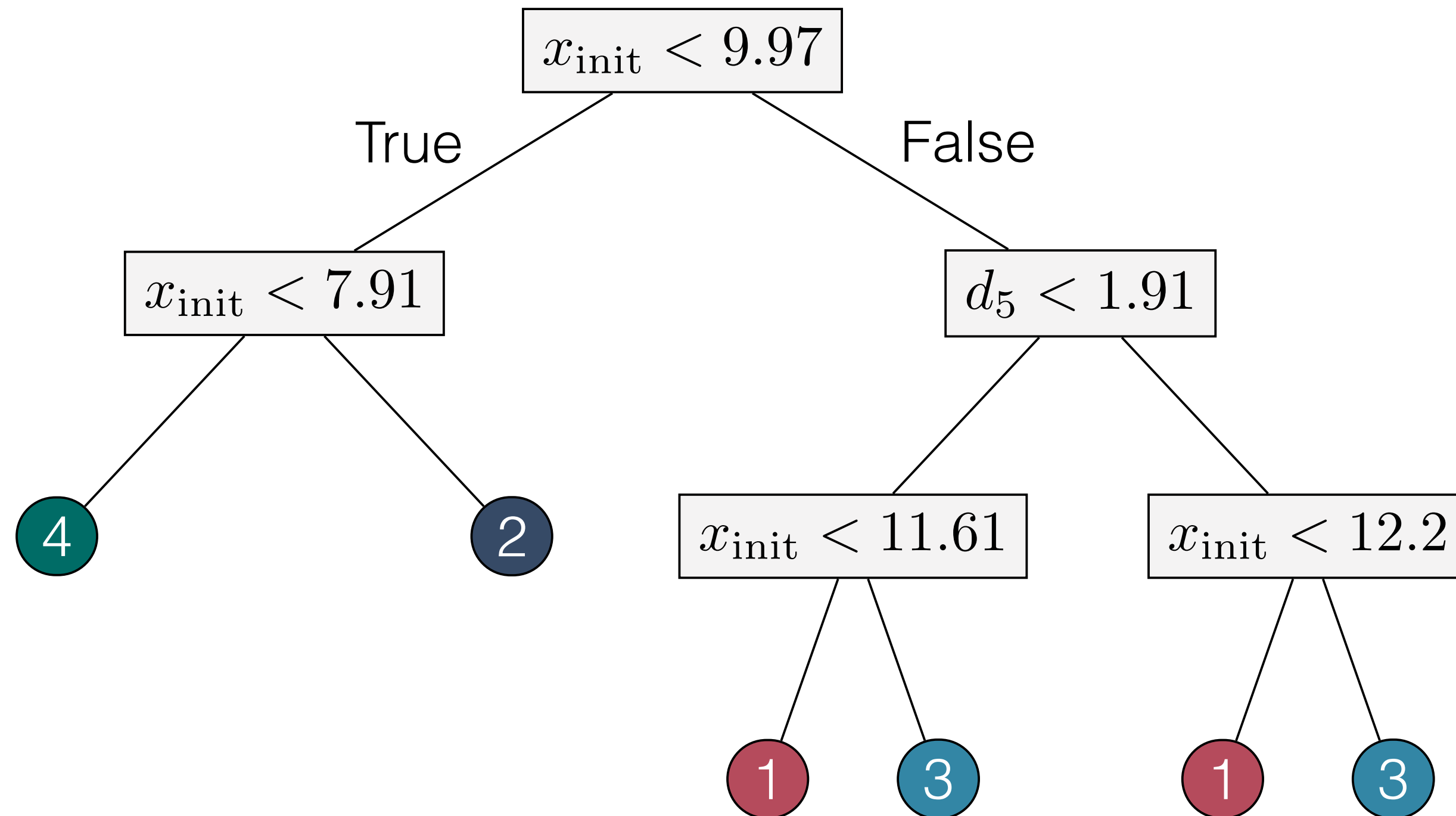
Inventory management

minimize $\sum_{t=0}^{T-1} h(x_t) + o(u_t)$
subject to $x_{t+1} = x_t + u_t - d_t$
 $x_0 = x_{\text{init}}$
 $0 \leq u_t \leq M$

inventory \nearrow
parameters \nearrow
order \uparrow
demand \uparrow

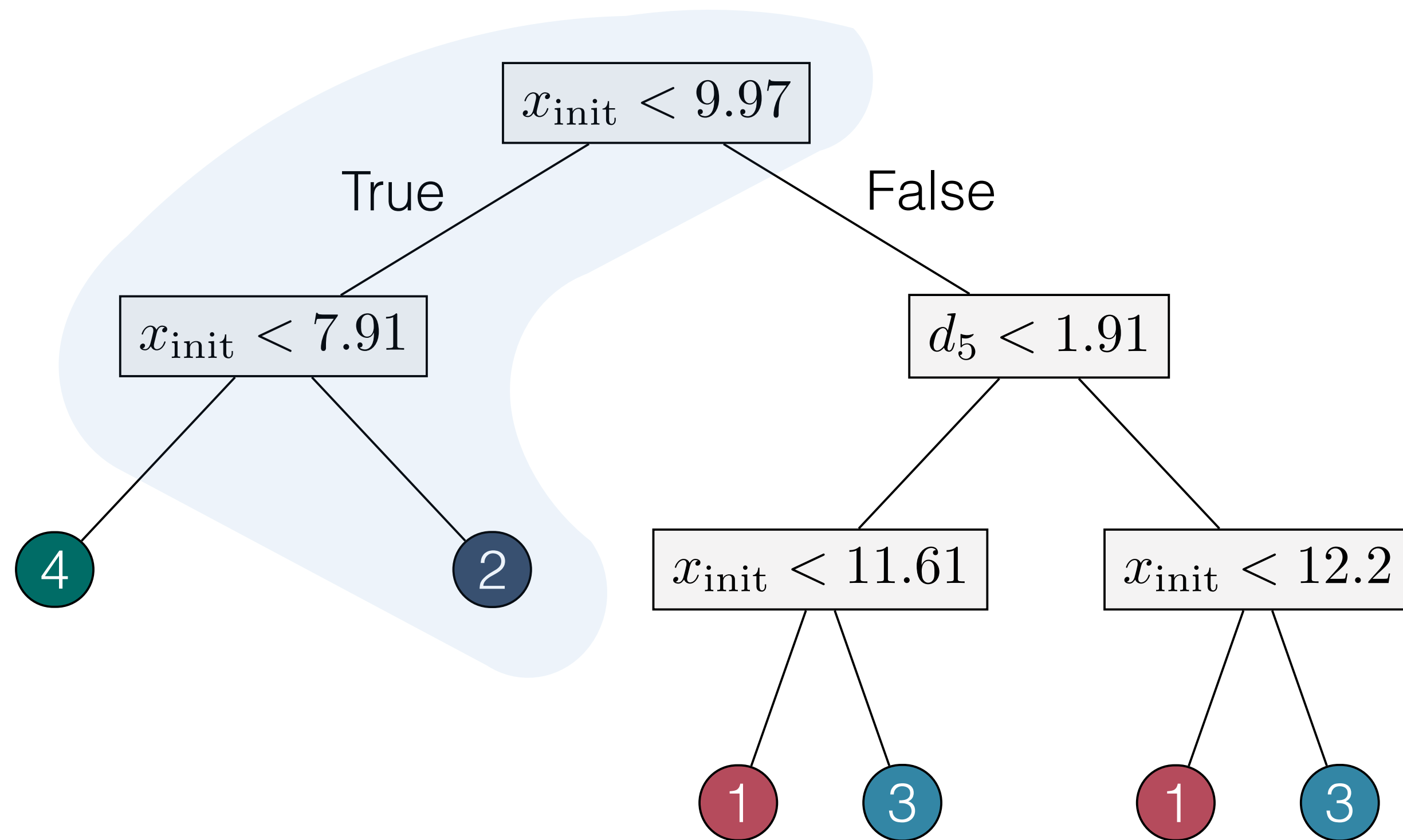


Inventory management strategies



minimize $\sum_{t=0}^{T-1} h(x_t) + o(u_t)$
 subject to $x_{t+1} = x_t + u_t - d_t$
 $x_0 = x_{\text{init}}$
 $0 \leq u_t \leq M$

Inventory management strategies



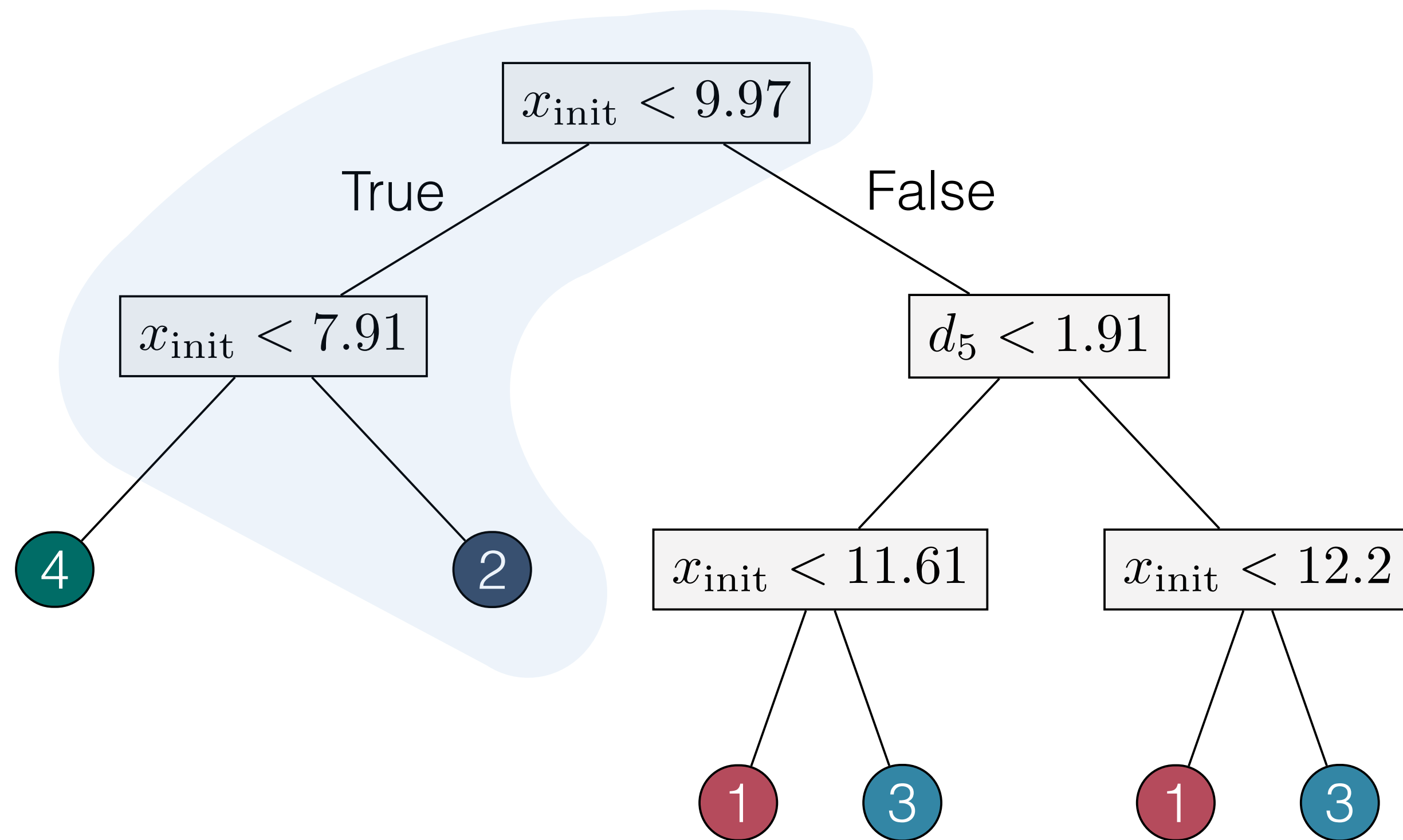
Strategy 2

$$u_t = 0 \quad t \leq 4$$

$$0 \leq u_t \leq M \quad t > 4$$

minimize $\sum_{t=0}^{T-1} h(x_t) + o(u_t)$
 subject to $x_{t+1} = x_t + u_t - d_t$
 $x_0 = x_{\text{init}}$
 $0 \leq u_t \leq M$

Inventory management strategies



Strategy 4

$$u_t = 0 \quad t \leq 3$$

$$0 \leq u_t \leq M \quad t > 3$$

Strategy 2

$$u_t = 0 \quad t \leq 4$$

$$0 \leq u_t \leq M \quad t > 4$$

minimize $\sum_{t=0}^{T-1} h(x_t) + o(u_t)$

subject to $x_{t+1} = x_t + u_t - d_t$

$x_0 = x_{\text{init}}$

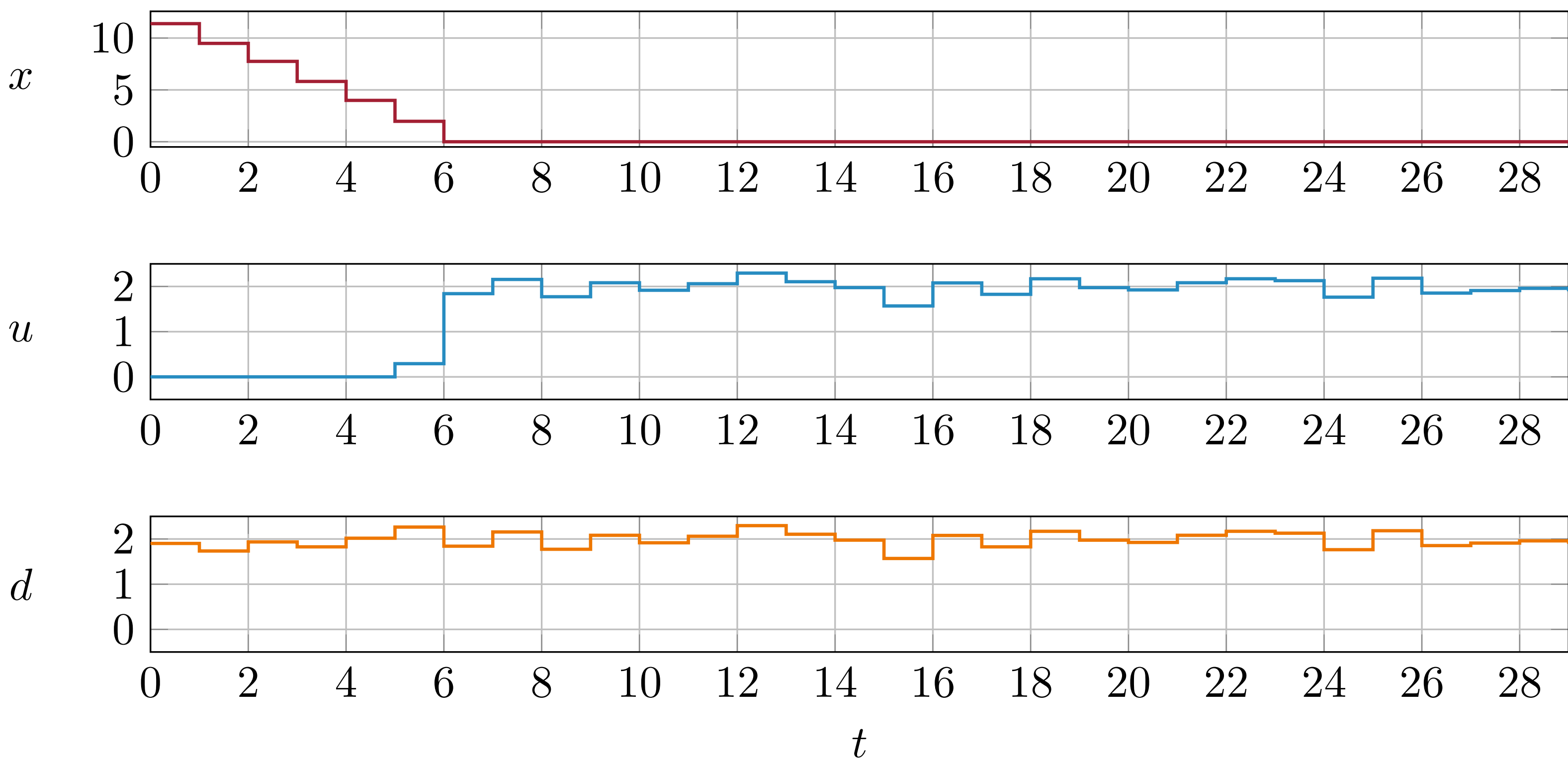
$0 \leq u_t \leq M$

Inventory management trajectory

Strategy 2

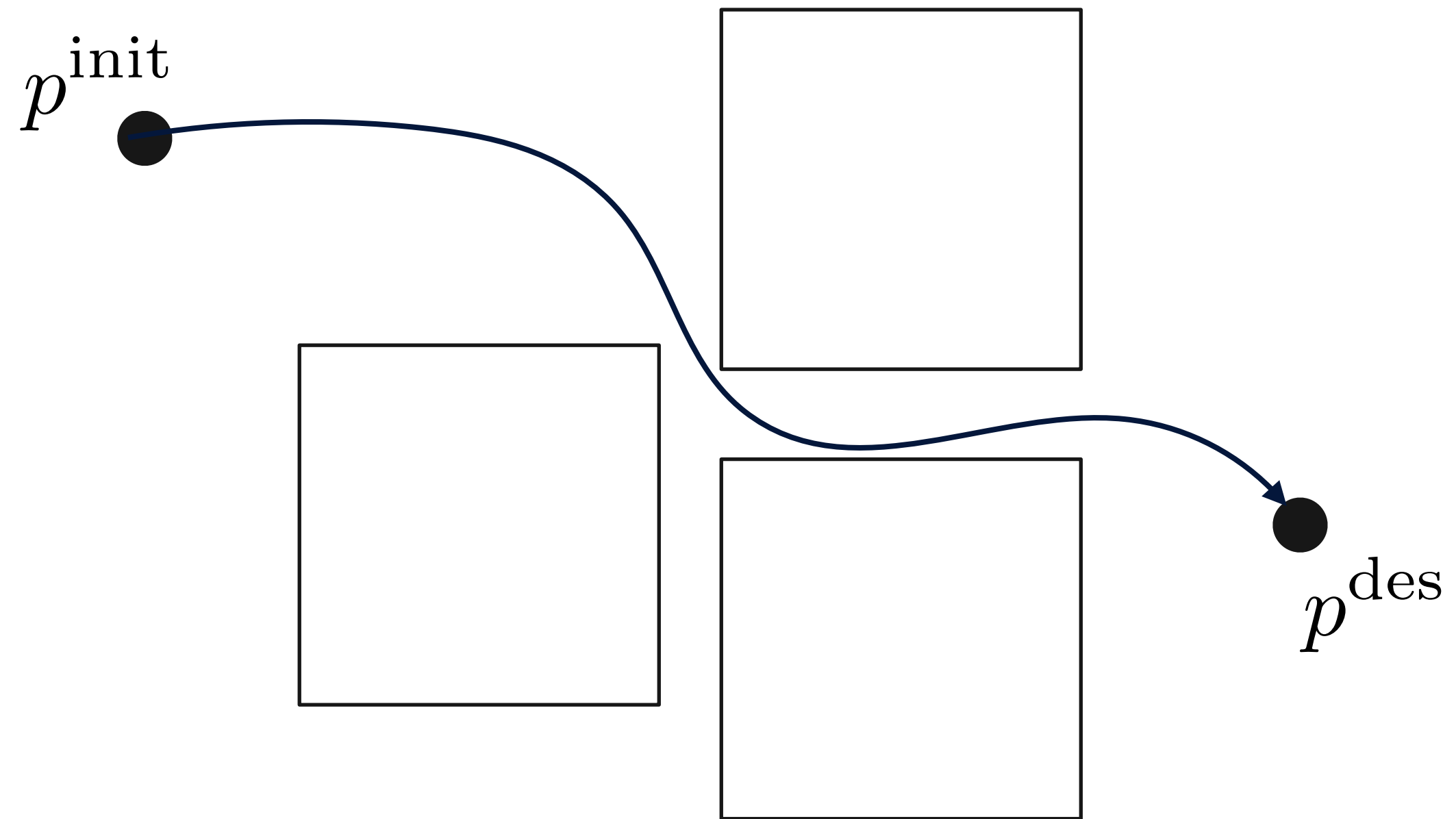
$$u_t = 0 \quad t \leq 4$$

$$0 \leq u_t \leq M \quad t > 4$$



Example

Motion planning with obstacles



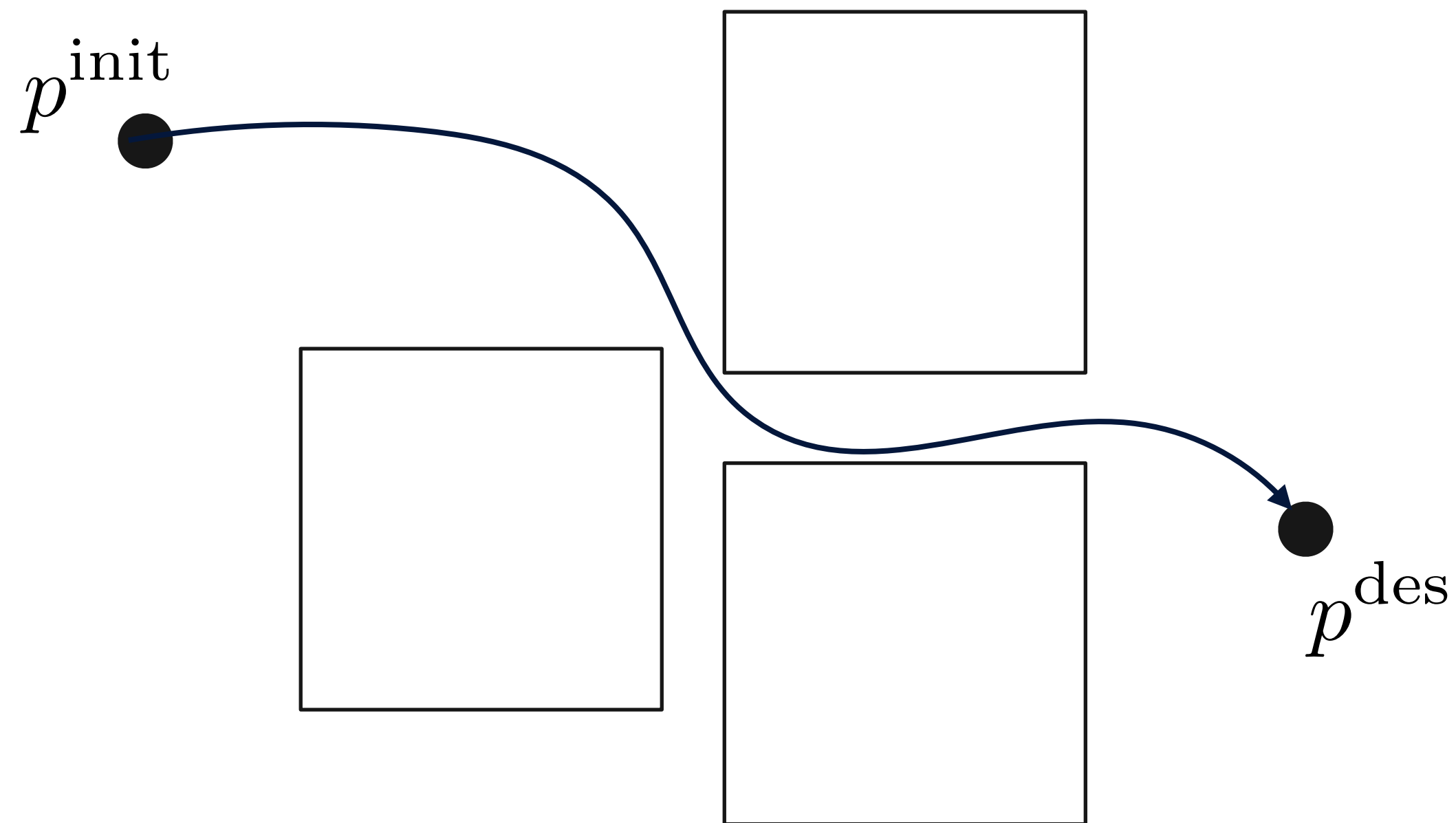
p_t position $\in \mathbf{R}^d$
 v_t velocity $\in \mathbf{R}^d$

p^{init} initial position
 v^{init} initial velocity

p^{des} desired position

Example

Motion planning with obstacles



p_t position $\in \mathbf{R}^d$
 v_t velocity $\in \mathbf{R}^d$

p^{init} initial position
 v^{init} initial velocity

p^{des} desired position

Obstacles

Obstacle i is a box $[\underline{o}^i, \overline{o}^i]$

Motion planning formulation

$$\text{minimize} \quad \|p_T - p^{\text{des}}\|_2^2 + \sum_{t=0}^{T-1} \|p_t - p^{\text{des}}\|_2^2 + \gamma \|u_t\|_2^2$$

Motion planning formulation

minimize $\|p_T - p^{\text{des}}\|_2^2 + \sum_{t=0}^{T-1} \|p_t - p^{\text{des}}\|_2^2 + \gamma \|u_t\|_2^2$

subject to $(p_{t+1}, v_{t+1}) = A(p_t, v_t) + Bu_t$
 $p_0 = p^{\text{init}}, \quad v_0 = v^{\text{init}}$

Dynamics

Motion planning formulation

\mathbb{R}^3 \mathbb{R}^2

minimize $\|p_T - p^{\text{des}}\|_2^2 + \sum_{t=0}^{T-1} \|p_t - p^{\text{des}}\|_2^2 + \gamma \|u_t\|_2^2$

subject to $(p_{t+1}, v_{t+1}) = A(p_t, v_t) + Bu_t$
 $p_0 = p^{\text{init}}, \quad v_0 = v^{\text{init}}$

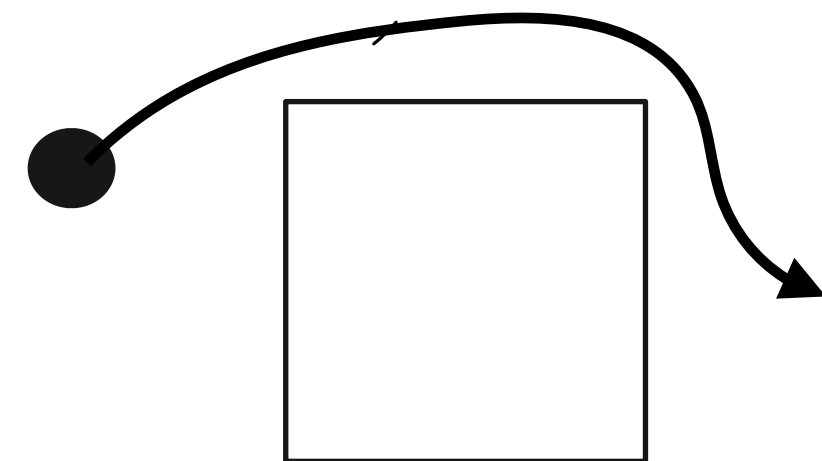
Dynamics

$$\bar{o}^i - M\bar{\delta}_t^i \leq p_t \leq \underline{o}^i + M\underline{\delta}_t^i, \quad i = 1, \dots, n_{\text{obs}}$$

$$\mathbf{1}^T \underline{\delta}_t^i + \mathbf{1}^T \bar{\delta}_t^i \leq 2d - 1$$

Obstacle avoidance

$$\bar{\delta}_t^i, \underline{\delta}_t^i \in \{0, 1\}^d, \quad i = 1, \dots, n_{\text{obs}}$$



Motion planning with obstacles

Worst-case timings

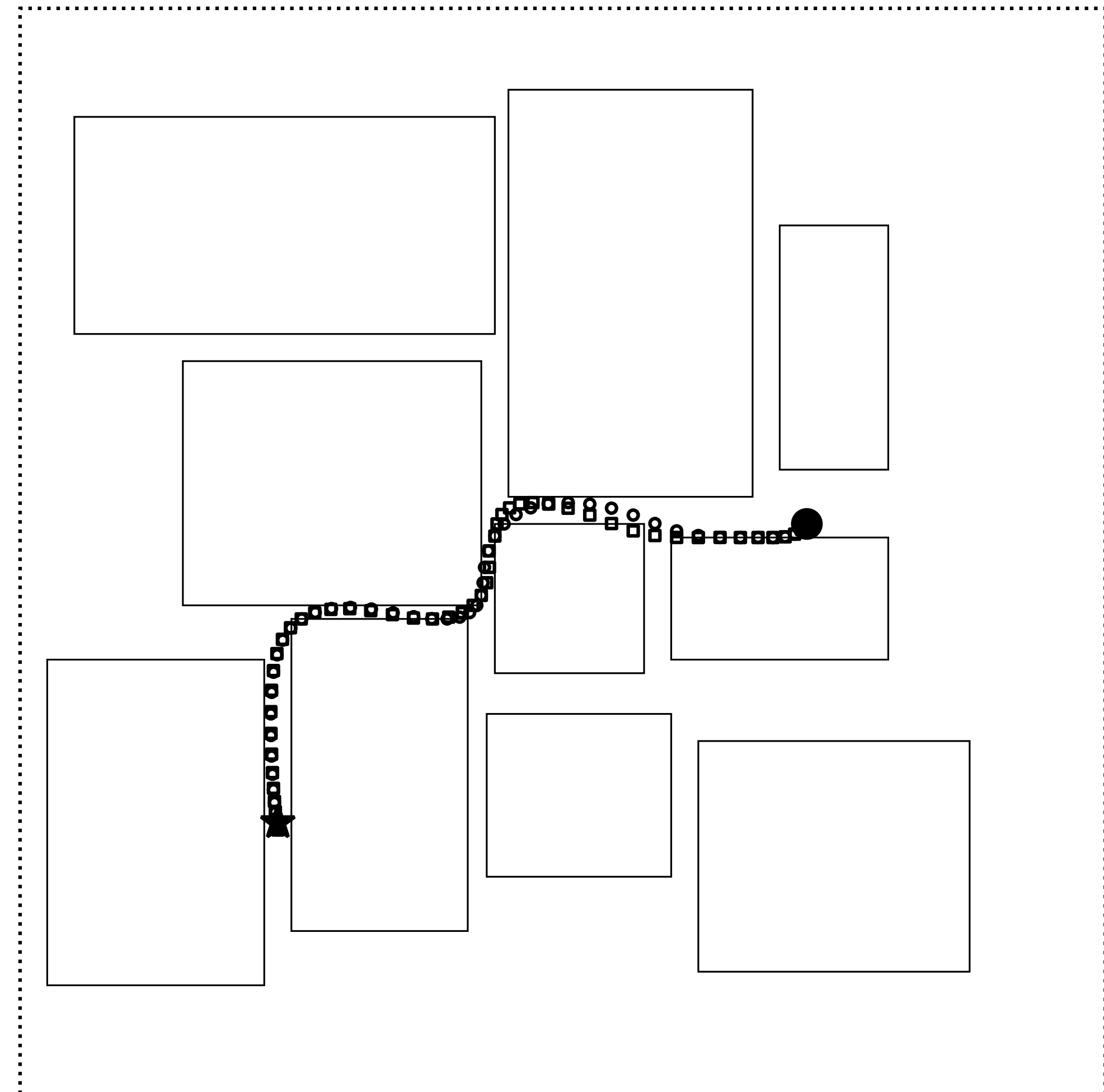
$n_{\text{obstacles}}$	n_{var}	n_{constr}	t_{max} MLOPT [s]	t_{max} Gurobi [s]	t_{max} Gurobi heuristic [s]	0-2 10%
2	1135	3773	0.4145	2.3776	2.2962	
4	1615	10133	0.1878	11.8172	8.1443	
6	2095	20333	0.3173	33.7869	11.5292	
8	2575	34373	0.2235	392.3073	128.4948	
10	3055	52253	0.2896	773.1476	206.4520	

2600x speedups

Motion planning with obstacles

Circles
optimal

Squares
MLOPT



Learning strategies in parametric optimization

Benefits

- Extremely fast
- Simple online method for nonconvex optimization
- It learns from your pool of problems

Downsides

- No optimality guarantees
- Relies on many offline solutions (expert demonstrations)

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Future directions

- Better NN architectures
- Optimality guarantees
- Reinforcement learning when we do not have offline solutions

Data-driven algorithms

Today, we learned recent research on data-driven algorithms:

- **Learning heuristics** in branch and bound search (global algorithm)
- **Learning strategies** in parametric optimization (heuristic algorithm)

Many more exciting directions

Differentiable optimization layers, reinforcement learning in optimization, learning-augmented first order methods, ...

Next lecture

- Course recap and conclusions