A Machine Learning Approach to Optimization

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MIT MANAGEMENT SLOAN SCHOOL → PRINCETON UNIVERSITY

ORFE Operations Research & Financial Engineering

MADDD seminar
UC Davis
June 9, 2020



TIMES
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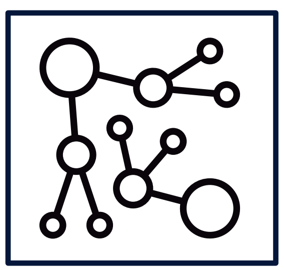
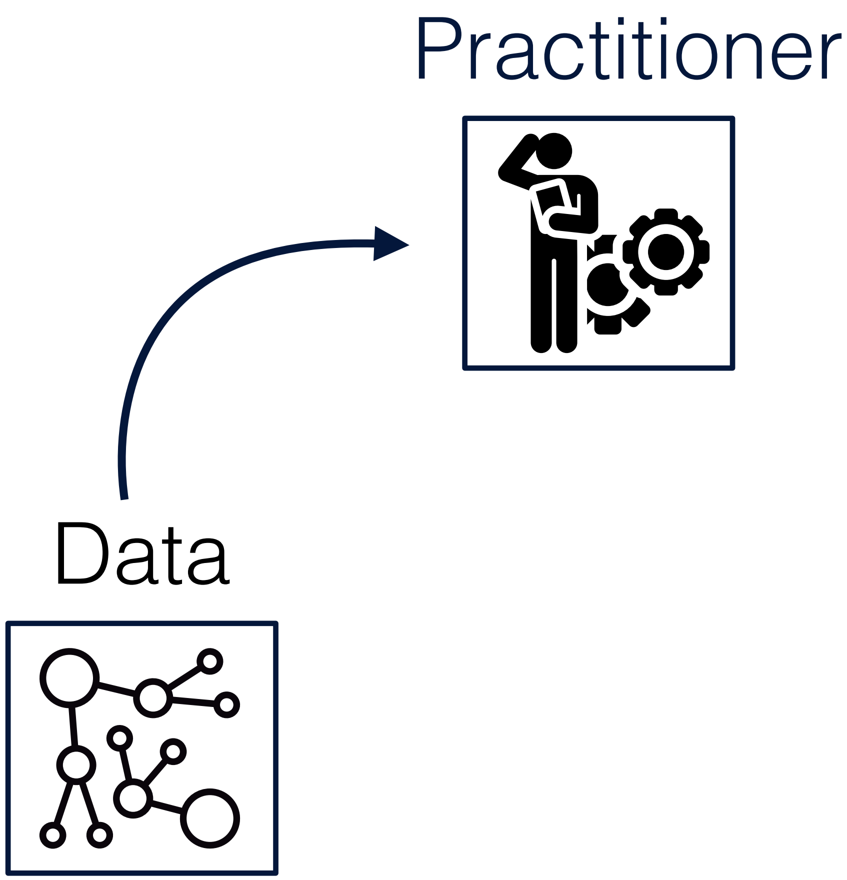
The decision-making workflow

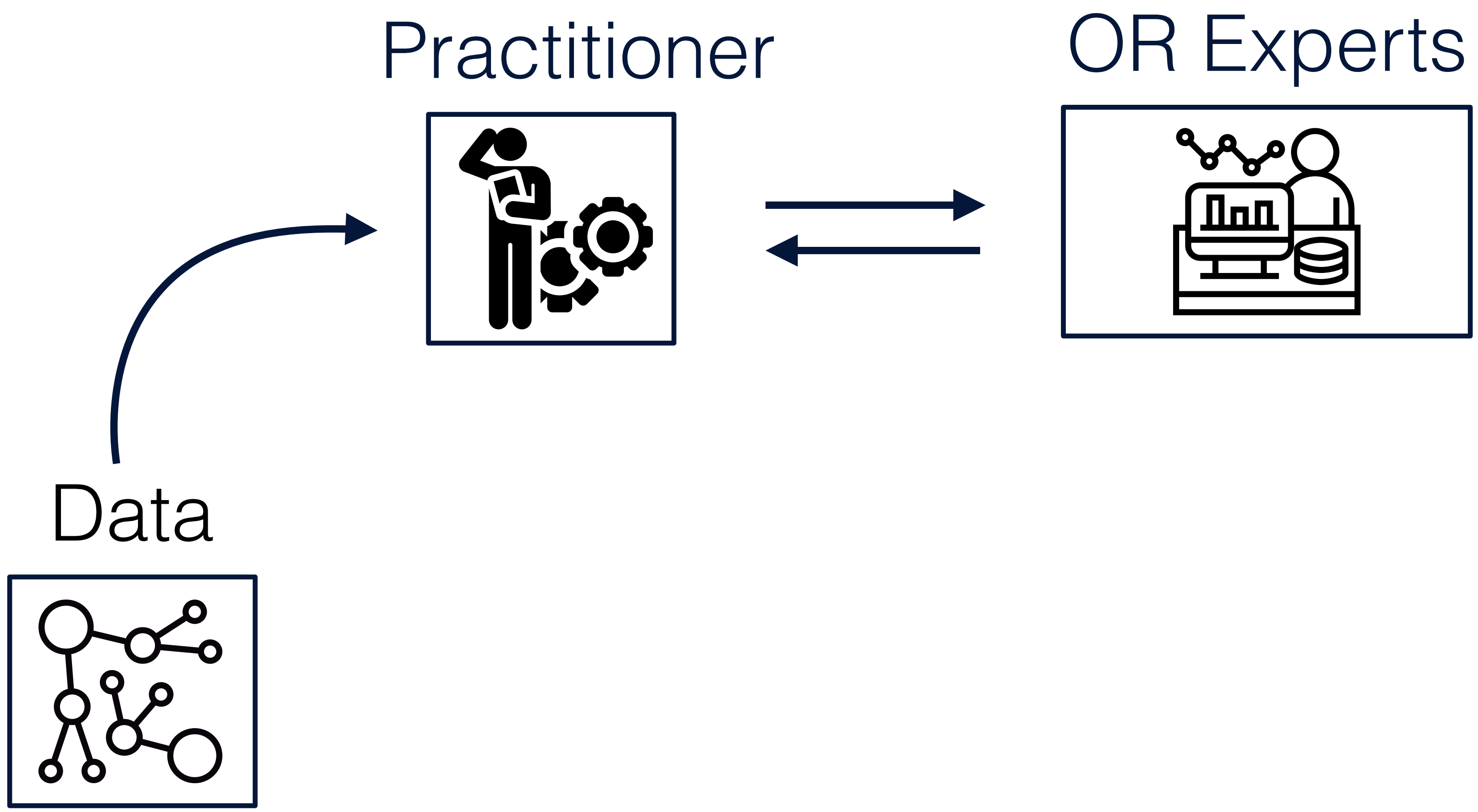
Data



The decision-making workflow



The decision-making workflow



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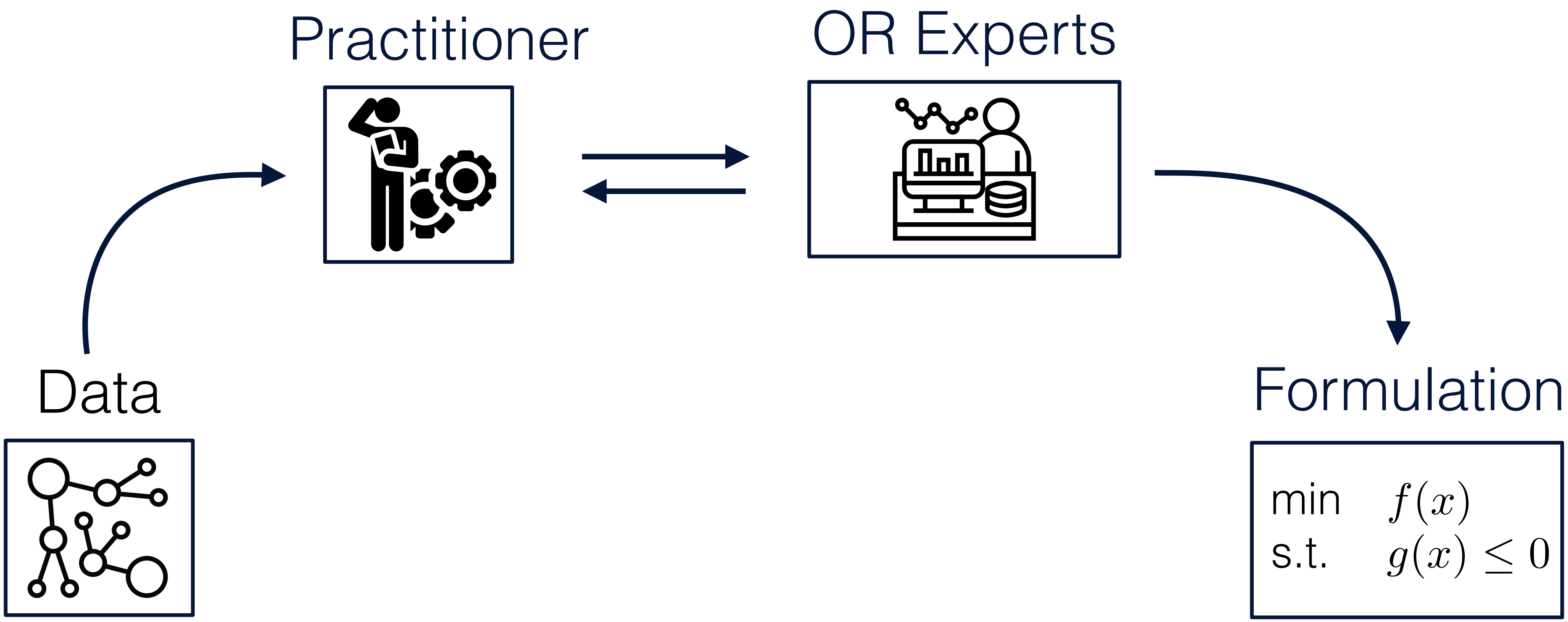

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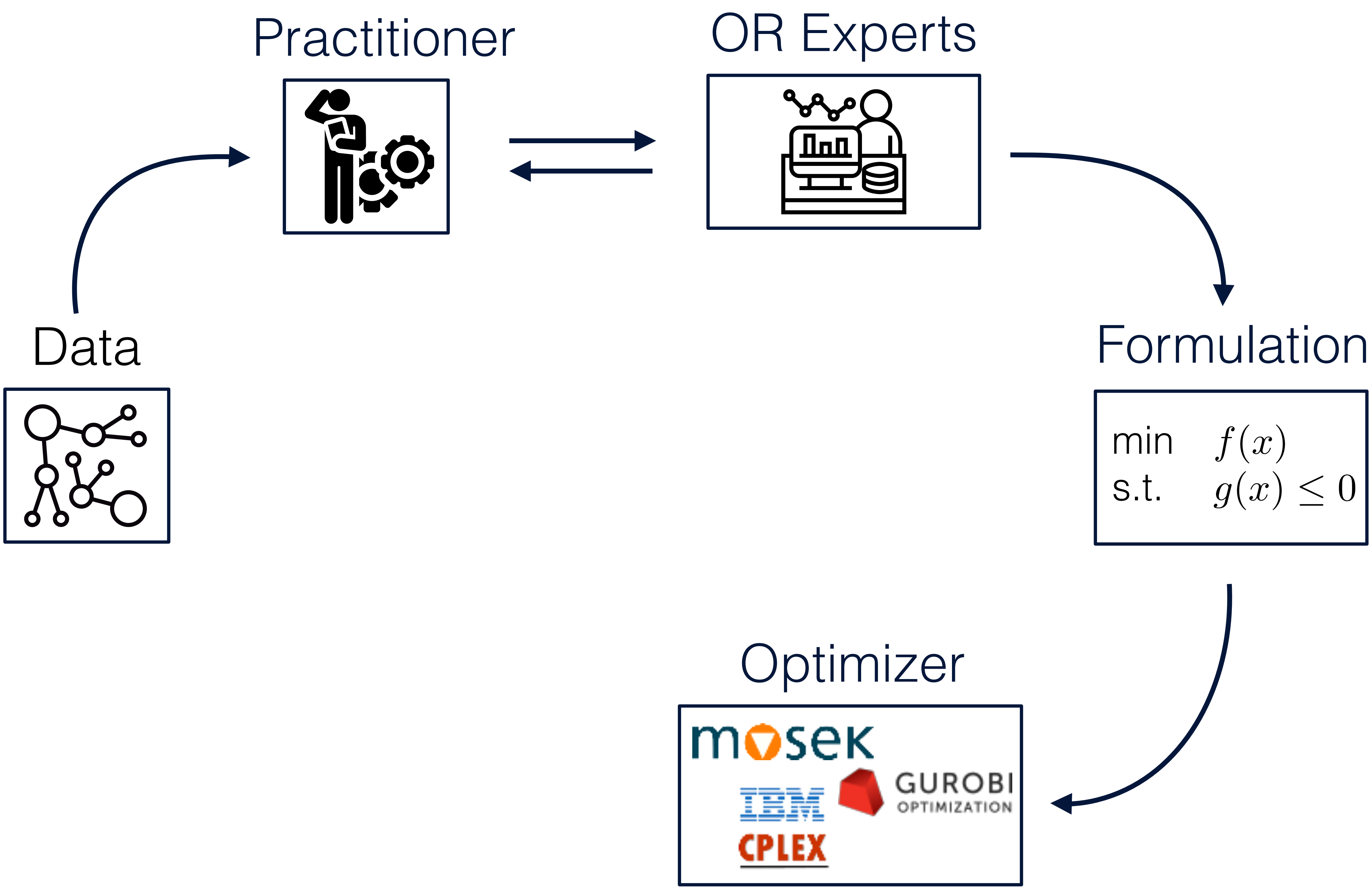

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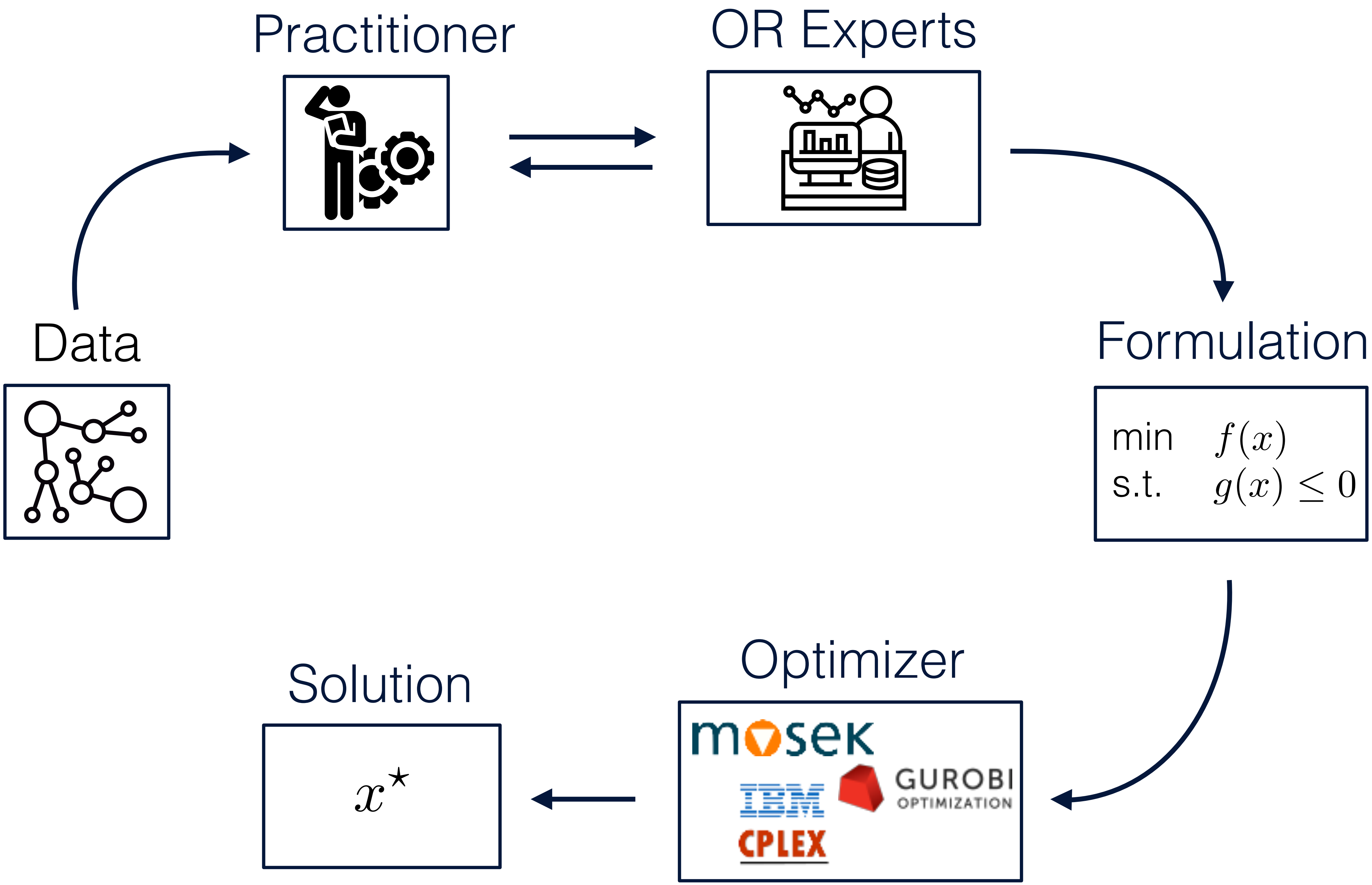

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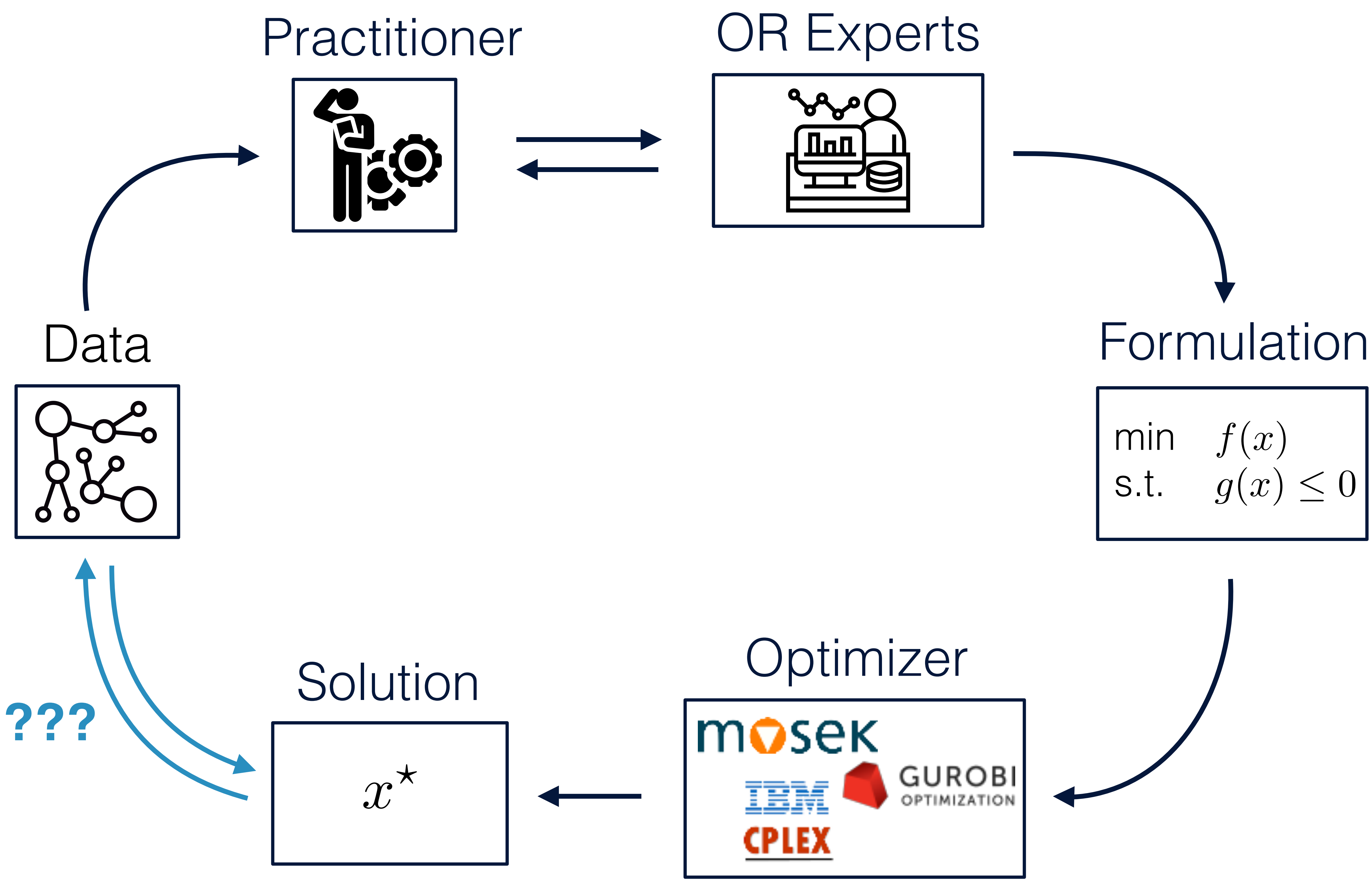
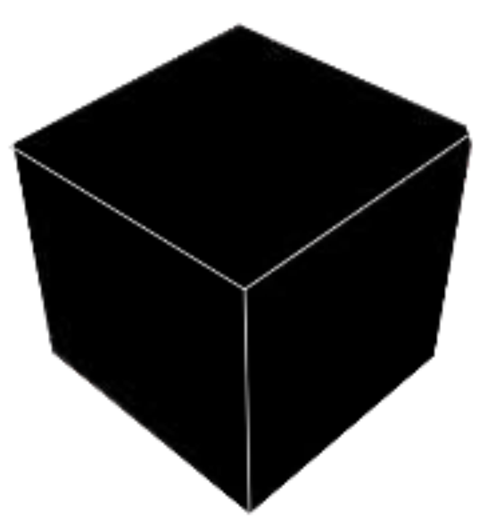


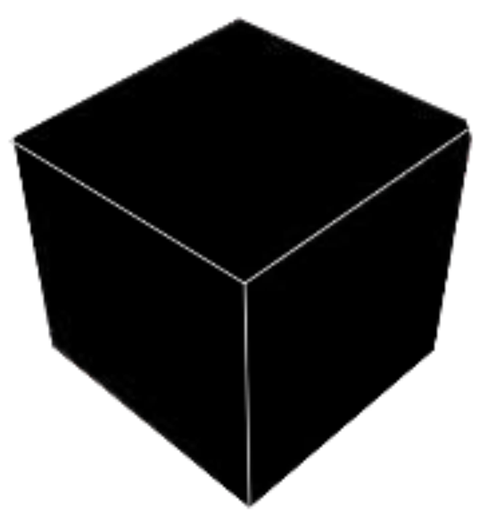
Limitations of traditional optimization

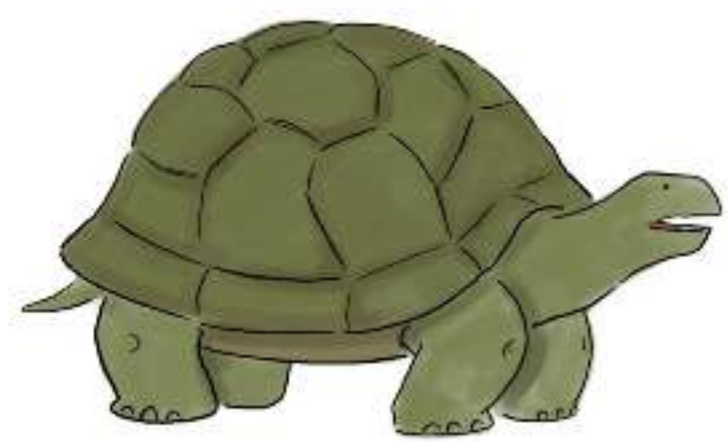
Limitations of traditional optimization

$\theta \longrightarrow$ **Optimization** $\longrightarrow x^\star$



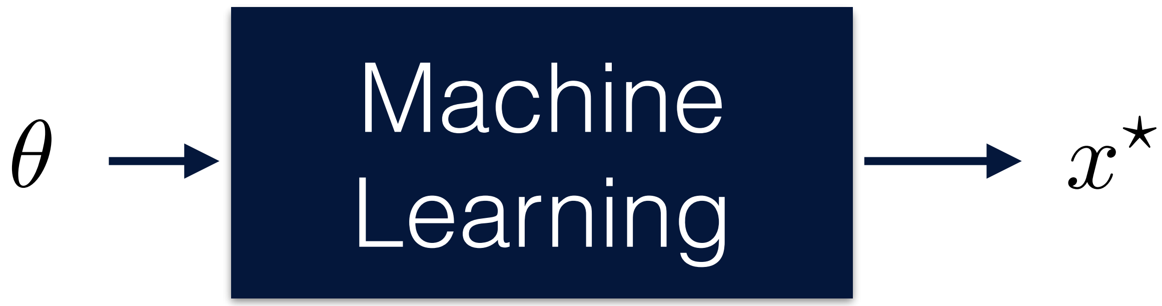
Limitations of traditional optimization





Existing methods

Machine learning for optimization



Comb. Opt: [Smith (1999)]
TSP: [Vinyals et al. (2017)]

Existing methods

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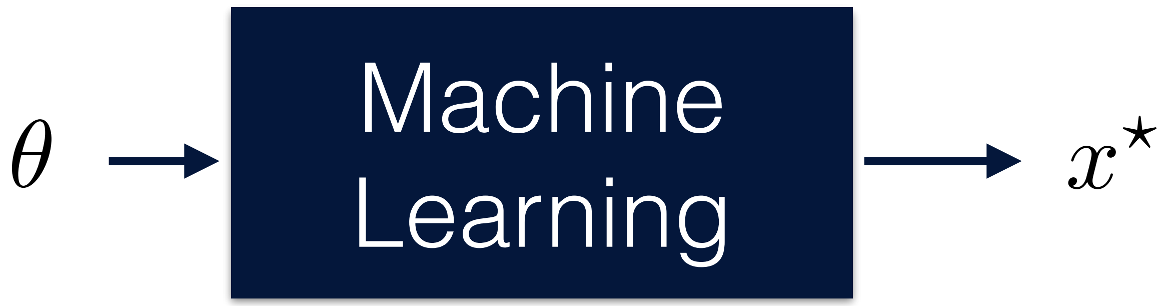

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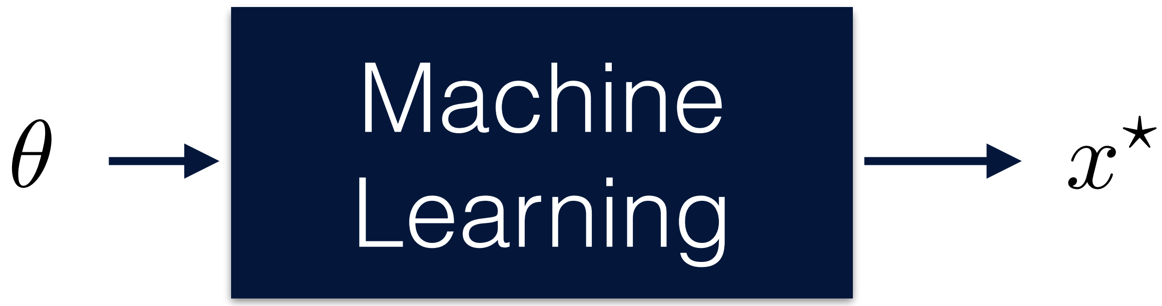
Very small problems

Imprecise

Existing methods

Machine learning for optimization



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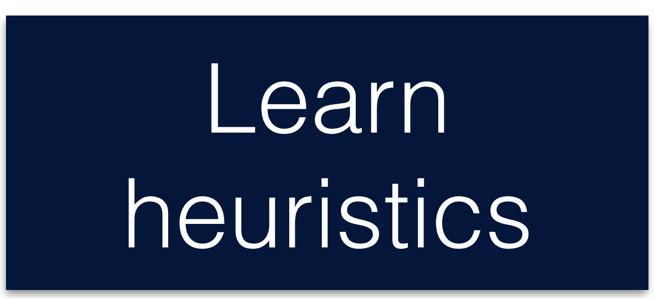
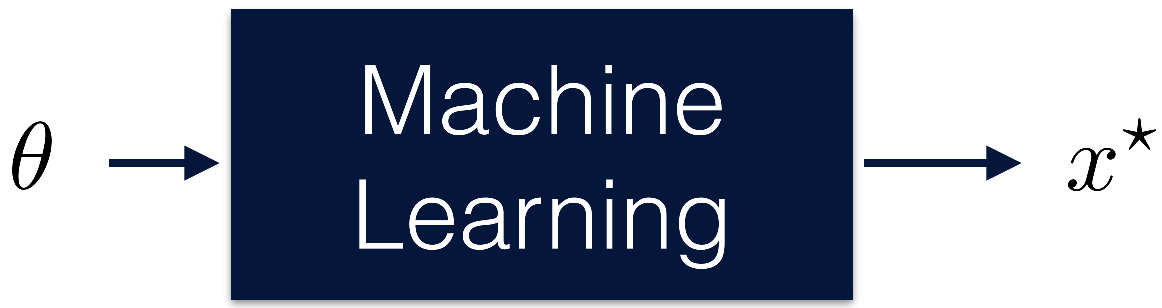


B&B: [Khalil et al. (2016)]
Decompositions [Bonami et al. (2018)]
TSP: [Khalil et al. (2017)]
Cuts: [Tang et a. (2020)]
Many more…

Existing methods

Machine learning for optimization



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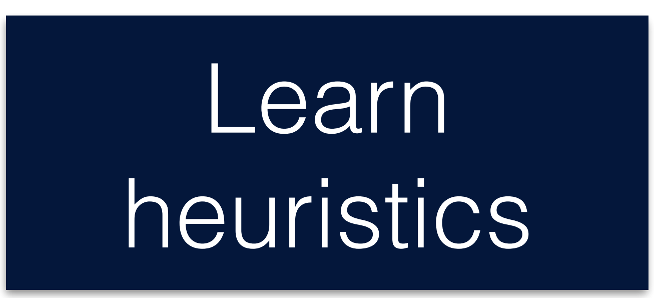

Still hard to solve

No parametric problems

B&B: [Khalil et al. (2016)]
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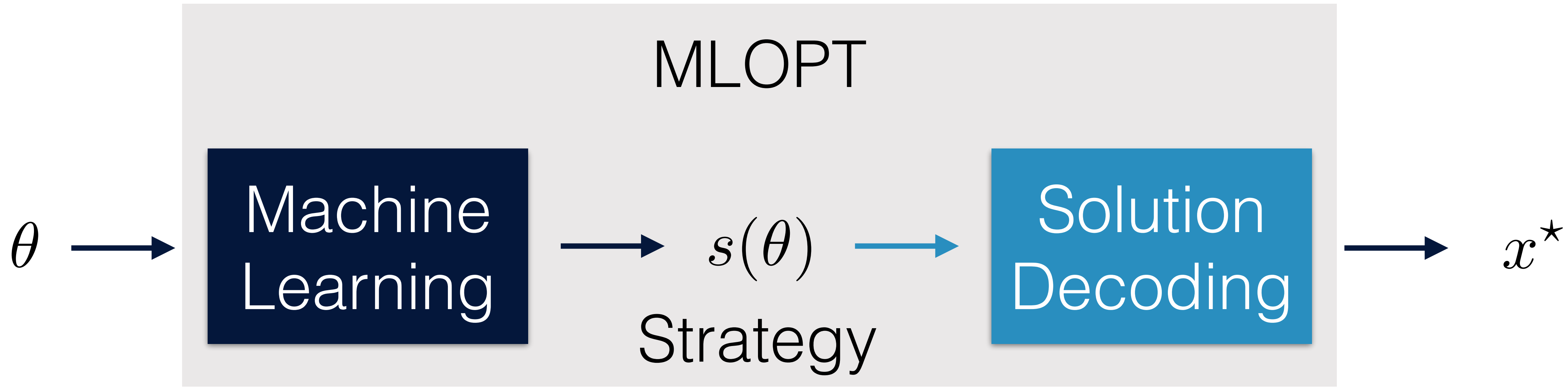
Many more…

Machine learning optimizer



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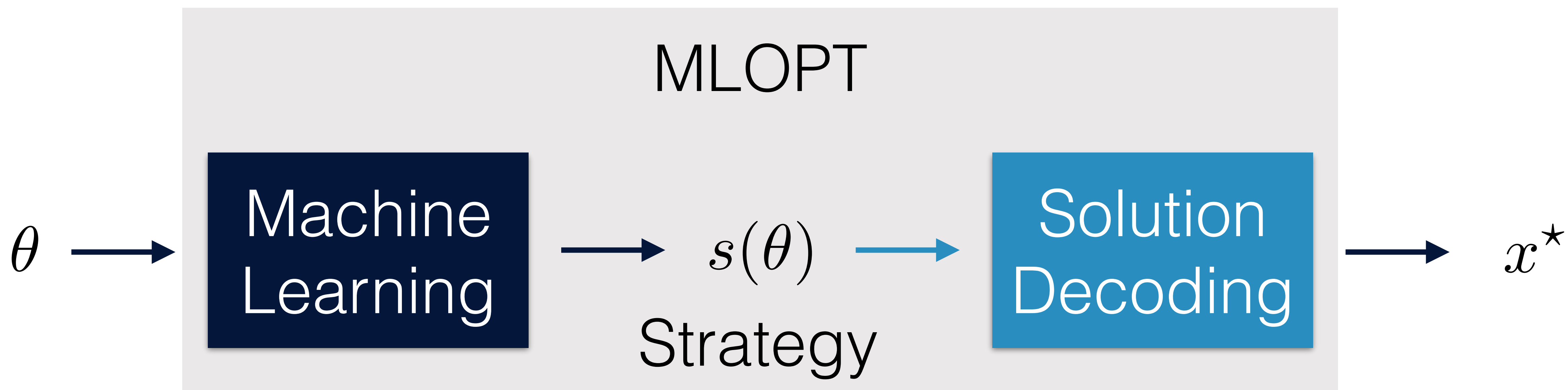

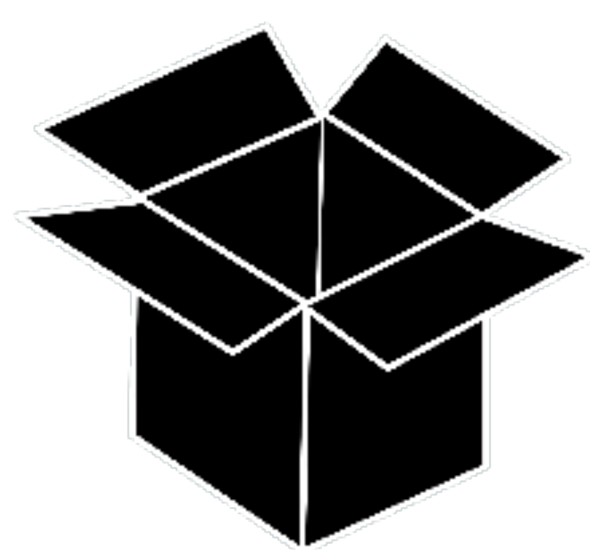

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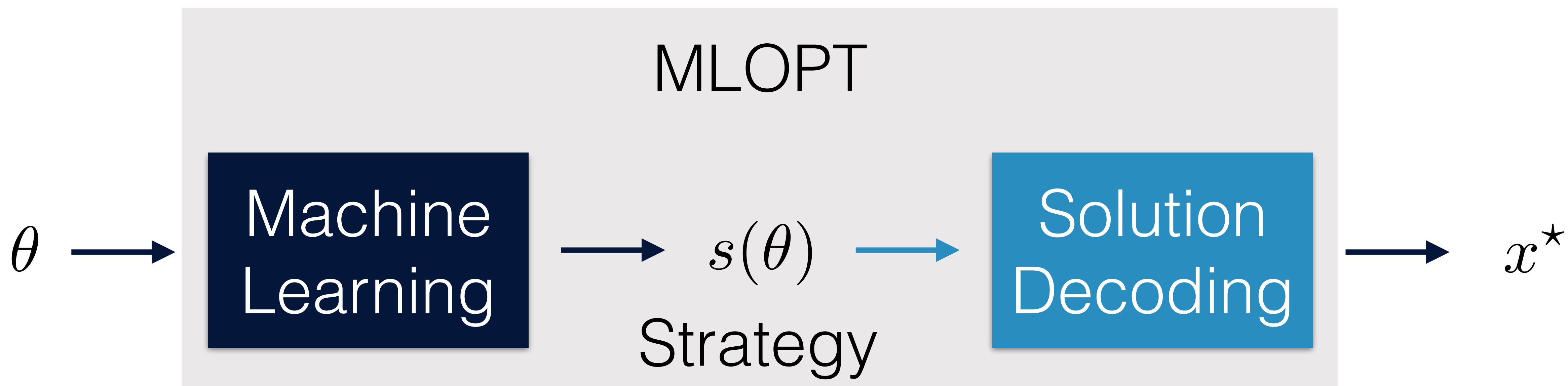
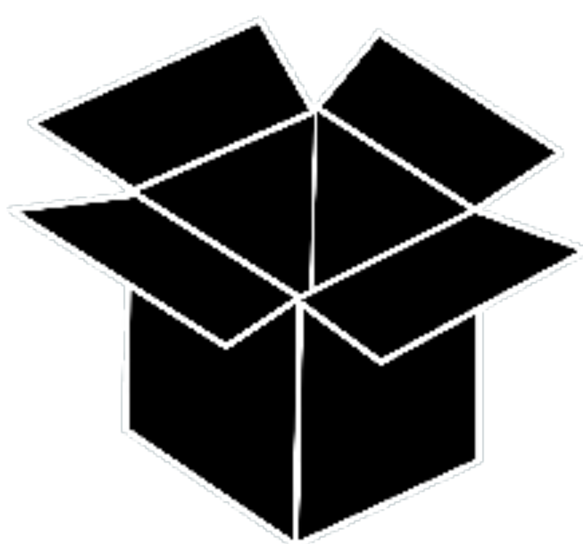




Machine learning optimizer

Optimal Strategies

Strategy Prediction

Strategy Exploration

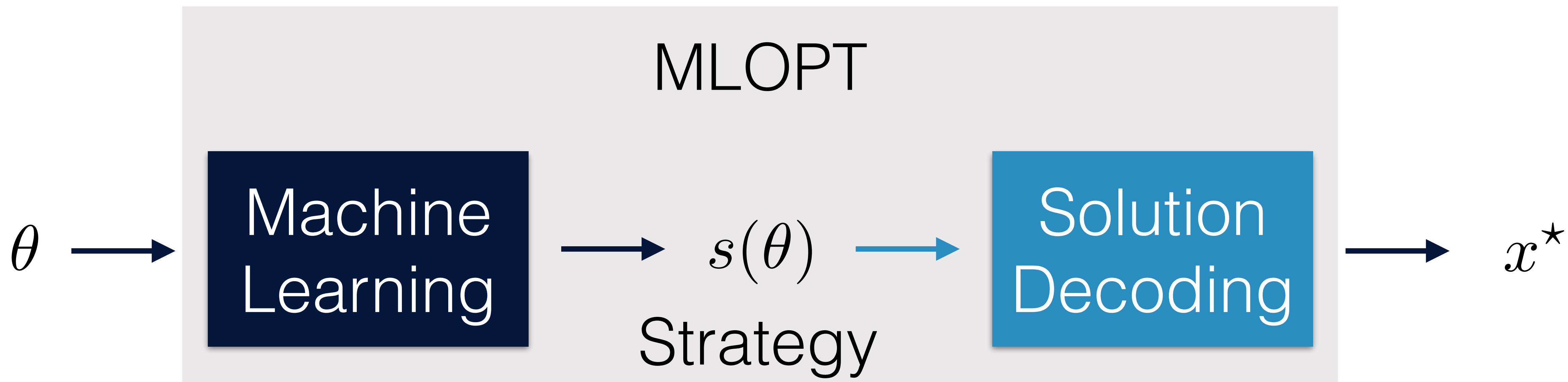
Speedups

Examples

Machine learning optimizer

- Optimal Strategies
- Strategy Prediction
- Strategy Exploration
- Speedups
- Examples

Machine learning optimizer



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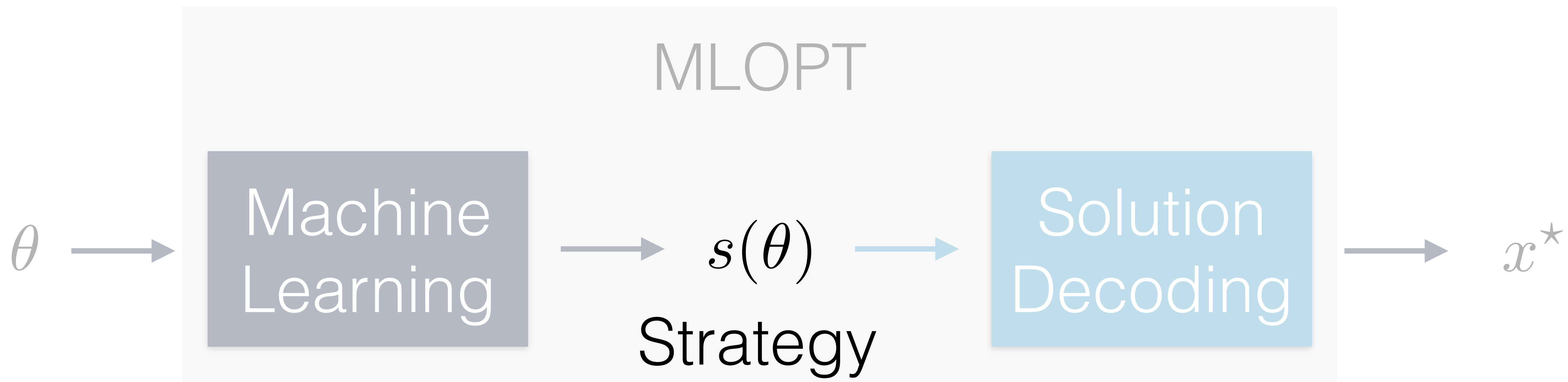
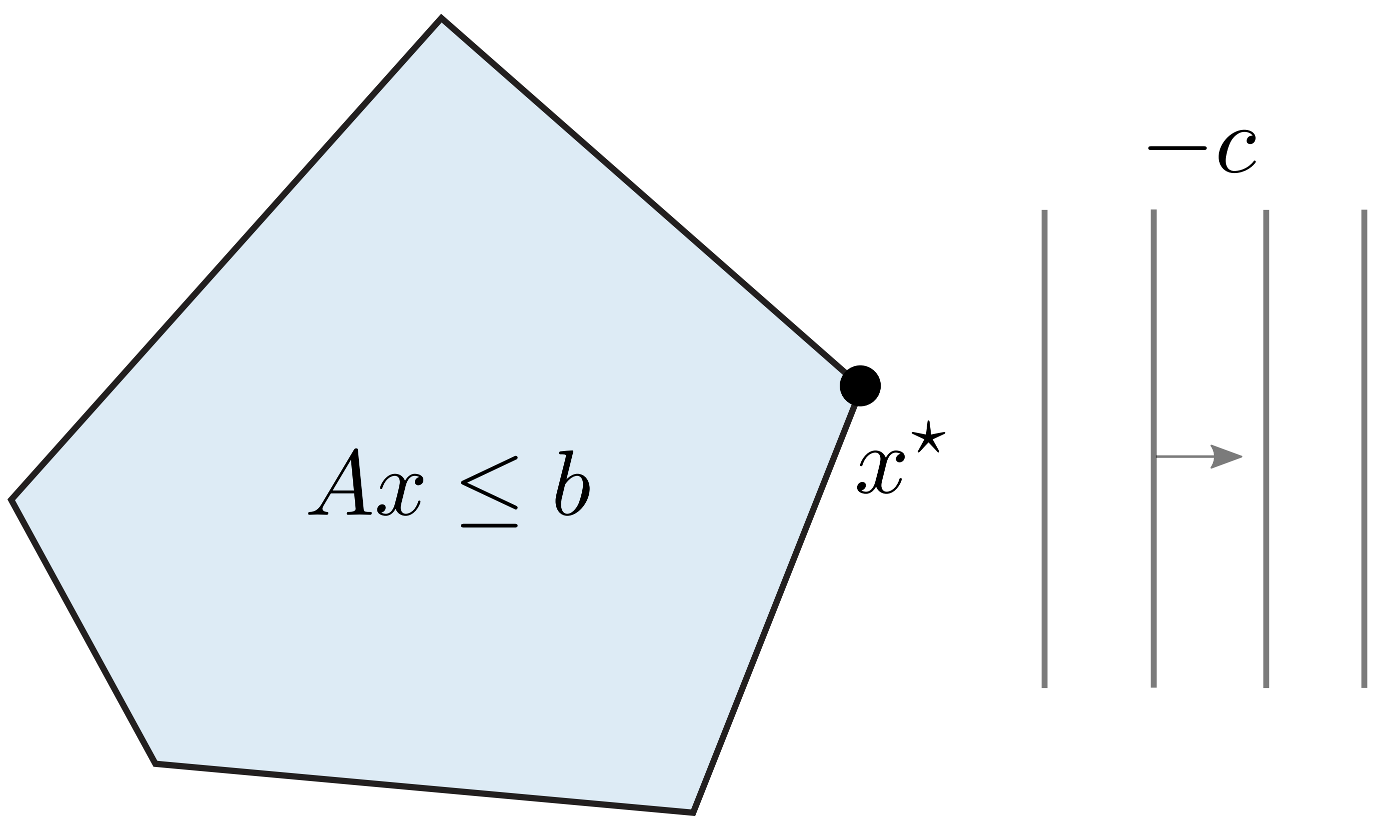


The complete information to efficiently get the optimal solution

$$s(\theta)$$

Linear optimization

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



Linear optimization

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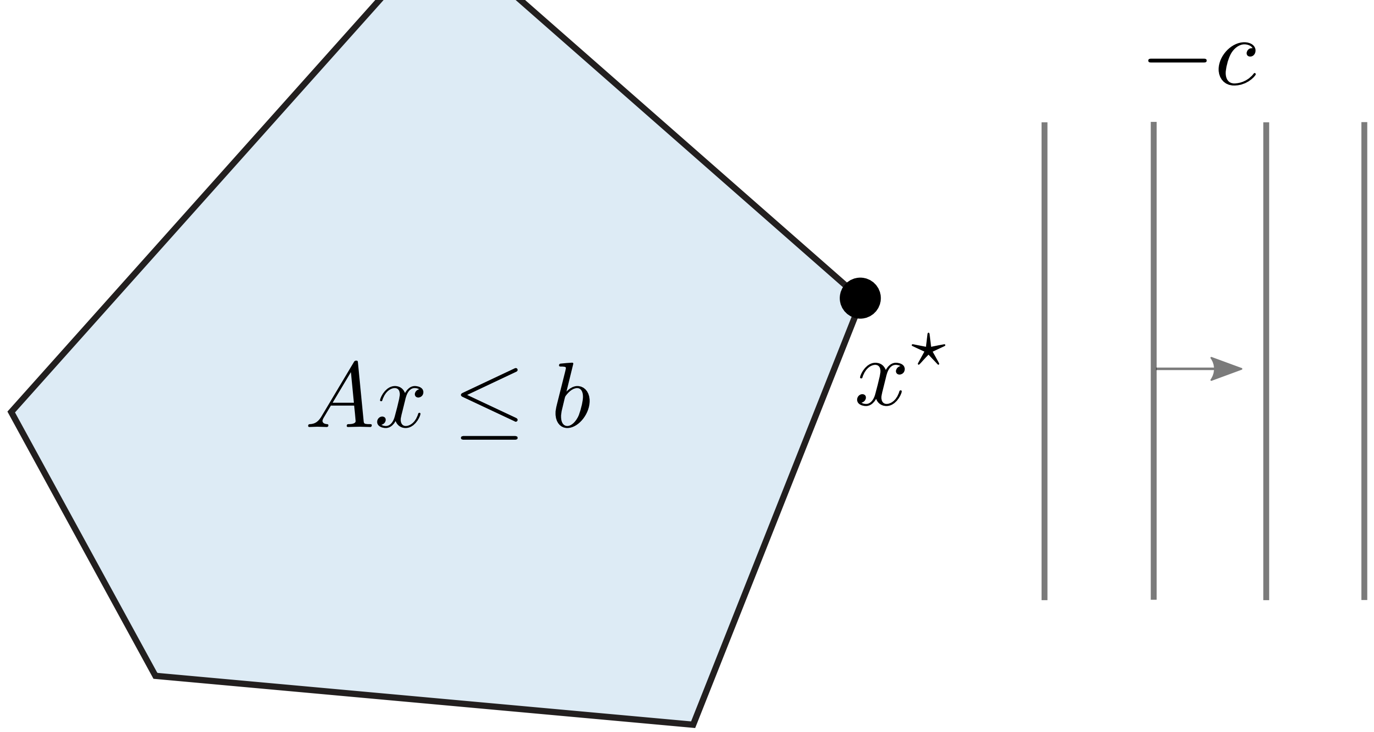
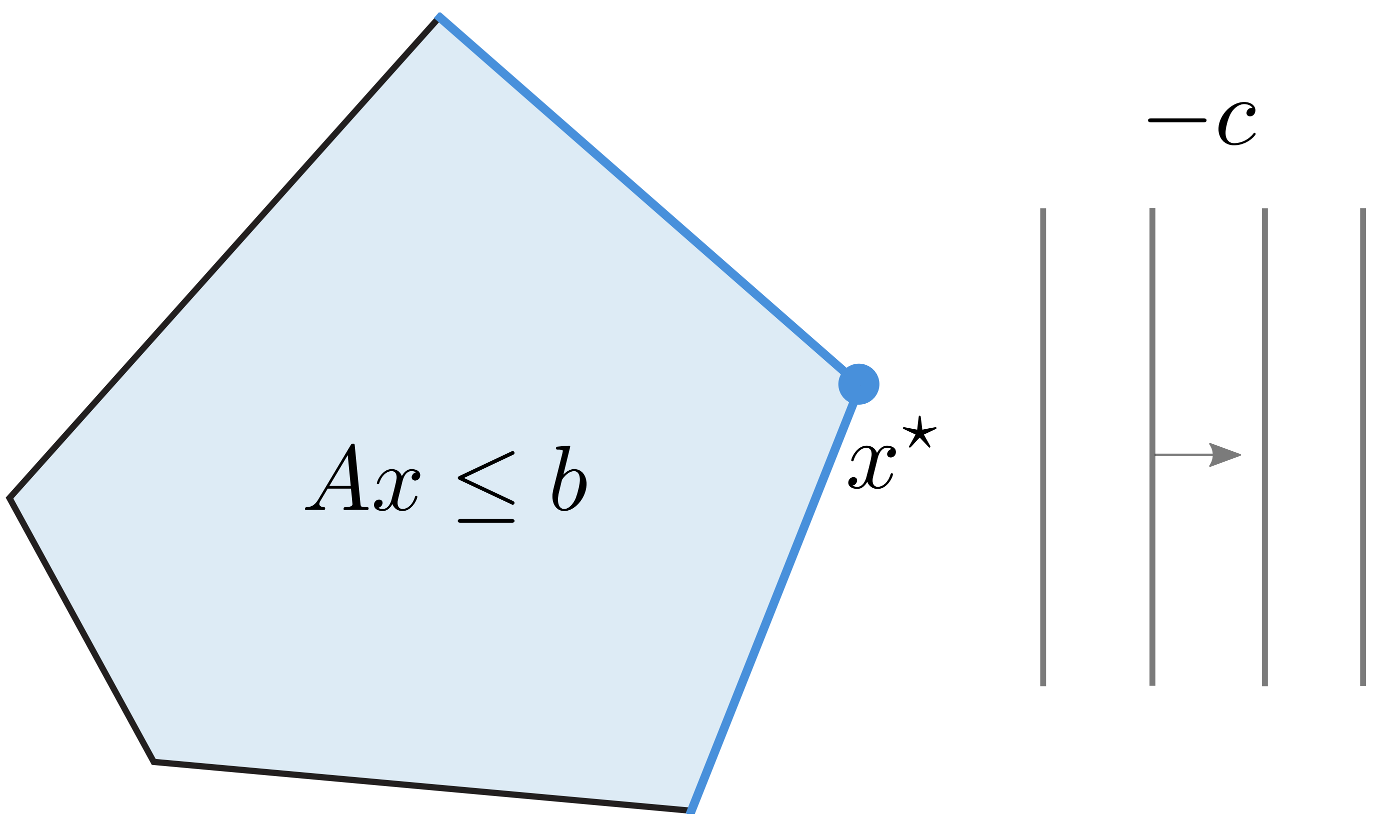
Parameters



Tight constraints

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



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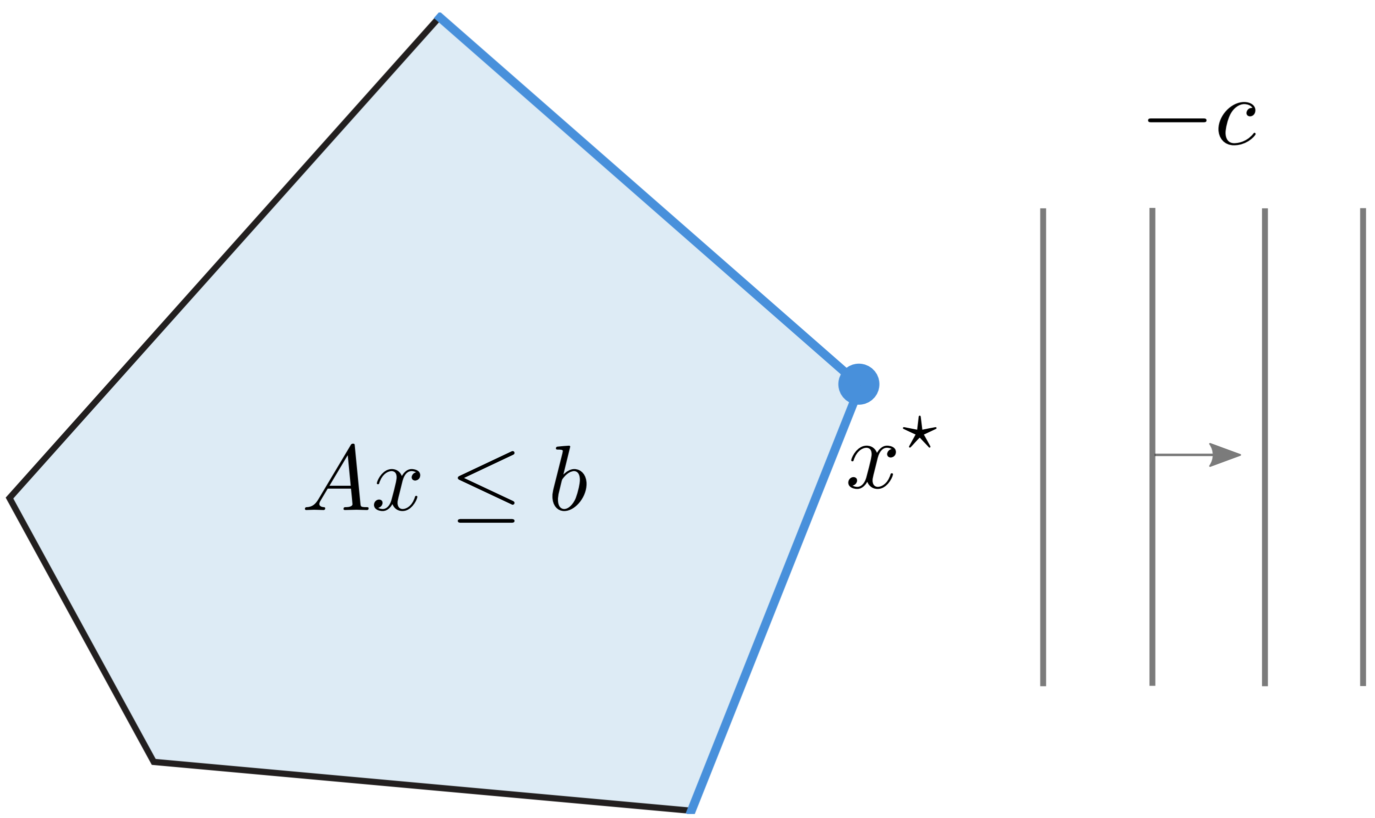

$|\mathcal{T}(\theta)| = \#$ variables   if non-degenerate

Tight constraints

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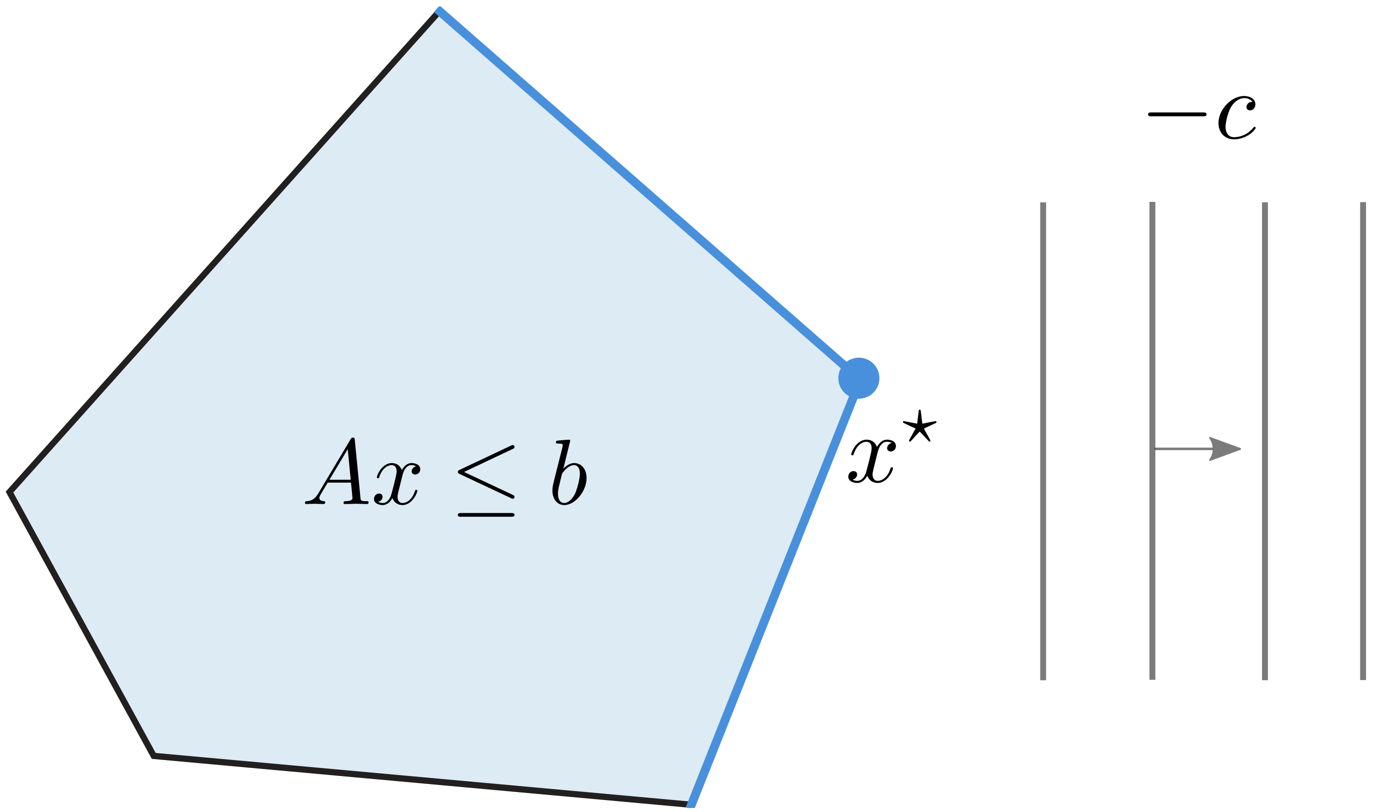
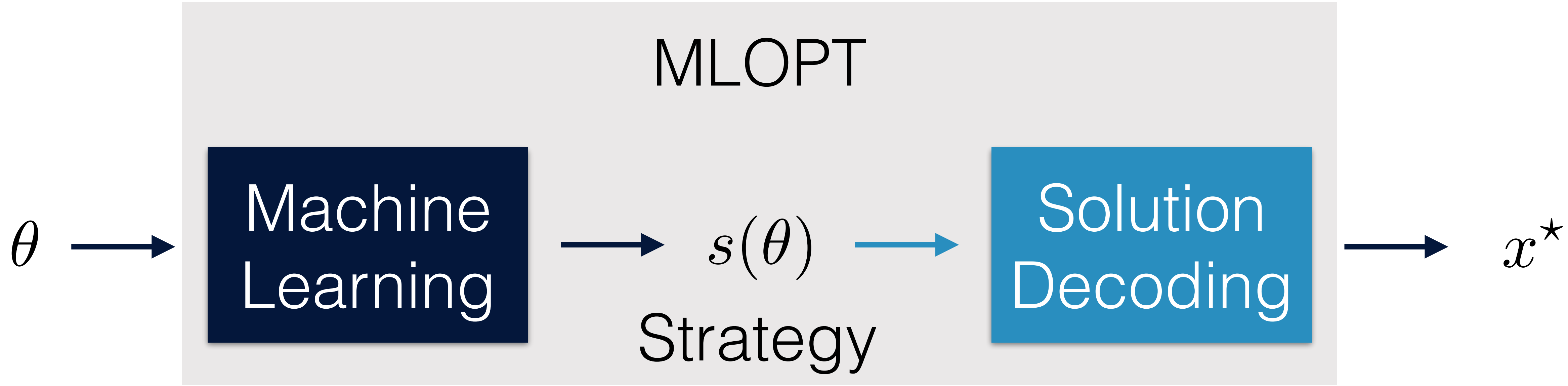


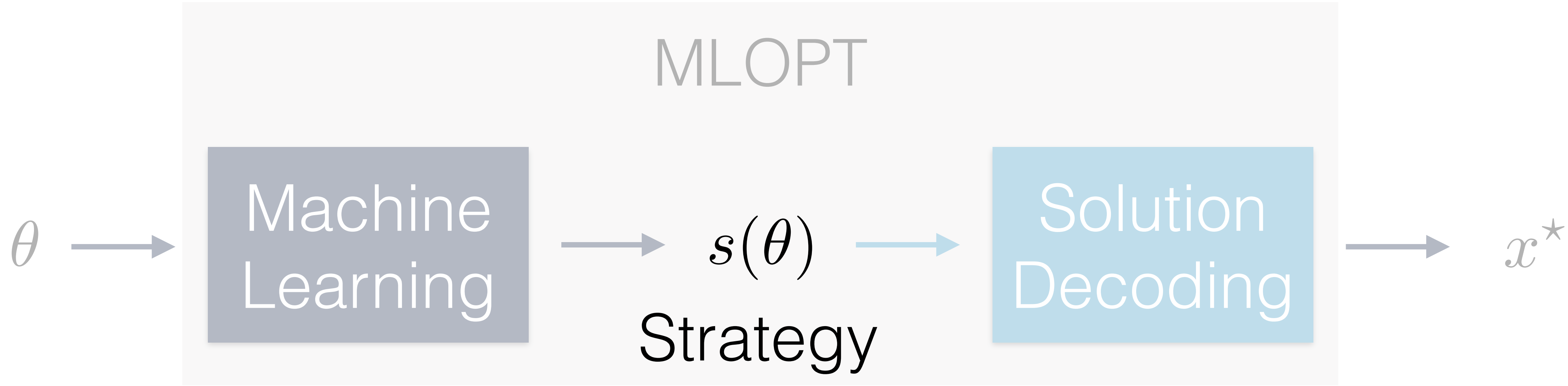
$|\mathcal{T}(\theta)| = \#$ variables if non-degenerate

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

Strategies for linear optimization



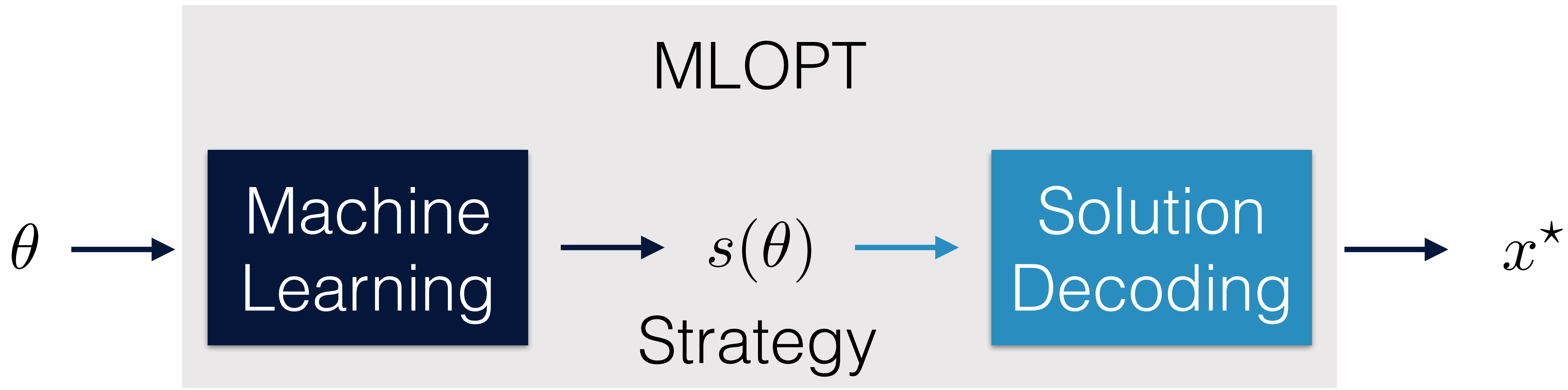
Strategies for linear optimization



The complete information to efficiently get the optimal solution

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

Computing the solution from the optimal strategy



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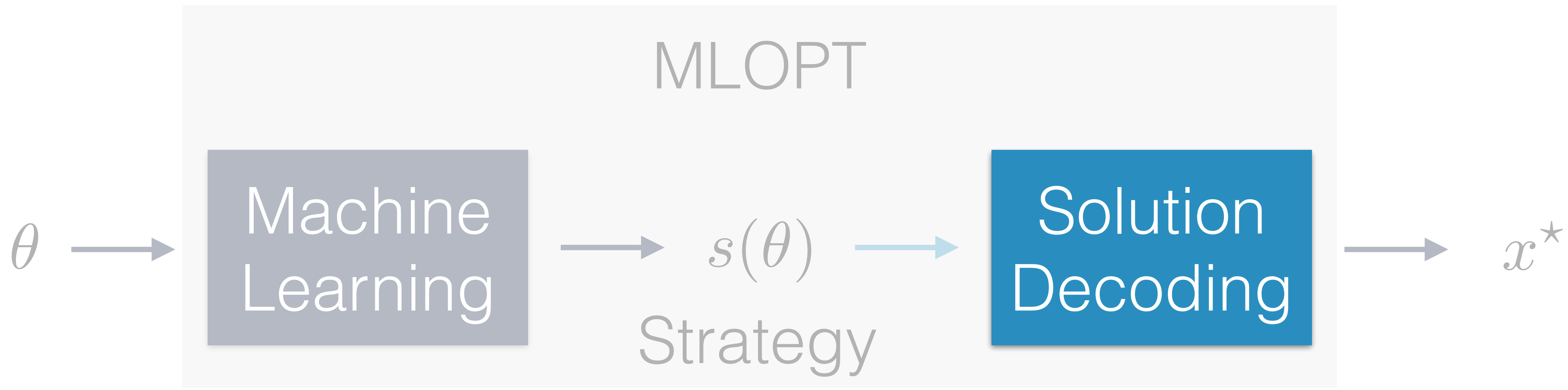


Computing the solution from the optimal strategy

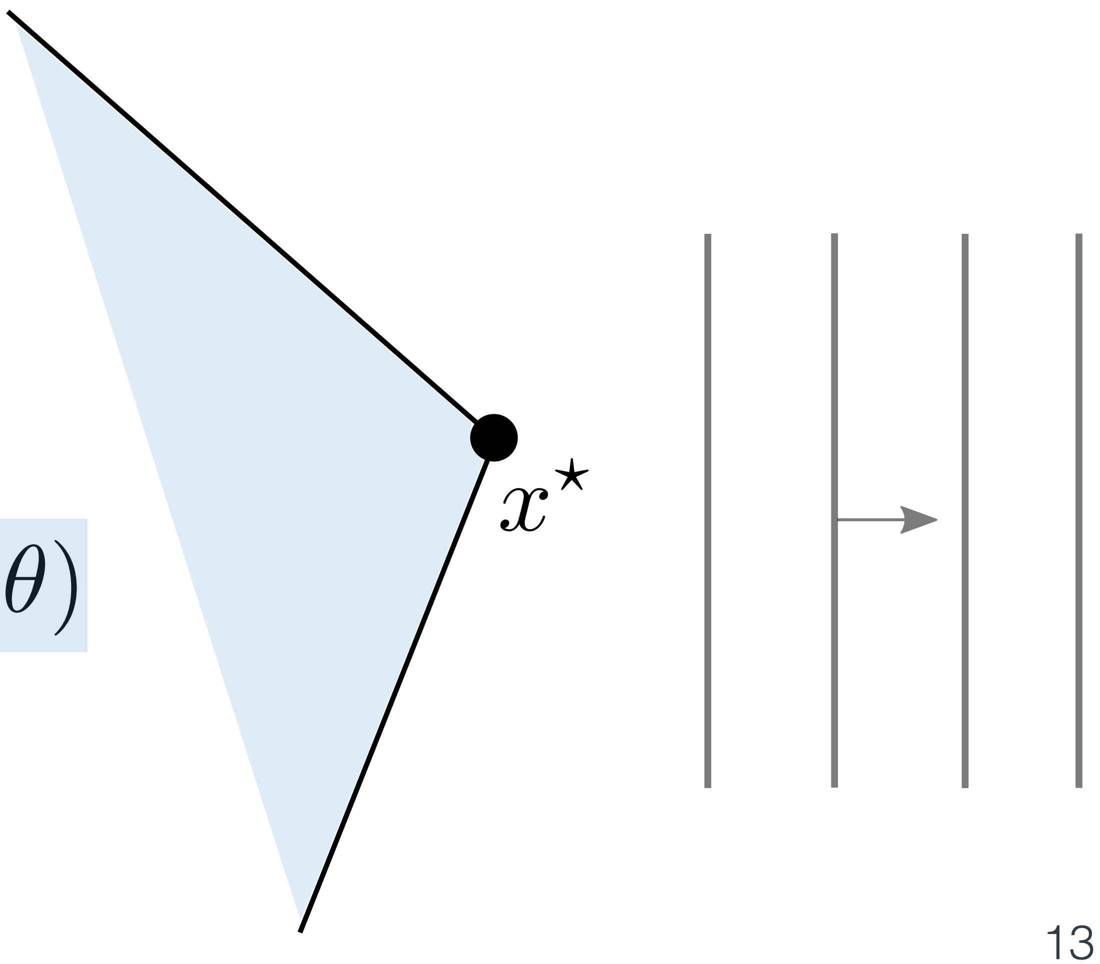
$$\begin{array}{ll} \text{minimize} & c(\theta)^T x \\ \text{subject to} & A(\theta)x \leq b(\theta) \end{array}$$

Computing the solution from the optimal strategy

minimize $\quad c(\theta)^T x$
subject to $\quad A(\theta)x \leq b(\theta)$

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

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



Inventory management

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

Inventory management

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Inventory

Inventory management

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Inventory

Order

Inventory management

$$
\begin{aligned}
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$$

Inventory (x_{t+1})

Order (u_t)

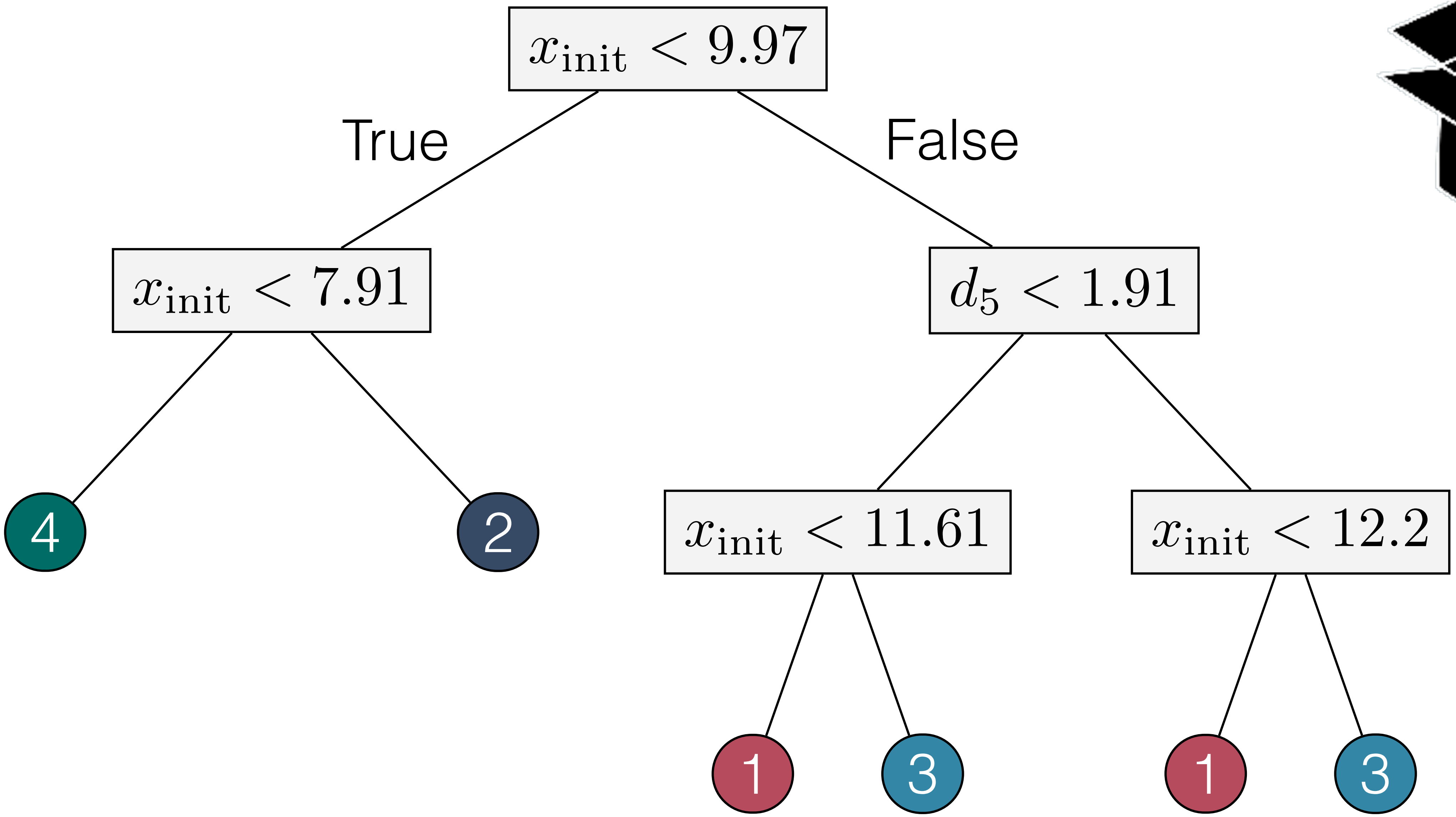
Demand (d_t)

Inventory management

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

Parameters

Strategy for inventory management



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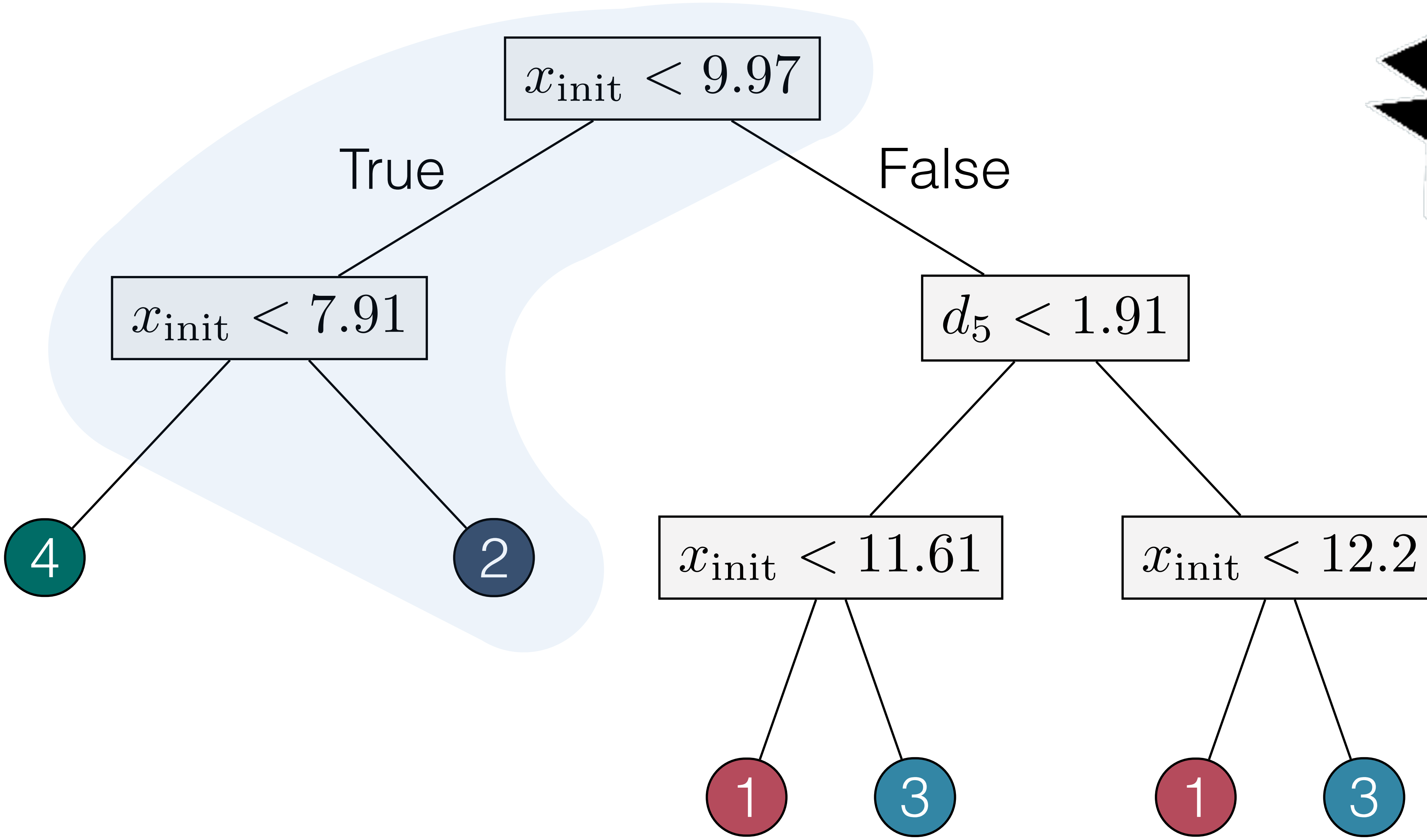
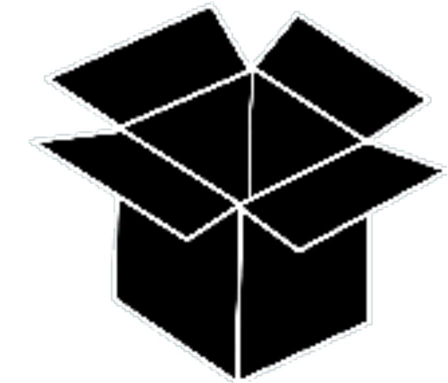
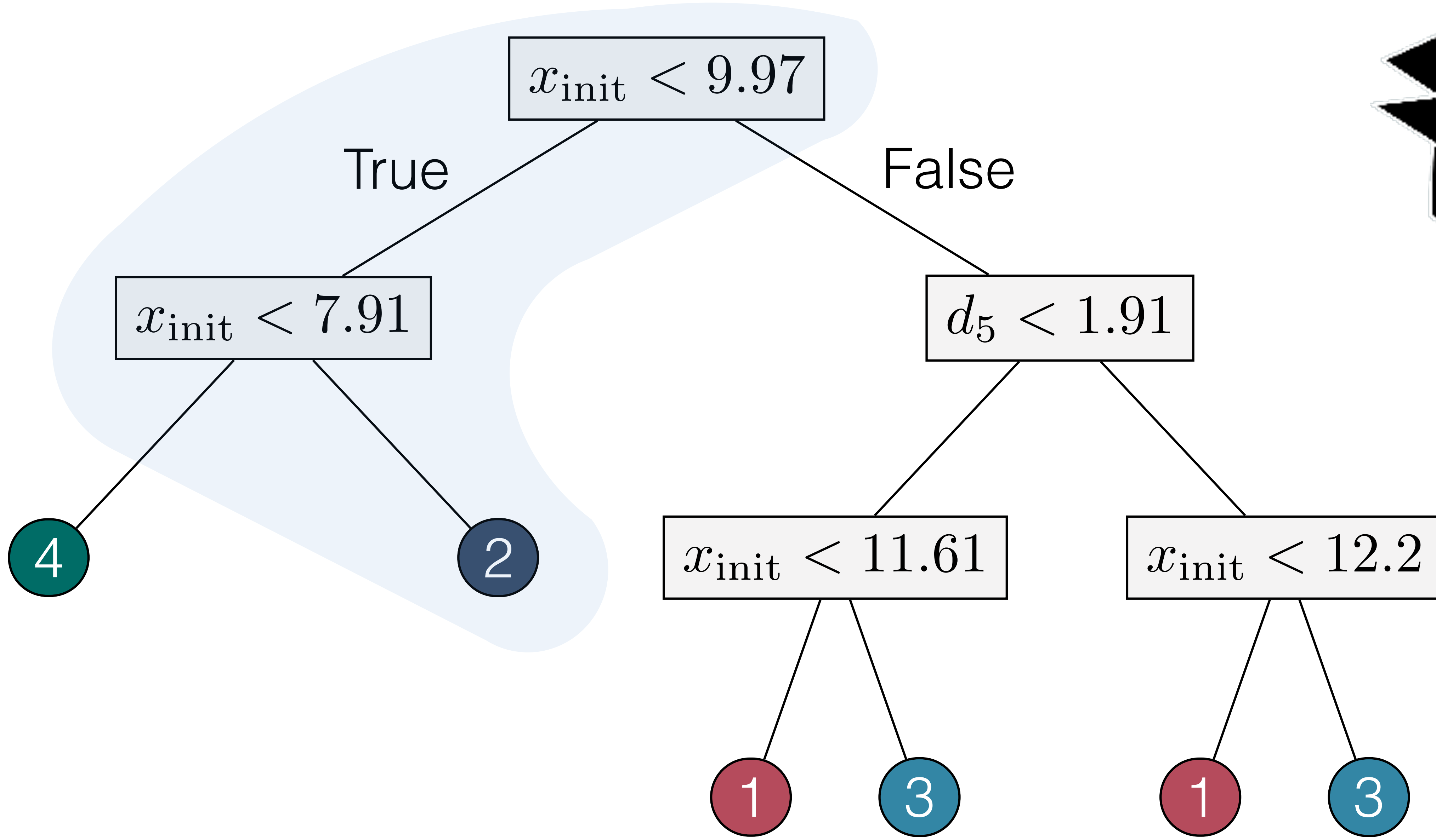


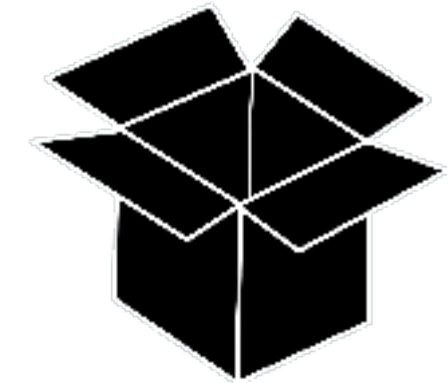


Strategy 2

$$u_t = 0 \qquad t \leq 4$$
$$0 \leq u_t \leq M \qquad t > 4$$

Strategy for inventory management





Strategy 4

$$u_t = 0 \qquad t \leq 3$$
$$0 \leq u_t \leq M \qquad t > 3$$

Strategy 2

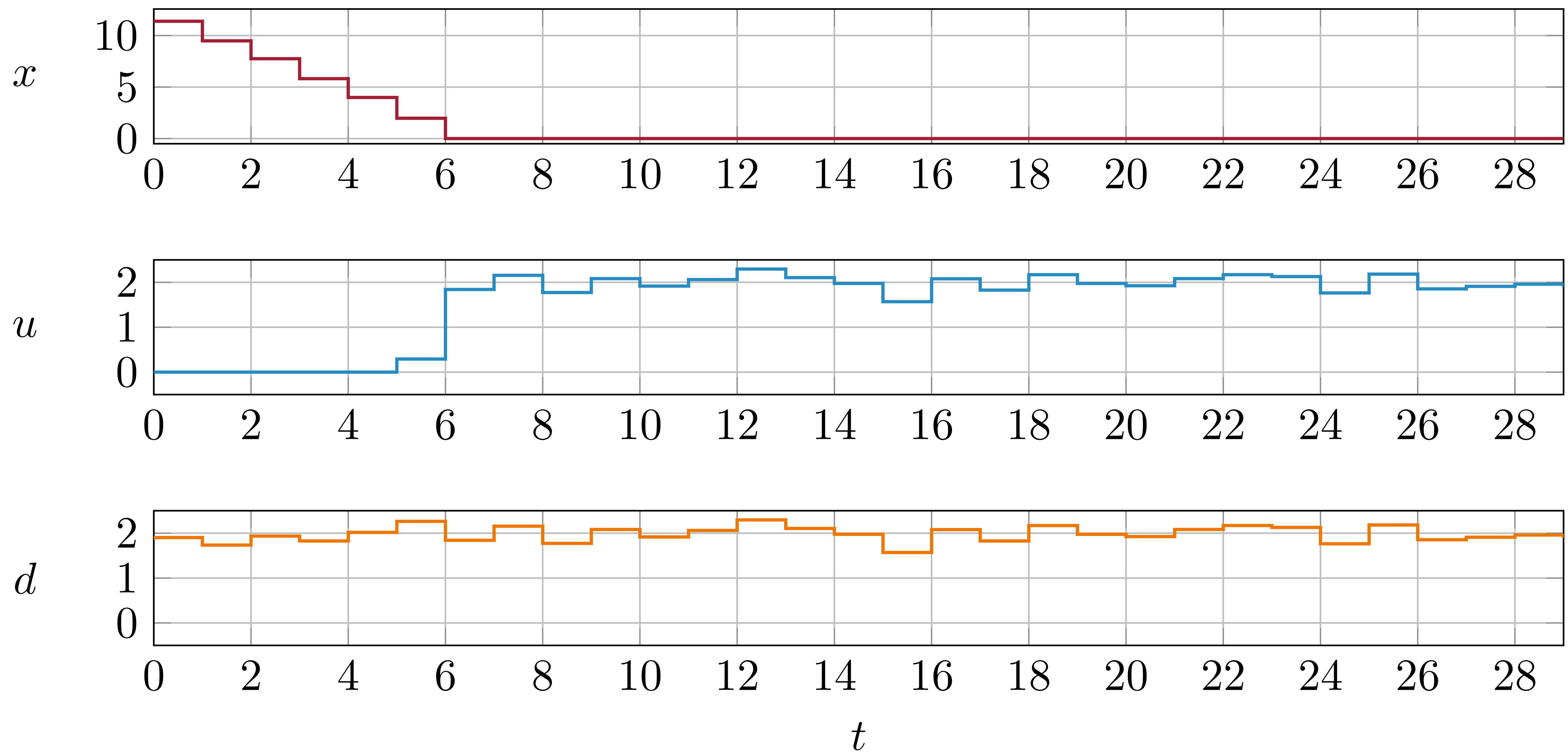
$$u_t = 0 \qquad t \leq 4$$
$$0 \leq u_t \leq M \qquad t > 4$$

Strategies for inventory management

Strategy 2

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

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



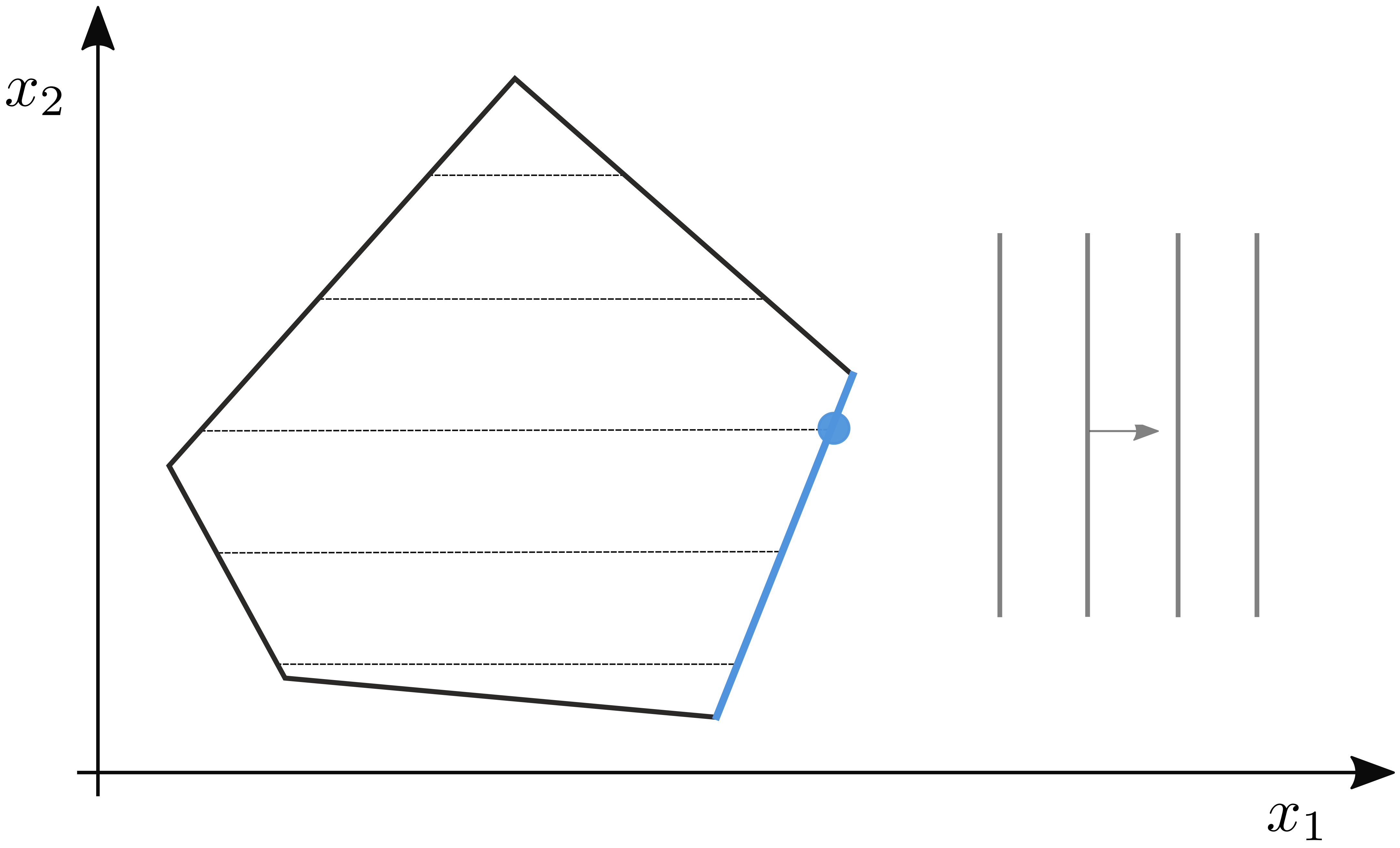
Mixed-integer optimization

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

Mixed-integer optimization

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

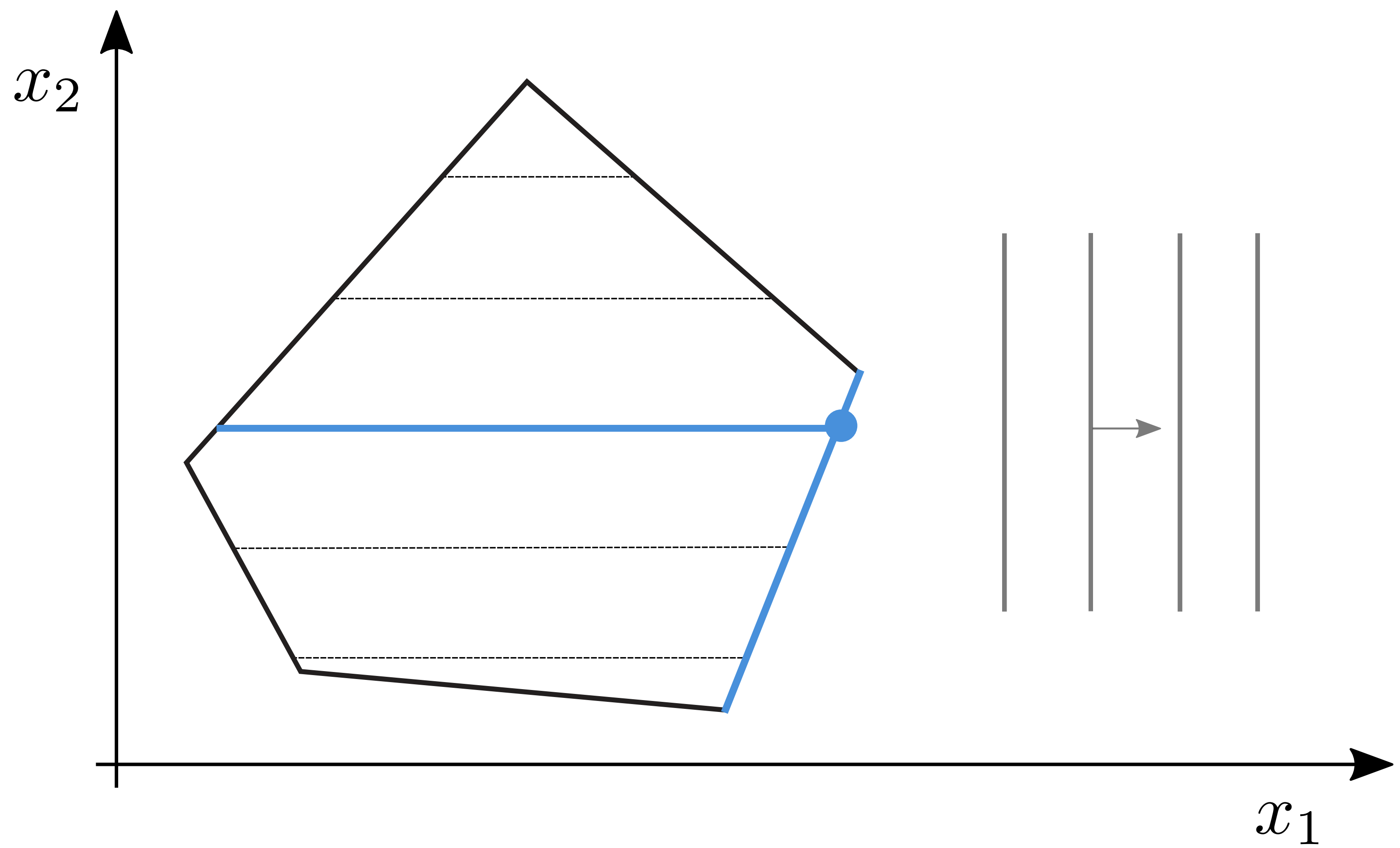
Tight constraints are not enough



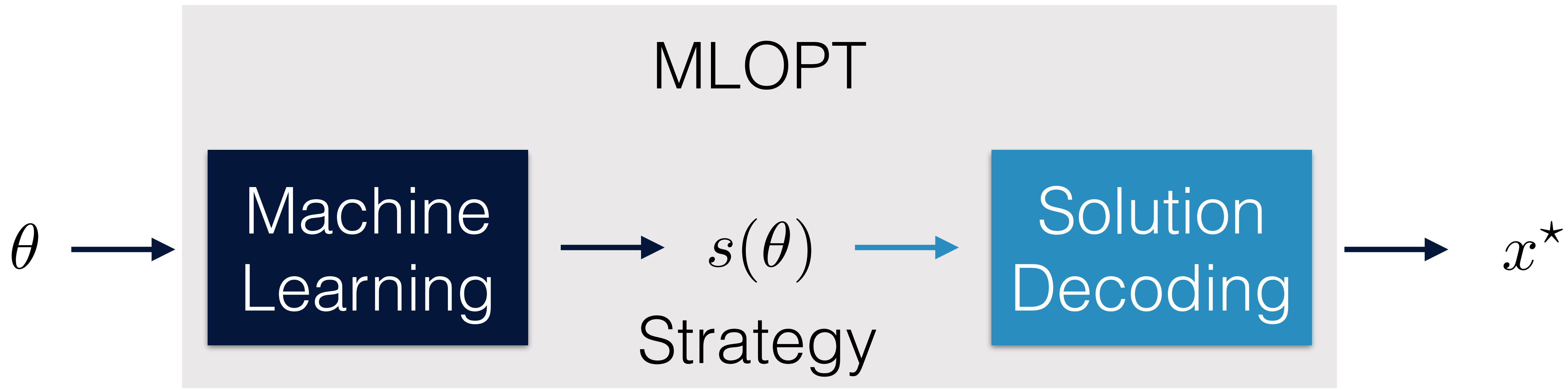
Strategy for mixed-integer optimization

$$s(\theta) = (\mathcal{T}(\theta), x^\star_{\mathcal{I}}(\theta))$$

Integer variables



Computing the solution from the optimal strategy



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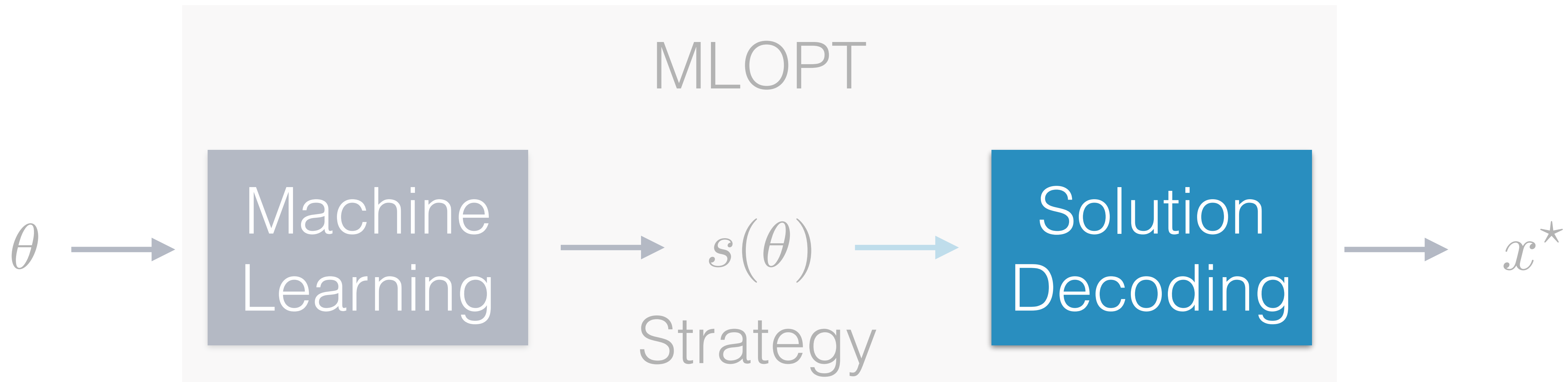


Computing the solution from the optimal strategy

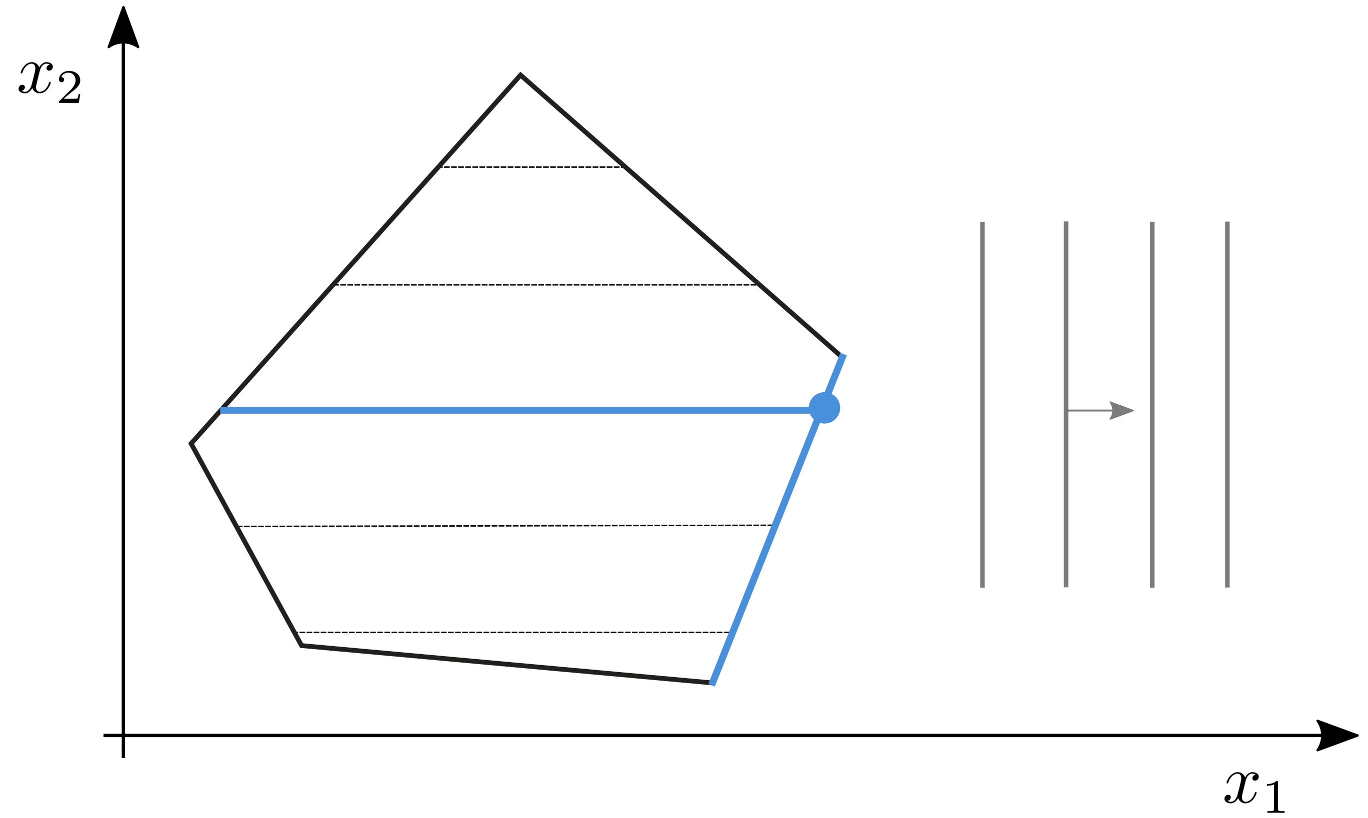
$$\begin{array}{ll} \text{minimize} & c(\theta)^T x \\ \text{subject to} & A(\theta)x \leq b(\theta) \\ & x_{\mathcal{I}} \in \mathbf{Z}^d \end{array}$$

Computing the solution from the optimal strategy

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

Strategy

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



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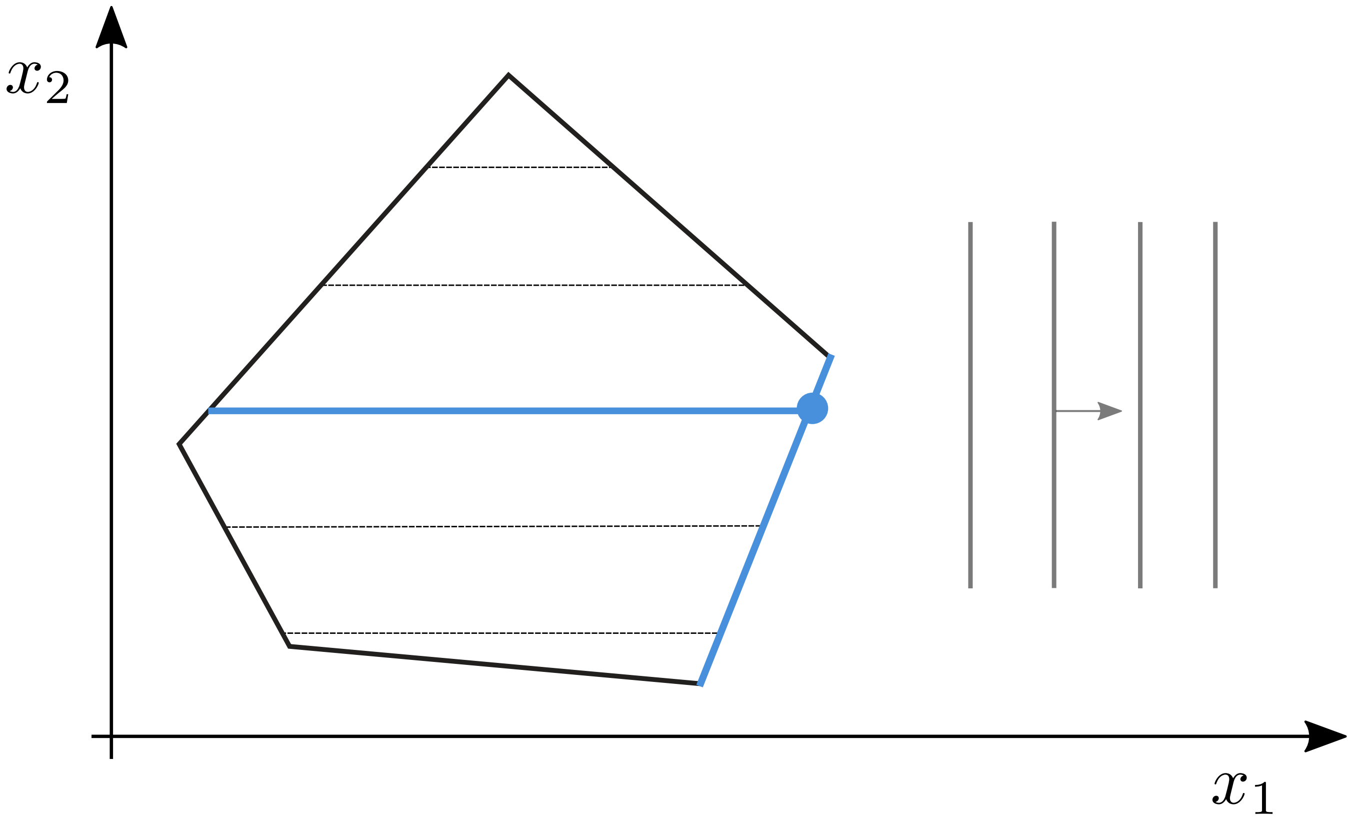
Strategy

$$s(\theta) = (\mathcal{T}(\theta), x^\star_{\mathcal{I}}(\theta))$$



$$\begin{array}{ll} \text{minimize} & c(\theta)^T x \\ \text{subject to} & A_i(\theta)x = b_i(\theta) \quad \forall i \in \mathcal{T}(\theta) \\ & x_{\mathcal{I}} = x^\star_{\mathcal{I}}(\theta) \end{array}$$

Integers

Knapsack

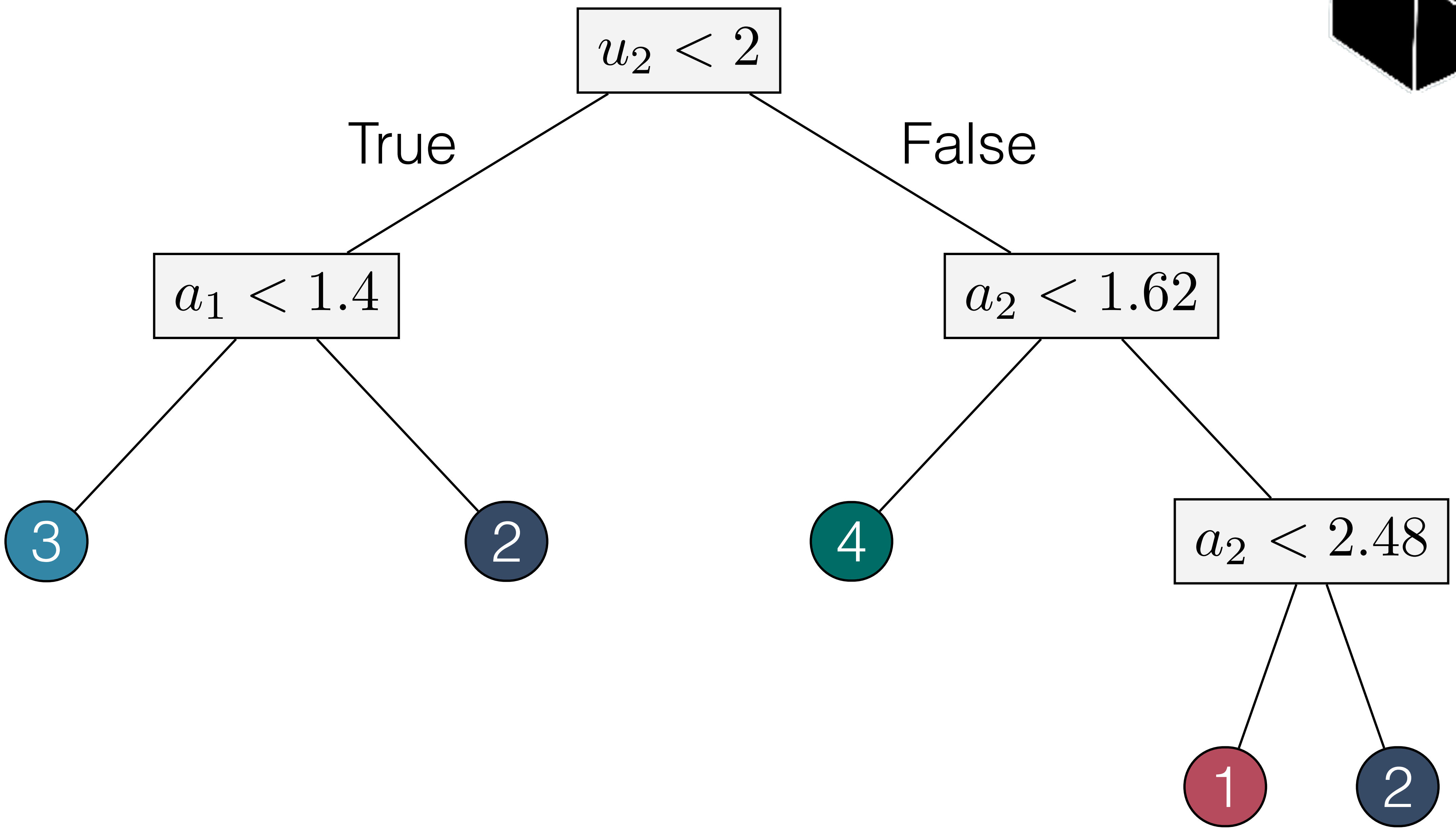
$$\begin{array}{ll} \text{maximize} & c^T x \\ \text{subject to} & a^T x \leq b \\ & 0 \leq x \leq u \\ & x \in \mathbf{Z}^n \end{array}$$

Knapsack

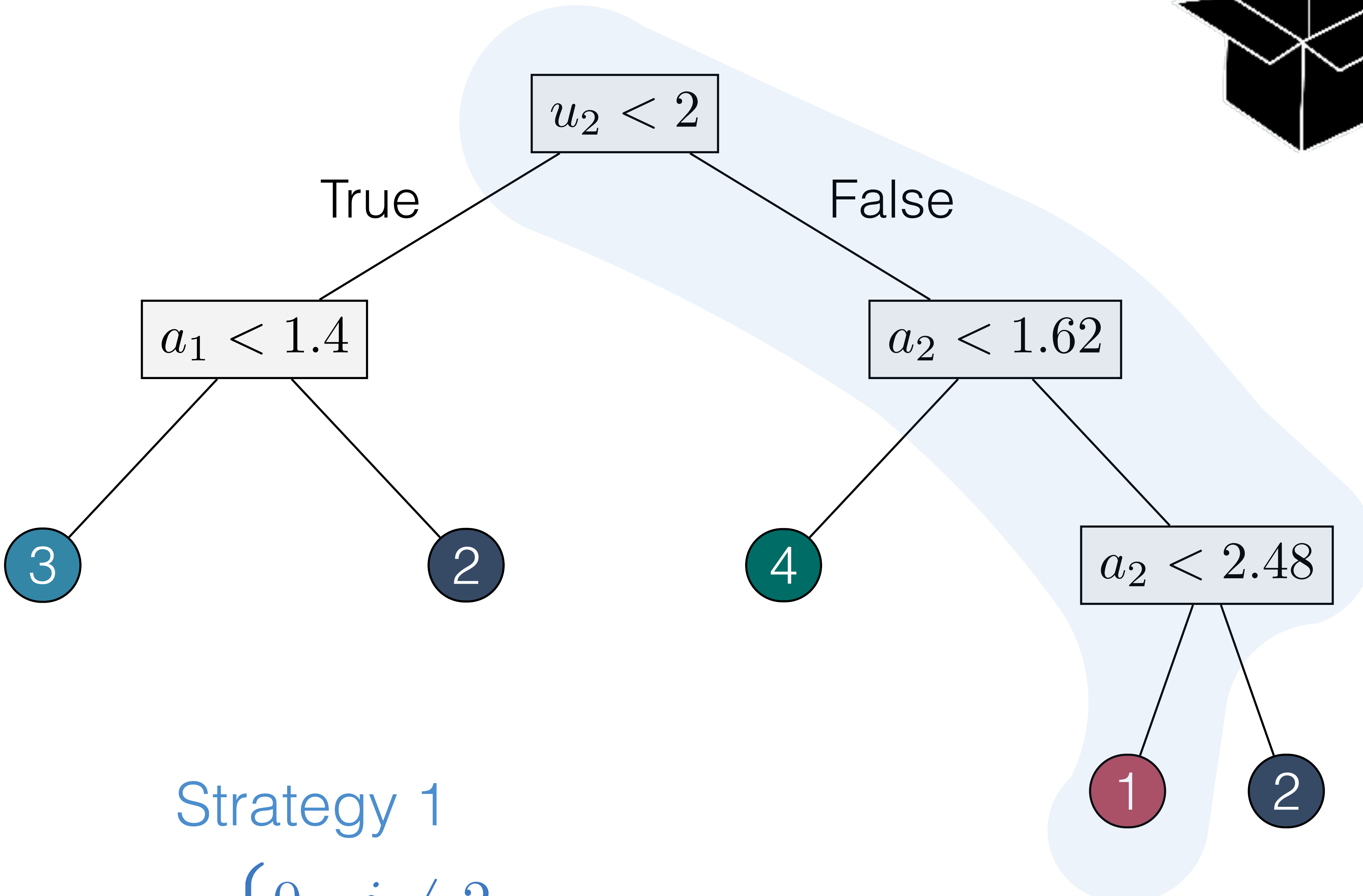
$$
\begin{aligned}
\text{maximize} \quad & c^T x \\
\text{subject to} \quad & a^T x \leq b \\
& 0 \leq x \leq u \\
& x \in \mathbf{Z}^n
\end{aligned}
$$

Parameters

Strategy selection for knapsack



Strategy selection for knapsack

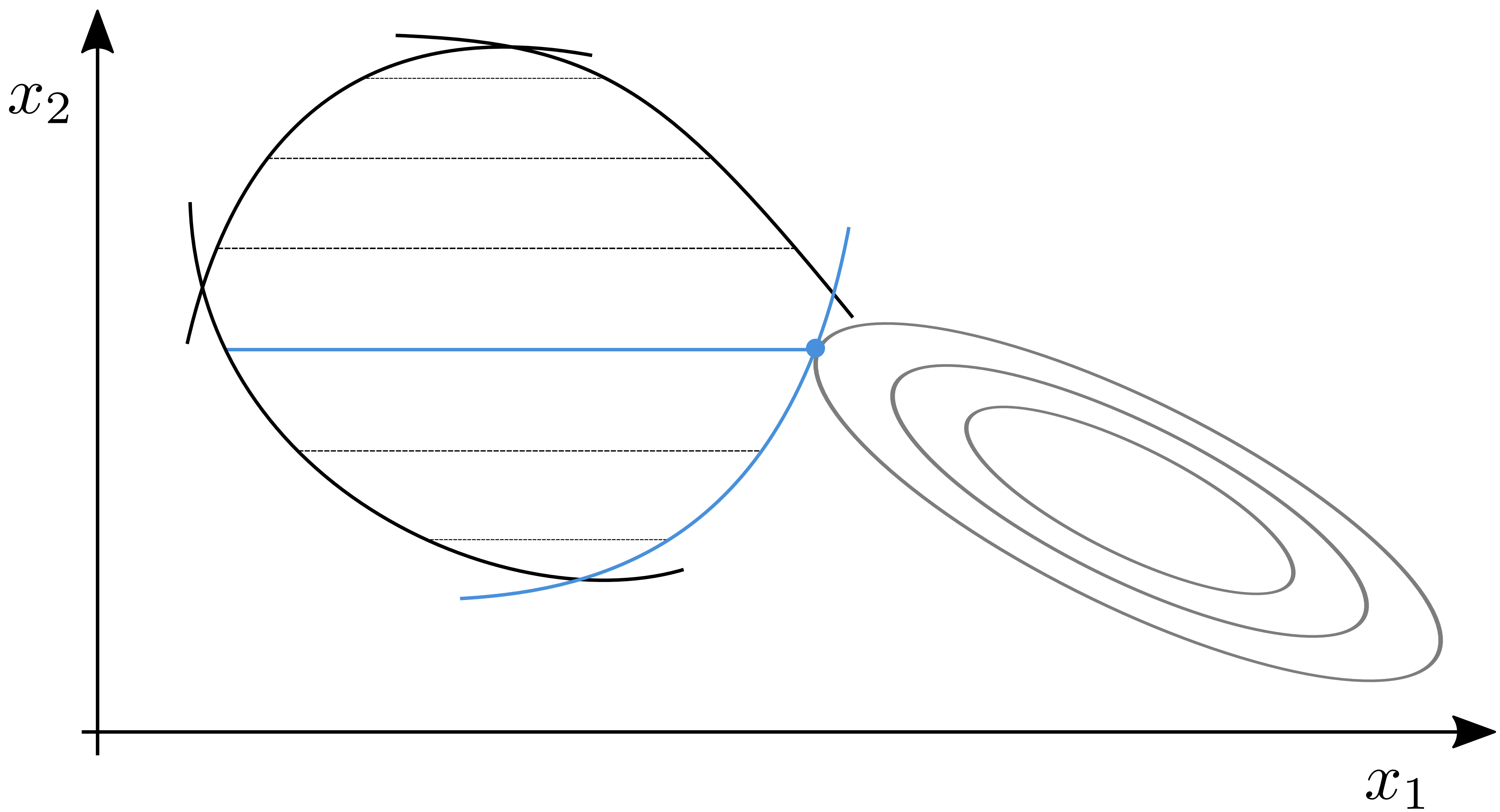


Strategy 1

$$x_i = \begin{cases} 0 & i \neq 2 \\ 2 & i = 2 \end{cases}$$

Mixed-integer convex optimization

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



[D. Bertsimas, B. Stellato, *The Voice of Optimization*, Machine Learning (to appear), (2020)]

Machine learning optimizer

- Optimal Strategies
- Strategy Prediction
- Strategy Exploration
- Speedups
- Examples
- Future Work

Machine learning optimizer

Optimal Strategies

Strategy Prediction

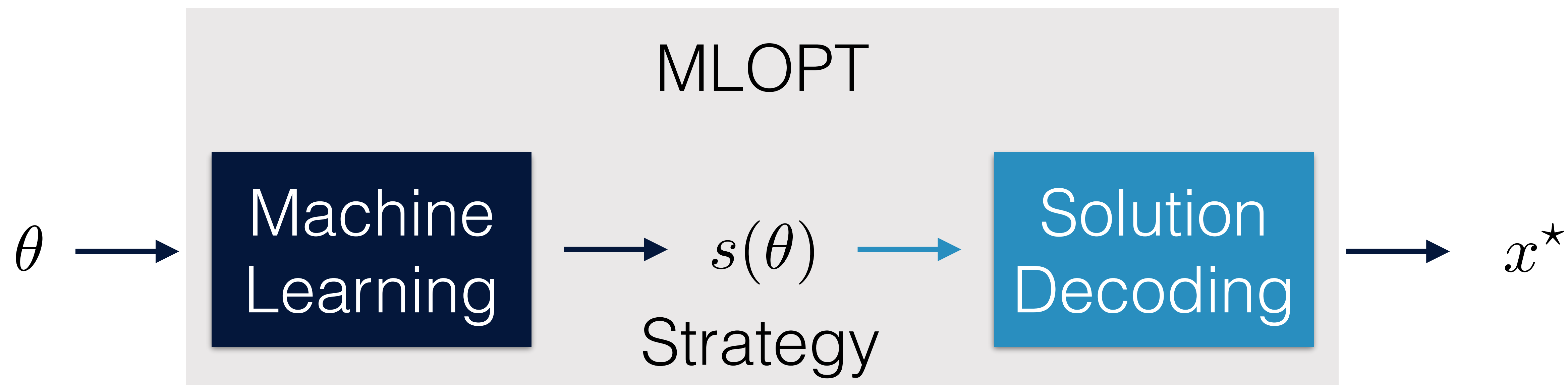
Strategy Exploration

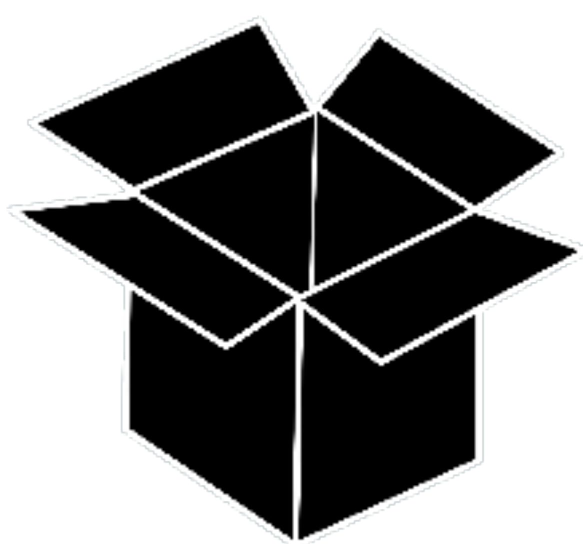
Speedups

Examples

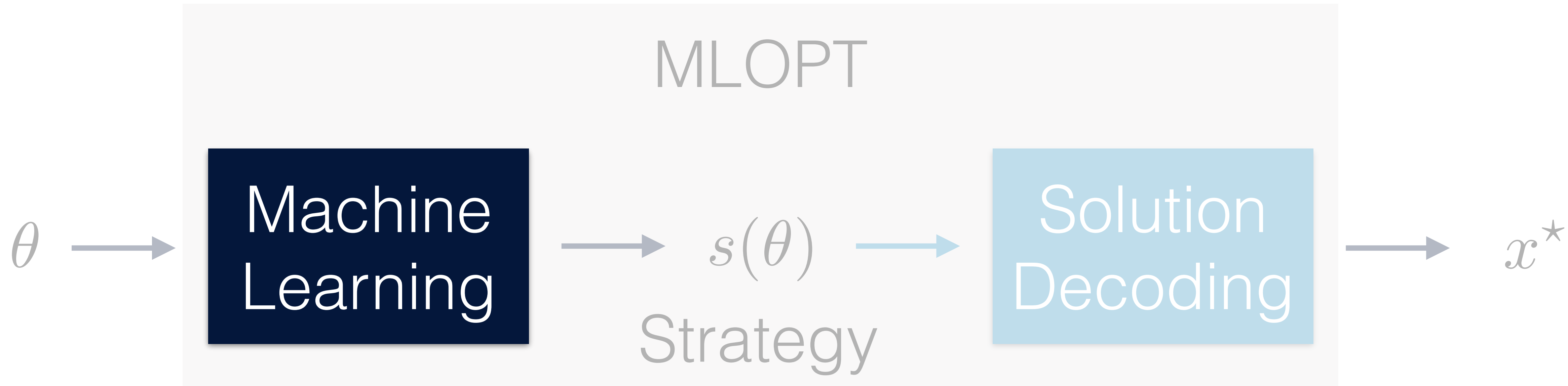
Future Work

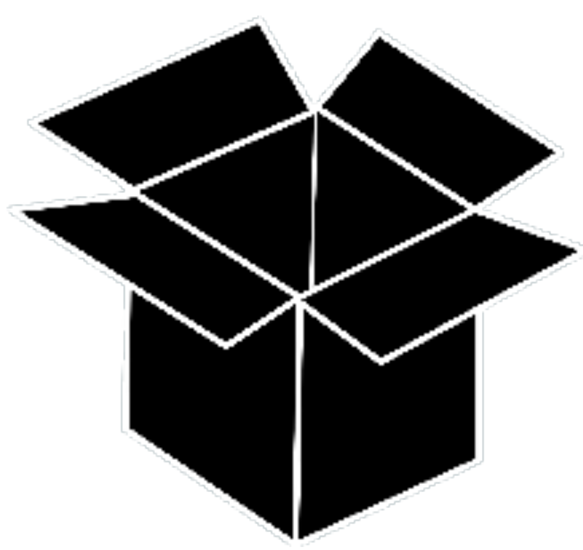
Machine learning optimizer



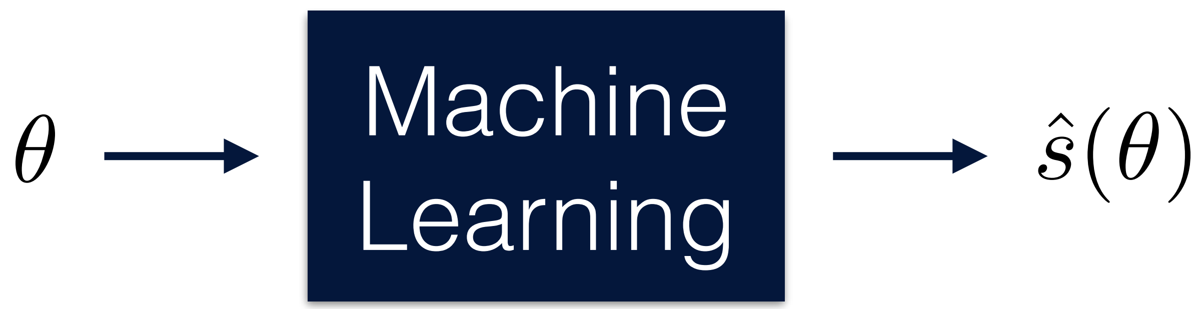


Machine learning optimizer





Selecting strategies is a classification problem



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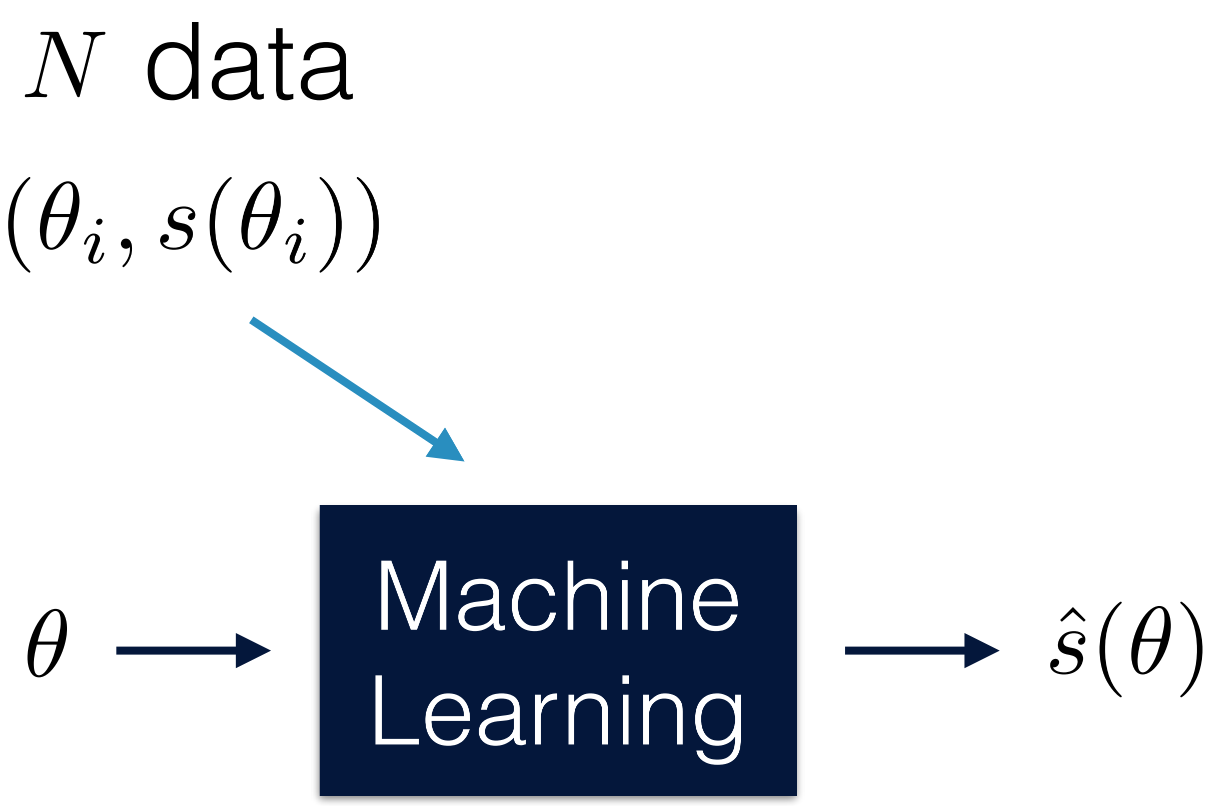

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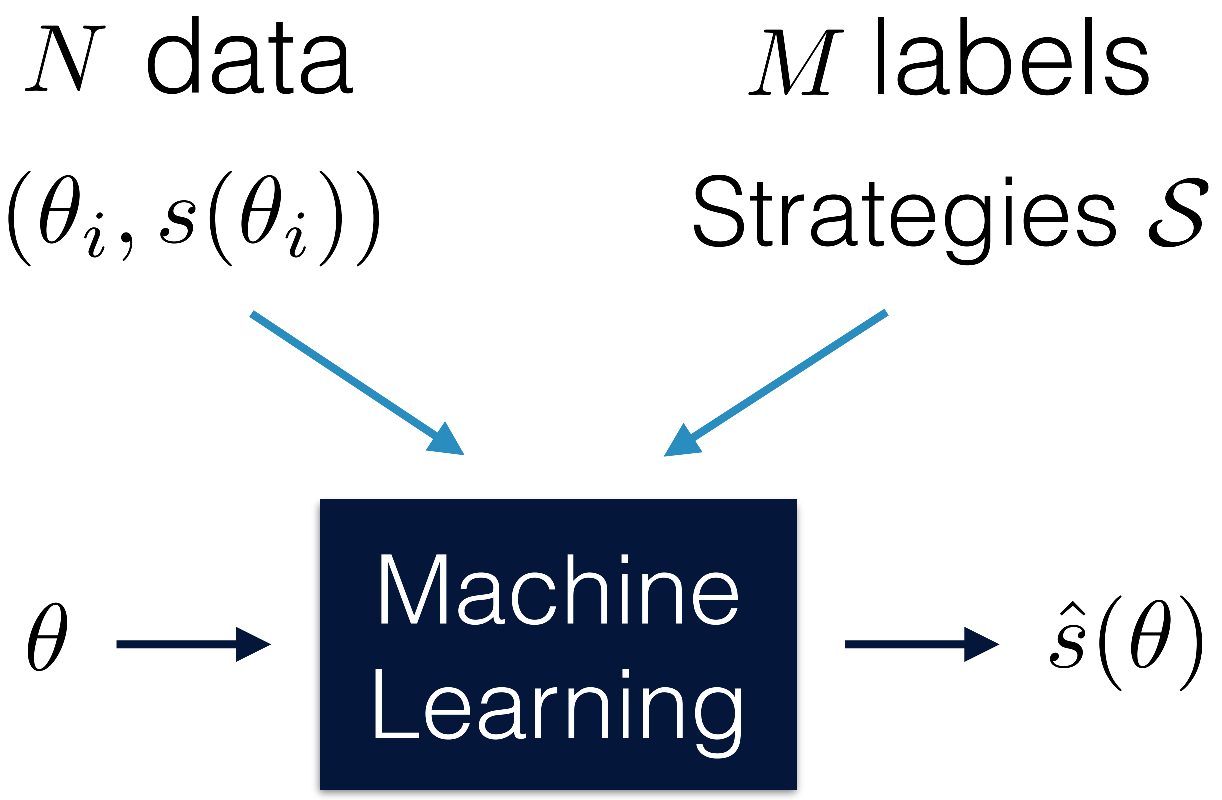

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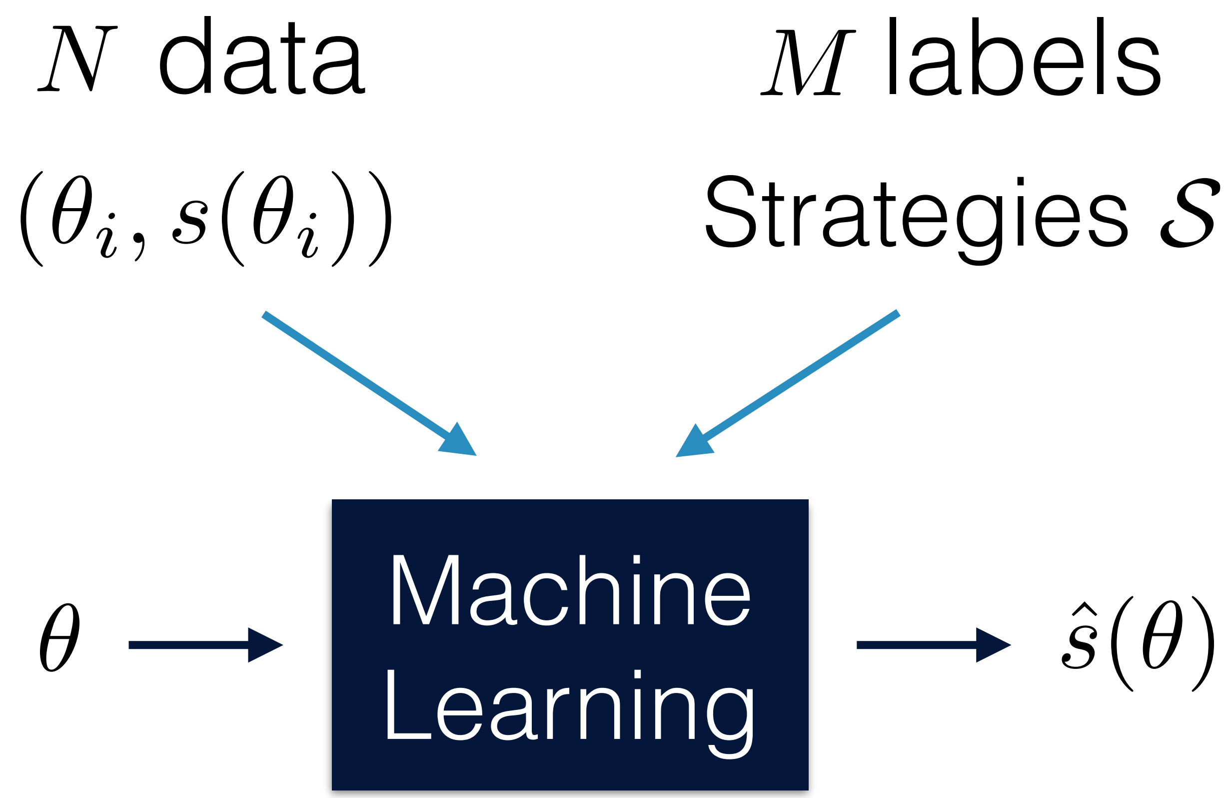
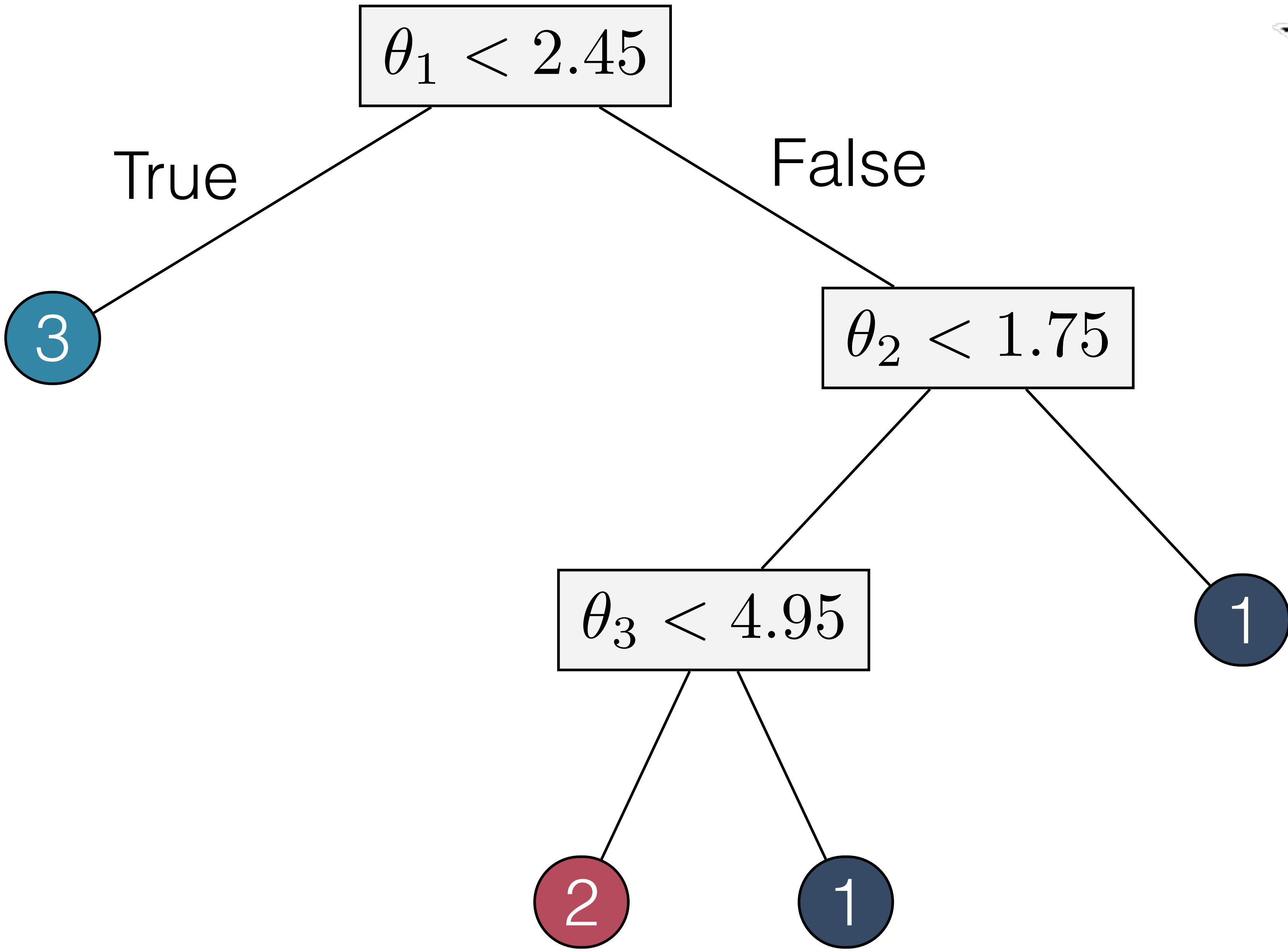
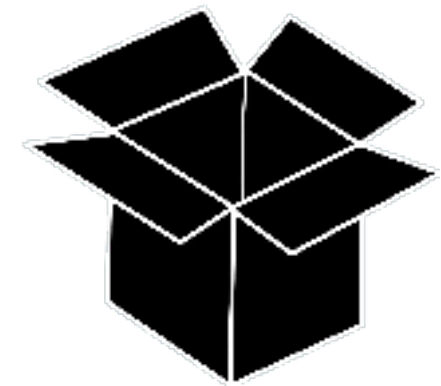


Optimal Trees

Neural Networks

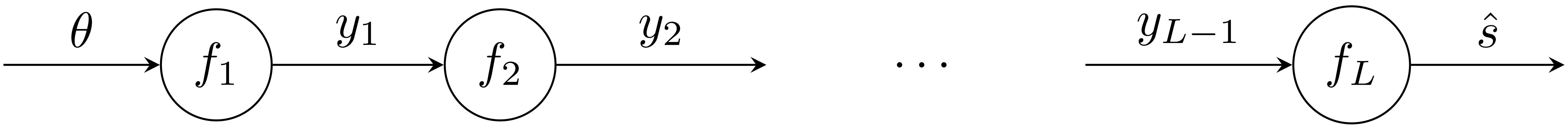
Optimal Classification Trees (OCT)





[Bertsimas and Dunn (2017)]

Neural Networks (NN)



Single layer

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

PyTorch

Machine learning optimizer

Optimal Strategies

Strategy Prediction

Strategy Exploration

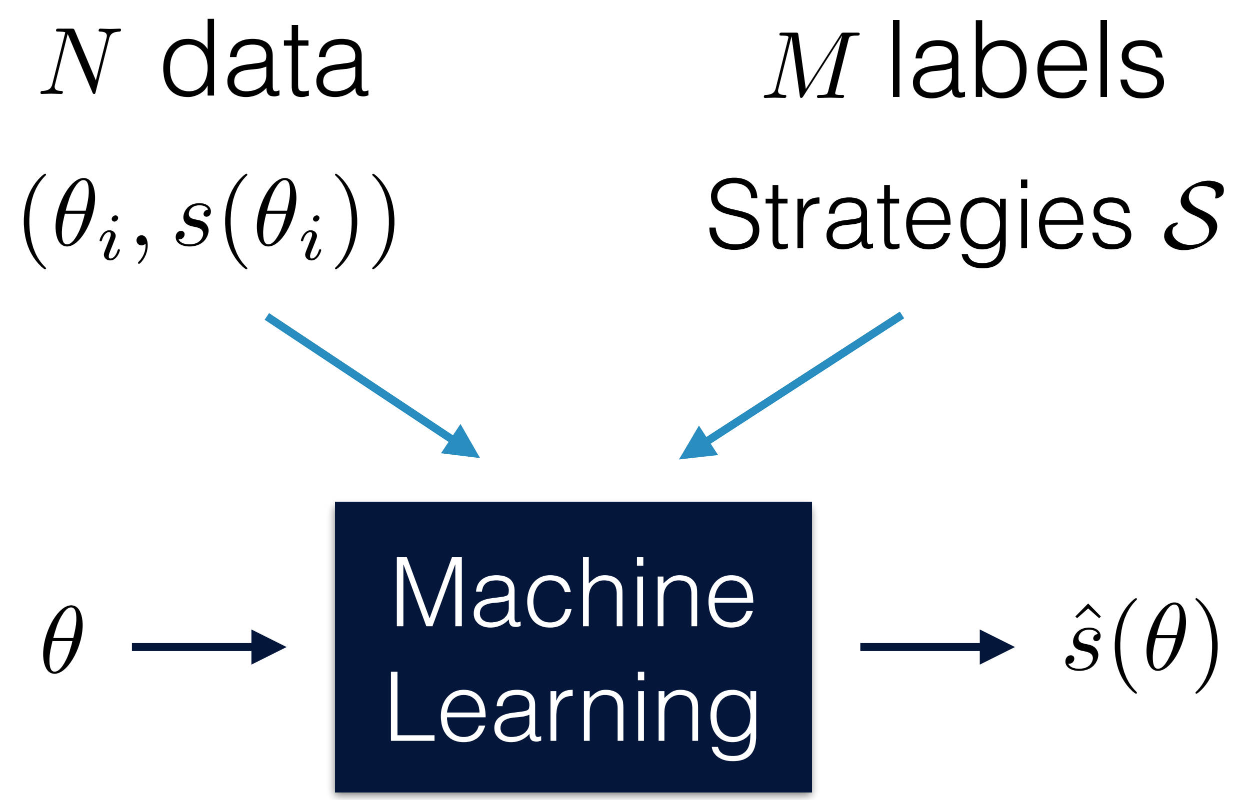
Speedups

Examples

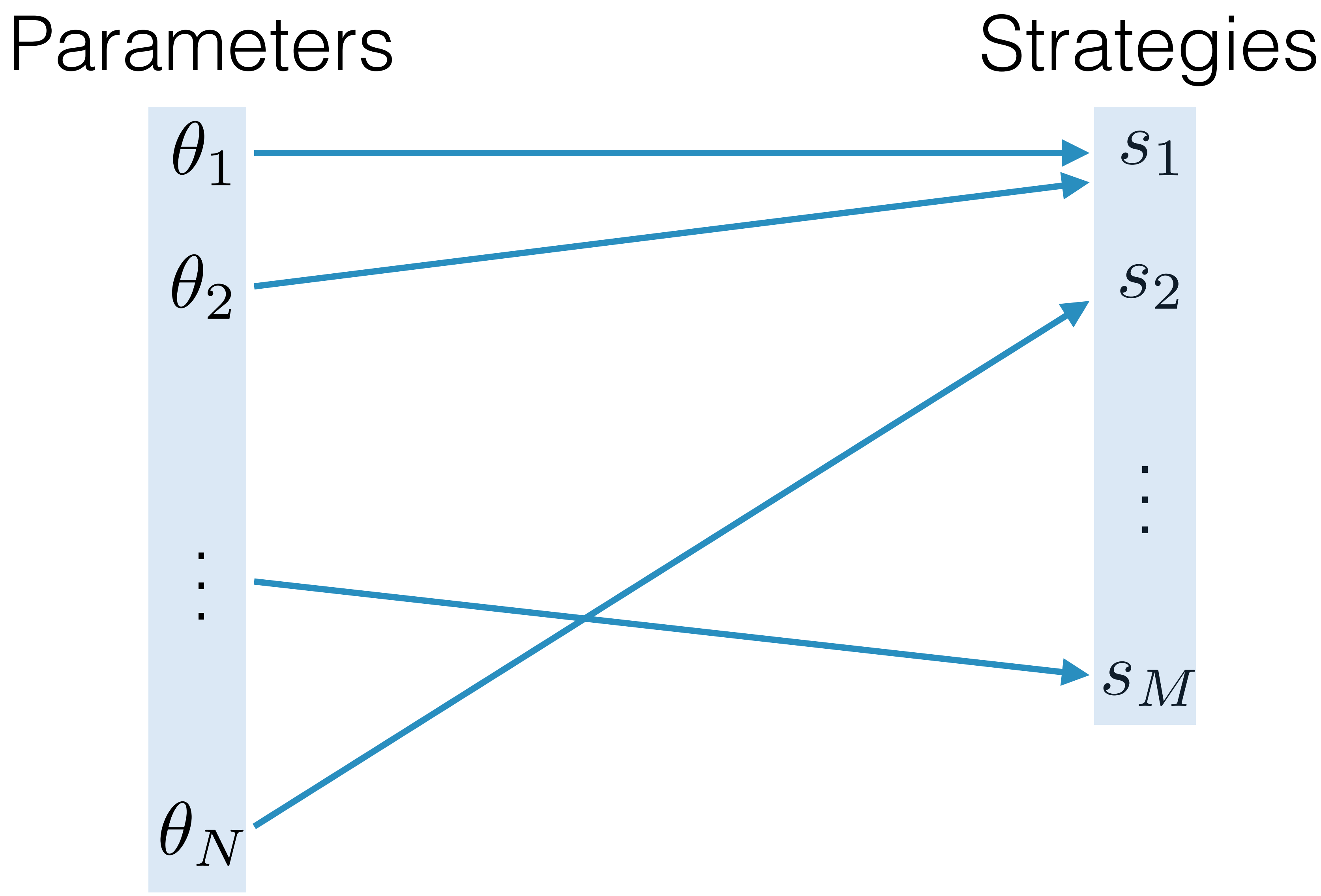
Machine learning optimizer

- Optimal Strategies
- Strategy Prediction
- **Strategy Exploration**
- Speedups
- Examples

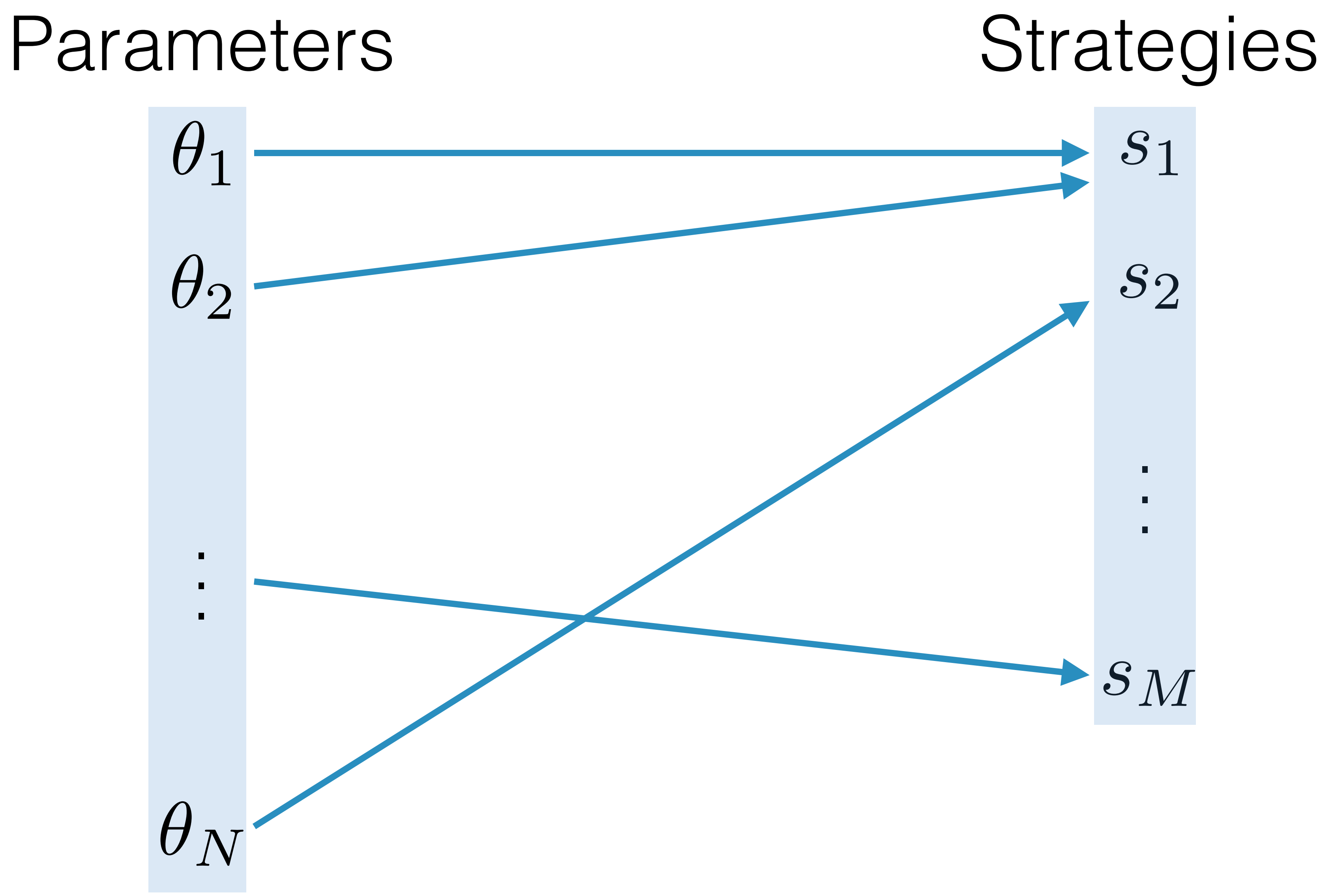
Have we seen enough data?



Will we find new strategies?

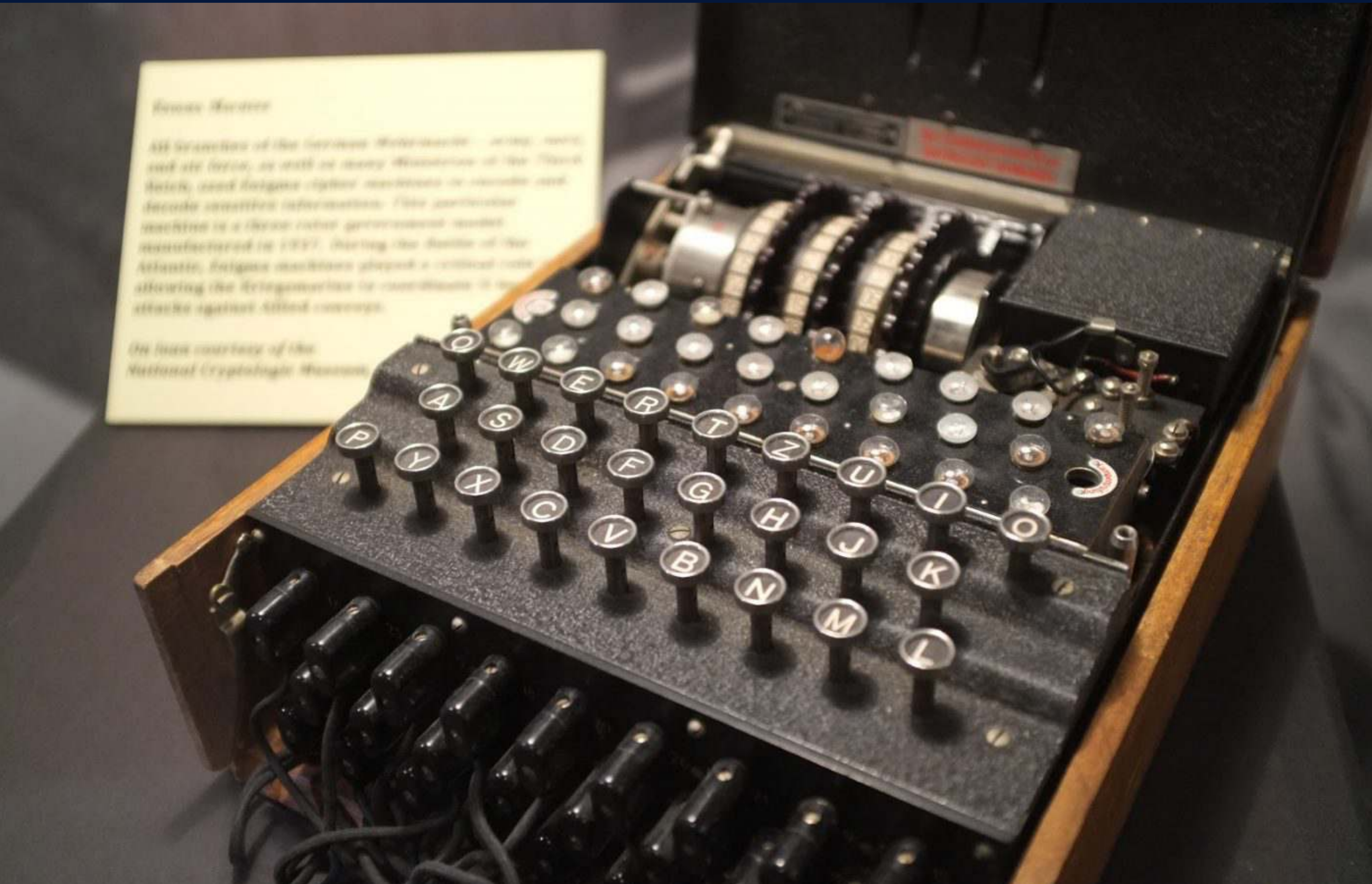


Will we find new strategies?



θ_{N+1}?

Alan Turing already knew that…



Good-Turing estimator

$N = 15$
$M = 5$

→

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

Good-Turing estimator

$N = 15$
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$$GT = \frac{N_1}{N} \approx \mathbf{P}(s(\theta_{N+1}) \notin \mathcal{S}(\Theta_N))$$

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Probability of unseen strategies

Good-Turing estimator

$$N = 15$$
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strategies appeared once

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Probability of unseen strategies

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Probability of unseen strategies

samples

Good-Turing estimator

$N = 15$
$M = 5$ →

s_1	6 times
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s_5	2 times

→ $GT = 1/15$

strategies appeared once

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

samples

Probability of unseen strategies

Good-Turing estimator

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

→

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s_2	3 times
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strategies appeared once

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

samples

Probability of unseen strategies

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

Good-Turing estimator

$N = 15$
$M = 5$

→

s_1	6 times
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s_5	2 times

→ $GT = 1/15$

\# strategies appeared once

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

Probability of unseen strategies

\# samples

Bound

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

[McAllester and Schapire (2001)]

Simple sampling scheme

Bound

Repeat until $GT + c\sqrt{(1/N)\ln(3/\beta)} \leq \epsilon$

1. sample θ_i from empirical distribution (history)
2. compute $s(\theta_i)$
3. update estimator $GT = \frac{N_1}{N}$

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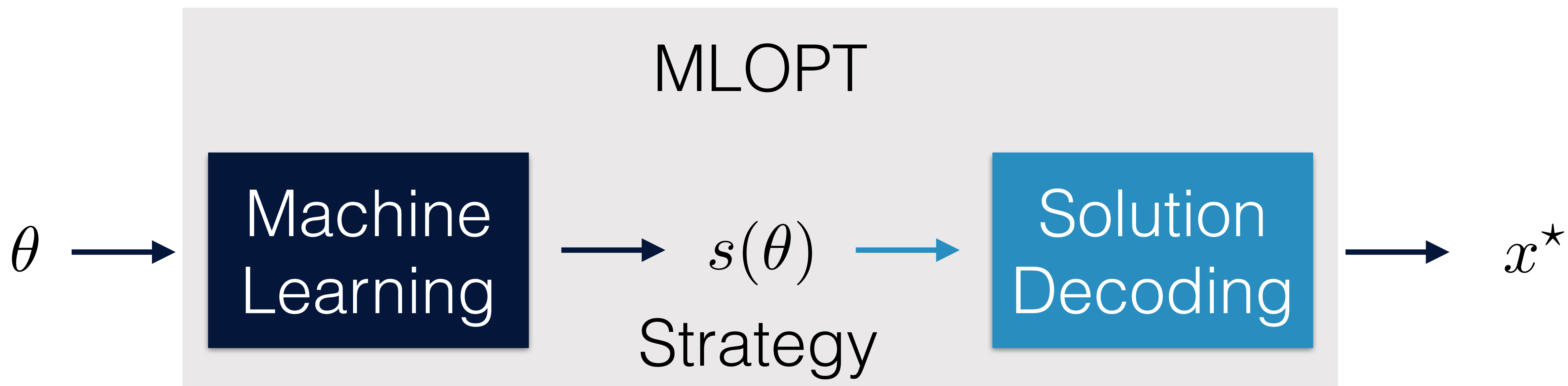
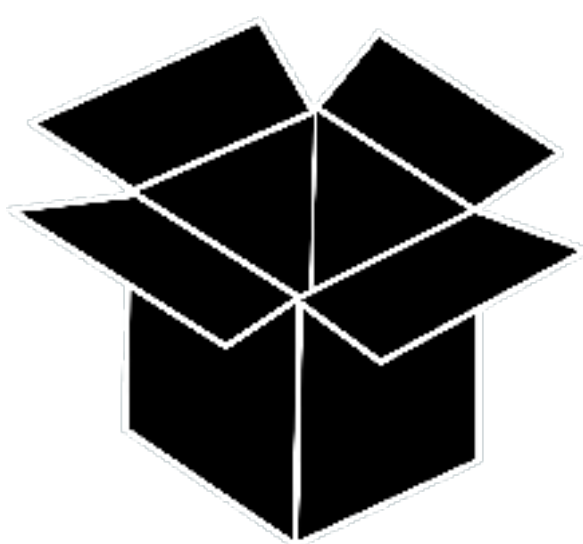
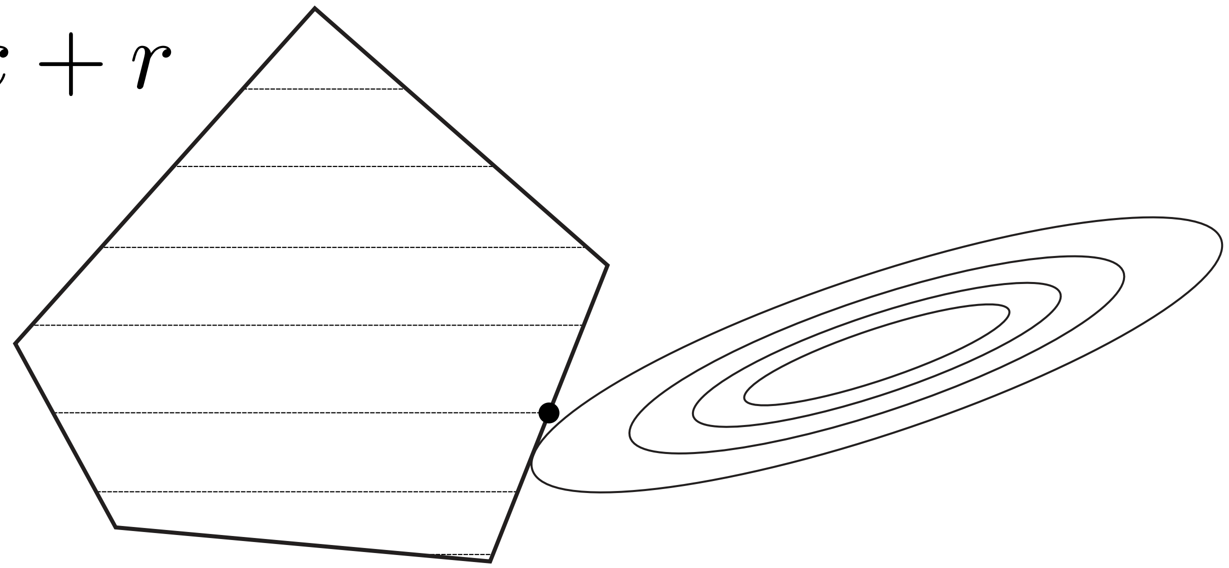




Mixed-integer quadratic optimization

$$\begin{array}{ll}\text{minimize} & (1/2)x^T P x + q^T x + r \\ \text{subject to} & Ax \leq b \\ & x_{\mathcal{I}} \in \mathbf{Z}^d\end{array}$$



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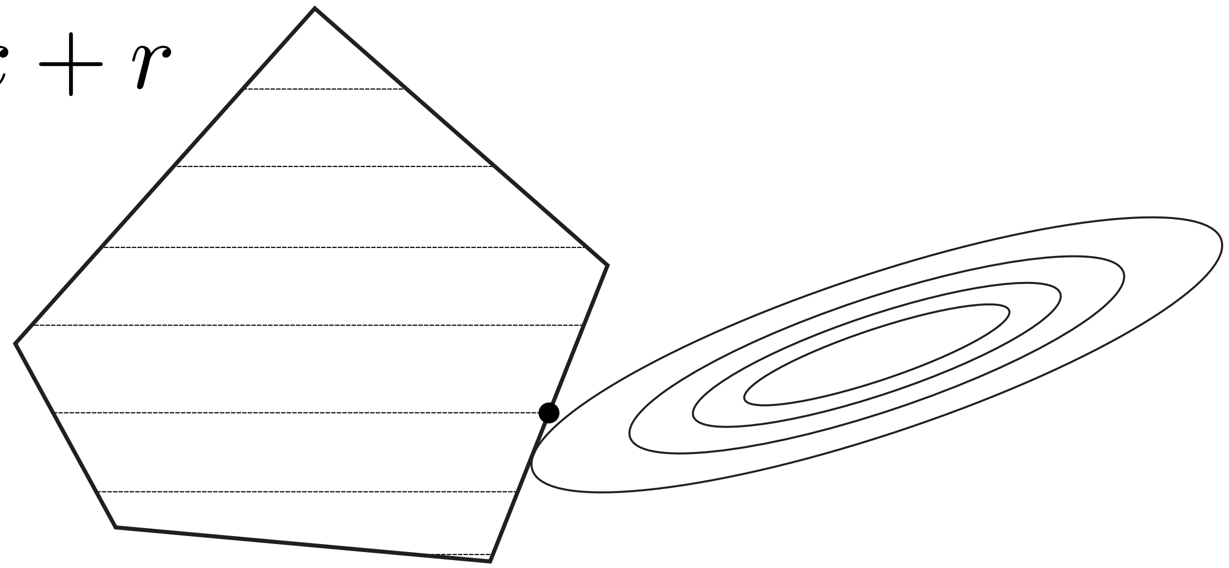

Strategy

$$\begin{array}{ll} \text{minimize} & (1/2)x^T P x + q^T x + r \\ \text{subject to} & A_{\mathcal{T}(\theta)} x = b_{\mathcal{T}(\theta)} \\ & x_{\mathcal{I}} = x_{\mathcal{I}}^{\star}(\theta) \end{array}$$

Equality Constrained QP

Quick online solution

KKT System

$$\begin{bmatrix} P & A_{\mathcal{T}(\theta)}^T & I_{\mathcal{I}}^T \\ A_{\mathcal{T}(\theta)} & & \\ I_{\mathcal{I}} & 0 & \end{bmatrix} \begin{bmatrix} x \\ \nu_A \\ \nu_I \end{bmatrix} = \begin{bmatrix} -q \\ b_{\mathcal{T}(\theta)} \\ x_{\mathcal{I}}^\star(\theta) \end{bmatrix}$$

[D. Bertsimas, B. Stellato, *Online Mixed-Integer Optimization in Milliseconds*, INFORMS Journal on Computing (under review), (2019)]

Quick online solution

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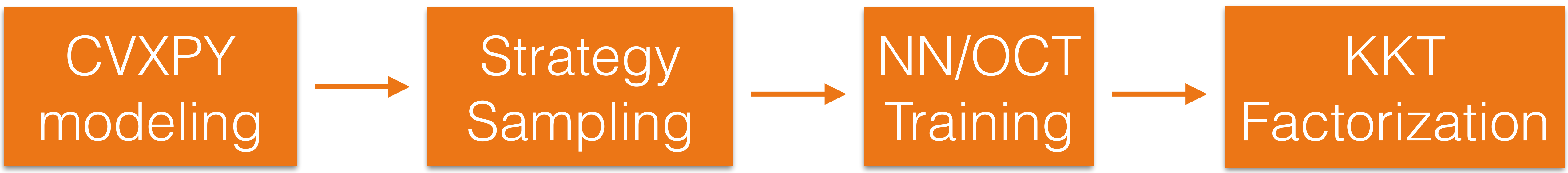
$\mathcal{NP}$-hard problem → Linear System

[D. Bertsimas, B. Stellato, *Online Mixed-Integer Optimization in Milliseconds*, INFORMS Journal on Computing (under review), (2019)]

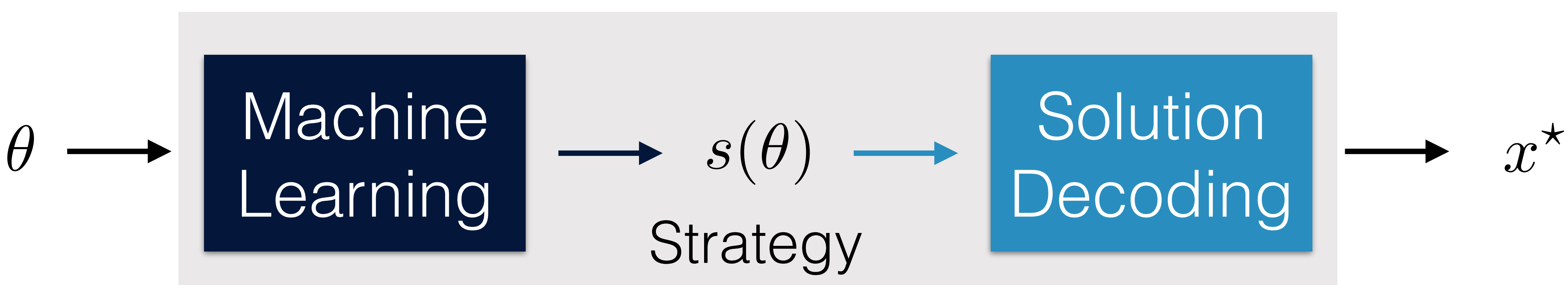
MLOPT: Machine Learning Optimizer

`github.com/bstellato/mlopt`

Offline Learning



Fast Online Optimization



[D. Bertsimas, B. Stellato, *The Voice of Optimization*, Machine Learning (to appear), (2020)]

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Sparse portfolio optimization

$$\begin{array}{ll} \text{maximize} & r^T w - \gamma w^T \Sigma w \\ \text{subject to} & \mathbf{1}^T w = 1 \\ & \mathbf{card}(w) \leq c \end{array}$$

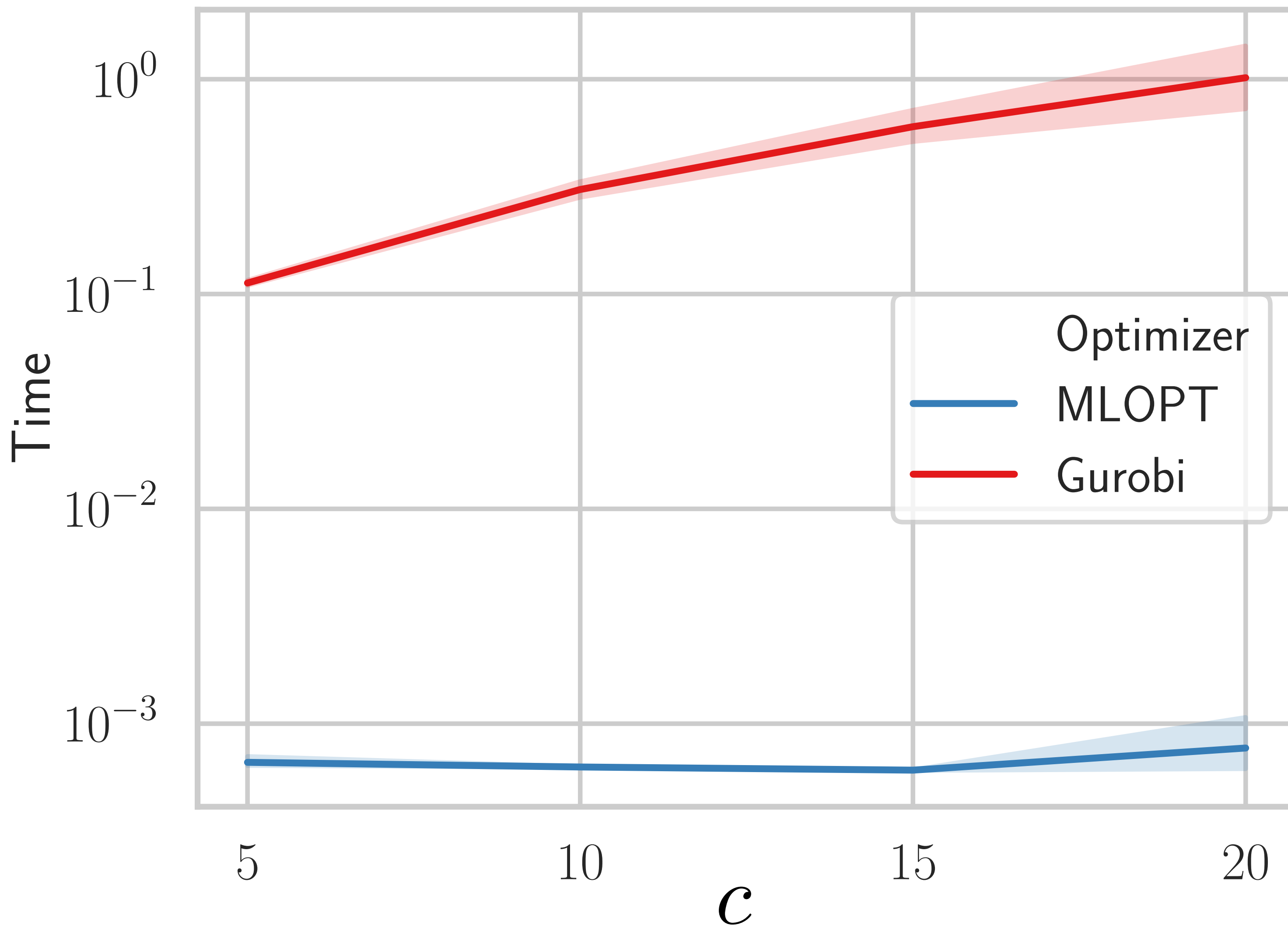
k-factor Risk Model

$$\Sigma = F \Sigma^k F^T + D$$

Parameters

$$\theta = (r, \Sigma^k, F, D)$$

S&P100 backtesting: high speed and accuracy



c	M	acc [%]	suboptimality	infeasibility
5	1027	99.11	9.88×10^{-3}	2.25×10^{-9}
10	1083	99.21	7.01×10^{-3}	8.19×10^{-7}
15	1120	99.30	1.92×10^{-2}	2.68×10^{-7}
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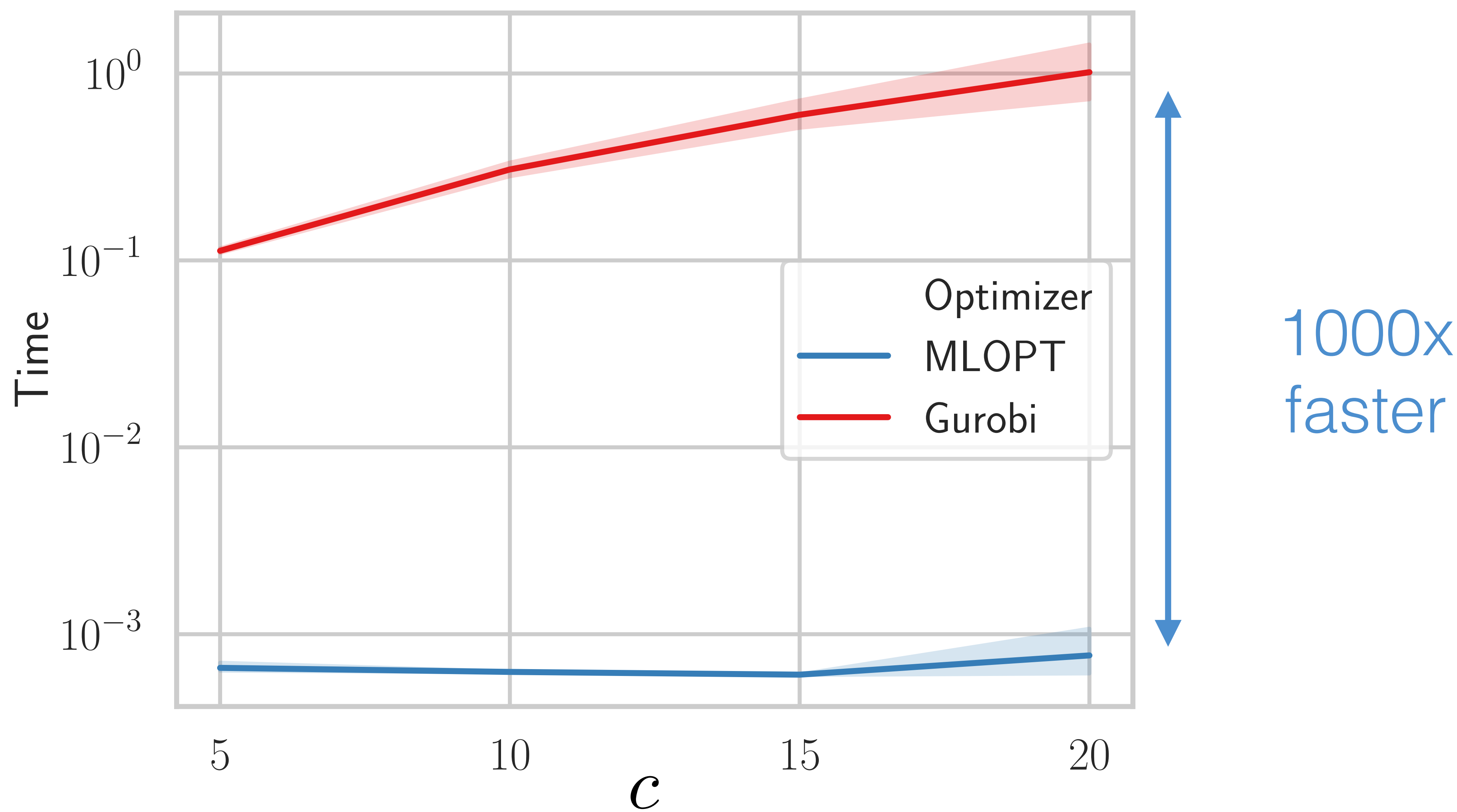

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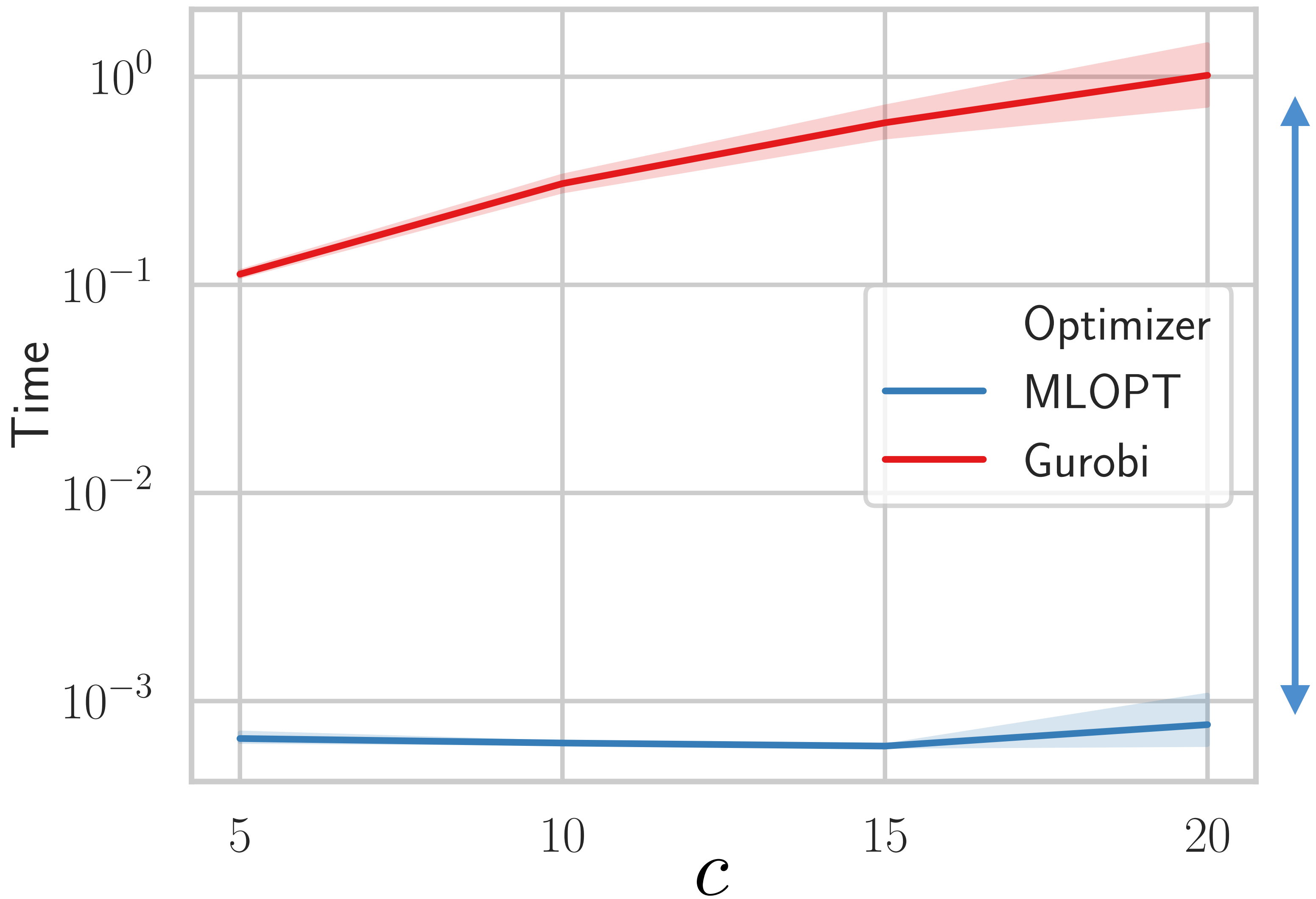

1000x faster

Low suboptimality and infeasibility

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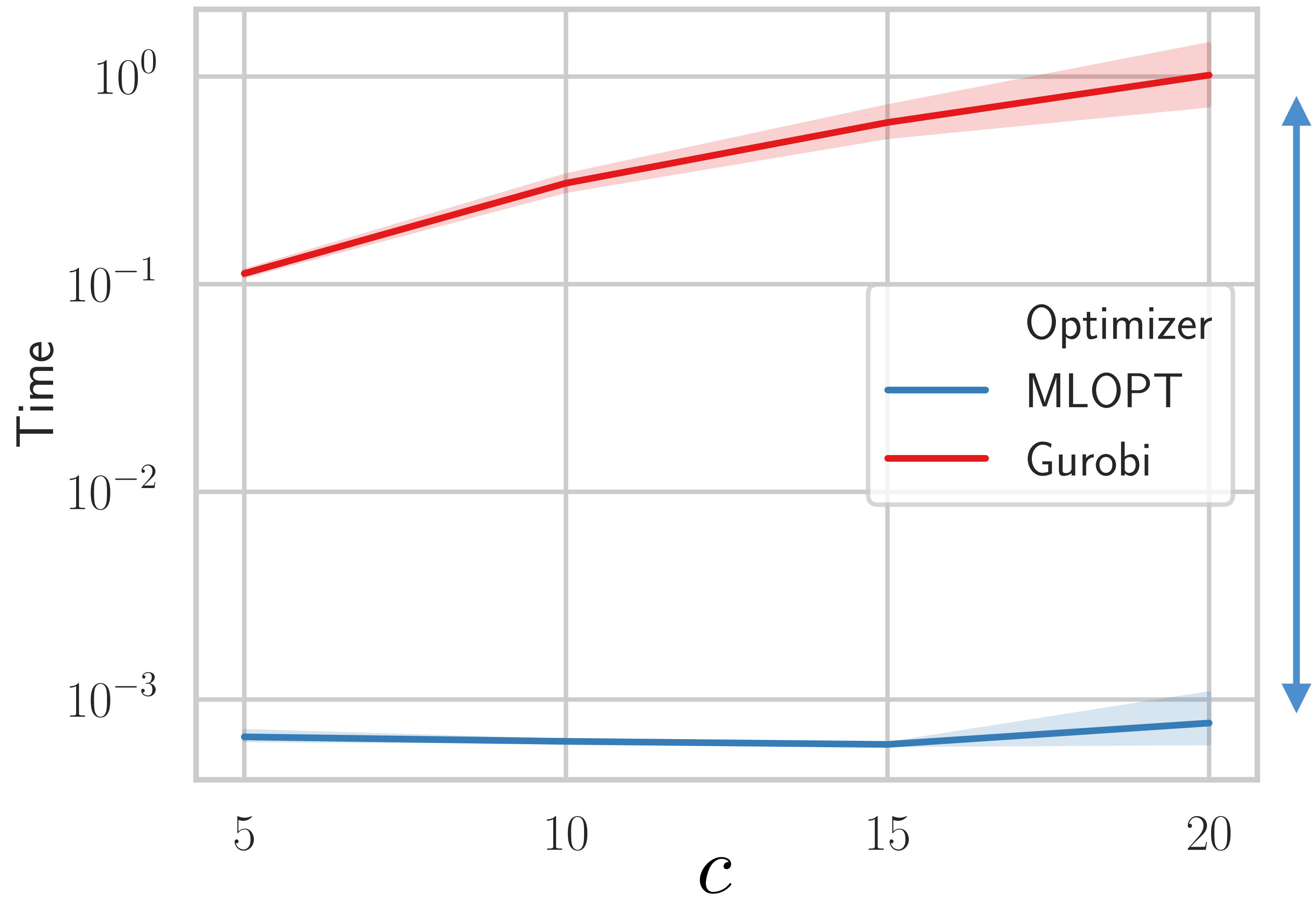

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High accuracy

Low suboptimality and infeasibility

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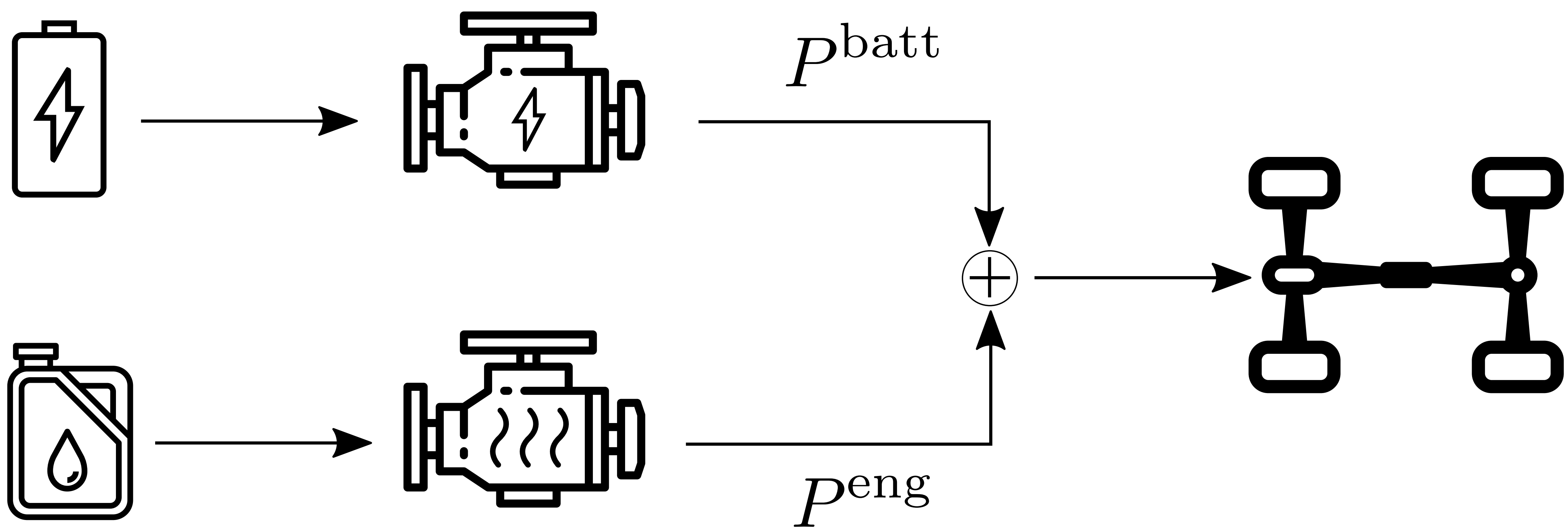
Hybrid-vehicle control



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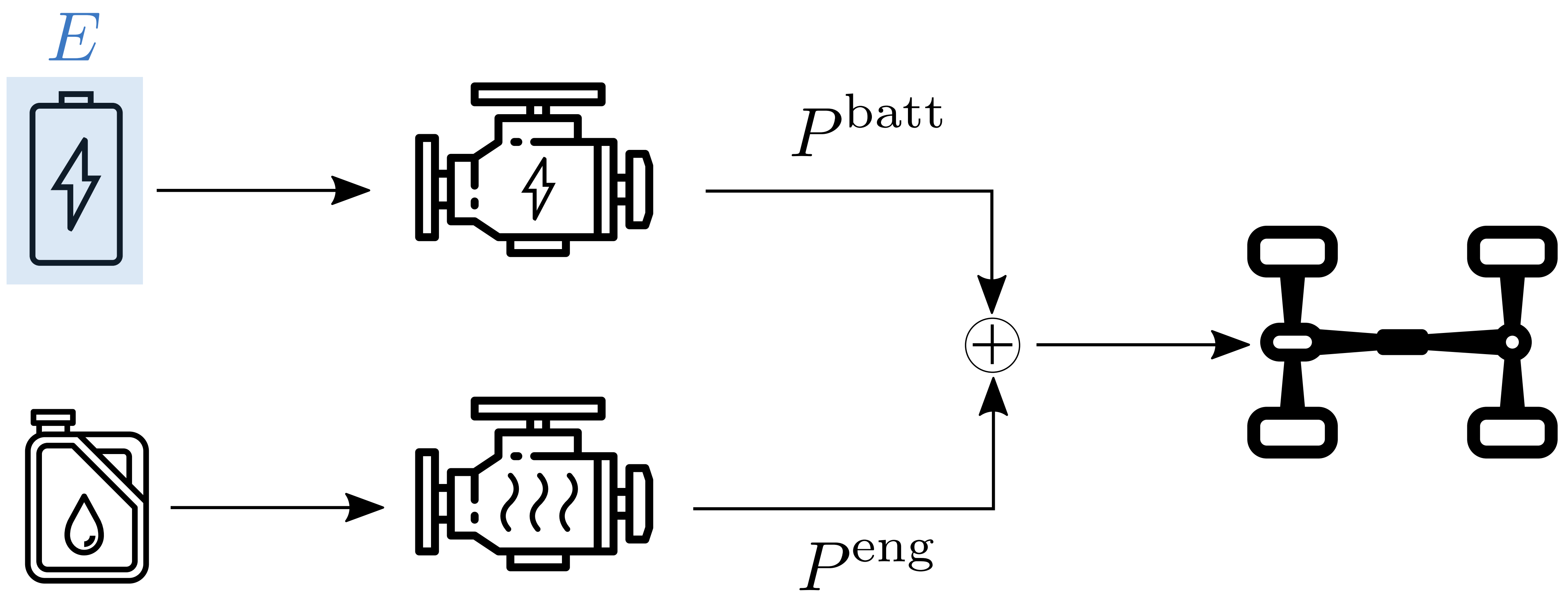


Hybrid-vehicle control

$$\begin{aligned}
\text{minimize} \quad & \sum_{t=0}^{T-1} f(P_t^{\text{eng}}, z_t) + \delta(z_t - z_{t-1})_+ \\
\text{subject to} \quad & P_t^{\text{batt}} + P_t^{\text{eng}} \geq P_t^{\text{des}} \\
& E_{t+1} = E_t - \tau P_t^{\text{batt}} \\
& E_0 = E_{\text{init}} \\
& z_t \in \{0, 1\}
\end{aligned}$$

Hybrid-vehicle control

minimize $\sum_{t=0}^{T-1} f(P_t^{\text{eng}}, z_t) + \delta(z_t - z_{t-1})_+$

subject to $P_t^{\text{batt}} + P_t^{\text{eng}} \geq P_t^{\text{des}}$ Desired Power

$E_{t+1} = E_t - \tau P_t^{\text{batt}}$

$E_0 = E_{\text{init}}$

$z_t \in \{0, 1\}$

Hybrid-vehicle control

$$\begin{aligned} \text{minimize} \quad & \sum_{t=0}^{T-1} f(P_t^{\text{eng}}, z_t) + \delta(z_t - z_{t-1})_+ \\ \text{subject to} \quad & P_t^{\text{batt}} + P_t^{\text{eng}} \geq P_t^{\text{des}} \\ & E_{t+1} = E_t - \tau P_t^{\text{batt}} \\ & E_0 = E_{\text{init}} \\ & z_t \in \{0, 1\} \end{aligned}$$

Desired Power

Battery Dynamics

Hybrid-vehicle control

minimize $$\sum_{t=0}^{T-1} f(P_t^{\text{eng}}, z_t) + \delta(z_t - z_{t-1})_+$$

subject to $$P_t^{\text{batt}} + P_t^{\text{eng}} \geq P_t^{\text{des}}$$ Desired Power

$$E_{t+1} = E_t - \tau P_t^{\text{batt}}$$
$$E_0 = E_{\text{init}}$$ Battery Dynamics

$$z_t \in \{0, 1\}$$ Engine Switch

Hybrid-vehicle control

$$\text{minimize} \quad \sum_{t=0}^{T-1} f(P_t^{\text{eng}}, z_t) + \delta(z_t - z_{t-1})_+$$

$$\text{subject to} \quad P_t^{\text{batt}} + P_t^{\text{eng}} \geq P_t^{\text{des}}$$

Desired Power

$$E_{t+1} = E_t - \tau P_t^{\text{batt}}$$

$$E_0 = E_{\text{init}}$$

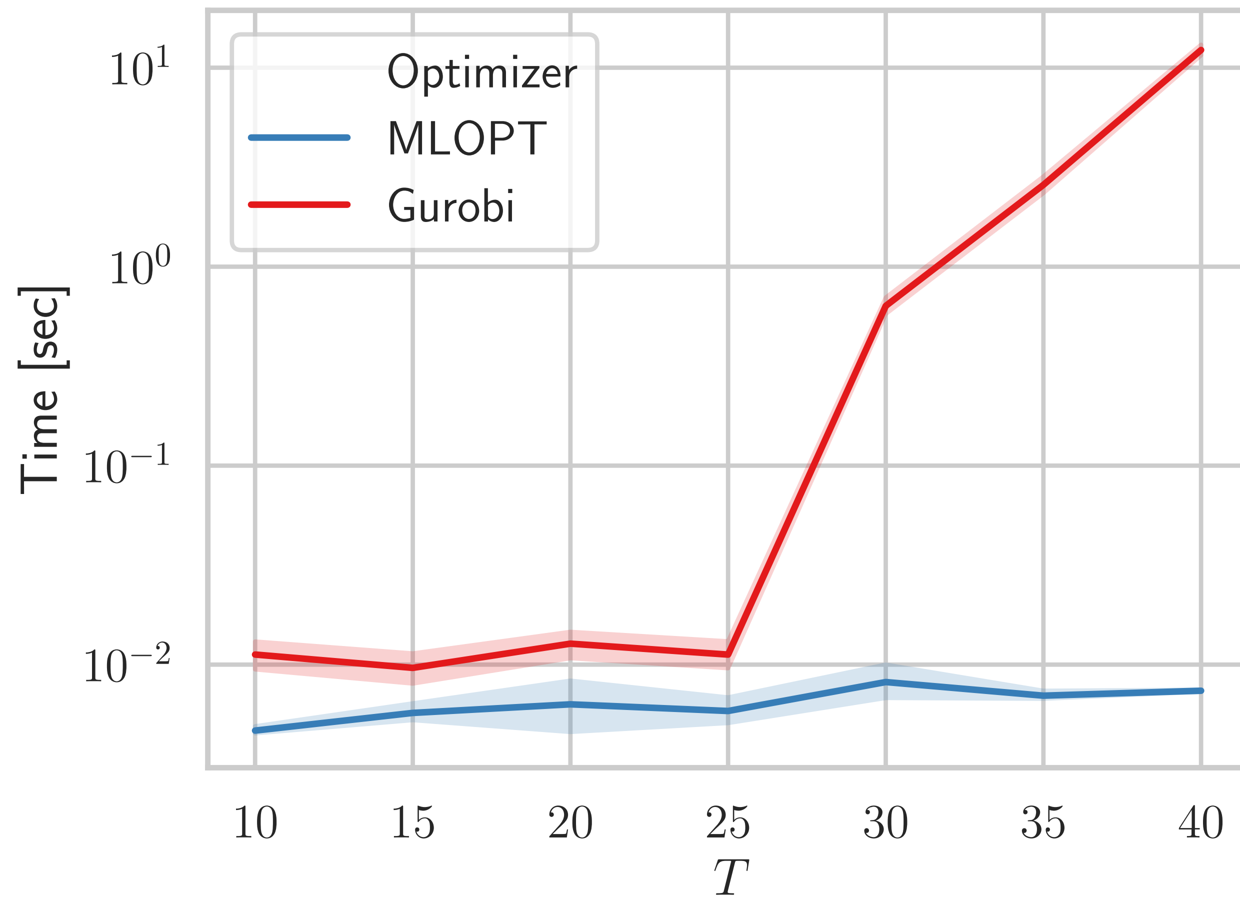
Battery Dynamics

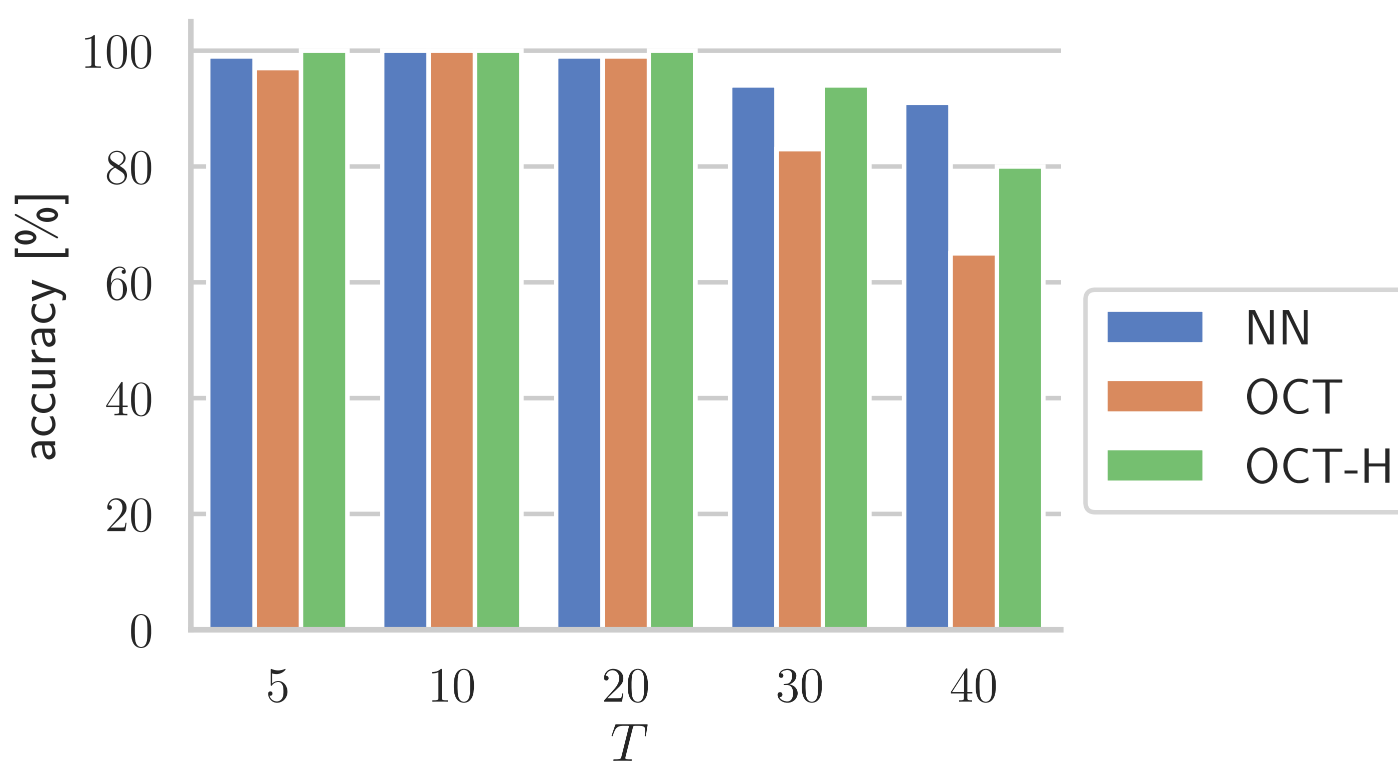
$$z_t \in \{0, 1\}$$

Engine Switch

Parameters

MPC results: high speed and accuracy





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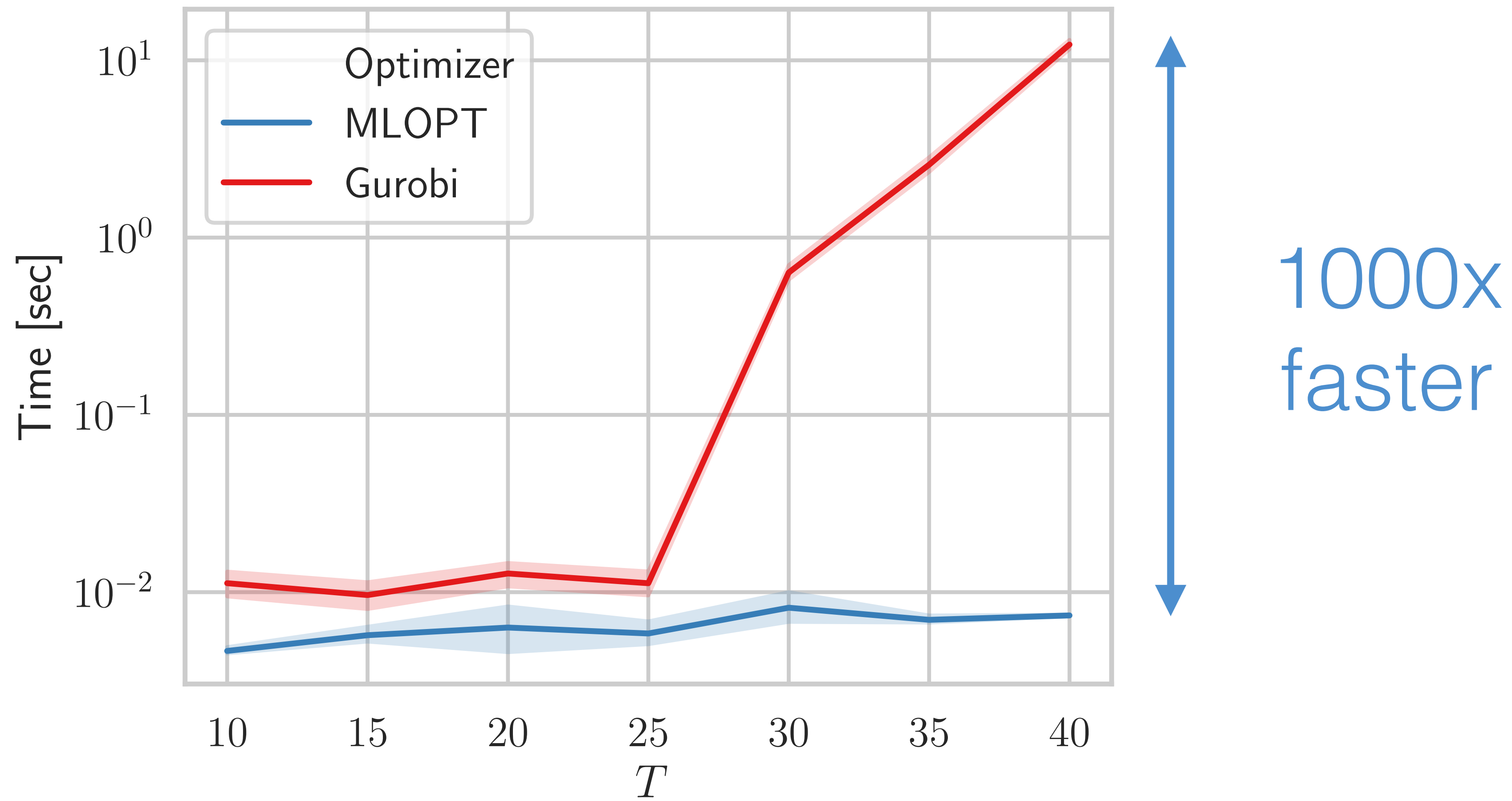

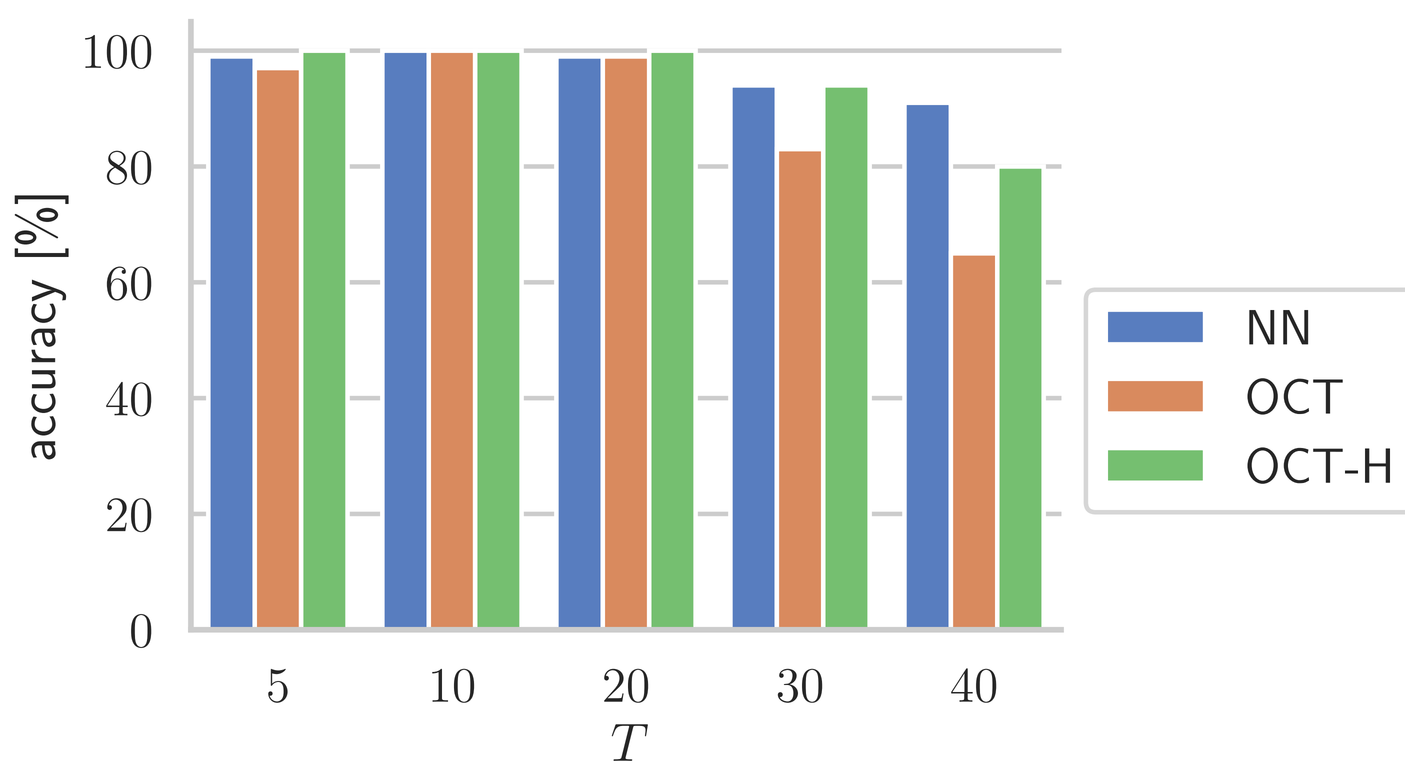

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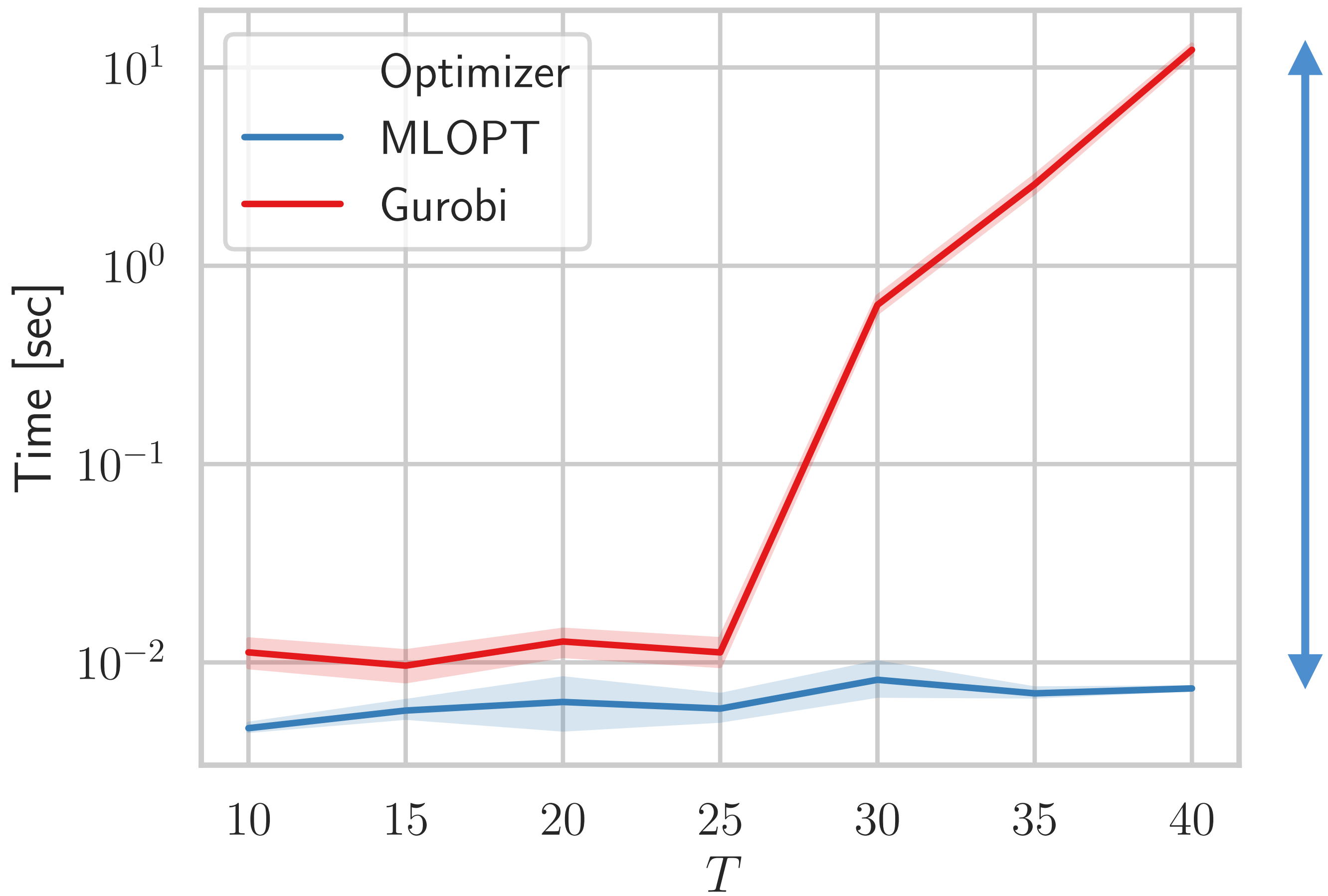
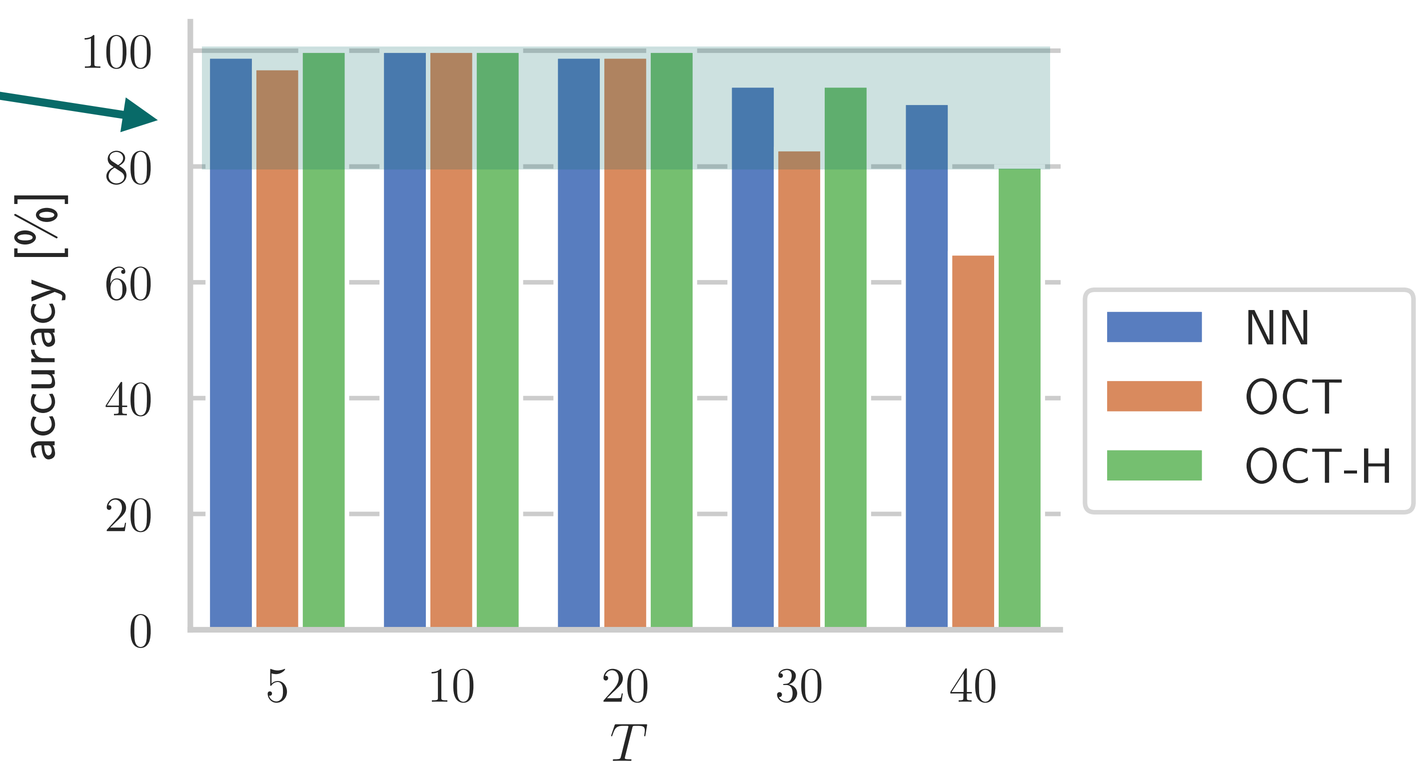
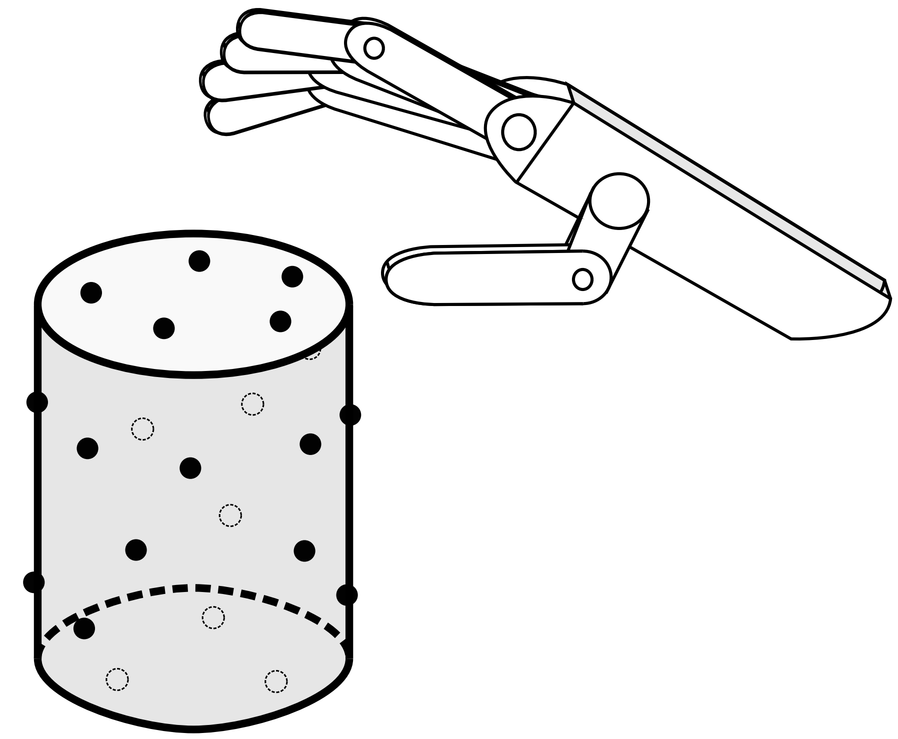


1000x faster

High accuracy



Dexterous Robotic Grasps



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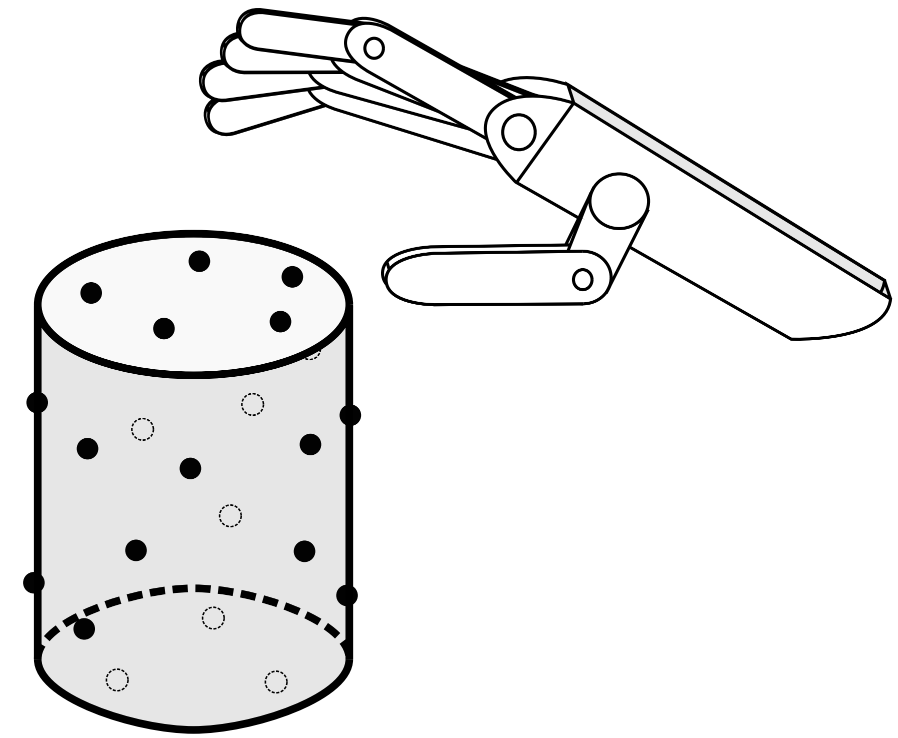


maximize α

subject to $Gf = \alpha \hat{F}$

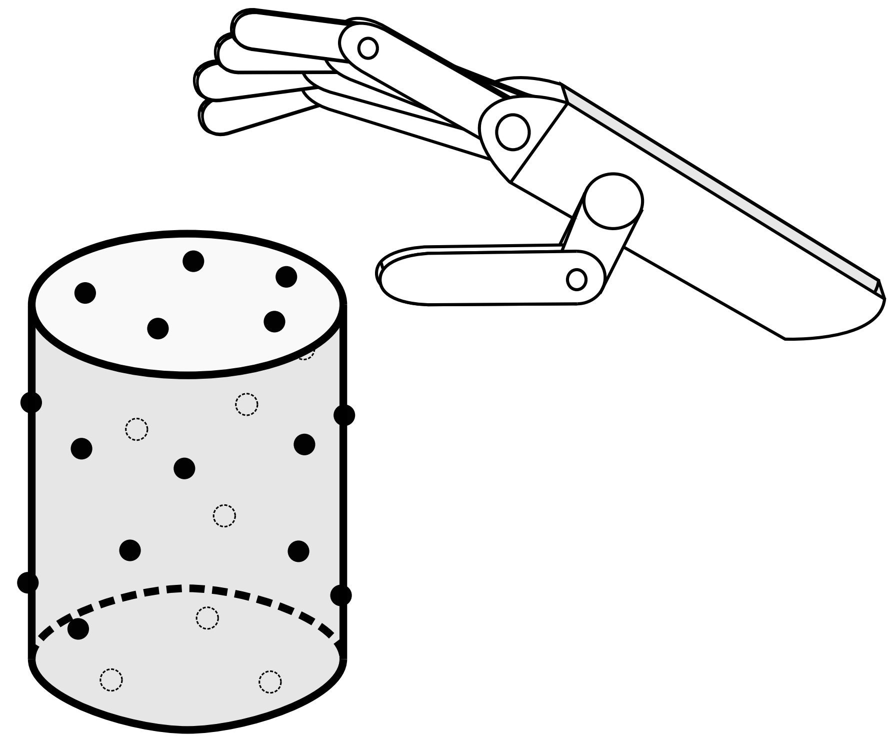
$$f_i \in \mathcal{K}^{(i)}, \quad i = 1, \dots P$$

$$f_i^z \leq \delta_i, \quad i = 1, \dots, P$$

$$\sum_{i=1}^{P} \delta_i \leq k$$

$$\delta \in \{0, 1\}^P$$

Dexterous Robotic Grasps



Grasp metric

maximize α

subject to $Gf = \alpha \hat{F}$

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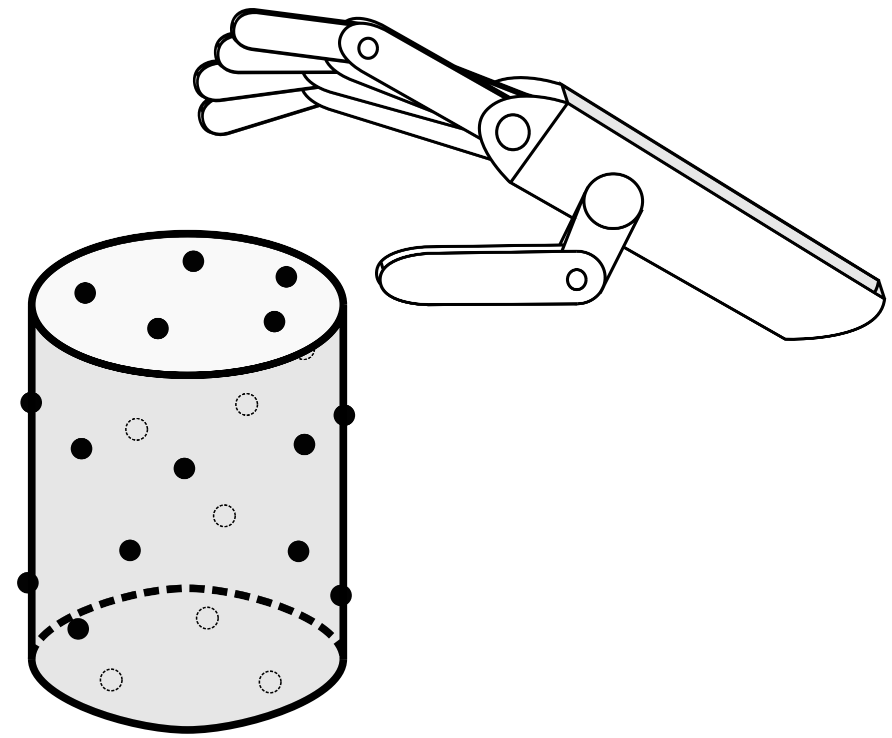
Dexterous Robotic Grasps



Grasp metric

maximize α

Task wrench

subject to $Gf = \alpha \hat{F}$

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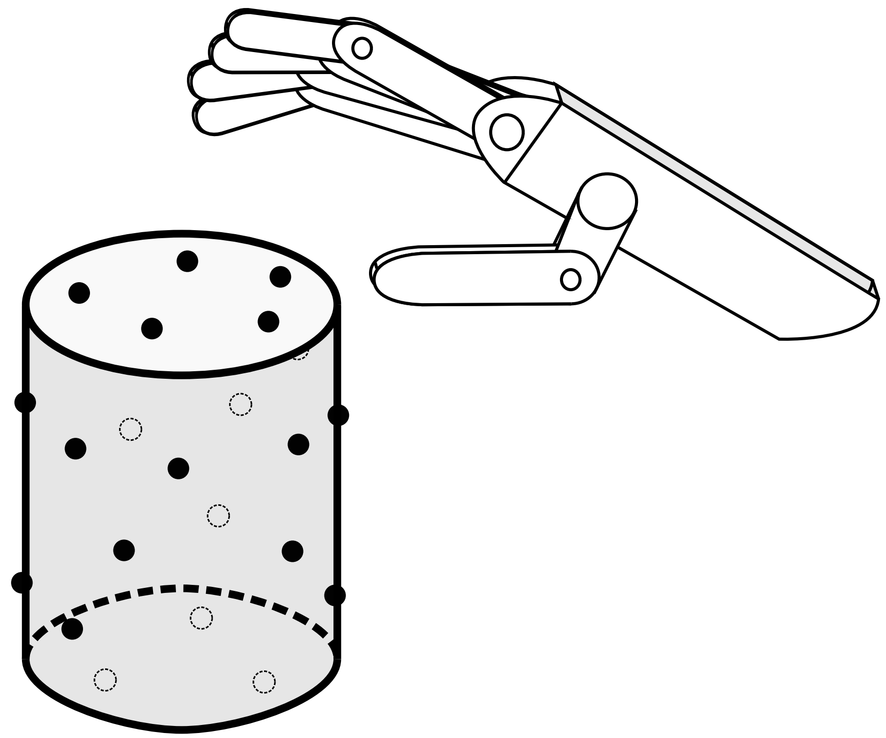

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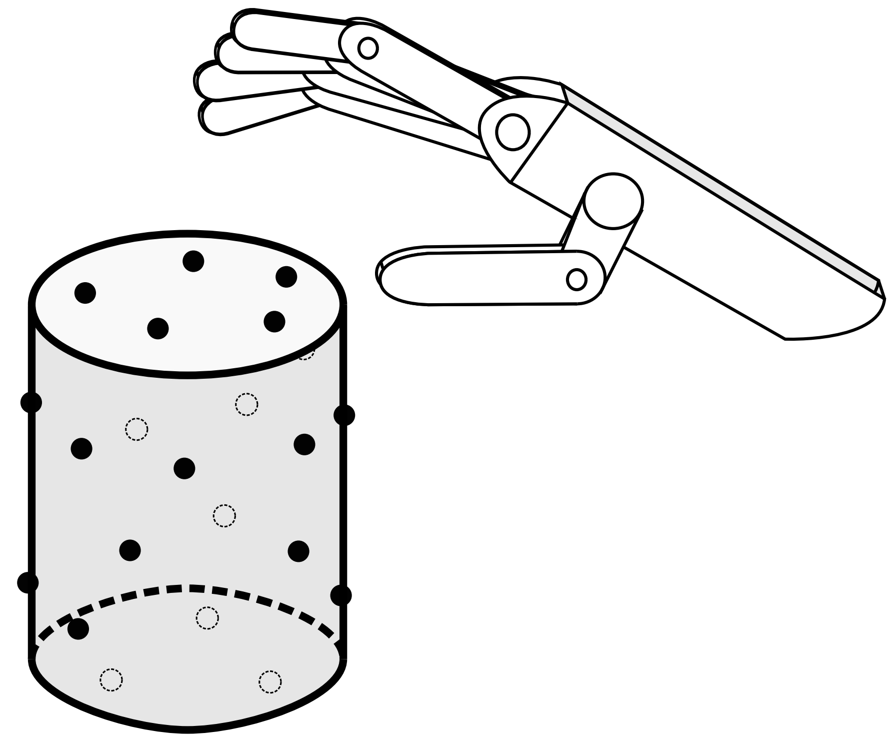
Dexterous Robotic Grasps



Grasp metric

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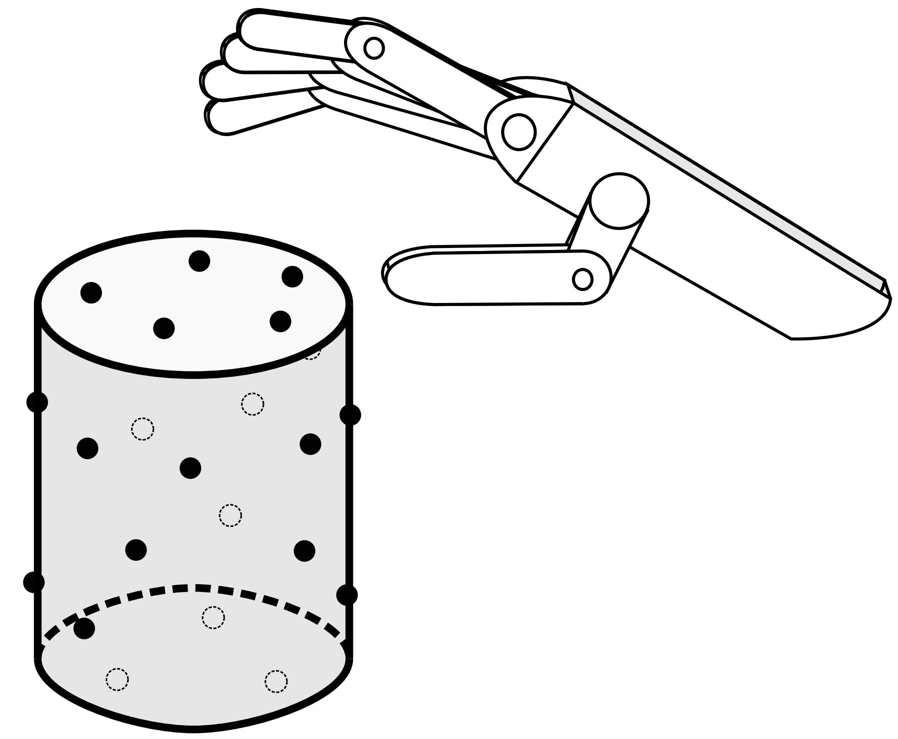
$$\sum_{i=1}^{P} \delta_i \leq k$$
$$\delta \in \{0, 1\}^P$$

Points Selection

Dexterous Robotic Grasps



Grasp metric

maximize α

Task wrench

subject to $Gf = \alpha \hat{F}$

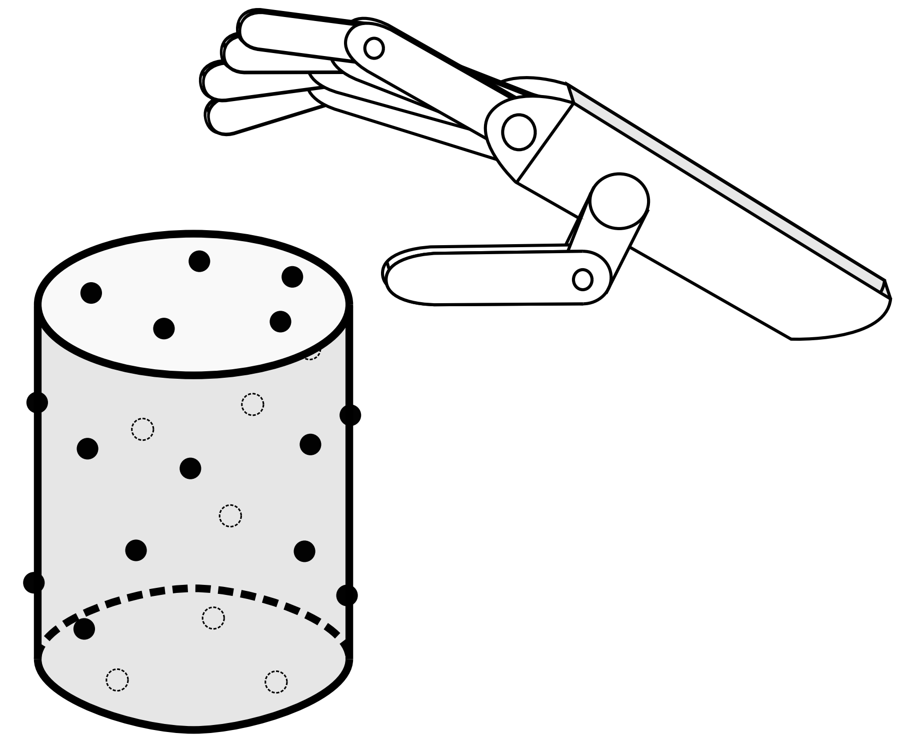
$f_i \in \mathcal{K}^{(i)}, \quad i = 1, \ldots P$ Friction Cone

$$f_i^z \leq \delta_i, \quad i = 1, \ldots, P$$
$$\sum_{i=1}^{P} \delta_i \leq k$$
$$\delta \in \{0, 1\}^P$$

Points Selection

MISOCP

Dexterous Robotic Grasps



Grasp metric

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Task wrench

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$f_i \in \mathcal{K}^{(i)}, \quad i = 1, \dots P$ Friction Cone

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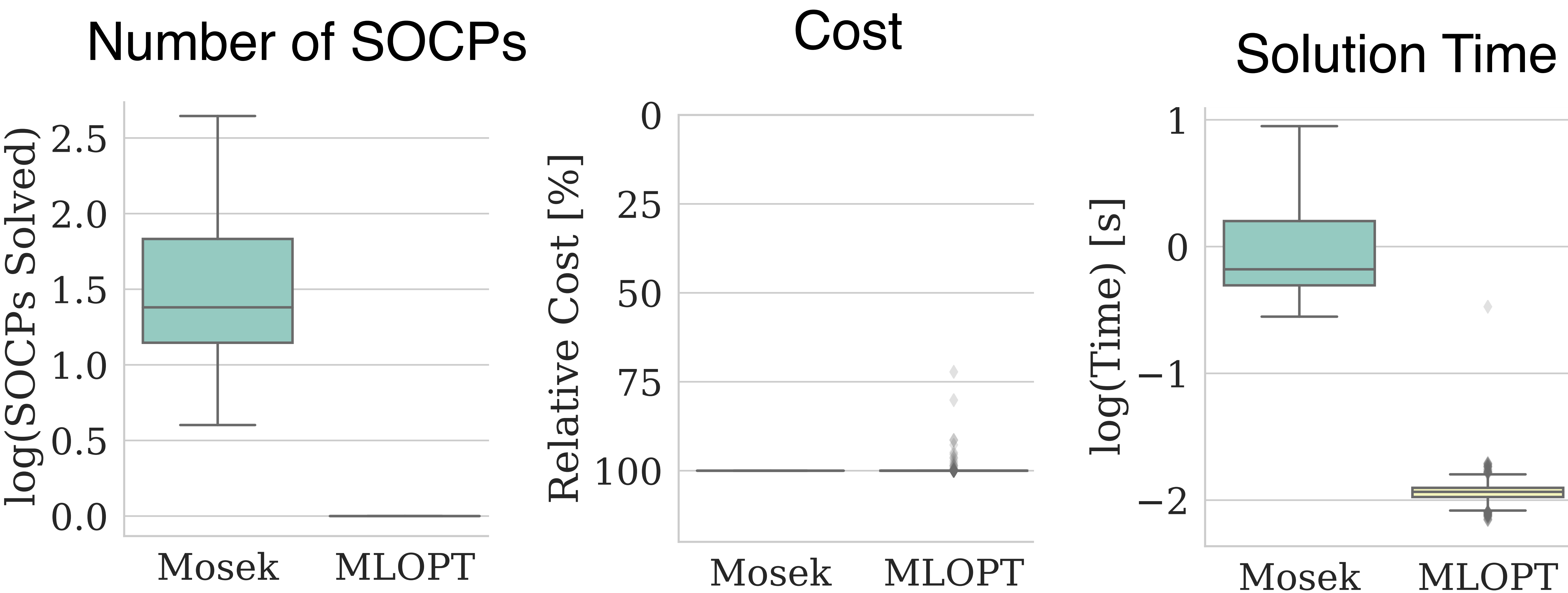
Points Selection

MISOCP

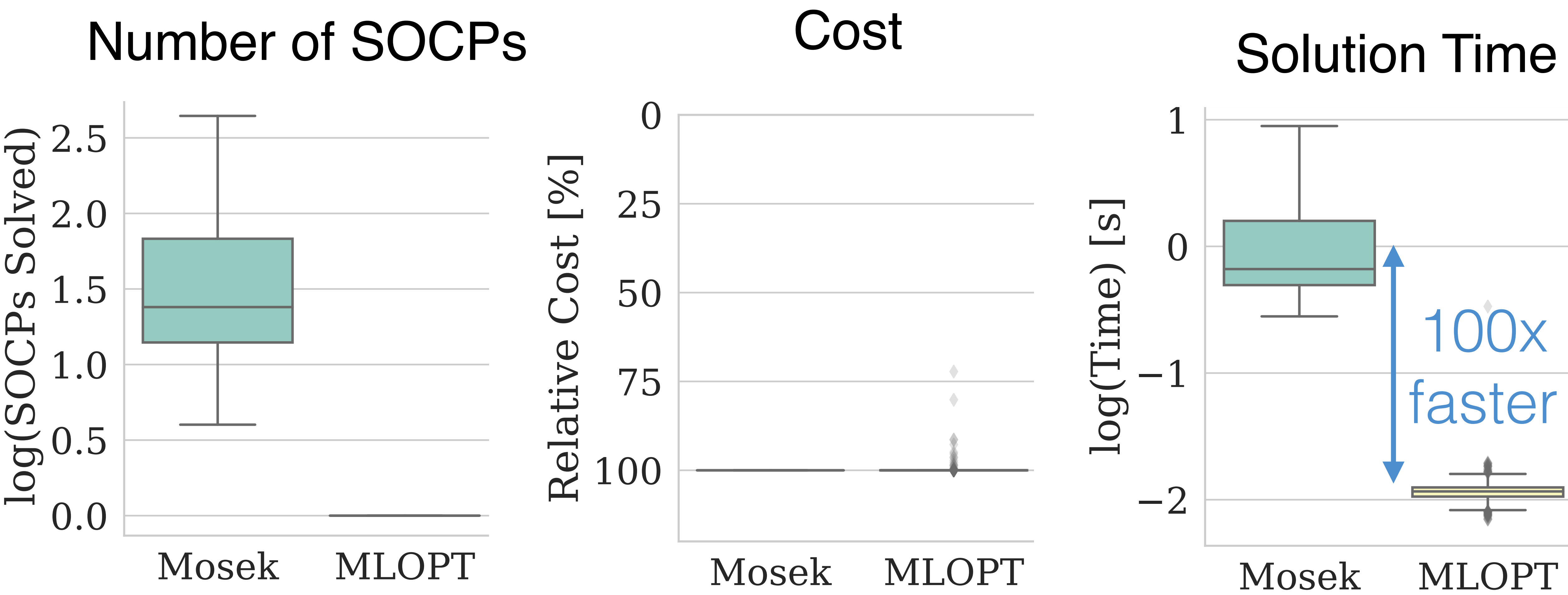
Parameters

High-speed Dexterous Robotic Grasps



[A. Cauligi, P. Culbertson, B. Stellato, D. Bertsimas, M. Schwager, M. Pavone, *Learning Mixed-Integer Convex Optimization Strategies for Robot Planning and Control*, arXiv:1907.02206, (2019)]

High-speed Dexterous Robotic Grasps



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Conclusions

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Machine Learning for Optimization

Optimization links data to decisions

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Understand it using ML

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Solve it very fast

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Backup

Sampling scheme

Algorithm 1 Strategies exploration

given $\epsilon, \beta, \Theta = \emptyset, \mathcal{S} = \emptyset, u = \infty$
for $k = 1, \ldots,$ **do**
  Sample θ_k and compute $s(\theta_k)$ ▷ Sample parameter and strategy.
  $\Theta \leftarrow \Theta \cup \{\theta_k\}$ ▷ Update set of samples.
  if $s(\theta_k) \notin \mathcal{S}$ **then**
    $\mathcal{S} \leftarrow \mathcal{S} \cup \{s(\theta_k)\}$ ▷ Update strategy set if new strategy found
  end if
  if $G + c\sqrt{(1/k)\ln(3/\beta)} \leq \epsilon$ **then** ▷ Break if bound less than ϵ
    break
  end if
end for
return $k, \Theta, \mathcal{S}$