Our contribution

Correctional Regret for Predict+Optimize with Unknown Objectives and Constraints

[Demirovı́ c et al., 2019a], [Elmachtoub and Grigas, 2022]

Work in progress -- IJCAI 2022 DSO Workshop

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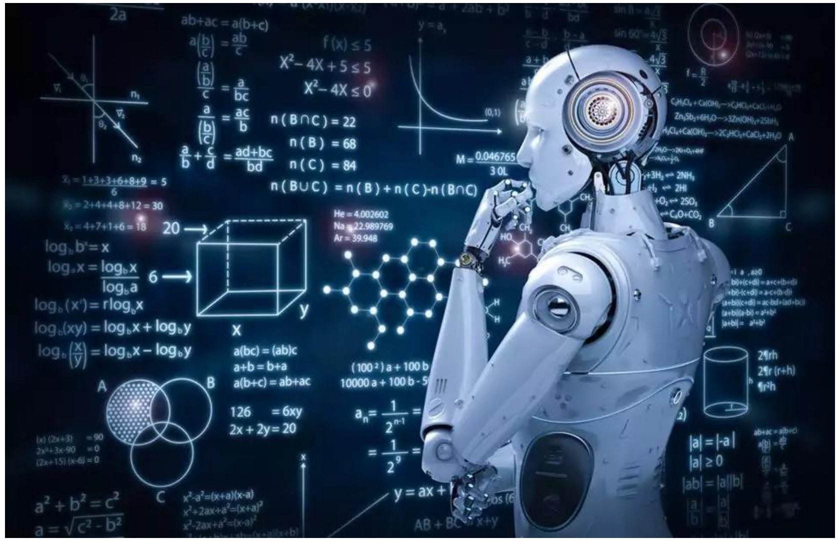
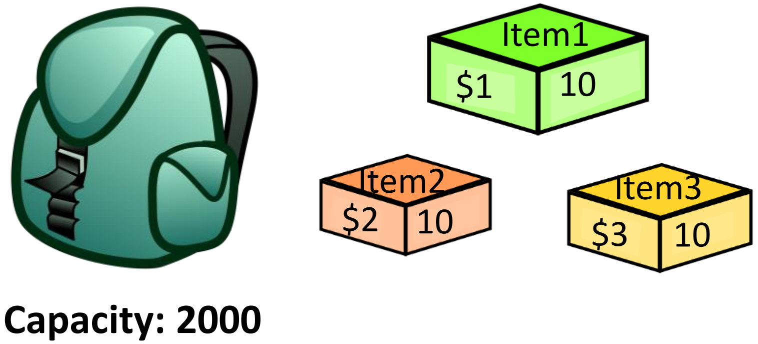




Machine learning

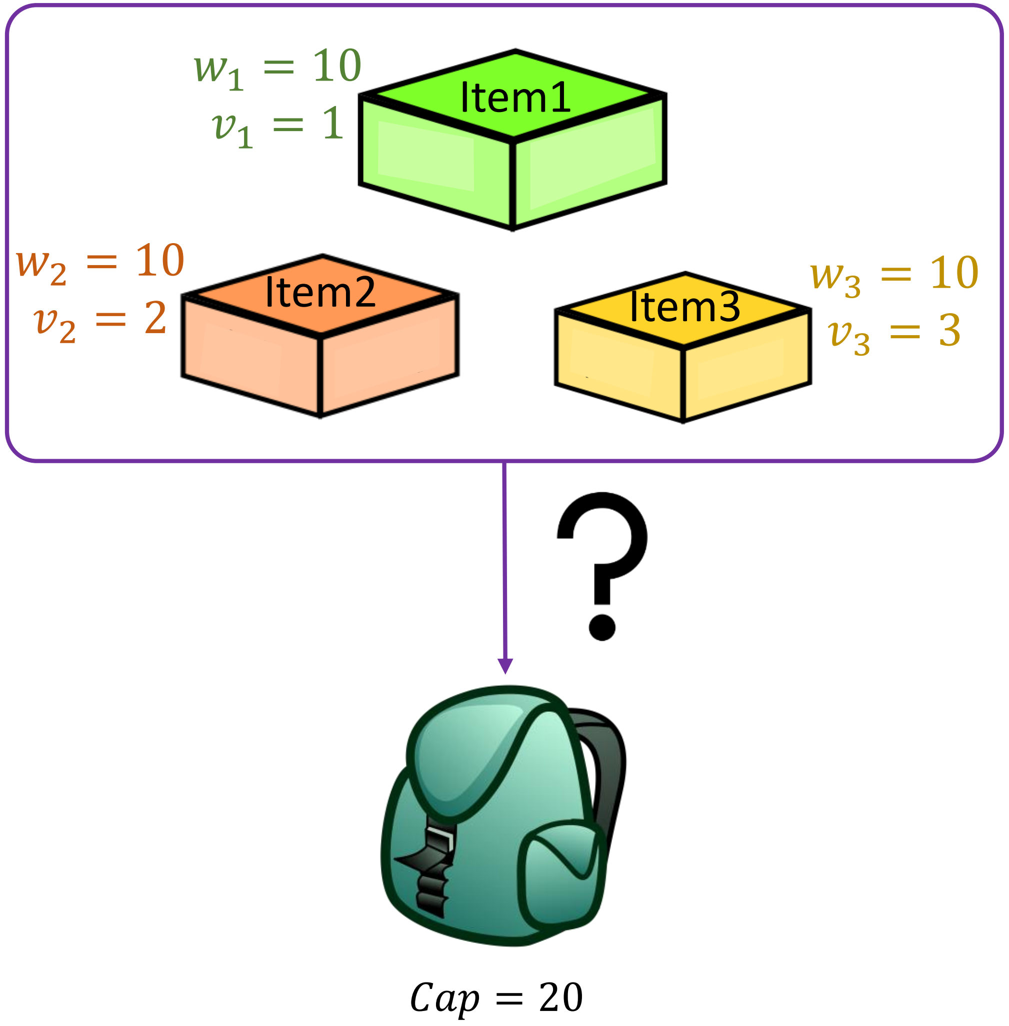
Constraint optimization

Predict+Optimize

Constraint Optimization Problems (COPs)
with unknown parameters

[Demirovĭ c et al., 2019a],
[Demirovĭ c et al., 2019b],
[Elmachtoub and Grigas, 2022]

Knapsack Problem



- 3 items, each with a weight w_i and a value v_i, the capacity Cap is limited.
- Select items so that
  - the total weight is no more than the capacity and
  - maximize the total value
- **Constraint Optimization Problem (COP):**

Decision variable

$$x_i = \begin{cases} 0, & \text{the } i\text{th item is not selected} \\ 1, & \text{the } i\text{th item is selected} \end{cases}$$

Objective function

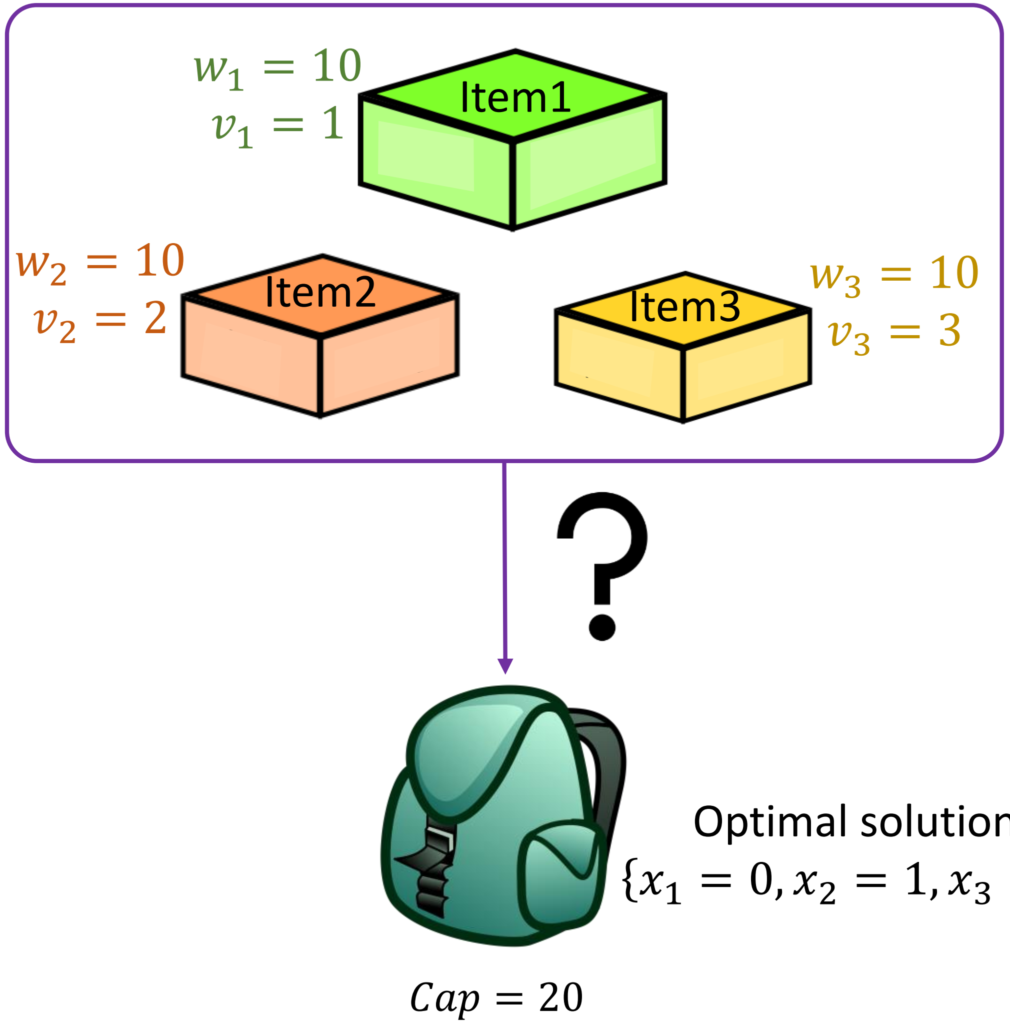
$$\boxed{\max_x x_1 + 2x_2 + 3x_3}$$

Constraints

$$\boxed{\begin{aligned} s.t.\, 10x_1 + 10x_2 + 10x_3 \leq 20 \\ x_i \in \{0,1\}\ \forall i \in \{1,2,3\} \end{aligned}}$$

A constraint is a condition of an optimization problem that the solution must satisfy.

Knapsack Problem



Optimal solution:
$\{x_1 = 0, x_2 = 1, x_3 = 1\}$

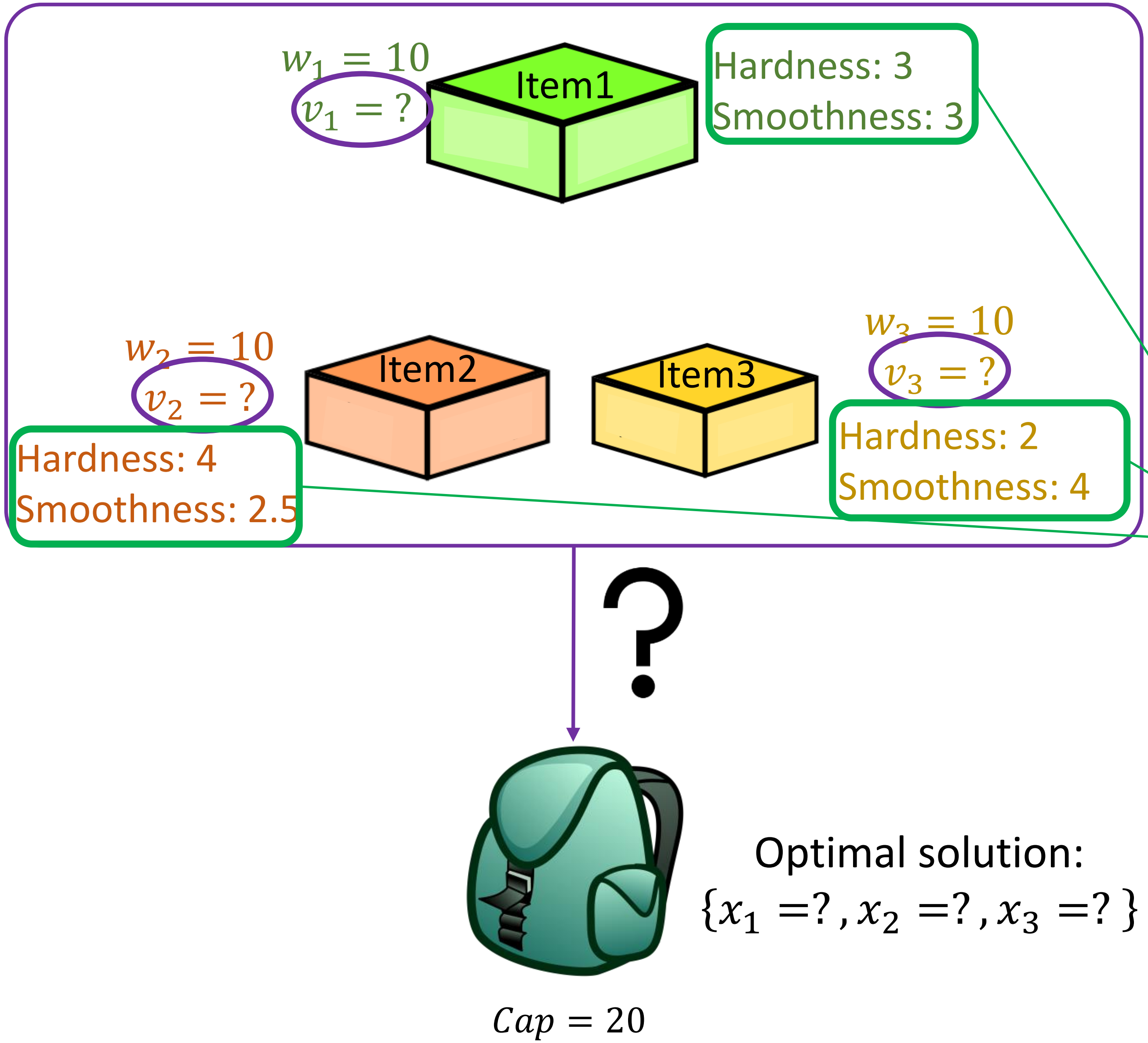
- 3 items, each with a weight w_i and a value v_i, the capacity Cap is limited.
- Select items so that
  - the total weight is no more than the capacity and
  - maximize the total value
- **Constraint Optimization Problem (COP):**

$$\max_x \sum_i v_i x_i$$
$$s.t. \sum_i w_i x_i \le Cap$$
$$x_i \in \{0,1\} \; \forall i \in \{1,2,3\}$$

Problem parameters

NP-hard

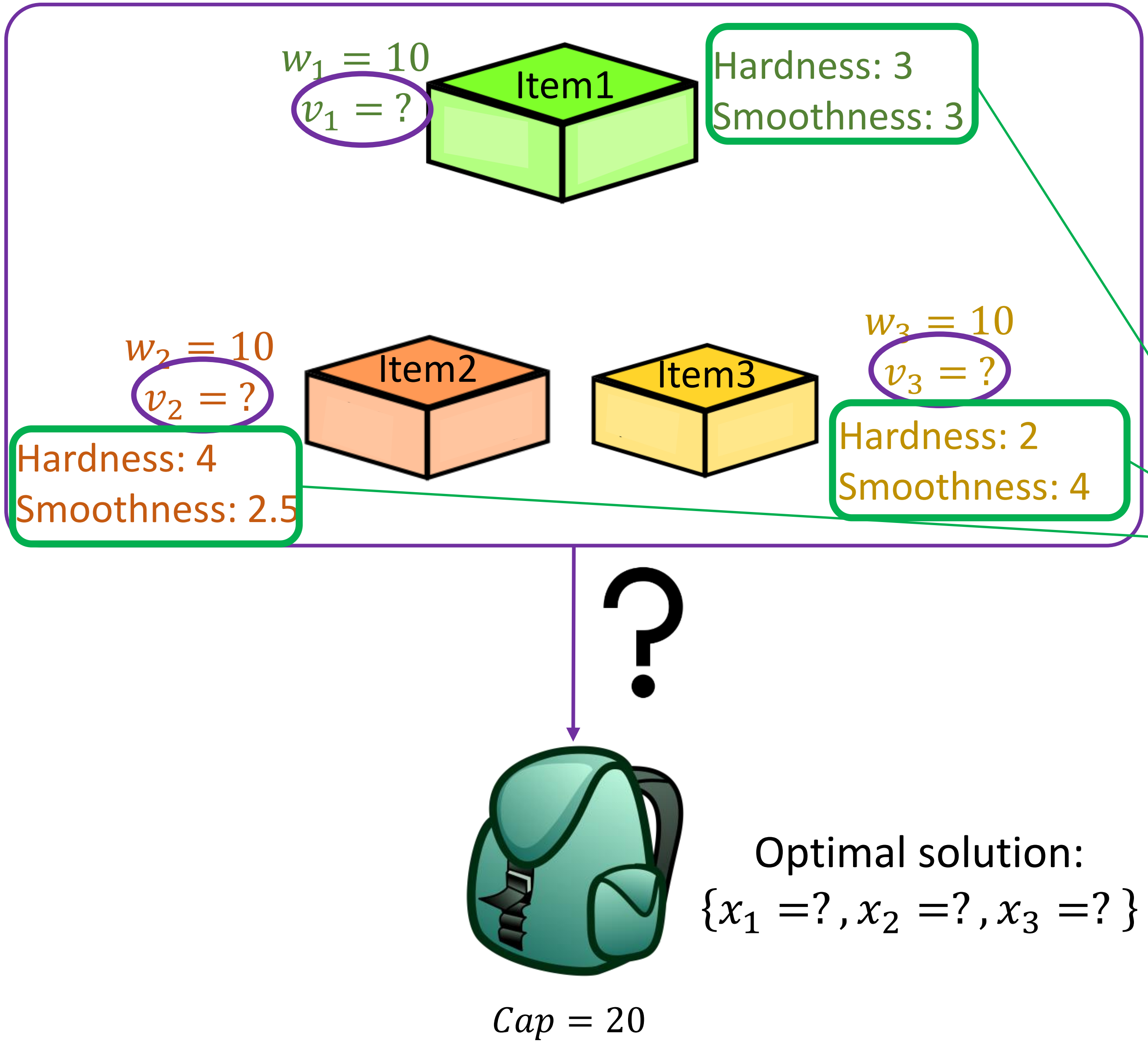
Some problem parameters may be unknown



- The value v_i is unknown.
- Select items so that
  - the total weight is no more than the capacity and
  - maximize the total value

- **COP with Unknown Parameters:**
  - θ: unknown parameters, e.g., $\theta = \{v_1, v_2, v_3\}$
  - A: feature matrix
    - Hardness
    - Smoothness
    - $A = \begin{bmatrix} 3 & 3 \\ 4 & 2.5 \\ 2 & 4 \end{bmatrix}$

Some problem parameters may be unknown



- The value v_i is unknown.
- Select items so that
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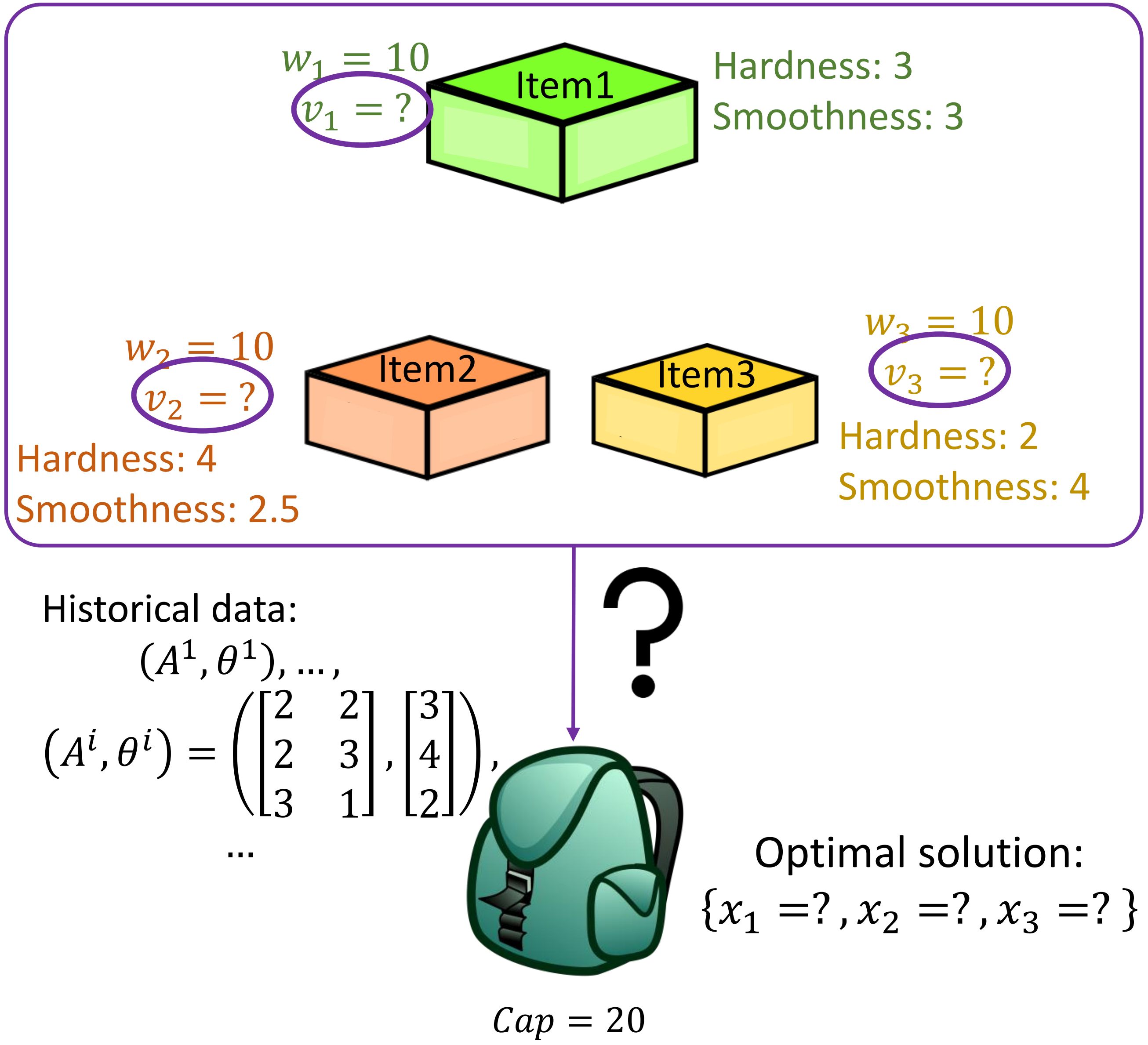
- **COP with Unknown Parameters:**
  - θ: unknown parameters, e.g., $\theta = \{v_1, v_2, v_3\}$
  - A: feature matrix
    - Hardness
    - Smoothness
    - $A = \begin{bmatrix} 3 & 3 \\ 4 & 2.5 \\ 2 & 4 \end{bmatrix}$
  - Historical data: $\{(A^1, \theta^1), (A^2, \theta^2), \dots, (A^k, \theta^k)\}$

$$(A^i, \theta^i) = \left(\overbrace{\begin{bmatrix} 2 & 2 \\ 2 & 3 \\ 3 & 1 \end{bmatrix}}^{\text{Historical features}}, \overbrace{\begin{bmatrix} 3 \\ 4 \\ 2 \end{bmatrix}}^{\text{True parameters}} \right)$$

Knapsack Problem



$w_1 = 10$

$v_1 = ?$

Item1

Hardness: 3

Smoothness: 3

$w_2 = 10$

$v_2 = ?$

Hardness: 4

Smoothness: 2.5

Item2

Item3

$w_3 = 10$

$v_3 = ?$

Hardness: 2

Smoothness: 4

Historical data:

$(A^1, \theta^1), \dots,$

$$(A^i, \theta^i) = \left(\begin{bmatrix} 2 & 2 \\ 2 & 3 \\ 3 & 1 \end{bmatrix}, \begin{bmatrix} 3 \\ 4 \\ 2 \end{bmatrix} \right),$$

…

Optimal solution:

$\{x_1 = ?, x_2 = ?, x_3 = ?\}$

$Cap = 20$

- Constraint Optimization Problem (COP):

$$\max_x \sum_i v_i x_i$$
$$s.t. \sum_i w_i x_i \le Cap$$
$$x_i \in \{0,1\} \ \forall i \in \{1,2,3\}$$

- COP with Unknown Parameters:

Unknown parameters

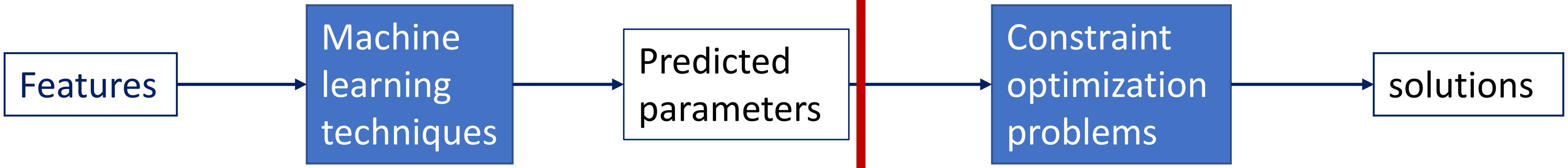
$$\max_x \sum_i \theta_i x_i$$
$$s.t. \sum_i w_i x_i \le Cap$$
$$x_i \in \{0,1\} \ \forall i \in \{1,2,3\}$$

- Aim:
  - learn a prediction function f
  - given current features, use f to generate predicted parameters $\hat{\theta}$
  - try to estimate optimal solution(s) of the COP by using $\hat{\theta}$

How to solve the problem

Predict

Optimize



Features

Machine learning techniques

Predicted parameters

Constraint optimization problems

solutions

Predict+Optimize VS Classical approaches
Main difference:
error measurement

[Demirovı́ c et al., 2020],
[Elmachtoub and Grigas, 2022],
[Guler et al., 2022]

Aim: good estimated solutions of the COP under the true parameters

Classical approaches: predict then optimize

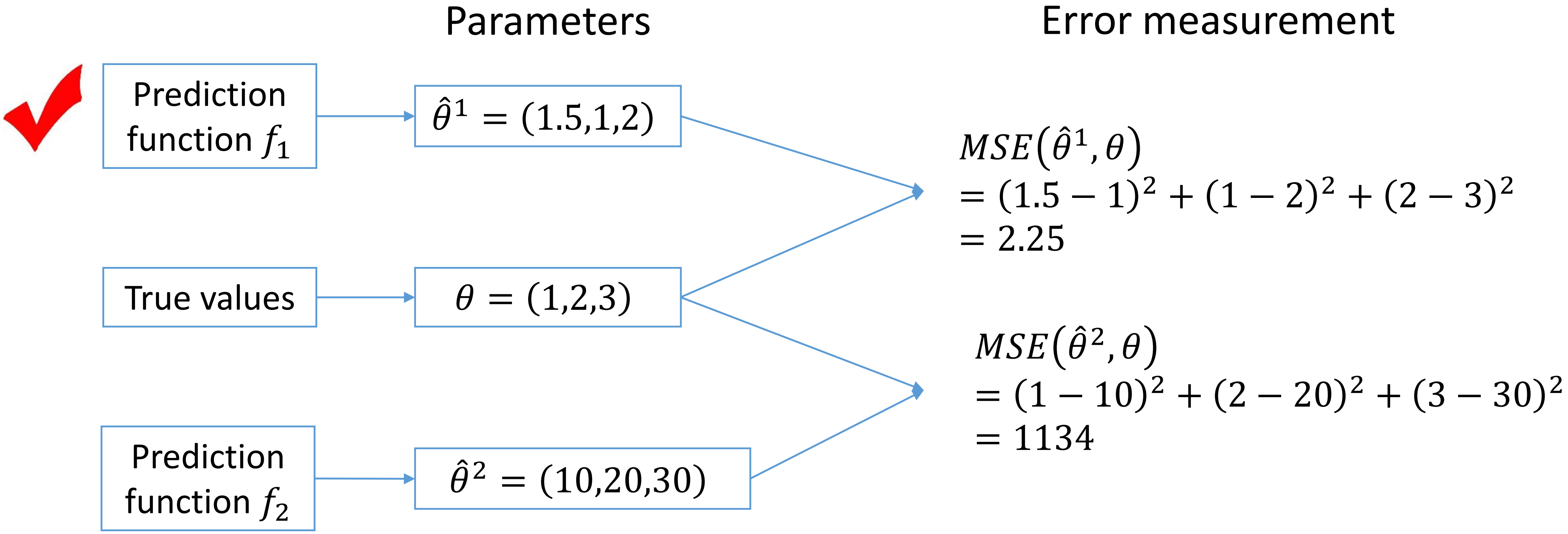
2 separated stage approach:

- Predict: Use standard machine learning techniques to estimate parameters independently of the COP;
  - Training: find a good prediction function that can make best forecast
- Optimize: Use these estimated parameters to solve the COP

Classical approaches: predict then optimize

2 separated stage approach:

- Predict: Use standard machine learning techniques to estimate parameters independently of the COP;
- Optimize: Use these estimated parameters to solve the COP



Parameters

Error measurement

✓ Prediction function f_1 → $\hat{\theta}^1 = (1.5,1,2)$

True values → $\theta = (1,2,3)$

Prediction function f_2 → $\hat{\theta}^2 = (10,20,30)$

$$MSE(\hat{\theta}^1, \theta)$$
$$= (1.5-1)^2 + (1-2)^2 + (2-3)^2$$
$$= 2.25$$

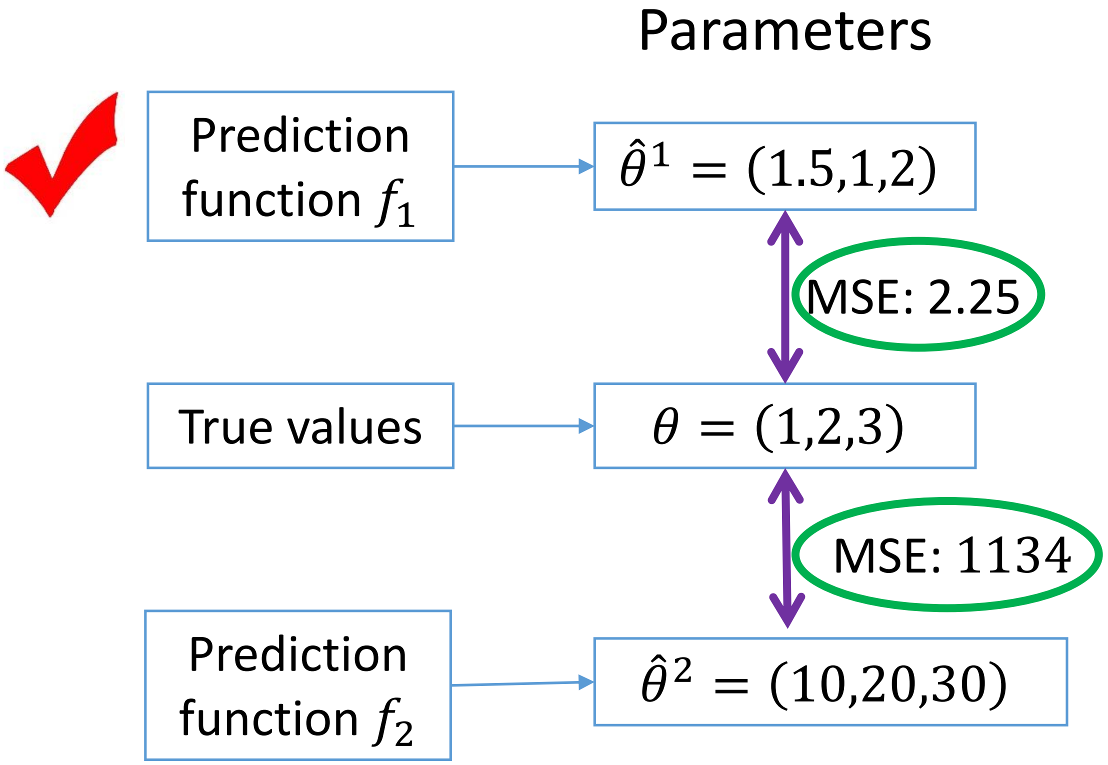
$$MSE(\hat{\theta}^2, \theta)$$
$$= (1-10)^2 + (2-20)^2 + (3-30)^2$$
$$= 1134$$

Classical approaches: predict then optimize

2 separated approach:

Predict: Use standard machine learning techniques to estimate parameters independently of the COP;

Optimize: Use these estimated parameters to solve the COP



Parameters
✓
Prediction function f_1
$\hat{\theta}^1 = (1.5,1,2)$
MSE: 2.25
True values
$\theta = (1,2,3)$
MSE: 1134
Prediction function f_2
$\hat{\theta}^2 = (10,20,30)$

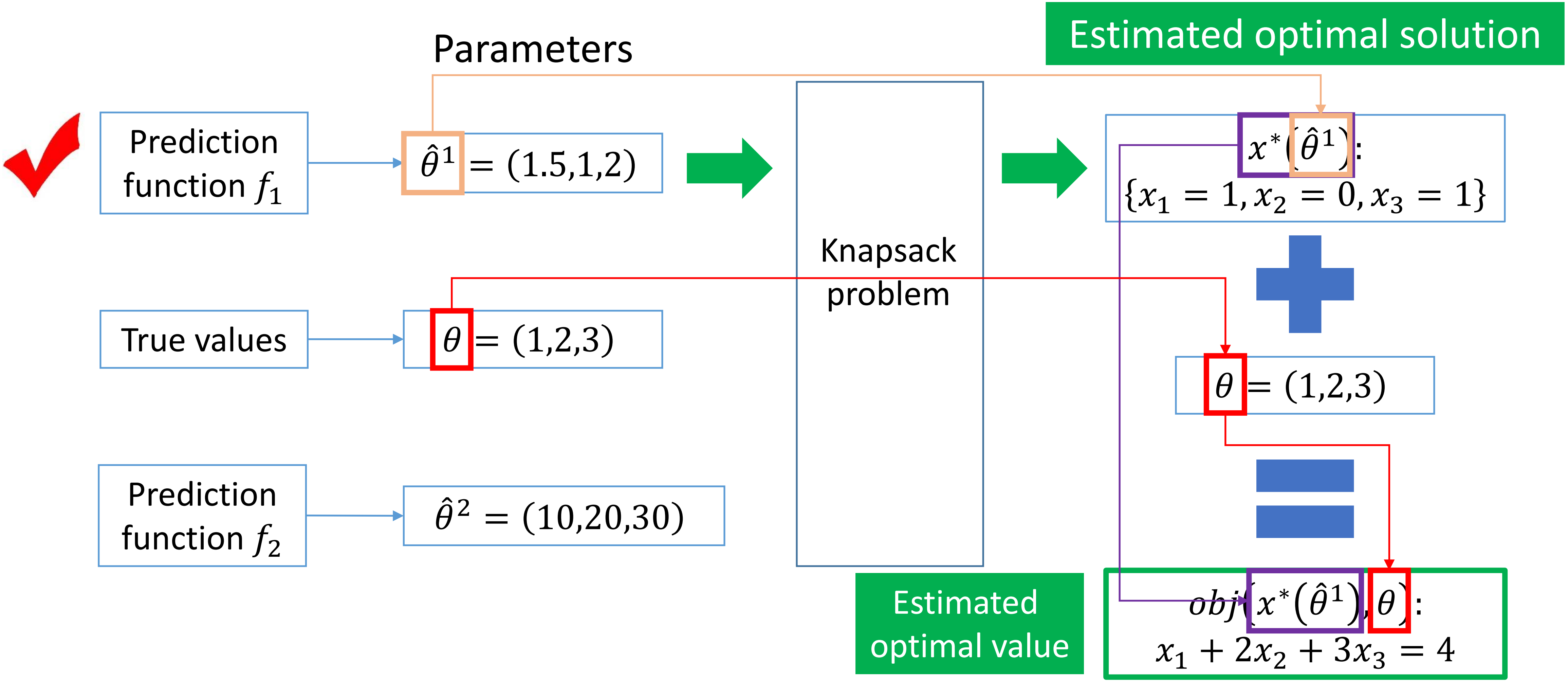
The prediction part is independent of the COP.

Classical approaches aim at minimizing the difference between estimated parameters values and true parameters values.

→ Prediction function f_1 is better.

However…

the best forecast may have a poor result when employed in the COP



Parameters

Estimated optimal solution

✓ Prediction function f_1 → $\hat{\theta}^1 = (1.5,1,2)$

True values → $\theta = (1,2,3)$

Prediction function f_2 → $\hat{\theta}^2 = (10,20,30)$

Knapsack problem

$x^*(\hat{\theta}^1)$:
$\{x_1 = 1, x_2 = 0, x_3 = 1\}$

+

$\theta = (1,2,3)$

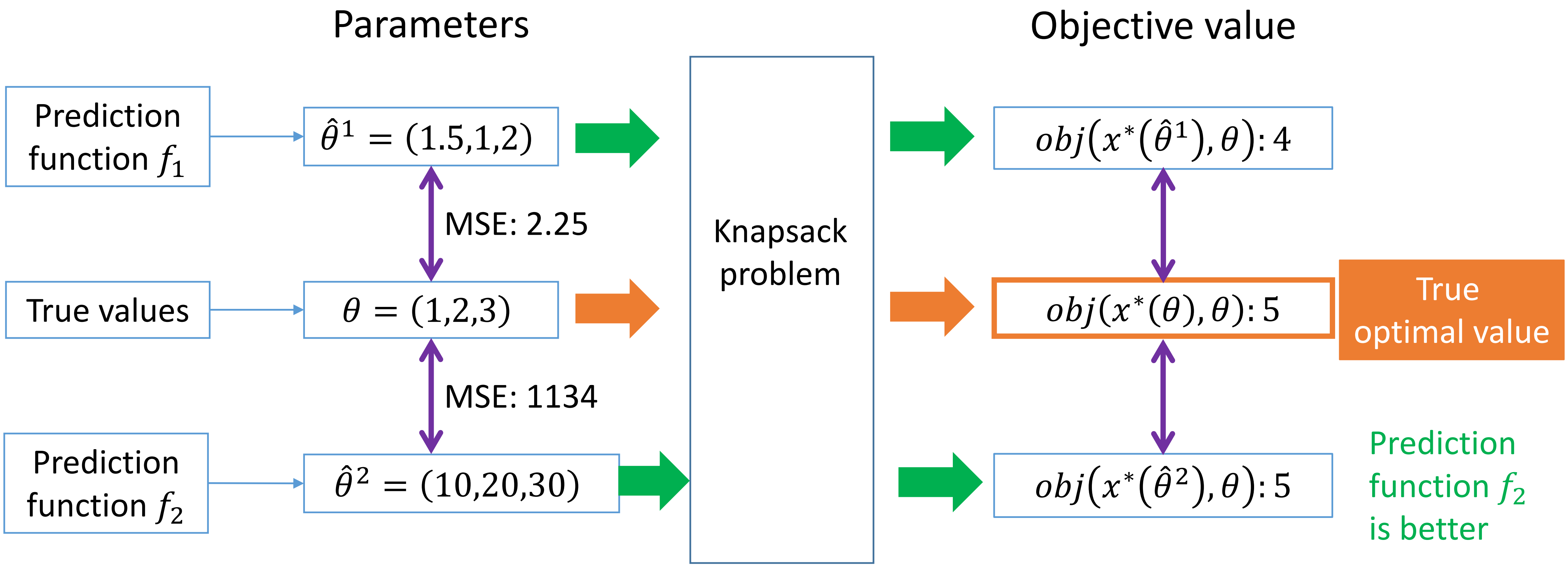
=

$obj(x^*(\hat{\theta}^1), \theta)$:
$x_1 + 2x_2 + 3x_3 = 4$

Estimated optimal value

However…

the best forecast may have a poor result when employed in the COP



Parameters

Objective value

Prediction function f_1

$\hat{\theta}^1 = (1.5,1,2)$

MSE: 2.25

True values

$\theta = (1,2,3)$

MSE: 1134

Prediction function f_2

$\hat{\theta}^2 = (10,20,30)$

Knapsack problem

$obj\left(x^*\left(\hat{\theta}^1\right), \theta\right): 4$

$obj\left(x^*(\theta), \theta\right): 5$

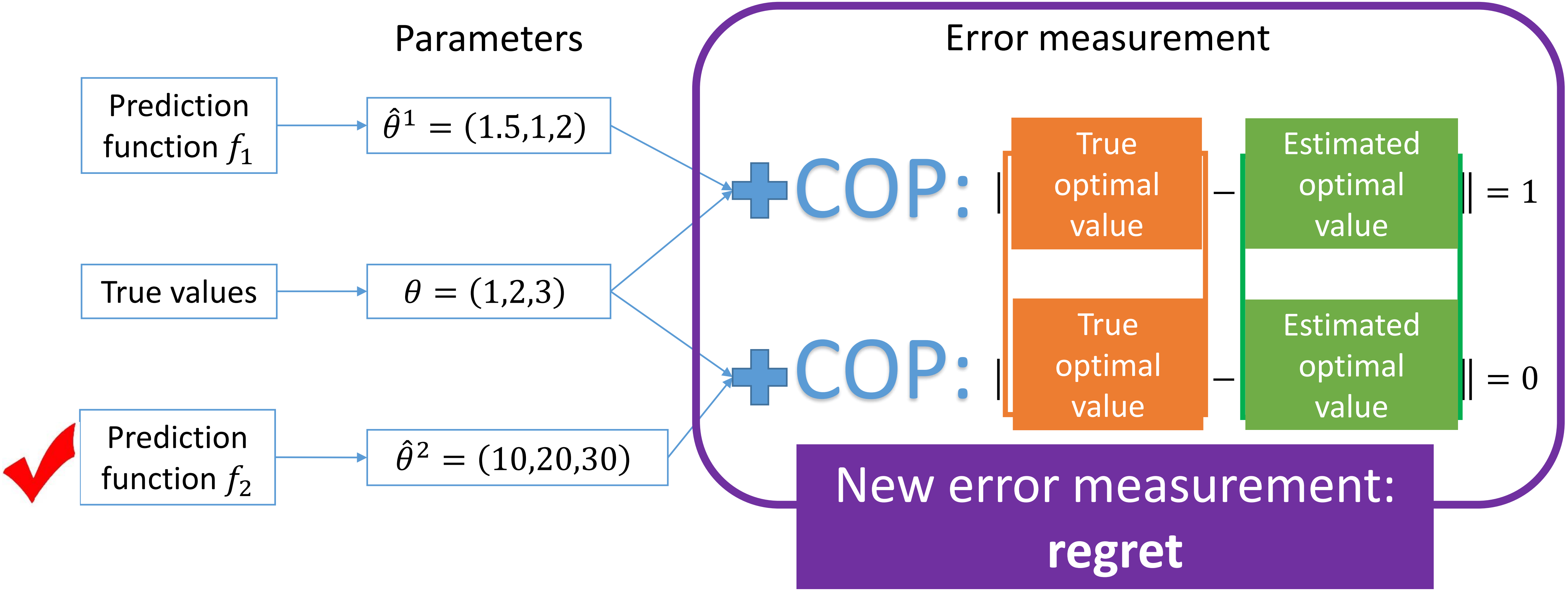
True optimal value

$obj\left(x^*\left(\hat{\theta}^2\right), \theta\right): 5$

Prediction function f_2 is better

Predict+Optimize

Take the COP into account when doing the prediction



Parameters

Error measurement

Prediction function f_1 → $\hat{\theta}^1 = (1.5,1,2)$

True values → $\theta = (1,2,3)$

Prediction function f_2 → $\hat{\theta}^2 = (10,20,30)$

+COP: $\|$ True optimal value $-$ Estimated optimal value $\| = 1$

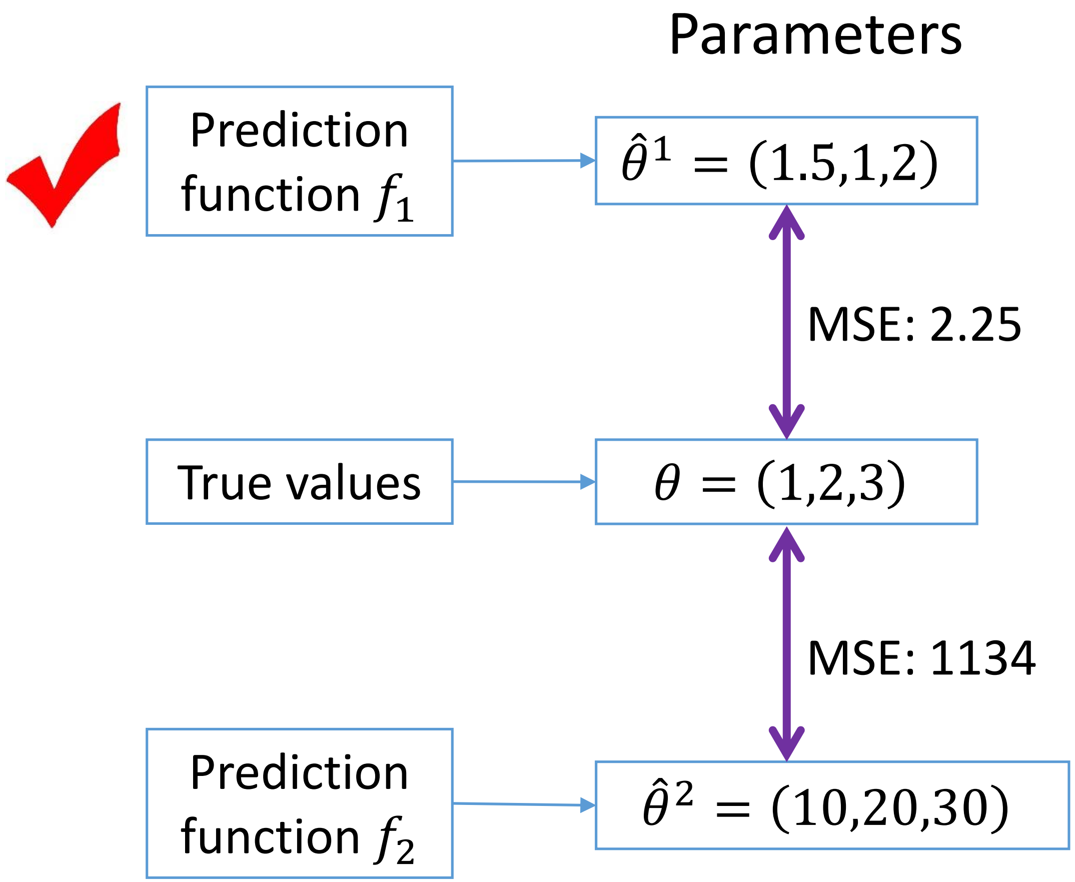
+COP: $\|$ True optimal value $-$ Estimated optimal value $\| = 0$

New error measurement: **regret**

[Demiroví c et al., 2019a], [Demiroví c et al., 2019b], [Guler et al., 2022]

Comparison

Classical approaches VS Predict+Optimize



Parameters

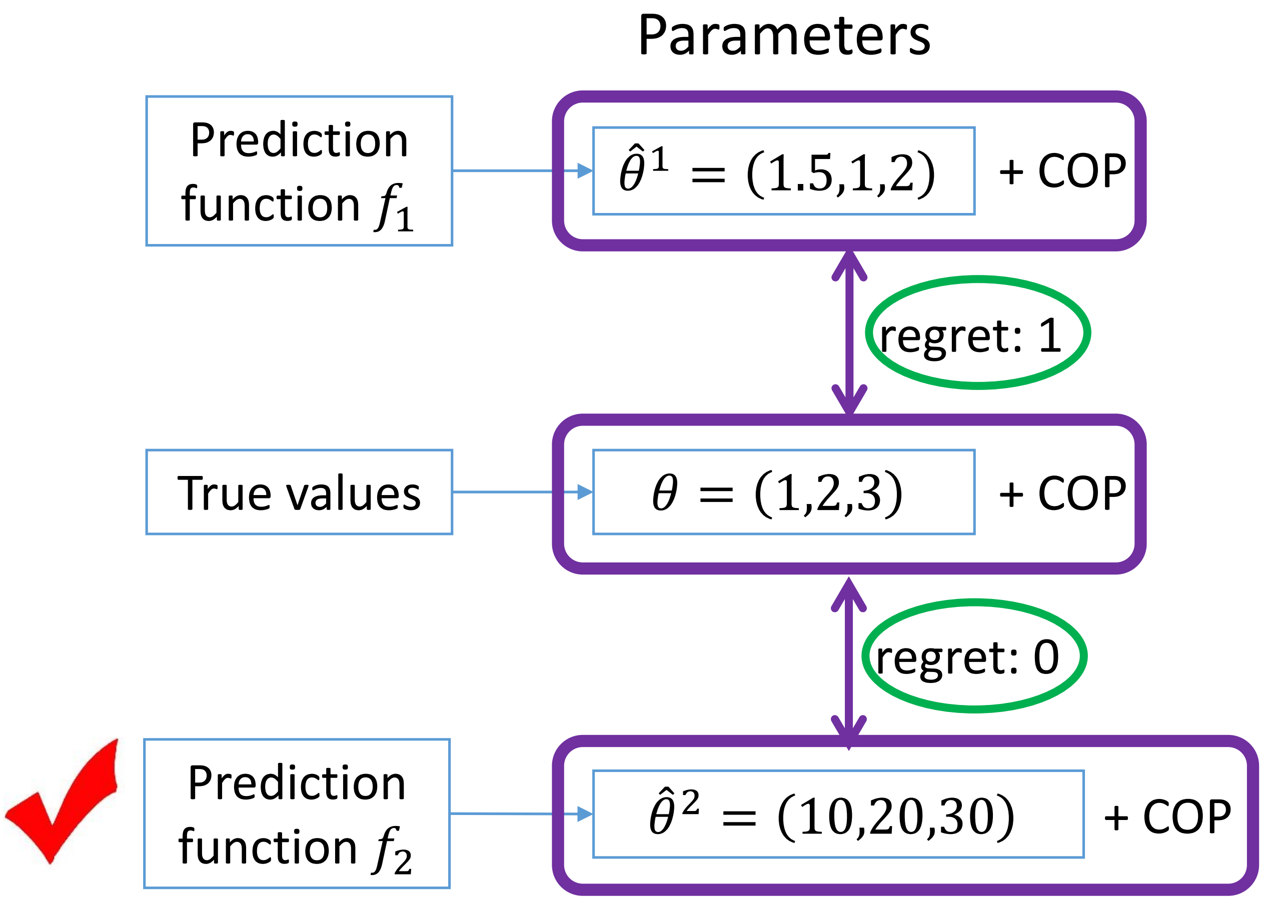
Prediction function f_1 → $\hat{\theta}^1 = (1.5,1,2)$

MSE: 2.25

True values → $\theta = (1,2,3)$

MSE: 1134

Prediction function f_2 → $\hat{\theta}^2 = (10,20,30)$



Parameters

Prediction function f_1 → $\hat{\theta}^1 = (1.5,1,2)$ + COP

regret: 1

True values → $\theta = (1,2,3)$ + COP

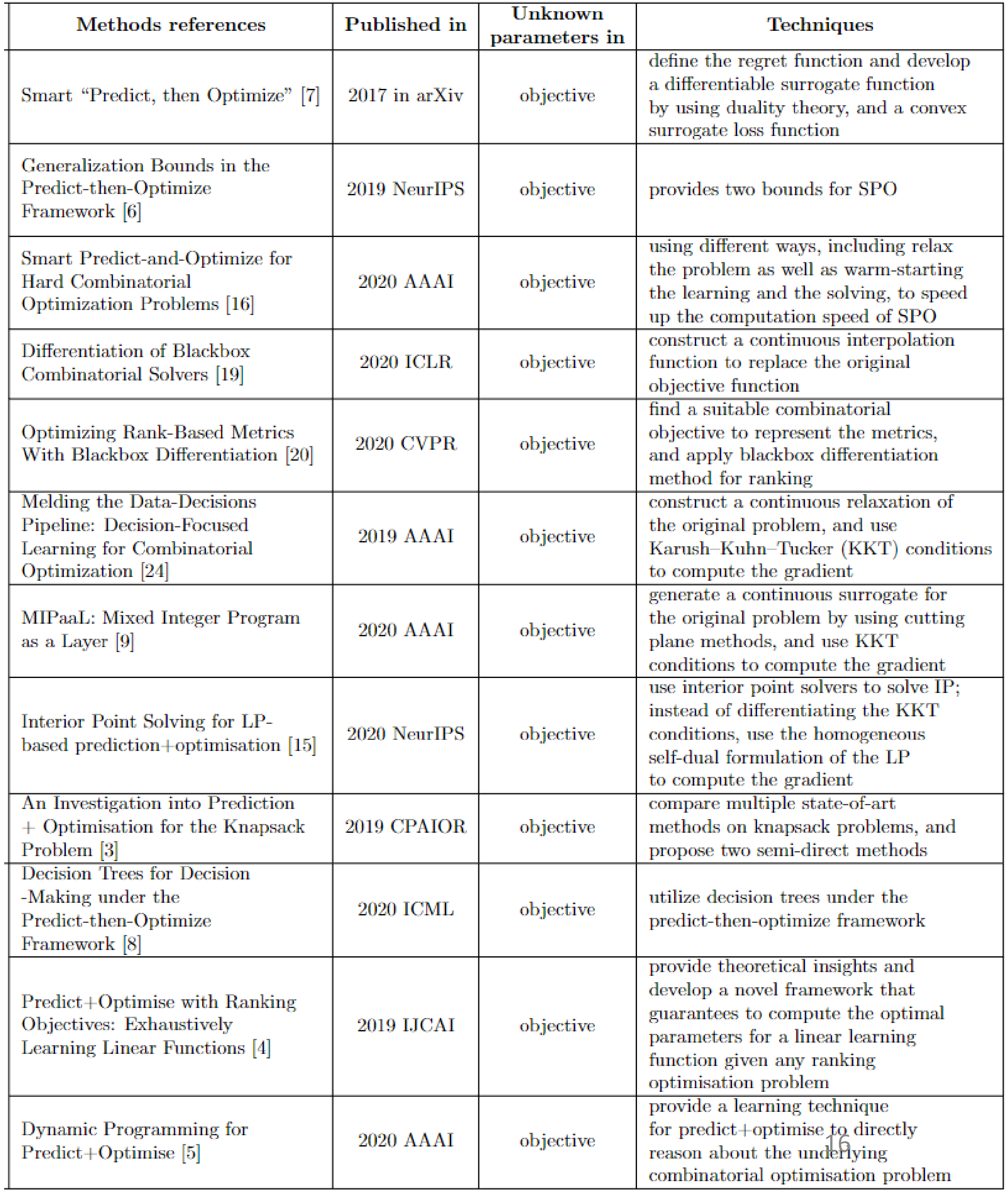
regret: 0

Prediction function f_2 → $\hat{\theta}^2 = (10,20,30)$ + COP

[Demirovi ́ c et al., 2019a], [Demirovi ́ c et al., 2019b], [Guler et al., 2022]

Related Works

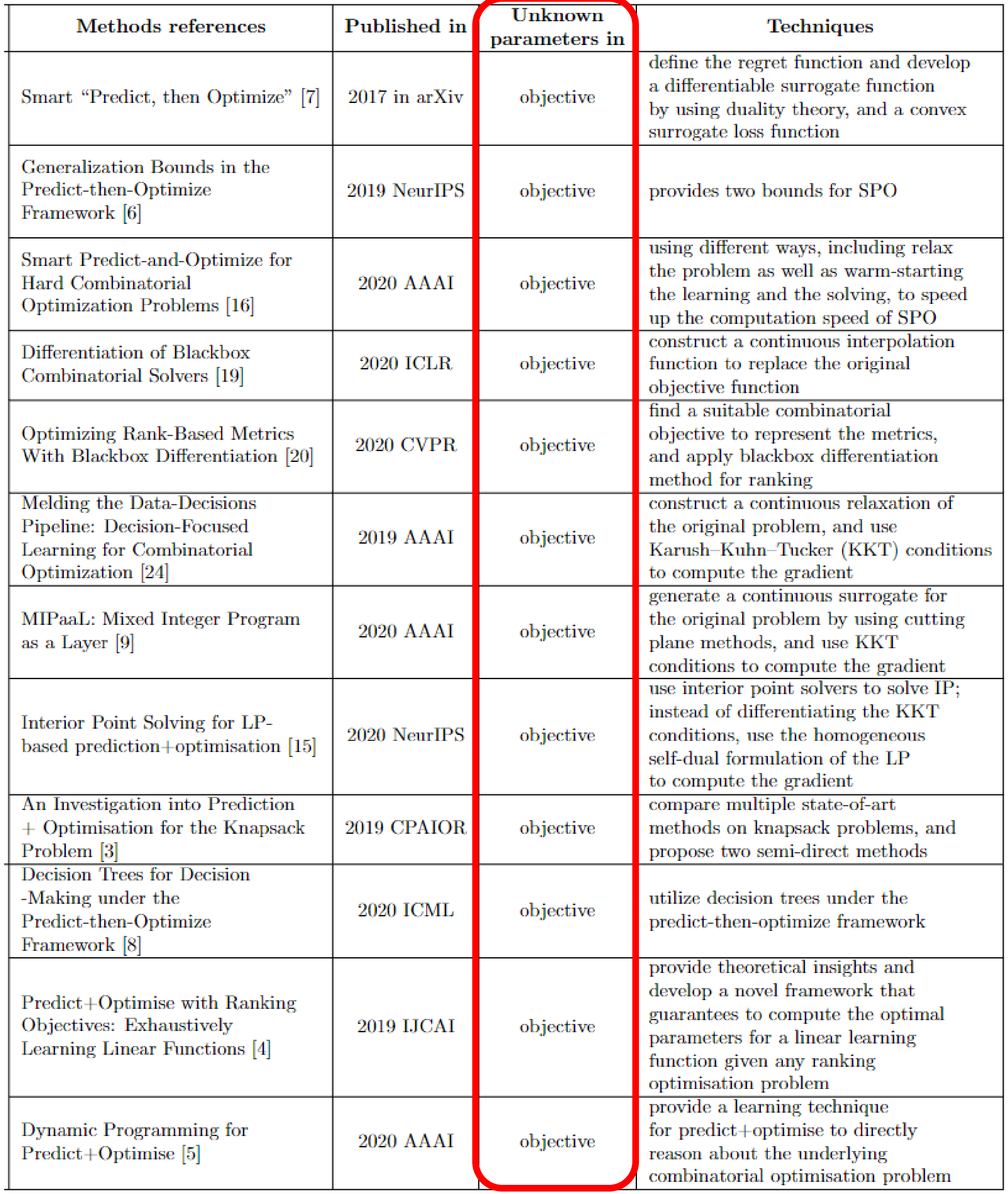
- The regret function is non-differentiable, which is unfriendly to any gradient-based learning process
- All of the related works focus on how to overcome the non-differentiability and train with the new loss.



Methods references	Published in	Unknown parameters in	Techniques
Smart "Predict, then Optimize" [7]	2017 in arXiv	objective	define the regret function and develop a differentiable surrogate function by using duality theory, and a convex surrogate loss function
Generalization Bounds in the Predict-then-Optimize Framework [6]	2019 NeurIPS	objective	provides two bounds for SPO
Smart Predict-and-Optimize for Hard Combinatorial Optimization Problems [16]	2020 AAAI	objective	using different ways, including relax the problem as well as warm-starting the learning and the solving, to speed up the computation speed of SPO
Differentiation of Blackbox Combinatorial Solvers [19]	2020 ICLR	objective	construct a continuous interpolation function to replace the original objective function
Optimizing Rank-Based Metrics With Blackbox Differentiation [20]	2020 CVPR	objective	find a suitable combinatorial objective to represent the metrics, and apply blackbox differentiation method for ranking
Melding the Data-Decisions Pipeline: Decision-Focused Learning for Combinatorial Optimization [24]	2019 AAAI	objective	construct a continuous relaxation of the original problem, and use Karush–Kuhn–Tucker (KKT) conditions to compute the gradient
MIPaaL: Mixed Integer Program as a Layer [9]	2020 AAAI	objective	generate a continuous surrogate for the original problem by using cutting plane methods, and use KKT conditions to compute the gradient
Interior Point Solving for LP-based prediction+optimisation [15]	2020 NeurIPS	objective	use interior point solvers to solve IP; instead of differentiating the KKT conditions, use the homogeneous self-dual formulation of the LP to compute the gradient
An Investigation into Prediction + Optimisation for the Knapsack Problem [3]	2019 CPAIOR	objective	compare multiple state-of-art methods on knapsack problems, and propose two semi-direct methods
Decision Trees for Decision -Making under the Predict-then-Optimize Framework [8]	2020 ICML	objective	utilize decision trees under the predict-then-optimize framework
Predict+Optimise with Ranking Objectives: Exhaustively Learning Linear Functions [4]	2019 IJCAI	objective	provide theoretical insights and develop a novel framework that guarantees to compute the optimal parameters for a linear learning function given any ranking optimisation problem
Dynamic Programming for Predict+Optimise [5]	2020 AAAI	objective	provide a learning technique for predict+optimise to directly reason about the underlying combinatorial optimisation problem

Related Works

What if the constraints also contain unknown parameters?



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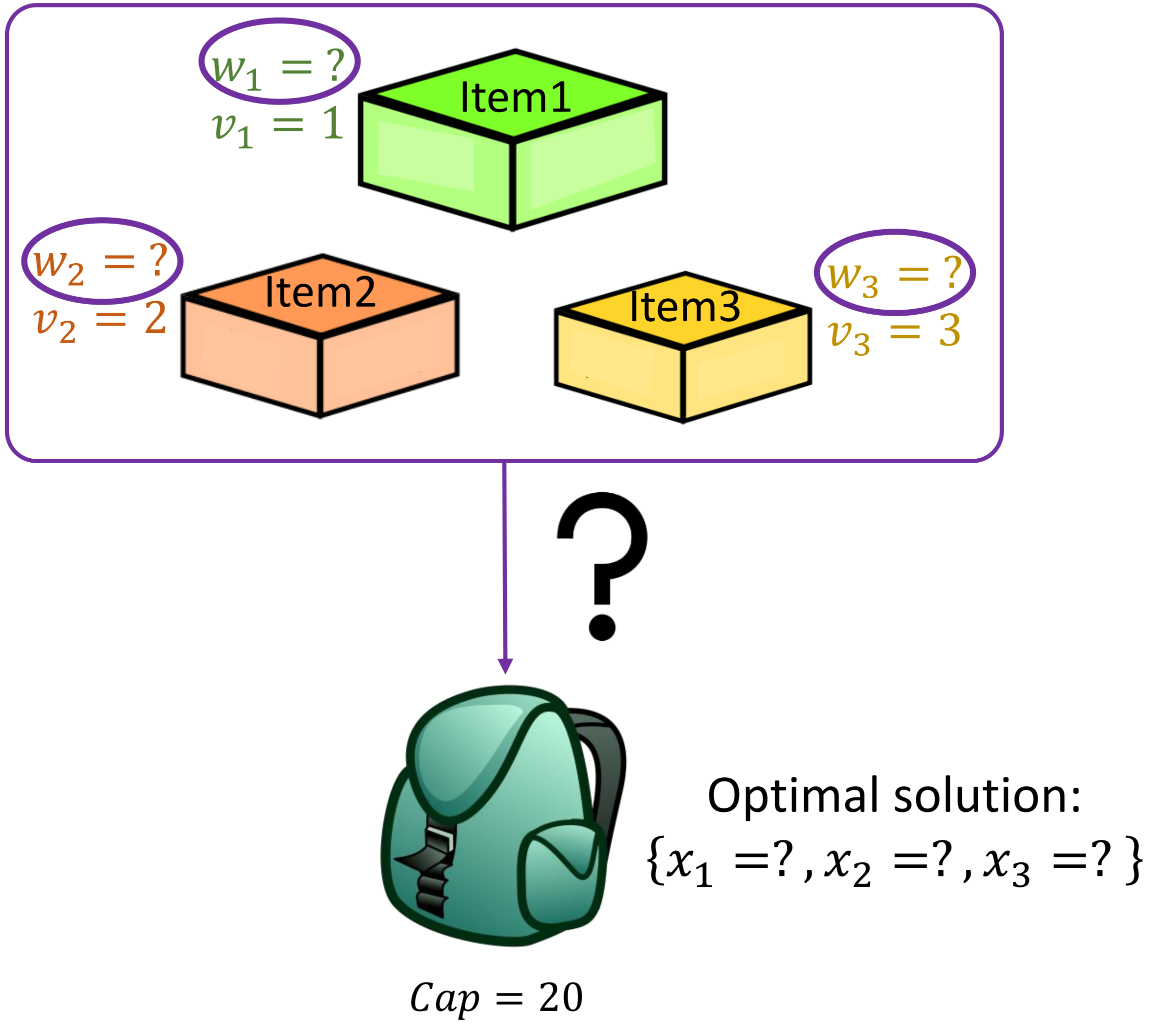
If the constraints contain unknown parameters



Optimal solution:
$\{x_1 = ?, x_2 = ?, x_3 = ?\}$

$Cap = 20$

- Knapsack with unknown weights

$$\max_x \sum_i v_i x_i$$
$$s.t. \sum_i \theta_i x_i \le Cap$$
$$x_i \in \{0,1\} \; \forall i \in \{1,2,3\}$$

Unknown parameters in constraints

- Eg.

Estimated weights: $\{\widehat{w_1} = \widehat{w_2} = \widehat{w_3} = 5\}$

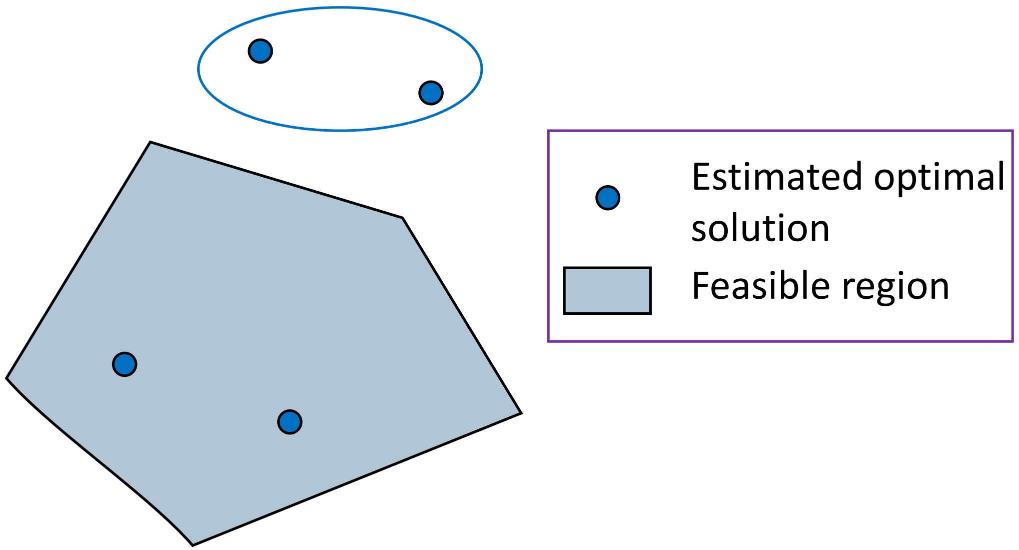
Estimated optimal solution:
$\{x_1 = x_2 = x_3 = 1\}$
(True weights: $\{w_1 = w_2 = w_3 = 10\}$)

infeasible

- The estimated optimal solution may be infeasible under the true parameters

Regret is inapplicable

- Unknown parameters appearing in constraints **(more complex)**
  - the estimated optimal solution may be out of the true solution space



- Regret: does not take feasibility into account

$$Regret(\hat{\theta},\theta) = \| \text{True optimal value} - \text{Estimated optimal value} \|$$

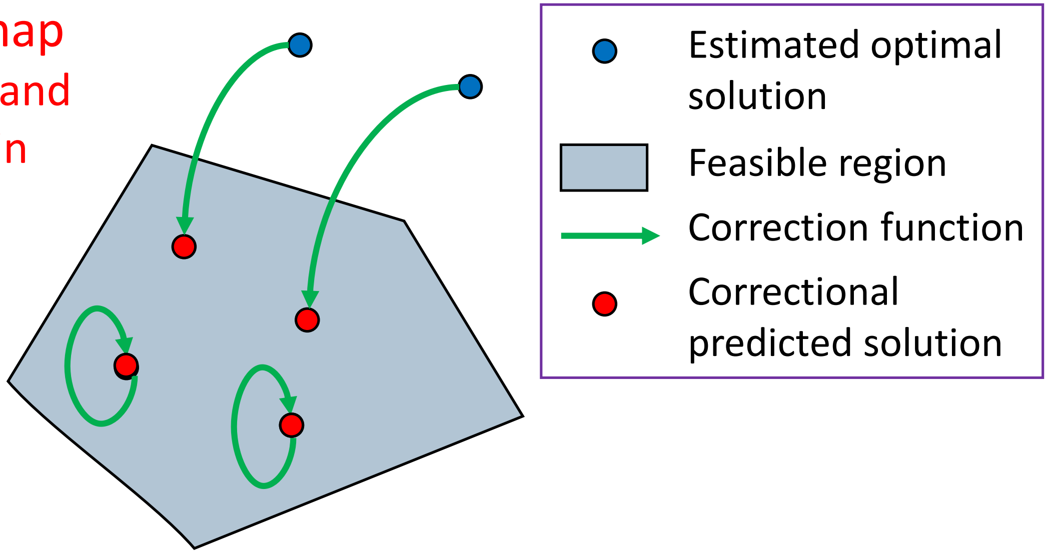
inapplicable

Our Work: Correction Function

Some applications:

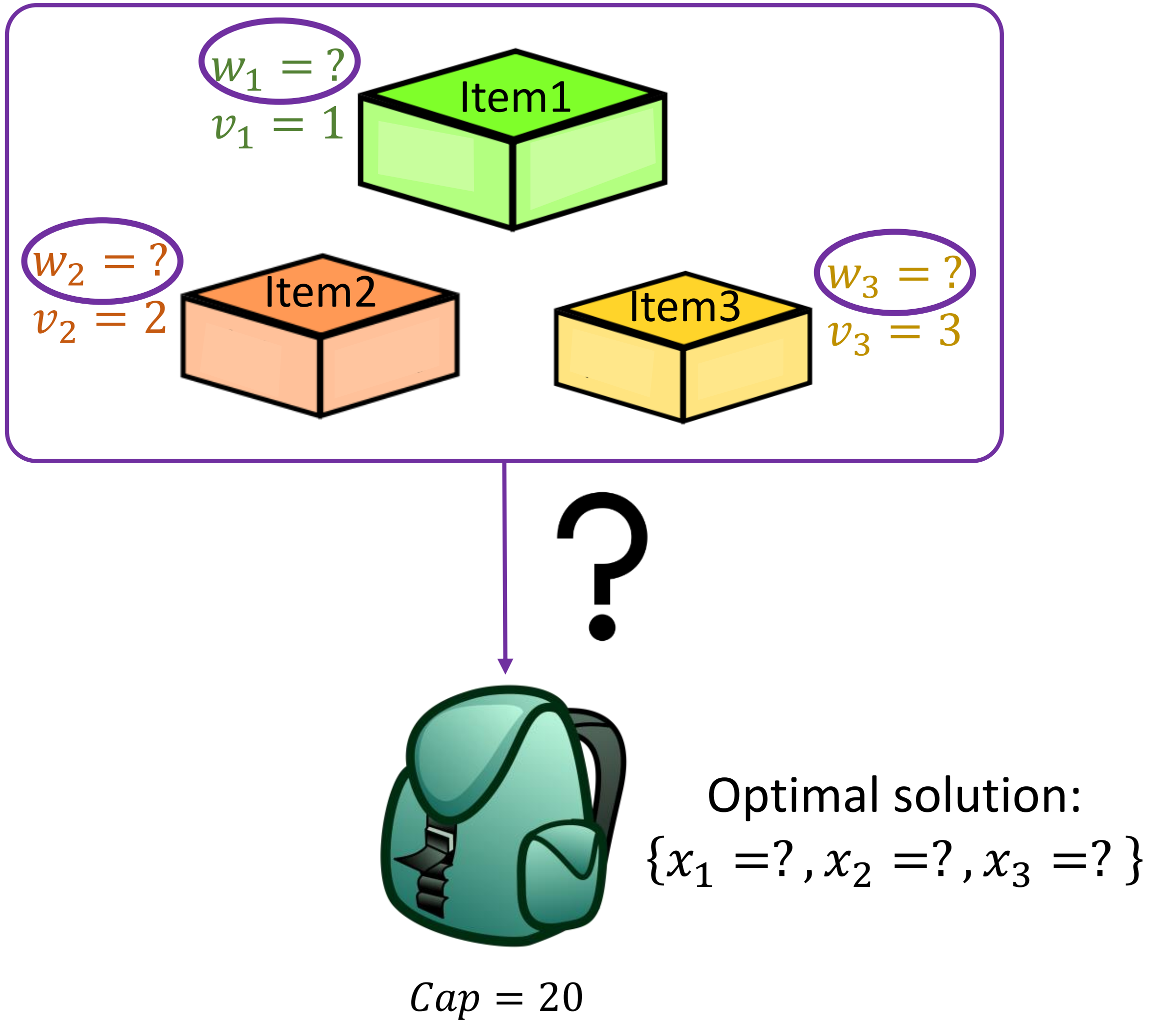
allow solution modification after true parameters are revealed

- **correction function** should map
  - (a) every feasible solution to itself and
  - (b) each infeasible solution to one in the feasible region



The space of possible correction functions : problem and application specific

Case Study 1: Knapsack



- If the weights are unknown?

$$\max_{x} \sum_{i} v_i x_i$$
$$s.t. \sum_i \theta_i x_i \leq Cap$$
$$x_i \in \{0,1\} \; \forall i \in \{1,2,3\}$$

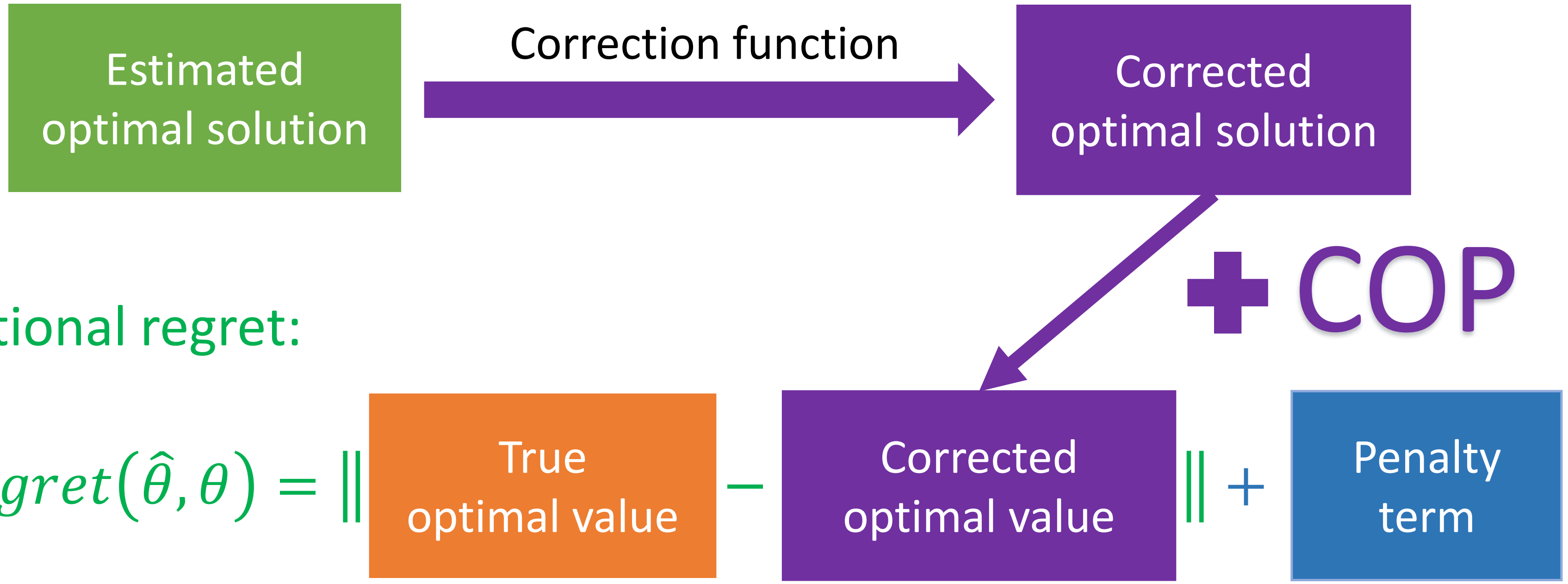
- When the total weight of the selected items exceeds the capacity:
  - Correction function 1: remove all items
  - Correction function 2: remove the items one by one in increasing order of values

Our Work: Correctional Regret

To cater for unknown parameters appearing in constraints

- Correction function:

- Correctional regret:



$CRegret(\hat{\theta}, \theta) = \|$ True optimal value $-$ Corrected optimal value $\| +$ Penalty term

E.g. knapsack problem with unknown weights: removal fee

Experiment Setting

Comparison algorithms

proposed

Comparison algorithms	Branch and learn (B&L) [Hu et al., 2022]	Branch and learn with correction (B&L-C)	Linear regression (LR)	k-nearest neighbors (k-NN)	Classification and regression tree (CART)	Random forest (RF)
Category	Predict+Optimize method	Extension of B&L	Classical regression methods			
Trained by	Regret	Correctional regret	Mean square error (MSE)			
Tested by	Correctional regret					

Experiment Setting

Maximum flow

- Unknown parameters in constraints
- 2 Real-life graphs
  - USANet, 24 vertices and 43 edges
  - GEANT, 40 vertices and 61 edges
- Artificial and real-life datasets

Minimum cost vertex cover

- Unknown parameters in **both** the objective and constraints
- 2 Real-life graphs
  - ABILENE, 12 vertices and 15 edges
  - GEANT, 11 vertices and 34 edges
- Artificial and real-life datasets

Experiment Dataset

Real life dataset

- ICON energy-aware scheduling competition
- Also used in previous works on Predict+Optimize
- Each parameter has 8 features

Artificial dataset

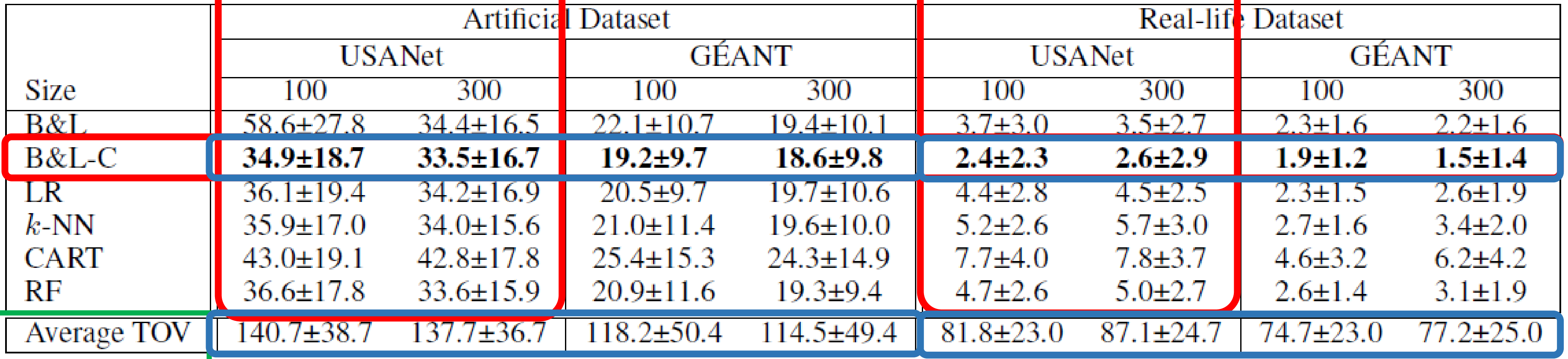
- $100 * \sin(a_1) * \sin(a_2) + 10 * \sin(a_3) * \sin(a_4)$

Highly nonlinear

Experiment Results: Maximum Flow

≥ 0.3% smaller correctional regret

≥ 25% smaller correctional regret



	Artificial Dataset				Real-life Dataset			
	USANet		GÉANT		USANet		GÉANT	
Size	100	300	100	300	100	300	100	300
B&L	58.6±27.8	34.4±16.5	22.1±10.7	19.4±10.1	3.7±3.0	3.5±2.7	2.3±1.6	2.2±1.6
B&L-C	**34.9±18.7**	**33.5±16.7**	**19.2±9.7**	**18.6±9.8**	**2.4±2.3**	**2.6±2.9**	**1.9±1.2**	**1.5±1.4**
LR	36.1±19.4	34.2±16.9	20.5±9.7	19.7±10.6	4.4±2.8	4.5±2.5	2.3±1.5	2.6±1.9
k-NN	35.9±17.0	34.0±15.6	21.0±11.4	19.6±10.0	5.2±2.6	5.7±3.0	2.7±1.6	3.4±2.0
CART	43.0±19.1	42.8±17.8	25.4±15.3	24.3±14.9	7.7±4.0	7.8±3.7	4.6±3.2	6.2±4.2
RF	36.6±17.8	33.6±15.9	20.9±11.6	19.3±9.4	4.7±2.6	5.0±2.7	2.6±1.4	3.1±1.9
Average TOV	140.7±38.7	137.7±36.7	118.2±50.4	114.5±49.4	81.8±23.0	87.1±24.7	74.7±23.0	77.2±25.0

TOV:
True Optimal Value

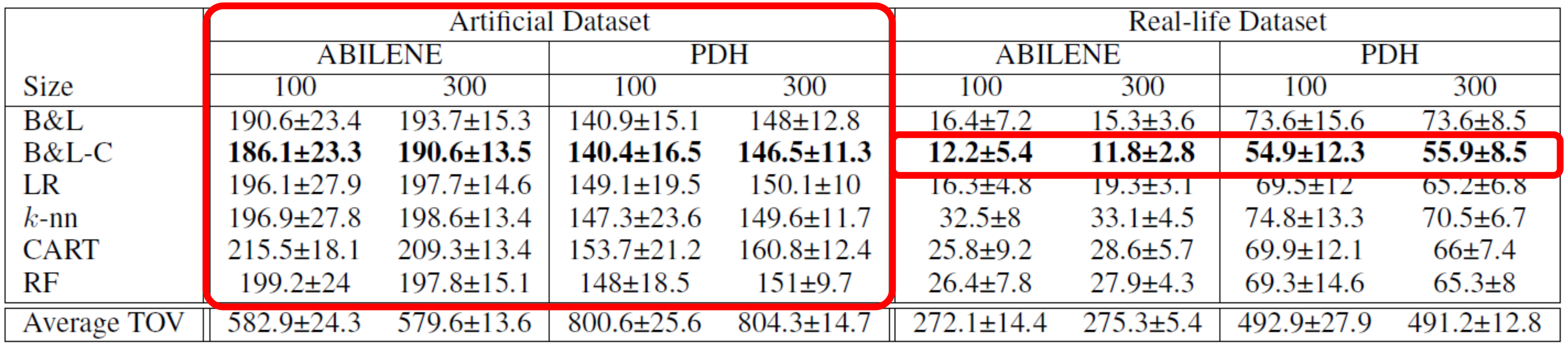
16-24% relative error

2-3% relative error

Table 1: Mean correctional regrets and standard deviations for MFP with unknown capacities.

- B&L-C achieves the best performance in all cases.
- The performance differences among different methods are larger in the real-life dataset, and the advantages of B&L-C are more obvious.
- All methods achieve better performance in the real-life dataset. This is consistent with how the artificial dataset is purposefully designed to be highly non-linear, and thus more difficult to estimate.

Experiment Results: Minimum Cost Vertex Cover



	Artificial Dataset				Real-life Dataset			
	ABILENE		PDH		ABILENE		PDH	
Size	100	300	100	300	100	300	100	300
B&L	190.6±23.4	193.7±15.3	140.9±15.1	148±12.8	16.4±7.2	15.3±3.6	73.6±15.6	73.6±8.5
B&L-C	**186.1±23.3**	**190.6±13.5**	**140.4±16.5**	**146.5±11.3**	**12.2±5.4**	**11.8±2.8**	**54.9±12.3**	**55.9±8.5**
LR	196.1±27.9	197.7±14.6	149.1±19.5	150.1±10	16.3±4.8	19.3±3.1	69.5±12	65.2±6.8
k-nn	196.9±27.8	198.6±13.4	147.3±23.6	149.6±11.7	32.5±8	33.1±4.5	74.8±13.3	70.5±6.7
CART	215.5±18.1	209.3±13.4	153.7±21.2	160.8±12.4	25.8±9.2	28.6±5.7	69.9±12.1	66±7.4
RF	199.2±24	197.8±15.1	148±18.5	151±9.7	26.4±7.8	27.9±4.3	69.3±14.6	65.3±8
Average TOV	582.9±24.3	579.6±13.6	800.6±25.6	804.3±14.7	272.1±14.4	275.3±5.4	492.9±27.9	491.2±12.8

Table 2: Mean correctional regrets and standard deviations for MCVC with unknown costs and edge values.

- B&L-C has the best performance in all cases with the real-life dataset.
- On the artificial dataset, all algorithms perform essentially the same.

Summary

- Predict+Optimize: unknown parameters in objectives + constraints
  - Challenge: estimated solutions may be infeasible
  - Correction function
  - Correctional regret

- Experiment results
  - Maximum flow problem: unknown capacities
  - Minimum cost vertex cover problem: unknown costs + edge values