Enhancing constraint programming with machine learning

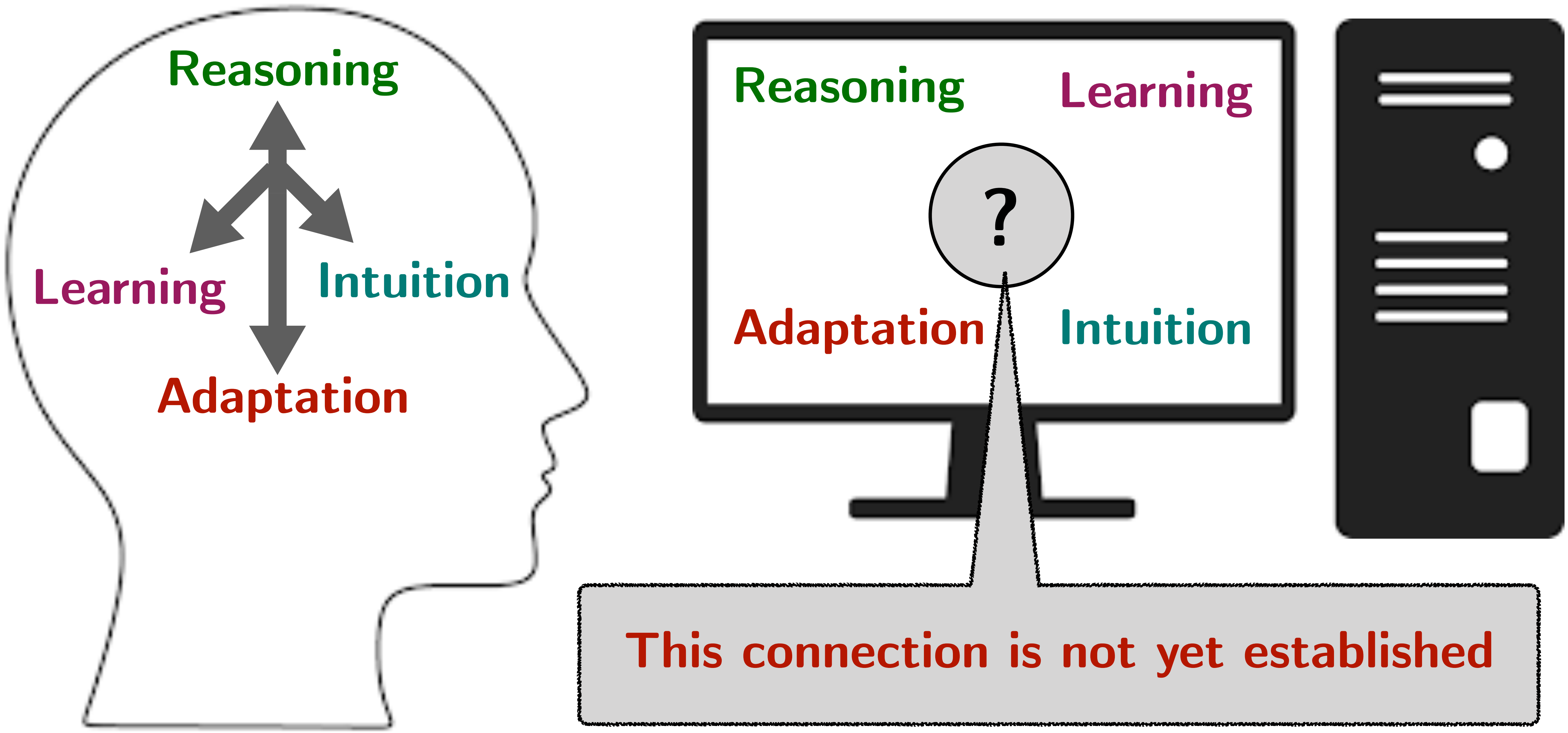
Current challenges and future opportunities

CP 2024 - Girona

Quentin Cappart

Human intelligence versus artificial intelligence

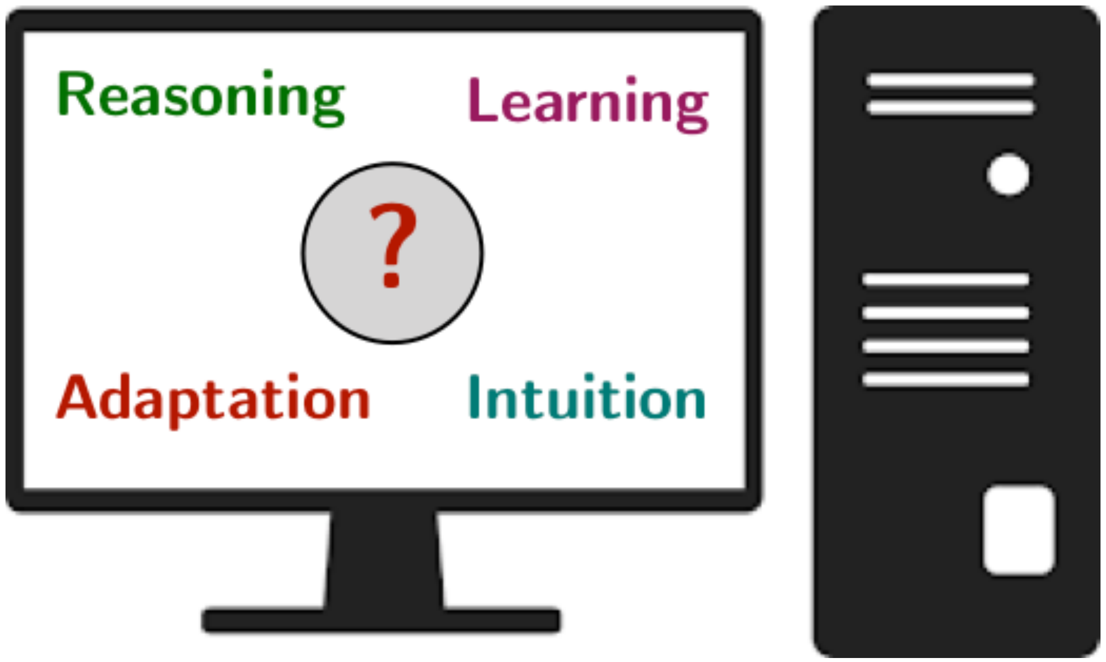
Human intelligence **Artificial intelligence**



Long-term research plan: building an AI with these connections

Goal: providing a better solving process for combinatorial problems

Constraint programming as a unifying framework



My research hypothesis

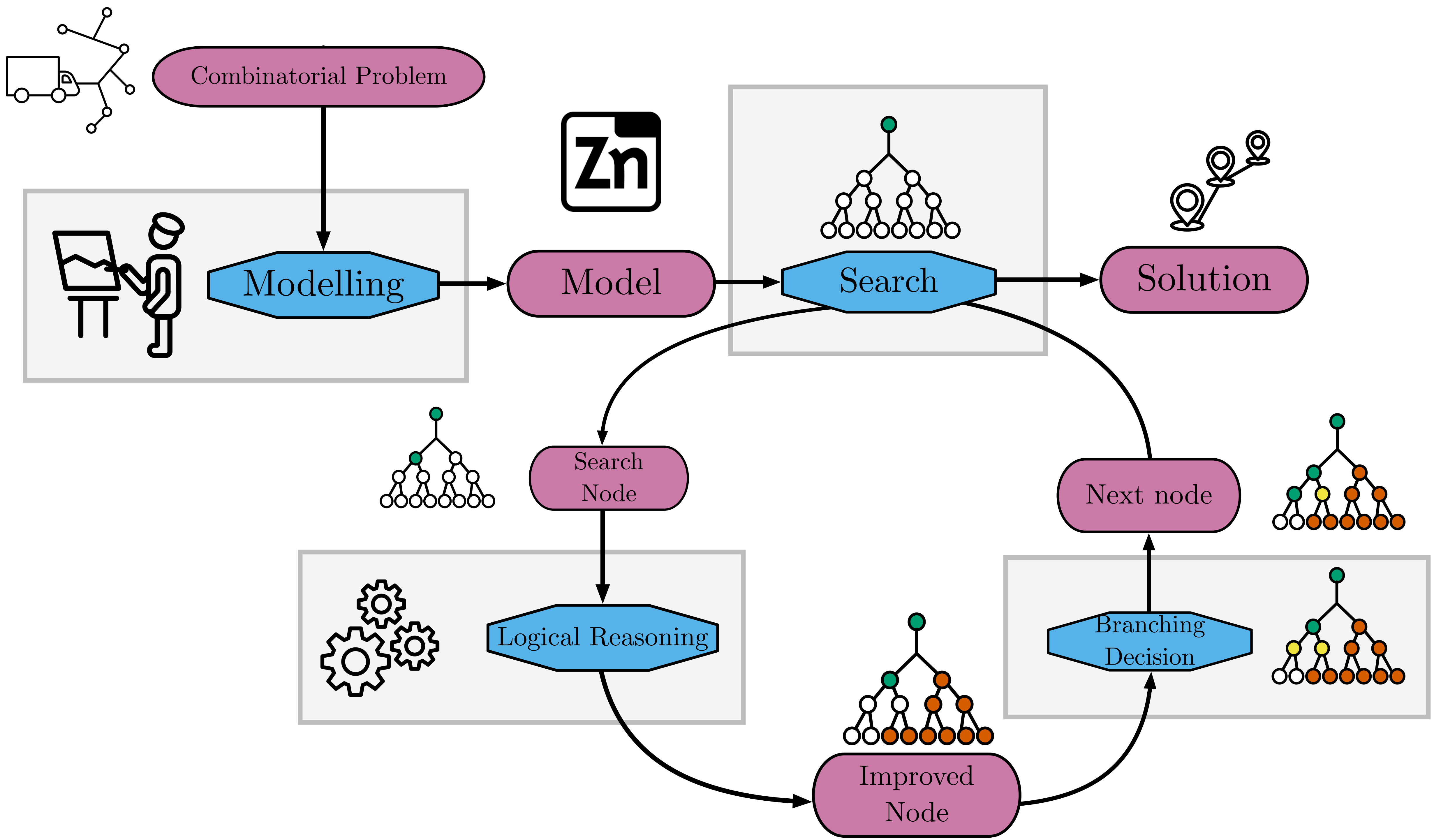
Constraint programming ***can be a hosting technology for building this hybrid AI***

CP = model + propagation + search + learning

- model: Huge flexibility
- propagation: Logical reasoning
- search: Following an intuition
- learning: Leveraging past knowledge

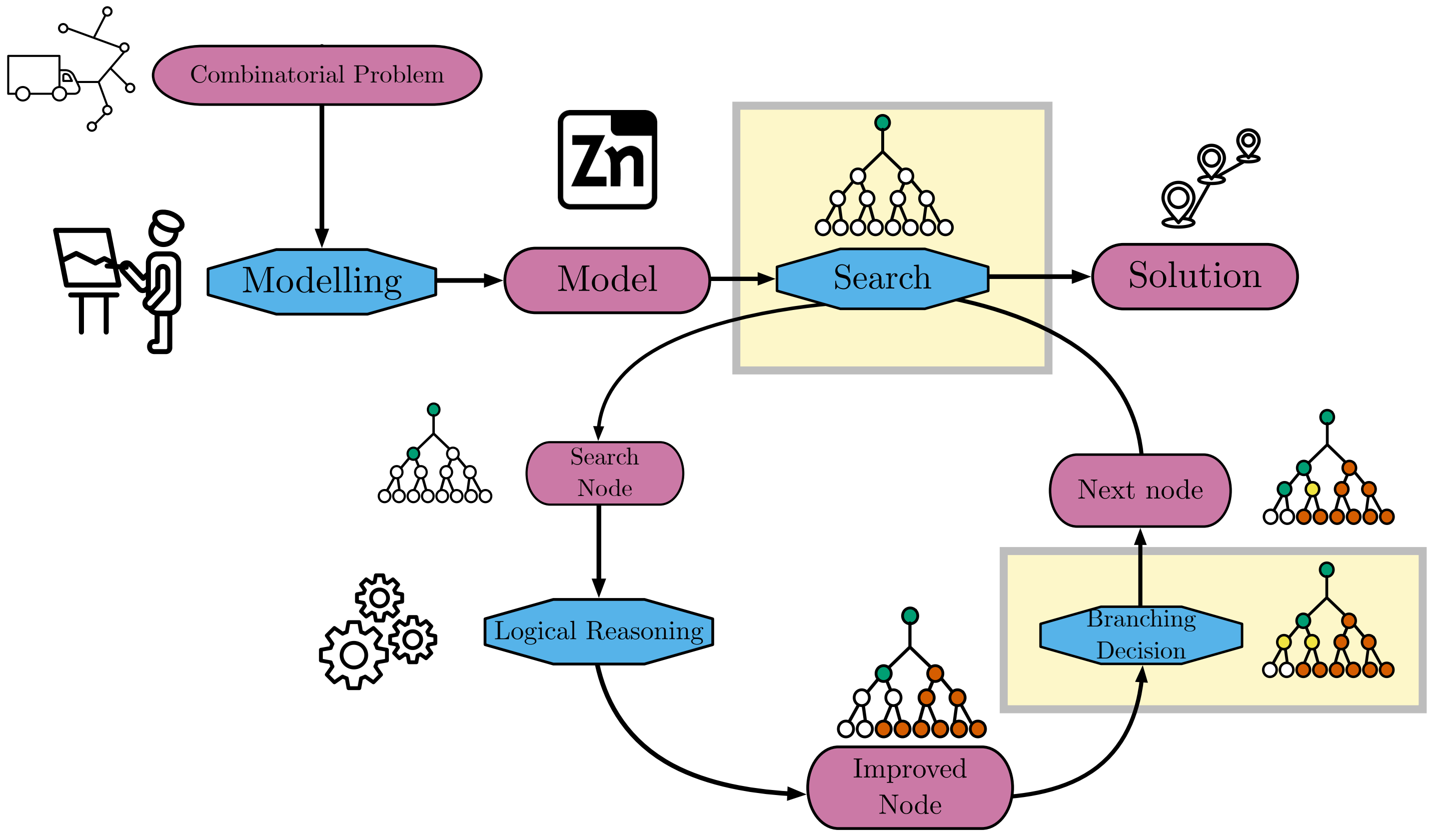
? How learning can be used to enhance the efficiency of CP solvers ?

Summary of the CP pipeline



Each decisional step has the potential to be improved with learning

Enhancing CP with learning



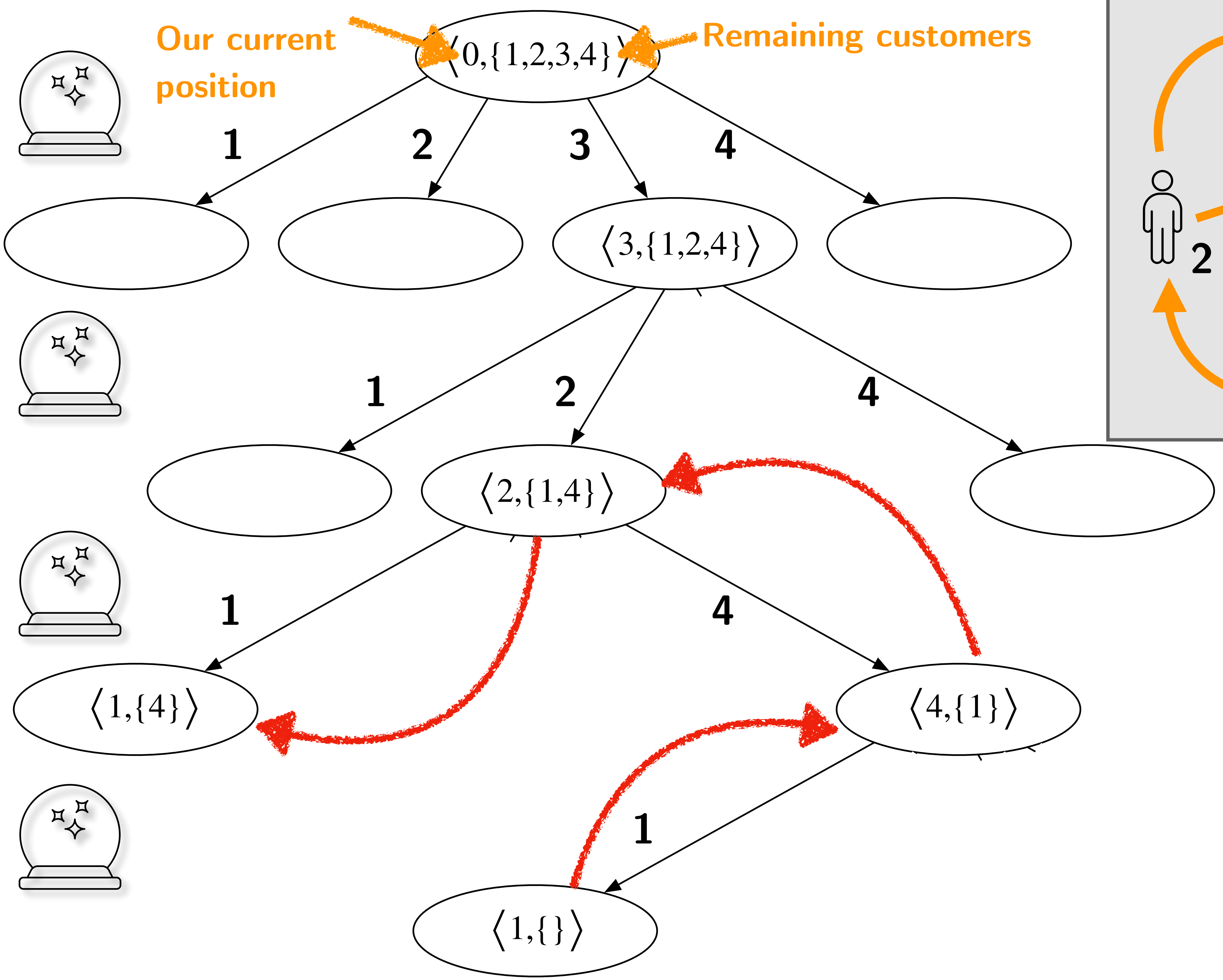
My first intuition: search is a good candidate as it heavily relies on imperfect heuristics

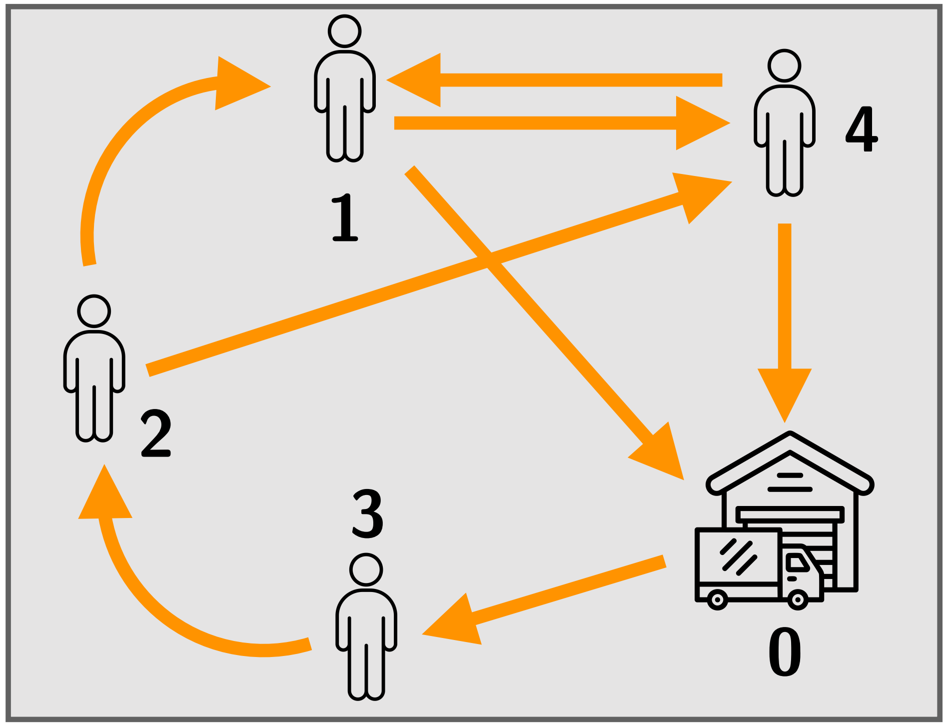
Consolidating argument: thanks to backtrack we can recover from bad predictions

Context: learning showed promising results for MIP (Gasse et al., Neurips 2019)

> *My first research direction was to learn appropriate value-selection heuristic*
>
> (with the intent to go further by learning variable-selection heuristics)

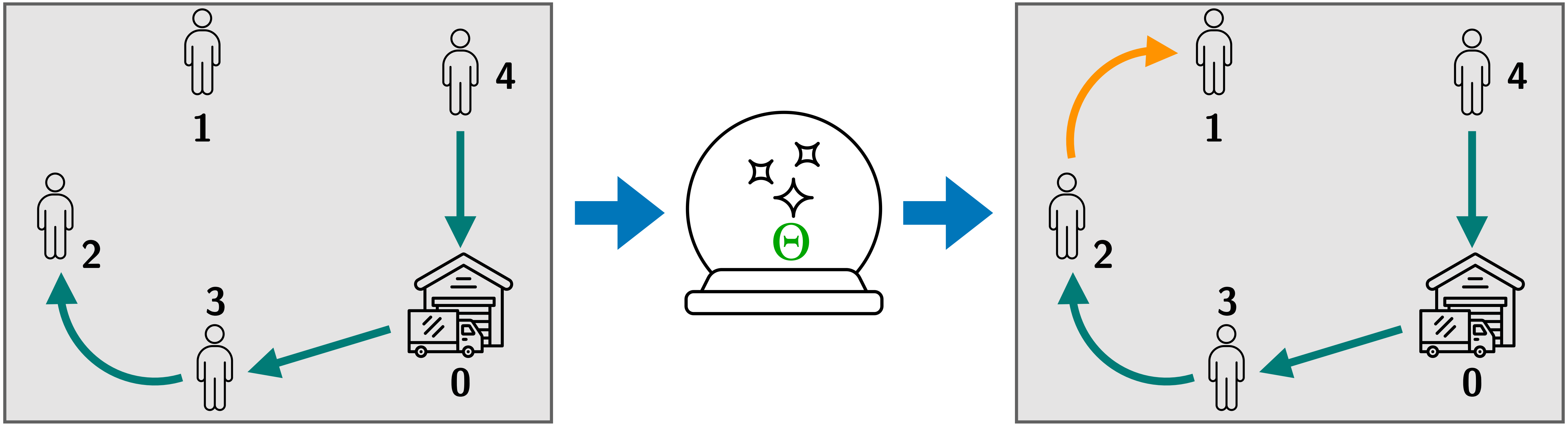
CP search with a learned heuristic on TSP





The ability to recover from bad decisions is fundamental for complete approaches

CP search with a learned heuristic on TSP



G, x

$f_{\Theta}(G, x)$

$d \sim D(x)$

Instance partially solved

Predictive model

Value to branch on

Variable to branch on

? **How can we build this predictive model (this magical crystal ball) ?**

Challenge 1: **we do not know what is the best choice (i.e., we do not have labels)**

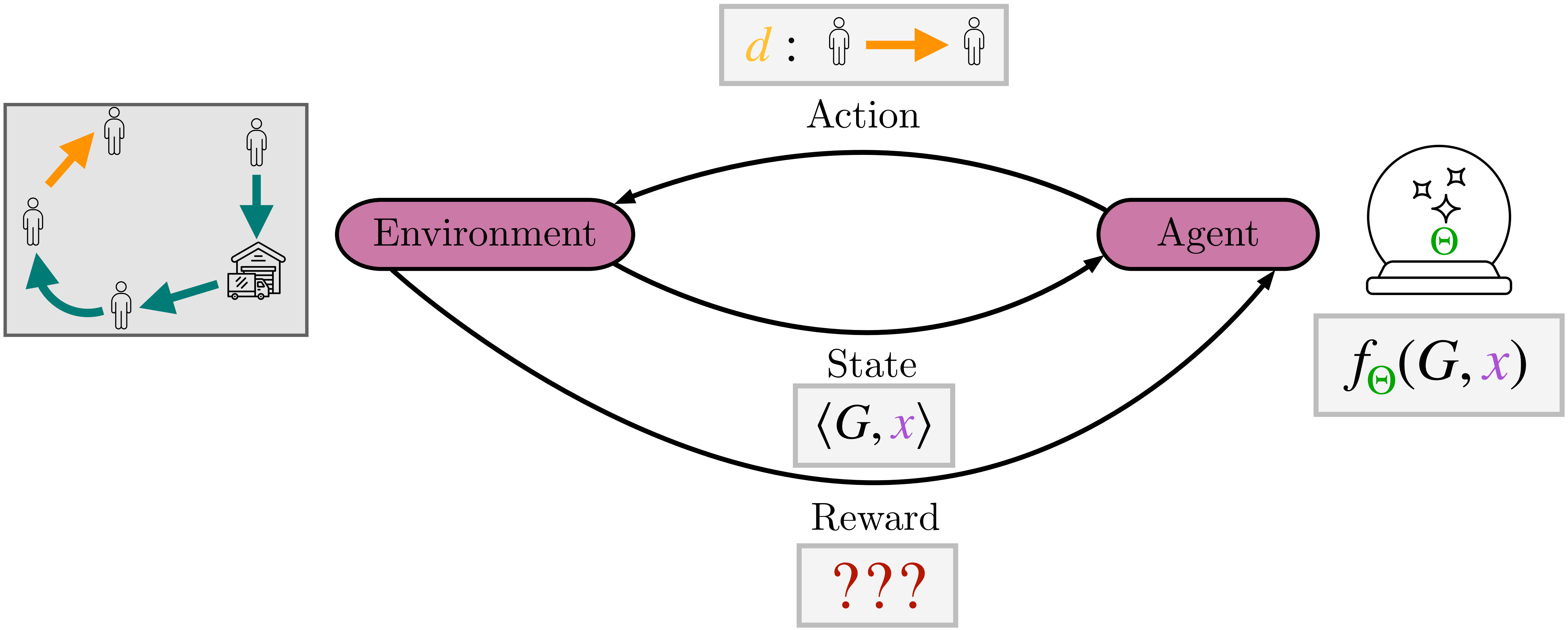
Challenge 2: **difficult to represent a combinatorial problem in a proper way for learning**

Tackling the first challenge (Cappart et al., AAAI 2021)

Challenge 1: we do not know what is the best choice

Consequence: tricky to rely on supervised learning

Our initial proposition: leverage reinforcement learning instead



Main idea: unveiling the connections of RL with CP through dynamic programming

Tricky part: it is not clear how to design the reward (what is a good assignment?)

Proposition of a reward function (Cappart et al., AAAI 2021)

? How to balance the fact that we want a feasible and optimal solution ?

Observation: feasibility is a prerequisite of optimality

Key idea 1: design a reward always prioritizing finding feasible solutions

Key idea 2: discriminate then feasible solutions by their quality

Reward for each action a at state s

$$= R(s,a) + \text{UB}$$

$$\text{UB} > R(s,a)$$

$R(s,a)$: direct increase in the objective function with assignment a

UB : strict upper bound on the optimal profit that can be reached

Intuition: solutions deeper in the tree are always more rewarded than shallower ones

Consequence 1: the first incentive is to go at the last depth (i.e., a feasible solution)

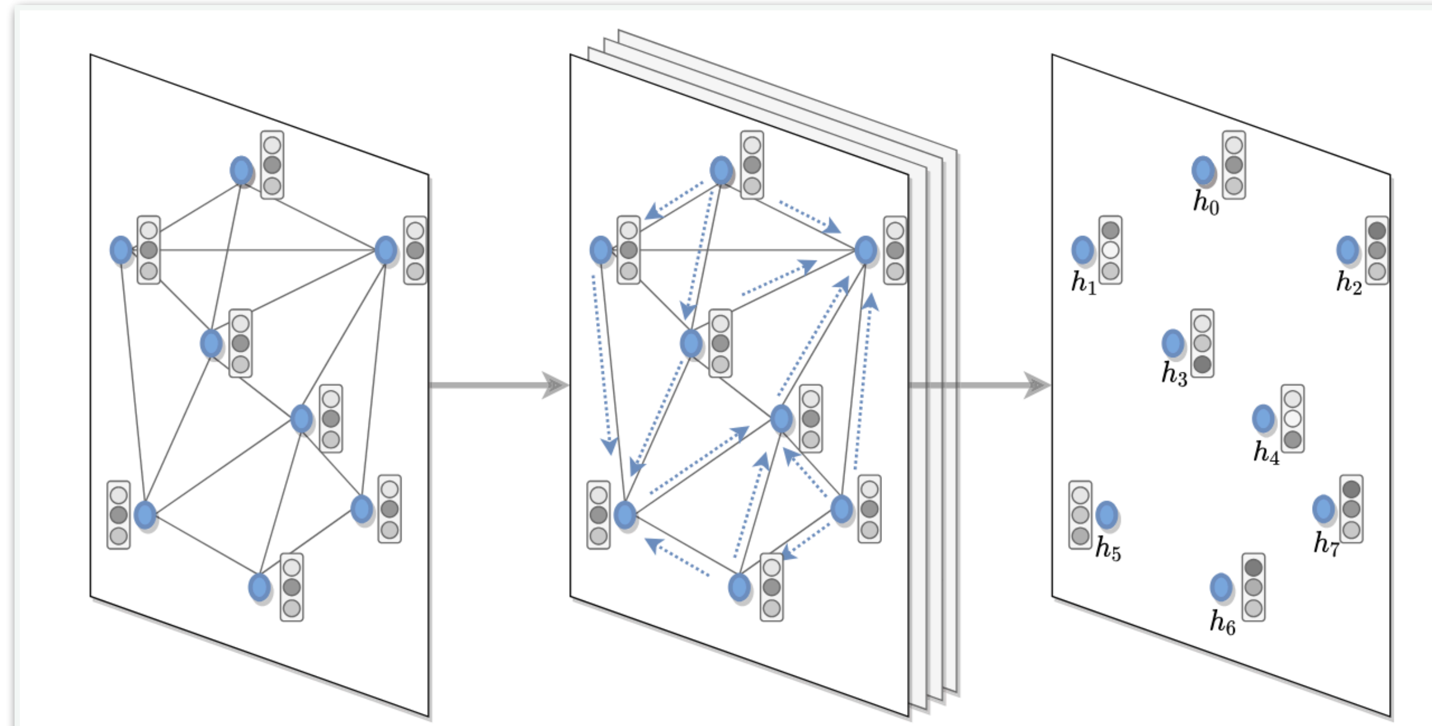
Consequence 2: solutions at the same depth are rewarded by their objective value

A first proof of concept (Cappart et al., AAAI 2021)

Algorithm 1: `BaB-DQN` Search Procedure.

▷ **Pre:** $\mathcal{Q}_p$ is a COP having a DP formulation.
▷ **Pre:** $\mathbf{w}$ is a trained weight vector.
$\langle \mathtt{X}, \mathtt{D}, \mathtt{C}, \mathtt{O} \rangle := \mathtt{CPEncoding}(\mathcal{Q}_p)$
$\mathcal{K} = \emptyset$
$\Psi := \mathtt{BaB\text{-}search}(\langle \mathtt{X}, \mathtt{D}, \mathtt{C}, \mathtt{O} \rangle)$
while Ψ is not completed **do**
  $\mathtt{s} := \mathtt{encodeStateRL}(\Psi)$
  $\mathtt{x} := \mathtt{takeFirstNonAssignedVar}(\mathtt{X})$
  if $\mathtt{s} \in \mathcal{K}$ **then**
    $v := \mathtt{peek}(\mathcal{K}, \mathtt{s})$
  else
    $v := \mathrm{argmax}_{u \in D(\mathtt{x})} \hat{Q}(\mathtt{s}, u, \mathbf{w})$
  end
  $\mathcal{K} := \mathcal{K} \cup \{\langle \mathtt{s}, v \rangle\}$
  $\mathtt{branchAndUpdate}(\Psi, \mathtt{x}, v)$
end
return $\mathtt{bestSolution}(\Psi)$

Challenge 2: how to represent a COP for learning?



Representing a problem as a graph, and feeding it to a graph neural network

Experiments: results showed that relevant branching decisions can be learned

Limitation: far below state-of-the-art results and limited to relatively small instances

Technical difficulty: not-so-efficient to embed learning into existing CP solvers

These first results showed the promise in this direction and drove my research

Improvements in learning to branch

(Chalumeau, Coulon et al., CPAIOR 2021)

SeaPearl.jl

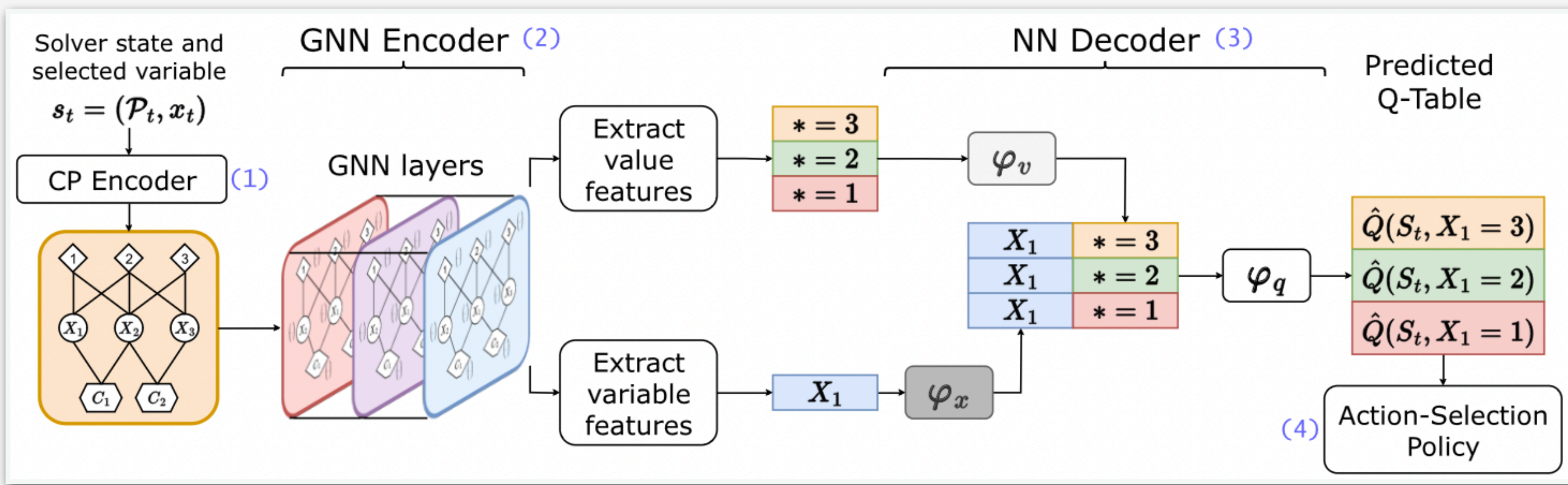
Seapearl: minimalist CP solver aiming to ease the integration of learning

Improvement: carrying out the learning inside the solver and not outside

Limitation 1: huge overhead in calling a GNN at each search node

Limitation 2: challenging to train (large resources, instability, etc.)

(Marty et al., CP 2023)



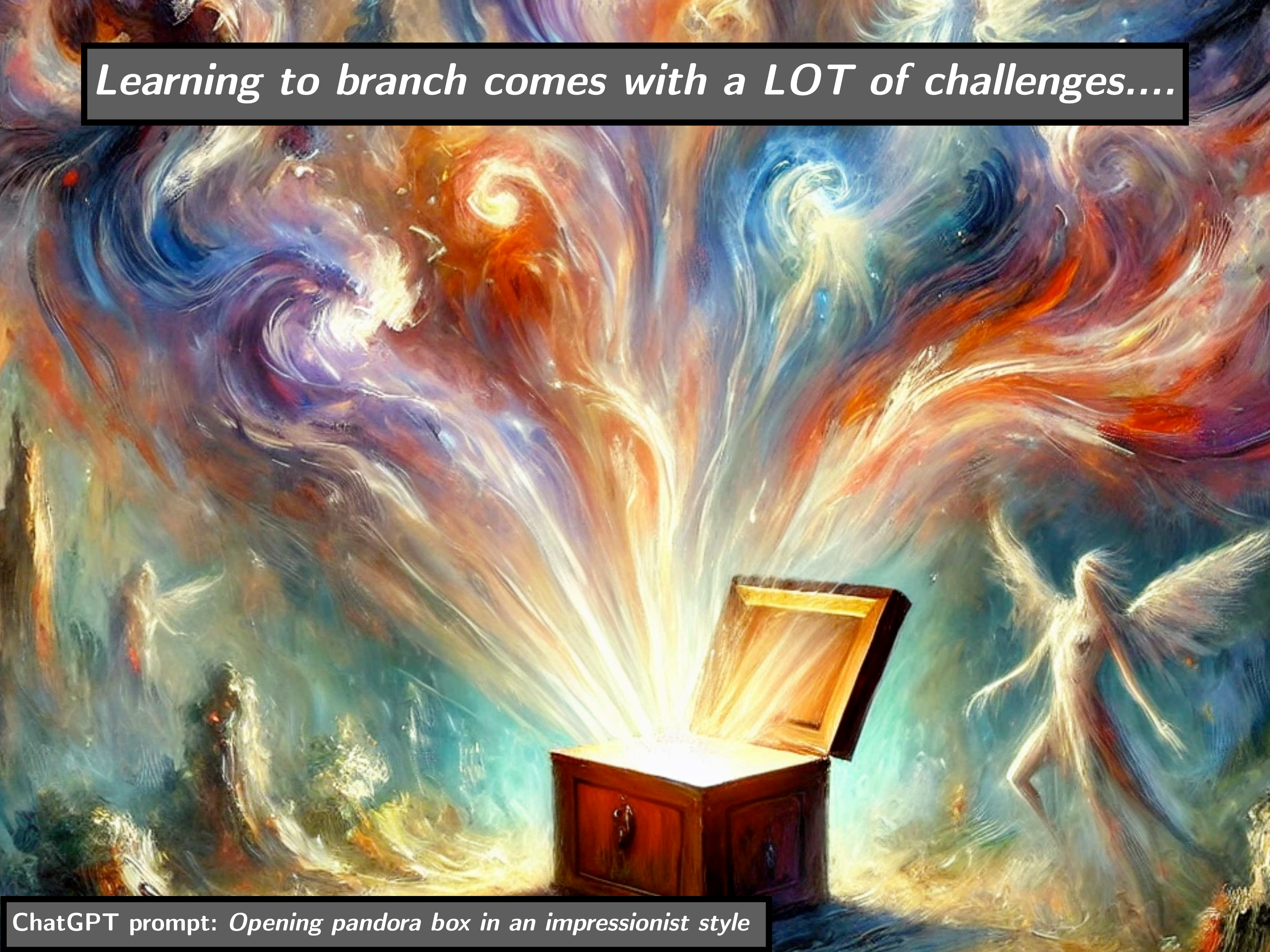
Main idea: mainly simplifying the framework!

Improvement: forget optimality proof (too difficult with value-selection heuristics)

New goal: finding quickly good solutions (redefining the reward function)

Limitation: still a huge overhead in calling often the GNN

Learning to branch comes with a LOT of challenges....



ChatGPT prompt: *Opening pandora box in an impressionist style*

My current thoughts in learning to branch

Learning branching heuristics comes with a LOT of challenges...

(1) **Overhead in calling a heavy model at each node** (compared to cheap heuristics)

(2) **Subjective choices in designing the reward** (feasibility, quality, optimality)

(3) A model good at the root node may be **poor at deeper levels** (*distributional shift*)

Here are few advices based on what worked the best for me

(1) **Do not use learning at each branching step** (too costly compared to heuristics)

(2) **Call the model only at the top of the tree** (where you likely have more samples)

(3) **Proving optimality may be out-of-range** (how to properly reward this?)

(4) **Focus on finding quickly good solutions** (in few nodes)

(5) **Prioritize hybrid approaches** (learning at the beginning, then use heuristics)

Going further with my thoughts...

Reinforcement learning may not be the best method for improving CP

Argument 1: much harder to train than supervised learning

Argument 2: indirectly require an unknown label (reward is an approximation of it)

Learning a value-selection heuristic may not be the best thing to do

Observation 1: learning is too costly and unstable to replace cheap heuristics

Observation 2: learning something does not always give practical improvements

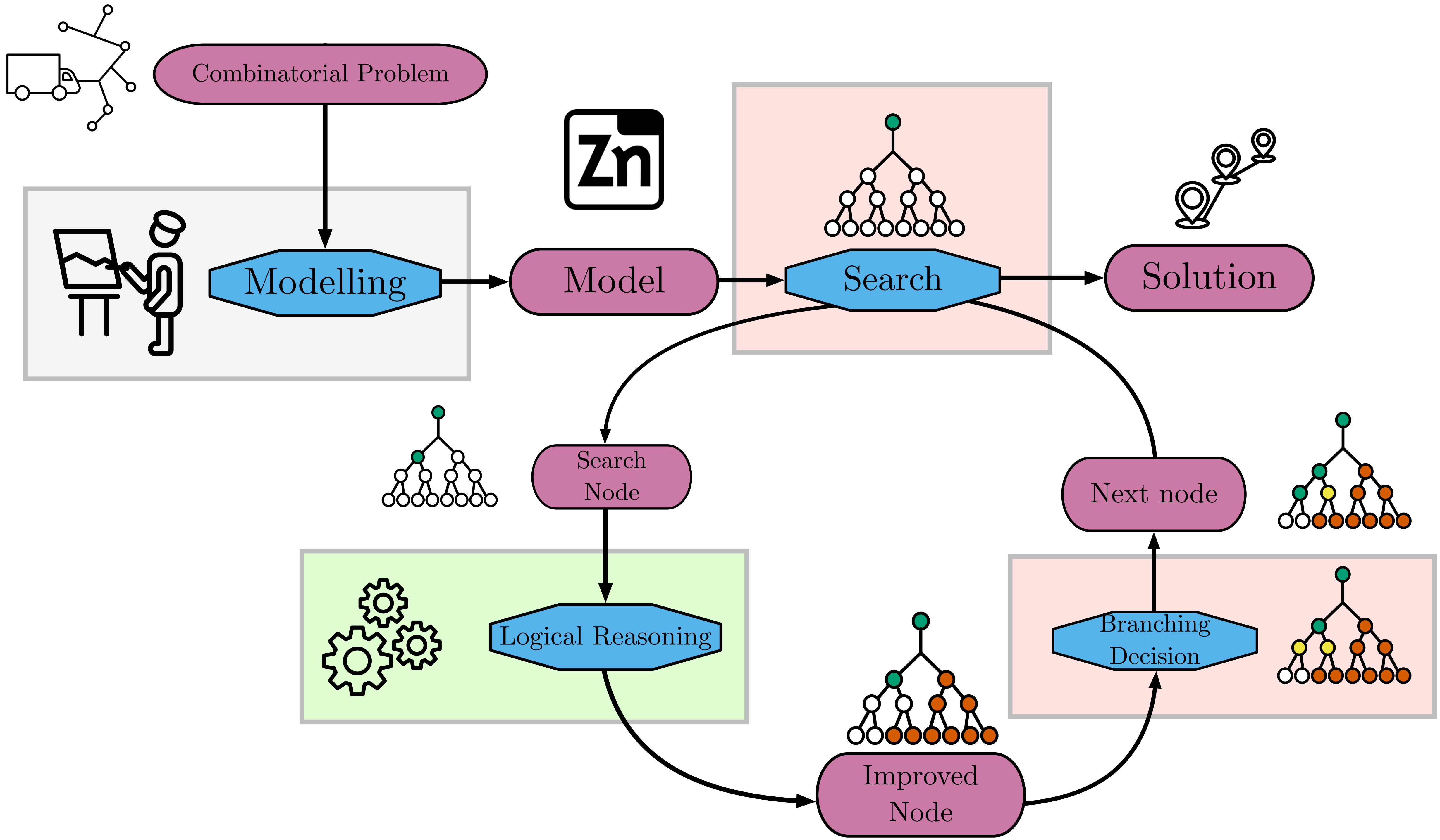
Note: please only see this as my personal opinion, and not as an irrevocable truth :-)

? What about learning a variable-selection heuristic for CP ?

My intuition: we will probably have similar challenges than for the value-selection

Ok, but what do you propose then ?

Can we learn something else?

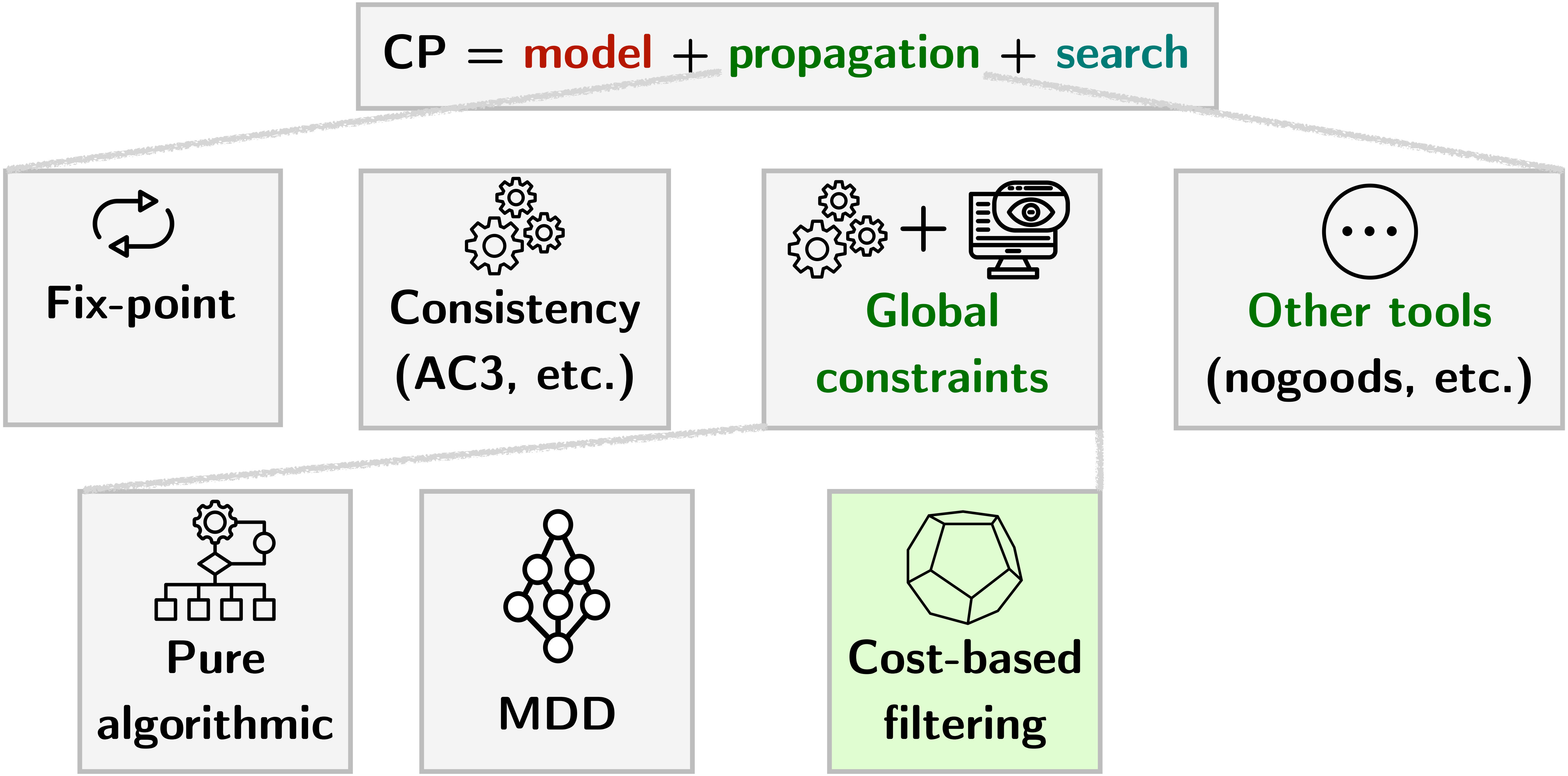


My main current research direction is to learn how to prune the search space

(Said differently, I plan to improve the quality of filtering)

Types of propagation in a CP solver

? But how to do that ? Propagation is mainly algorithmic



Some propagators relies on tricky-to-get information that we propose to learn

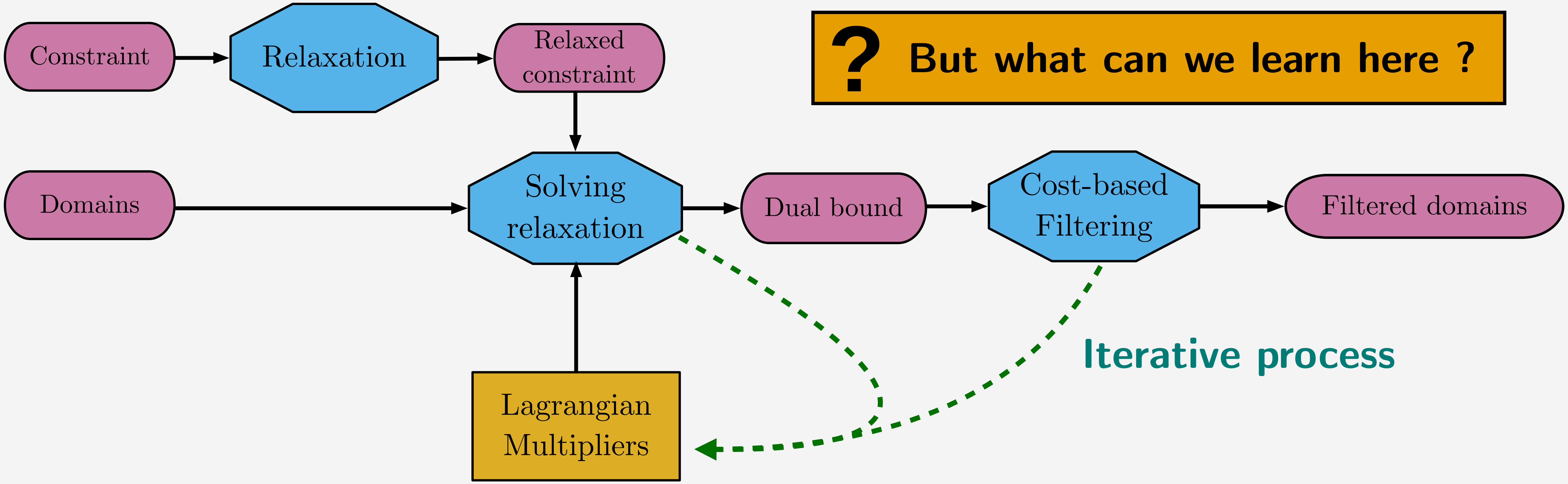
Cost-based filtering (Focacci et al., CP 1999)

Cost-based filtering leverages relaxation to improve the filtering of a constraint

Step 1: a **valid relaxation** is embedded into the global constraint

Step 2: the relaxed problem is solved to get **a dual bound** on the cost

Step 3: the bound is used to **prune** the search space



? But what can we learn here ?

Trick: the quality of the relaxation depends on **Lagrangian multipliers**

Bad news: **determining the best values of the multipliers is generally costly**

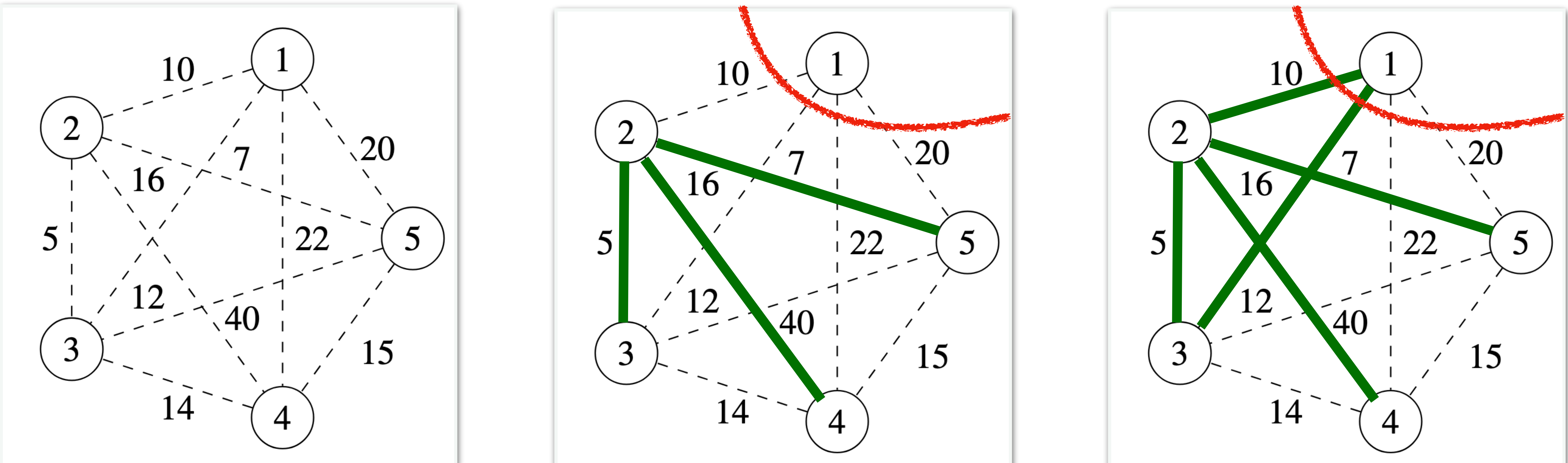
We propose to obtain the multipliers through self-supervised learning

Learning Lagrangian Multipliers for the TSP

WeightedCircuit(X, G, d) : **ensure that variables X form a TSP tour in G of cost $\leq d$**

1-tree relaxation(X, G) : **allows the TSP to go twice in a specific node**

- **Step 1:** **ensure that variables X form a minimum spanning tree in $G \backslash \{v_1\}$**
- **Step 2:** **link the remaining node v_1 to the tree with the two cheapest edges**



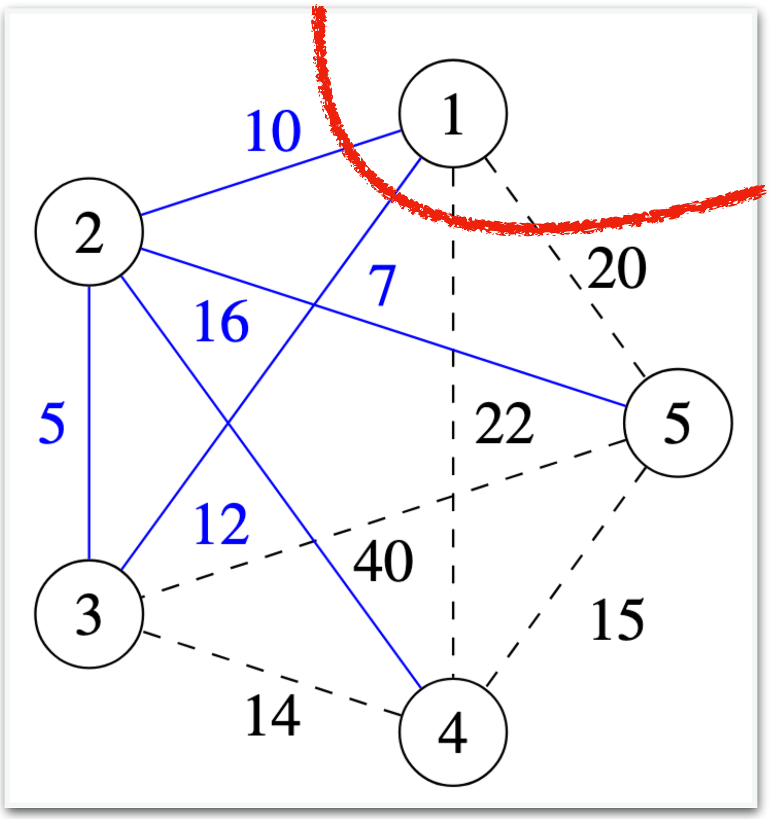
Optimal TSP cost: 62

Relaxation cost: 50

We have here a example of how a specific constraint can be relaxed

Learning Lagrangian Multipliers for the TSP

? The bound is not very tight, could we improve it ?



Relaxation cost: 50

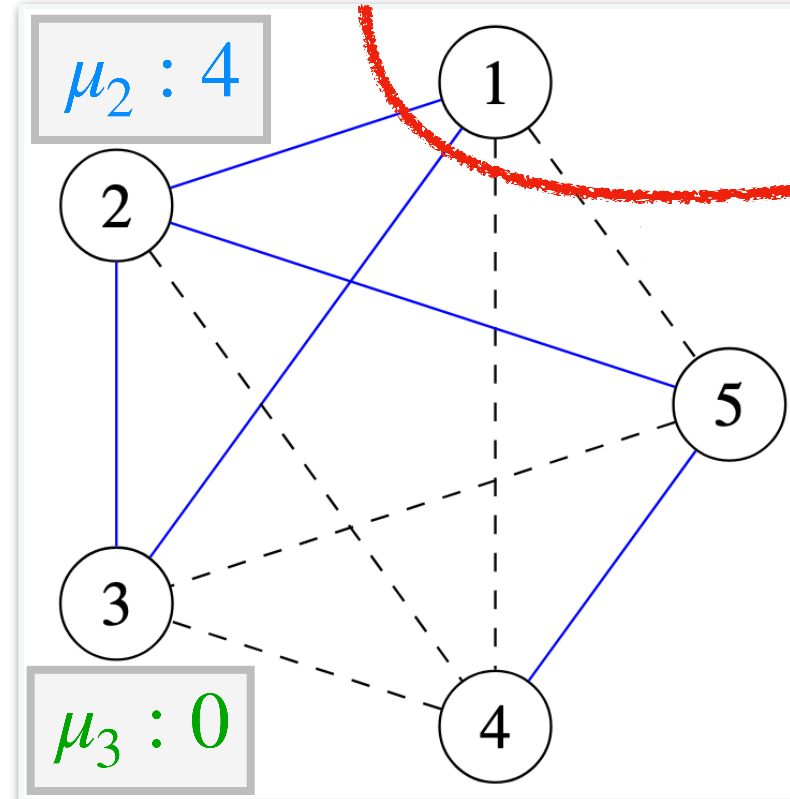
Lagrangian Multipliers

$\langle \mu_1, \mu_2, \mu_3, \mu_4, \mu_5 \rangle$

$$c'_{u,v} = c_{u,v} + \mu_u + \mu_v$$

$$c'_{2,3} = c_{2,3} + \mu_2 + \mu_3$$

$$9 = 5 + 4 + 0$$



Relaxation cost: 59

Main idea: perturbate the cost of each edge with values called Lagrangian multipliers

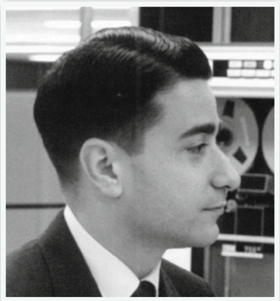
Lagrangian multiplier: value associated with each node

Perturbation: change the cost of each edge based on the multipliers of its nodes

Nice property 1: the optimal TSP tour is invariant under this perturbation

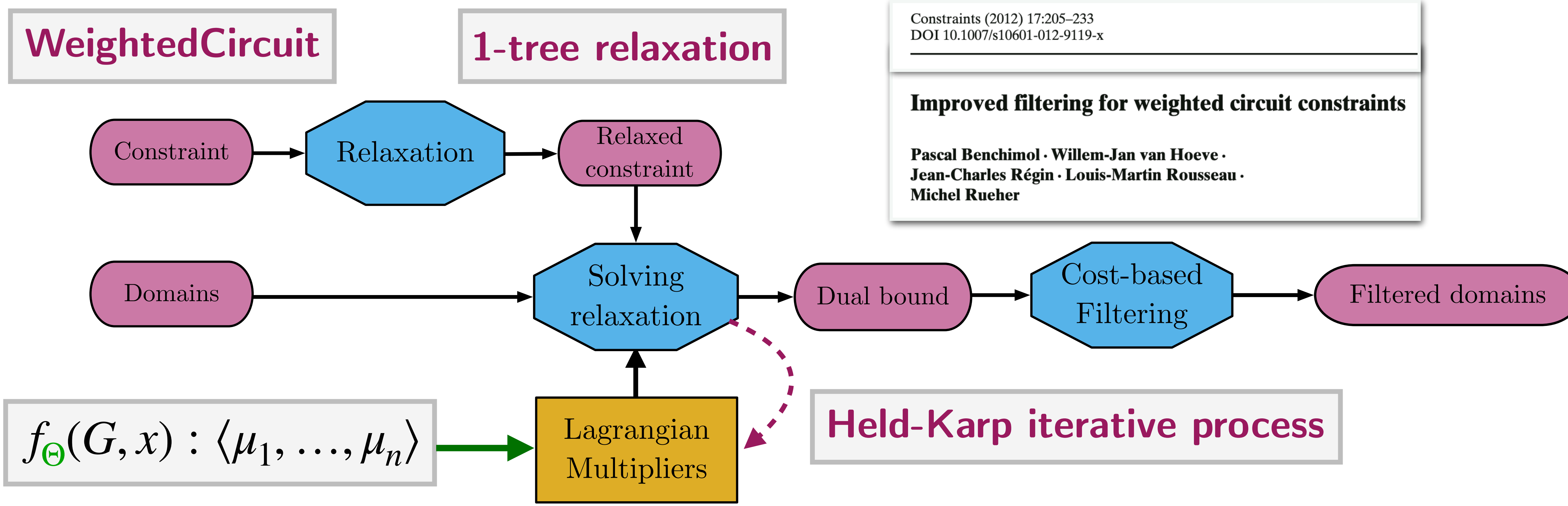
Nice property 2: better bounds generally result in a much better filtering

Learning Lagrangian Multipliers for the TSP



? But how can we find good values for the multipliers ?

Held and Karp, 1970: proposed an iterative algorithm for that



Constraints (2012) 17:205–233
DOI 10.1007/s10601-012-9119-x

Improved filtering for weighted circuit constraints

Pascal Benchimol · Willem-Jan van Hoeve ·
Jean-Charles Régin · Louis-Martin Rousseau ·
Michel Rueher

Bad news: the iterative adjustment of the multipliers is computationally expensive

Parjadis et al. (CP 2024): use learning to initialize the multipliers

Idea: use a GNN to predict multipliers (one per node) from a TSP instance

Results: better filtering achieved on random and symmetric TSPs

Observation: replacing HK process with learning was not successful

Types of propagation in a CP solver

? Can we learn a more general bounding mechanism in CP ?

CP = model + propagation + search

Fix-point

Consistency (AC3, etc.)

Global constraints

Other tools (nogoods, etc.)

Pure algorithmic

MDD

Cost-based filtering

Lagrangian decomposition

We extend the idea to learn multipliers to CP-based Lagrangian decomposition

Lagrangian decomposition (Guignard and Kim, 1987)

Lagrangian decomposition splits the problem into independent and easier subproblems

Step 1: each variable in each constraint is duplicated, except for the first constraint

Step 2: a constraint linking the values is added for each new variable

Step 3: these constraints are moved into the objective function with a penalty term

$$\begin{aligned} \max \quad & f(X_1, X_2, X_3) \\ \textbf{s.t.} \quad & C_1(X_1, X_2, X_3) \\ & C_2(X_2, X_3) \\ & X_1, X_2, X_3 \in \mathbb{N}^+ \end{aligned}$$

$$\begin{aligned} \max \quad & f(X_1, X_2, X_3) \\ \textbf{s.t.} \quad & C_1(X_1, X_2) \\ & \boxed{C_2(Y_2, Y_3)} \\ & Y_2 = X_2, \; Y_3 = X_3 \\ & X_1, X_2, Y_2, X_3, Y_3 \in \mathbb{N}^+ \end{aligned}$$

$$\max \quad f(X_1, X_2, X_3) + \boxed{\mu_2} \cdot (Y_2 - X_2) + \boxed{\mu_3} \cdot (Y_3 - X_3)$$

Again, we have Lagrangian multipliers, but in a more generic way than before

Lagrangian decomposition (Guignard and Kim, 1987)

$$\mathscr{B}(\mu_2, \mu_3) = \begin{cases} \max & f(X_1, X_2, X_3) + \mu_2 \cdot (X_2 - Y_2) + \mu_3 \cdot (X_3 - Y_3) \\ \textbf{s.t.} & C_1(X_1, X_2, X_3) \\ & C_2(Y_2, Y_3) \\ & X_1, X_2, Y_2, X_3, Y_3 \in \mathbb{N}^+ \end{cases}$$

Solving this relaxed problem will give a dual bound

? But, is it easy to solve ?

Observation: by construction, each constraint has its own set of variables

Consequence: each constraint can be solved independently

$$\mathscr{B}(\mu_2, \mu_3) = \boxed{\begin{array}{l} \max \left(f(X_1, X_2, X_3) + \mu_2 \cdot X_2 + \mu_3 \cdot X_3 \right) \\ \textbf{s.t. } C_1(X_1, X_2, X_3) \\ \quad X_1, X_2, X_3 \in \mathbb{N}^+ \end{array}} + \boxed{\begin{array}{l} \max \left(-\mu_2 \cdot Y_2 - \mu_3 \cdot Y_3 \right) \\ \textbf{s.t. } C_2(Y_2, Y_3) \\ \quad Y_2, Y_3 \in \mathbb{N}^+ \end{array}}$$

Given some multipliers, we can obtain a bound by solving several subproblems

Lagrangian decomposition in CP (Hà et al. CP 2015)

$$\mathcal{B}(\mu_2,\mu_3) = \boxed{\begin{array}{ll} \max \Big(f(X_1,X_2,X_3) + \mu_2 \cdot X_2 + \mu_3 \cdot X_3\Big) \\ \textbf{s.t. } C_1(X_1,X_2,X_3) \\ \quad X_1,X_2,X_3 \in \mathbb{N}^+ \end{array}} + \boxed{\begin{array}{ll} \max \big(-\mu_2 \cdot Y_2 - \mu_3 \cdot Y_3\big) \\ \textbf{s.t. } C_2(Y_2,Y_3) \\ \quad Y_2,Y_3 \in \mathbb{N}^+ \end{array}}$$

? How to set the values of the multipliers ?

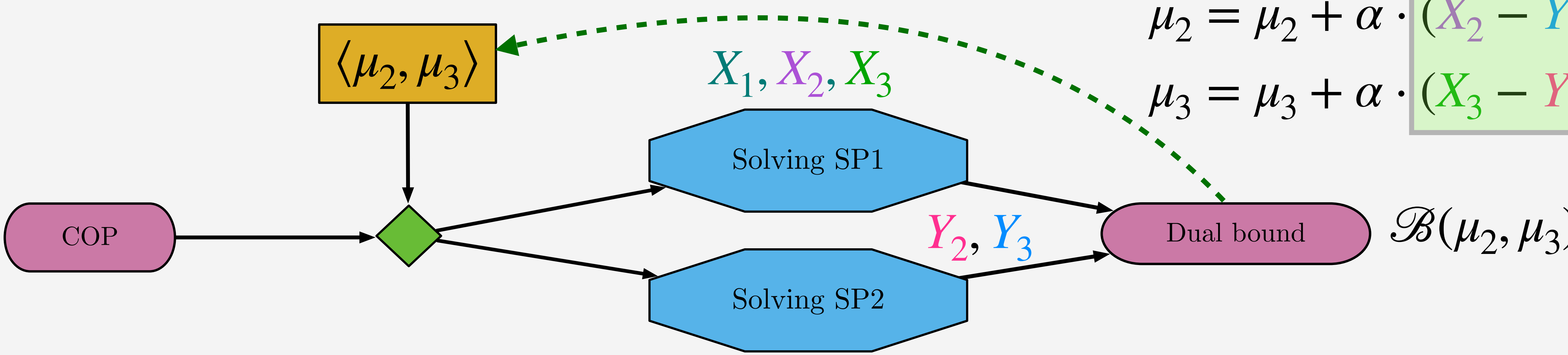
Initialization: we set the multipliers to an arbitrary value

Step 1: we solve all subproblems with these values (we get a dual bound)

Step 2: we update the multipliers with sub-gradient (we improve the bound)

Main loop: we repeat steps 1 and 2 for *x* iterations

$$\mu_2 = \mu_2 + \alpha \cdot \boxed{(X_2 - Y_2)}$$
$$\mu_3 = \mu_3 + \alpha \cdot \boxed{(X_3 - Y_3)}$$



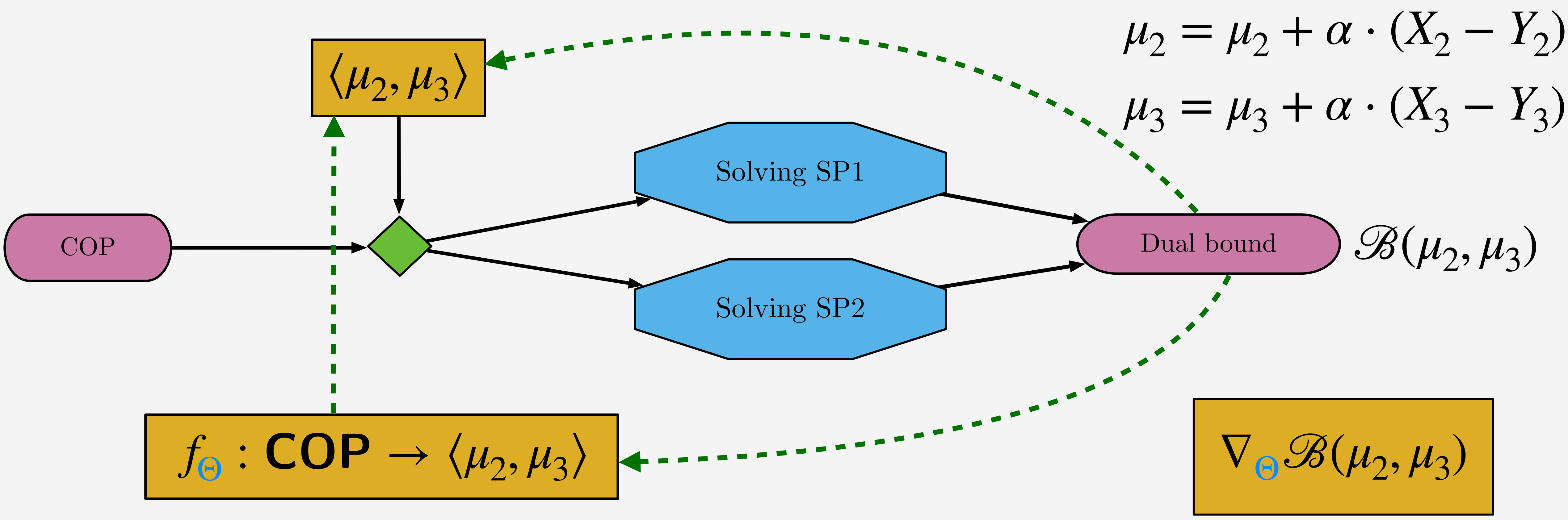
Learning multipliers for Lagrangian decomposition

This process is very costly as it requires solving few subproblems at each iteration

We propose a self-supervised learning approach to compute them

Step 1: multipliers are now obtained by a differentiable predictive model

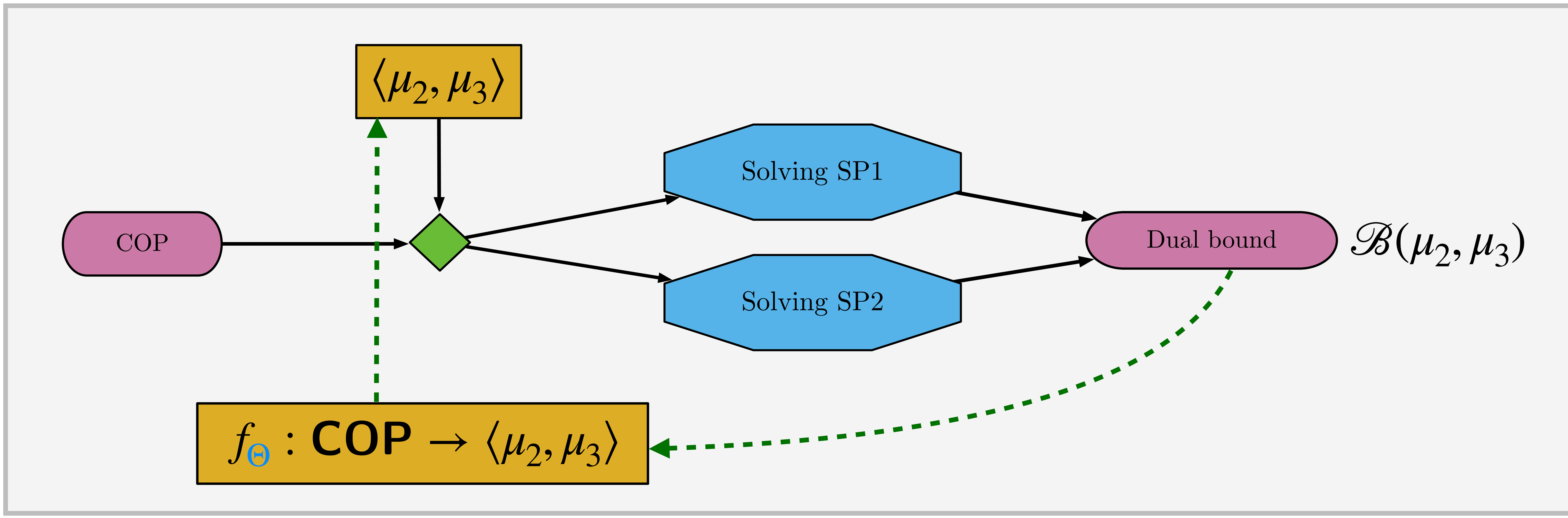
Step 2: the model is trained end-to-end by differentiating the bound



Intuition: the optimisation process is carried out offline during a training phase

Learning multipliers for Lagrangian decomposition

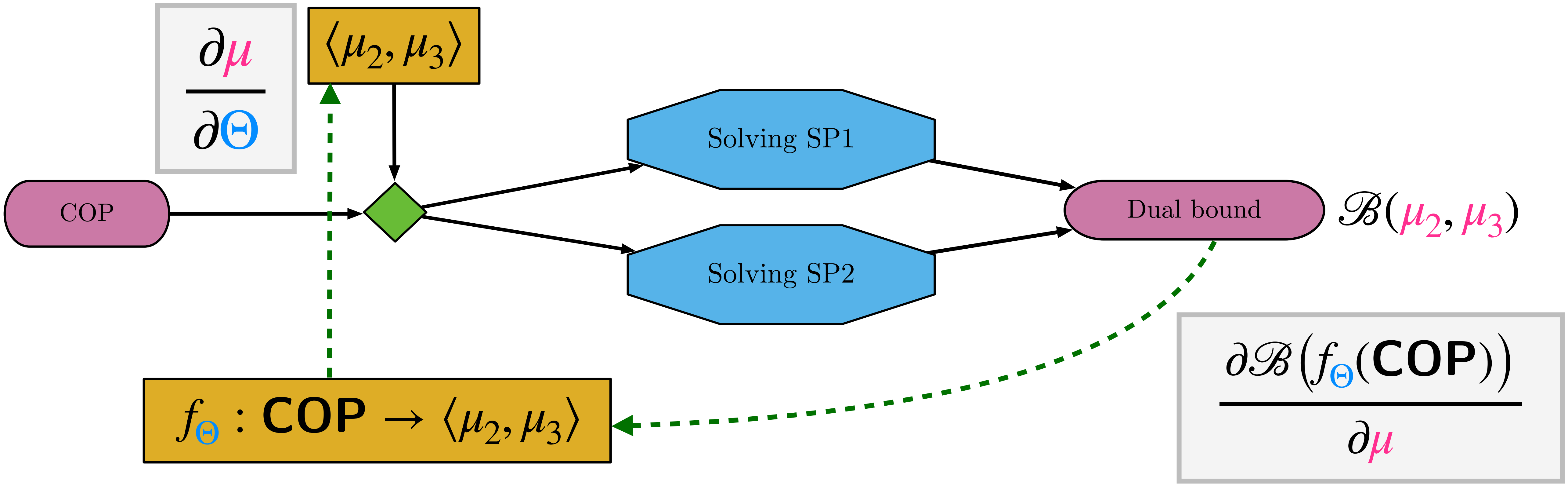
$$\mathscr{B}(\mu_2, \mu_3) = \boxed{\begin{array}{l} \max \left(f(X_1, X_2, X_3) + \mu_2 \cdot X_2 + \mu_3 \cdot X_3 \right) \\ \textbf{s.t. } C_1(X_1, X_2, X_3) \\ \qquad X_1, X_2, X_3 \in \mathbb{N}^+ \end{array}} + \boxed{\begin{array}{l} \max \left(-\mu_2 \cdot Y_2 - \mu_3 \cdot Y_3 \right) \\ \textbf{s.t. } C_2(Y_2, Y_3) \\ \qquad Y_2, Y_3 \in \mathbb{N}^+ \end{array}}$$



Gradient: $\nabla_\Theta \mathscr{B}(\mu)$

? How to compute the gradient of this bound ?

Learning multipliers for Lagrangian decomposition



$$\nabla_\Theta \mathscr{B}(\mu) = \frac{\partial \mathscr{B}\left(f_\Theta(\mathbf{COP})\right)}{\partial \mu} \times \frac{\partial \mu}{\partial \Theta} \quad = (X - Y) \times \frac{\partial \mu}{\partial \Theta}$$

Step 1: we use the chain-rule to uncover dependencies

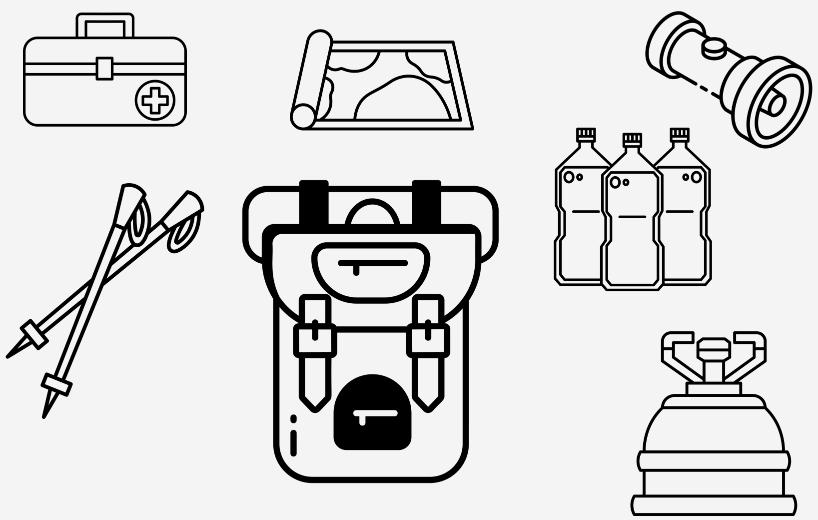
Step 2: right-term is a simple backpropagation in the predictive model

Step 3: left-term reuses the initial sub-gradient expression

Training: differentiating on training instances (no need to have labels)

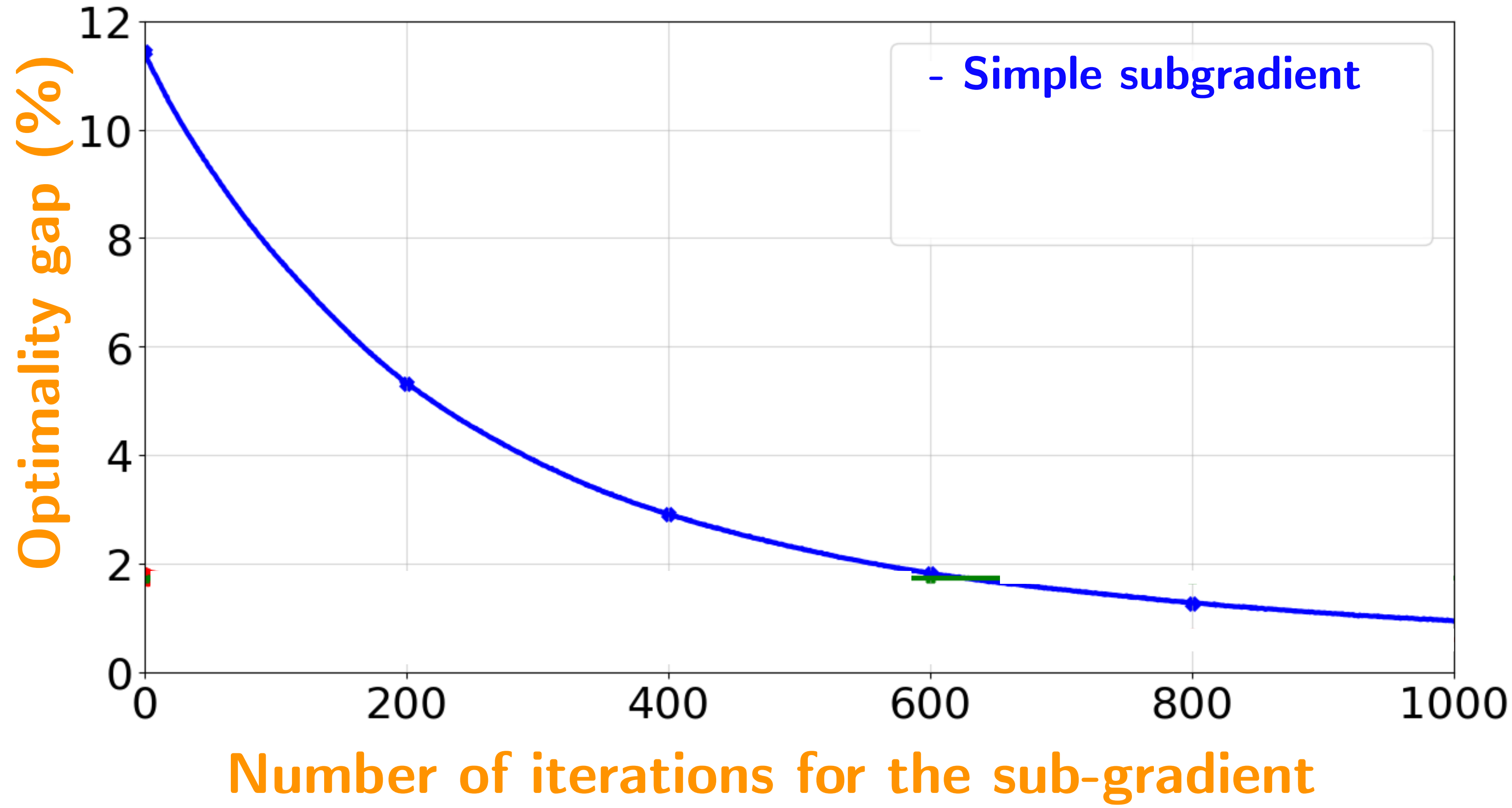
Qualitative results

Multidimensional knapsack



Size: 100 items

Dimension: 5 constraints



Metric: quality of the dual bound obtained at the root node

Observation 1: simple subgradient requires a lot of iterations to find good bounds

Observation 2: learning alone manages to get directly good bounds

Observation 3: learning to initialize sub-gradient quickly gives better bounds

Our results showed both the interest of learning alone or with sub-gradient

My current thoughts in learning to bound

I think that learning to bound in CP is a promising direction

(1) The lack of generic relaxation is a shortcoming of CP (compared to MIP solvers)

(2) Lagrangian relaxation (or decomposition) ensures the validity of the bound

(3) Learning can fully replace the subgradient (less filtering but cheaper)

(4) Learning can also only initialize subgradient (better filtering but more expensive)

(5) Results are encouraging in terms of execution time (more than for branching)

But there are still questions and challenges to address...

(1) Which predictive model should we use? (is GNN a right choice?)

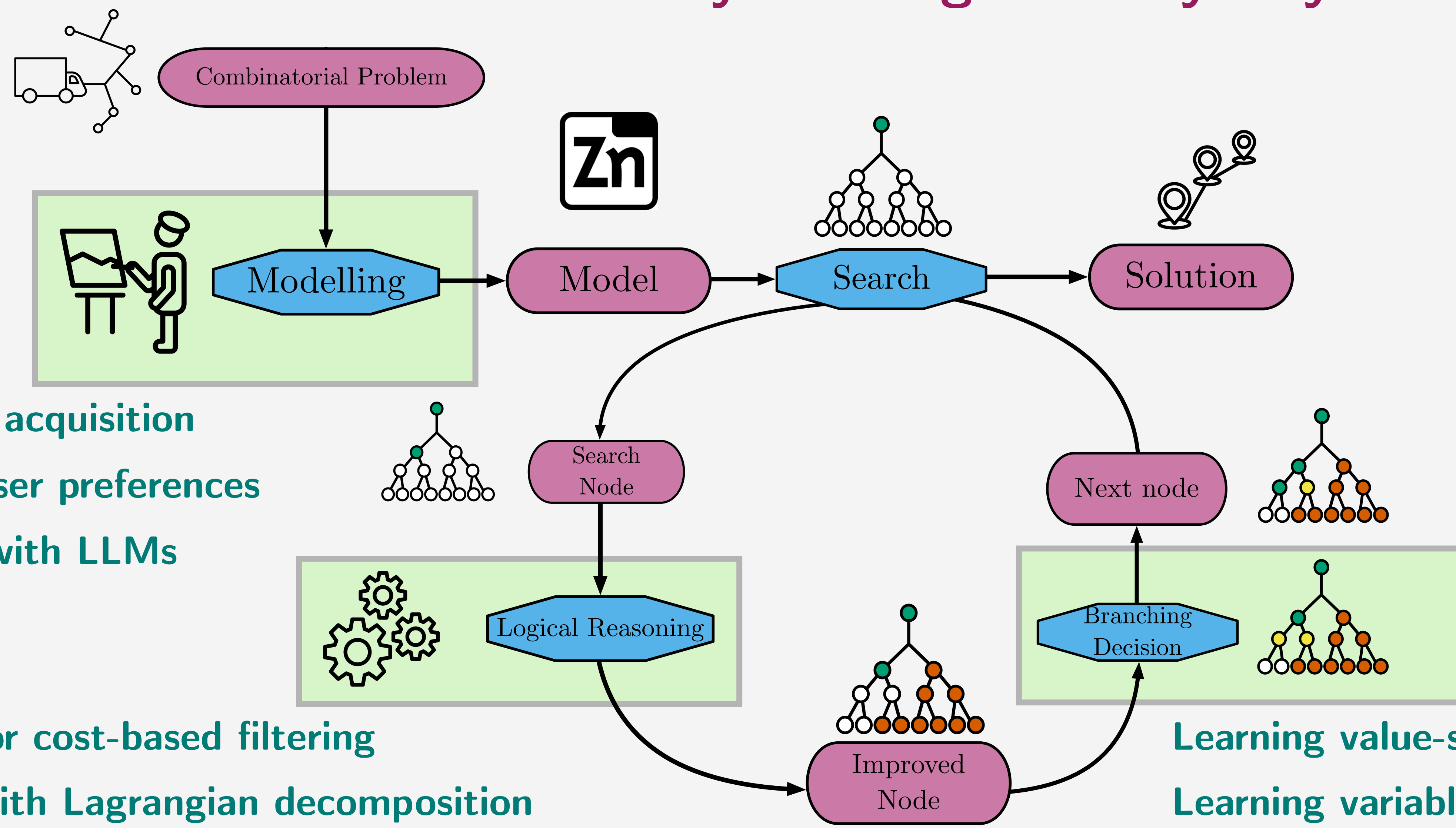
(2) Can we have a generic representation of any COP (Boisvert et al., CPAIOR 2024)

(3) How to handle problems with only few representative instances?

(4) There are still the subproblems that need to be solved efficiently

Conclusion with my final notes

CP can be enhanced by learning in many ways...



Constraint acquisition

Learning user preferences

Modeling with LLMs

Learning for cost-based filtering

Learning with Lagrangian decomposition

Learning value-selection

Learning variable-selection

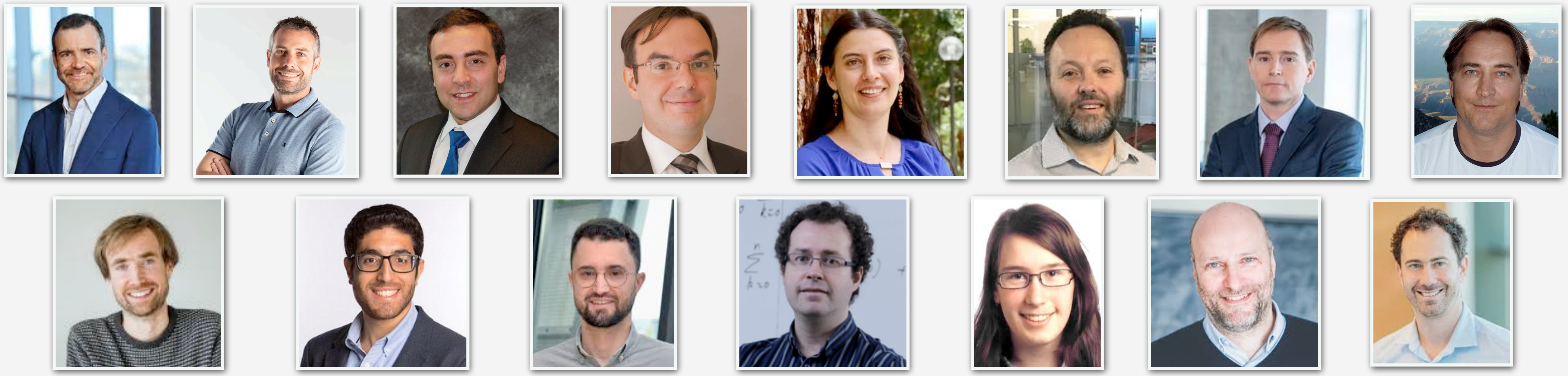
My take-home messages

(1) **Learning something meaningful does not always result in improved performances**

(2) **Combining learning with existing tools mitigate the shortcomings of learning**

(3) **Promising research direction, but a lot of challenges to handle for a practical use**

Many thanks!!



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SNCF
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mitacs

POLYTECHNIQUE MONTRÉAL
UNIVERSITÉ D'INGÉNIERIE
CIRRELT
Mila
CORAIL
Combinatorial Optimization and Reasoning in Artificial Intelligence Laboratory

Reference list (work we carried out)

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Learning to bound

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Learning to model and graph neural networks

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Please reach me if you know other works using learning to get dual bounds :-)

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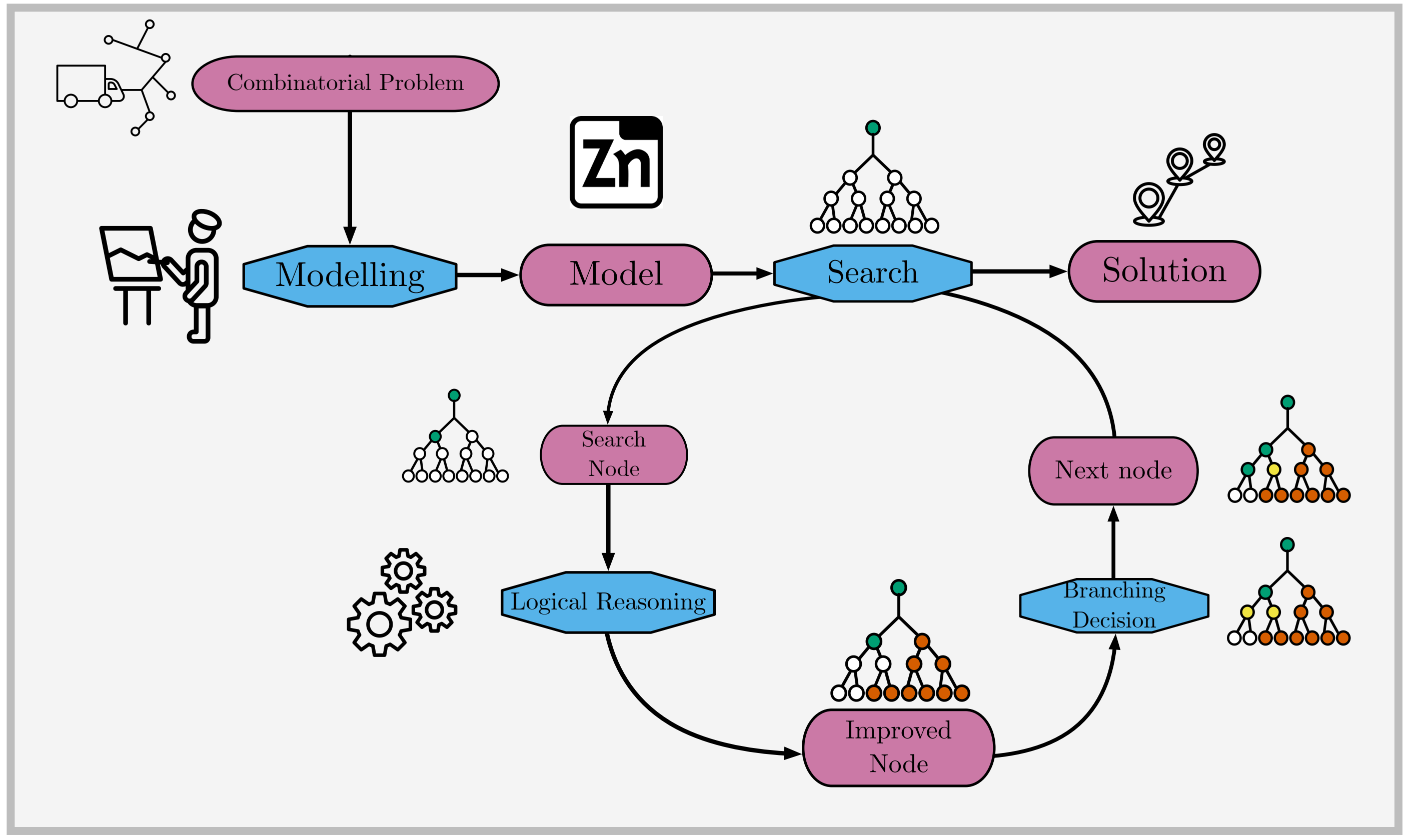

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