Learning a value-selection heuristic inside a constraint programming solver

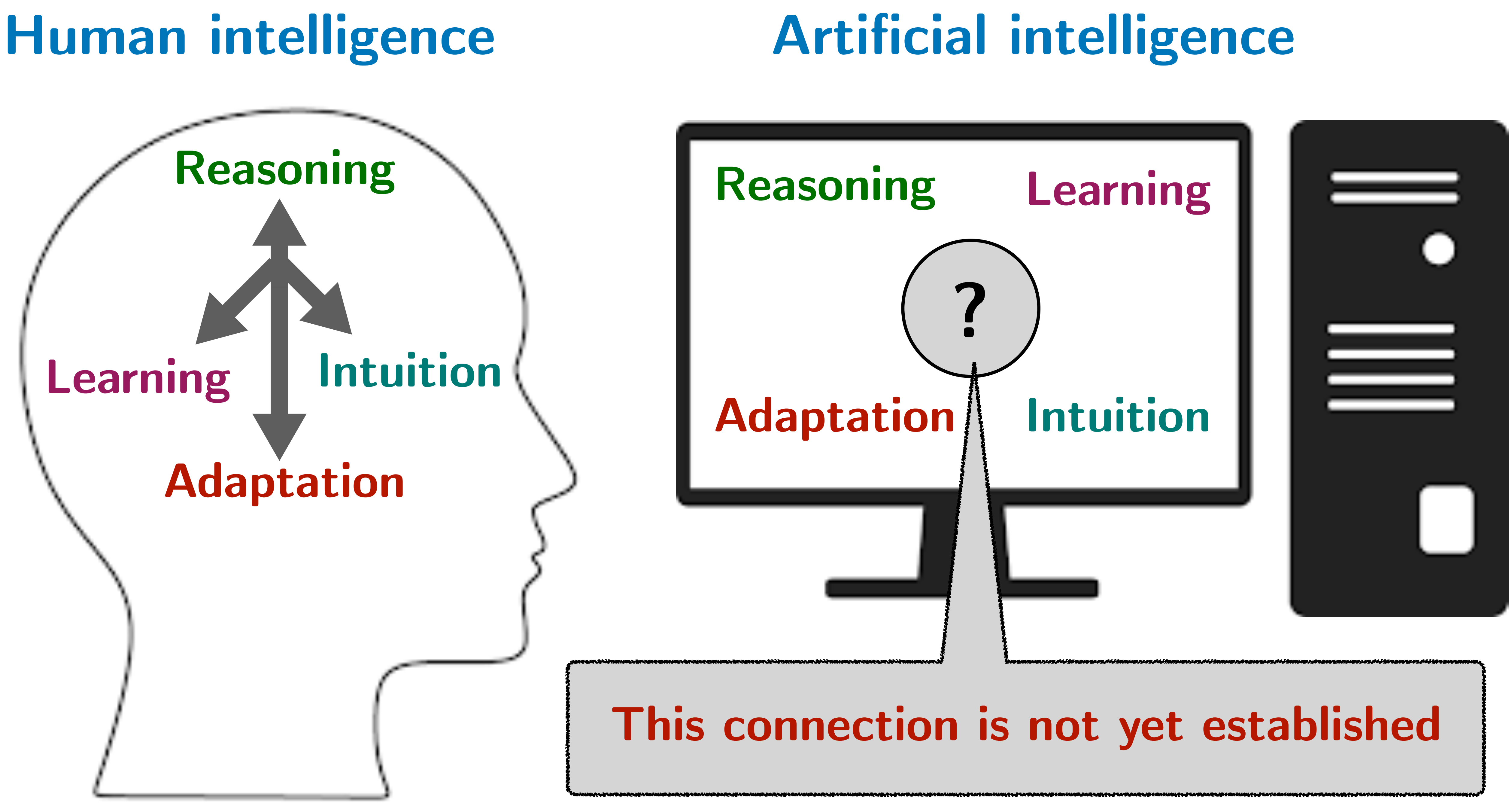
ACP Summer School 2023 - Leuven

POLYTECHNIQUE MONTRÉAL

Combinatorial Optimization and Reasoning in Artificial Intelligence Laboratory

Quentin Cappart

Human intelligence versus artificial intelligence



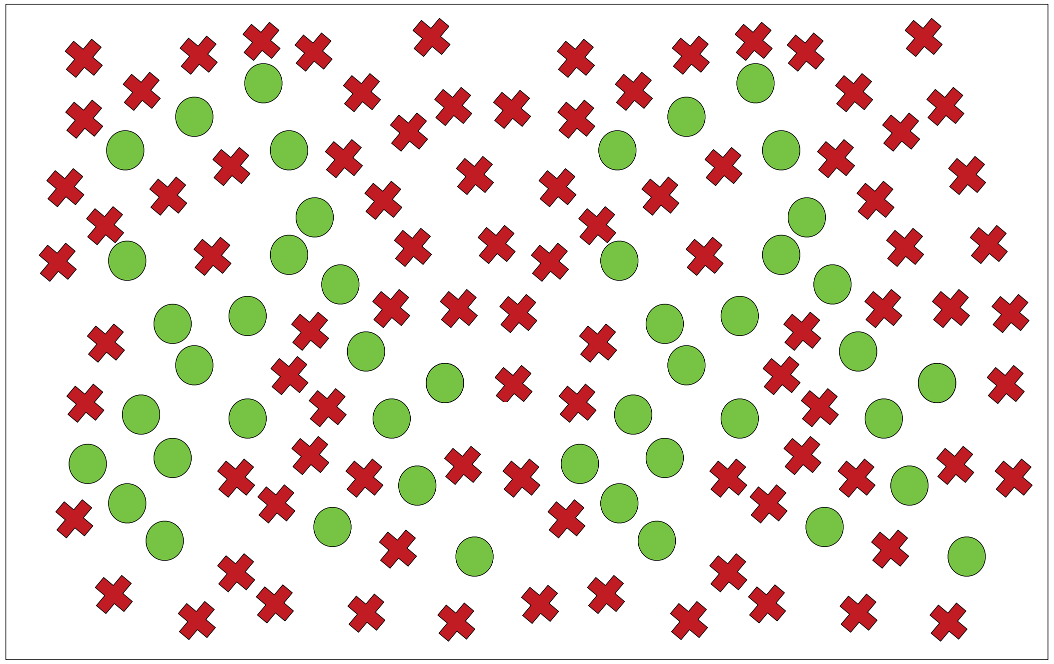
Long-term research plan: building an AI with these connections

Goal: providing a better solving process for combinatorial problems

Combinatorial problems

What is a combinatorial problem ?

Combinatorial satisfaction problem (CSP)



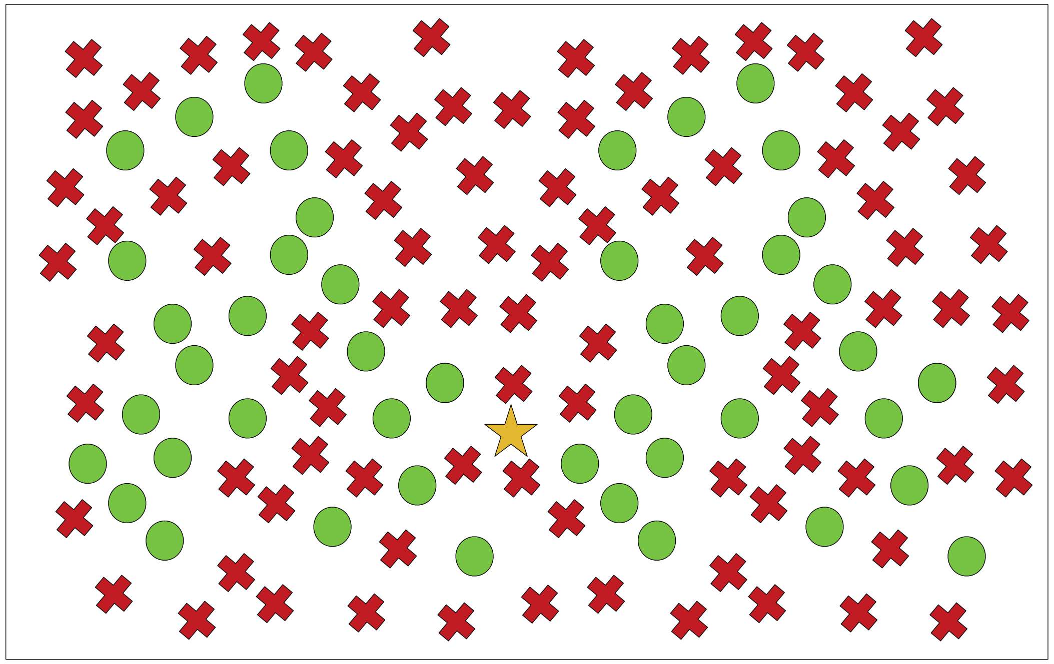
Finding a feasible solution from a finite set of solutions

Finding a needle in a haystack

Building a schedule satisfying a set of constraints

Servicing a set of customers without delays

Combinatorial optimization problem (COP)



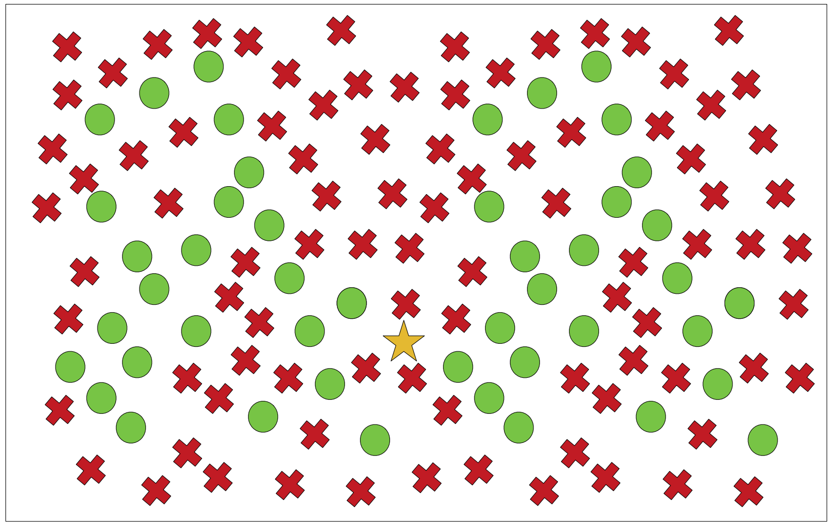
Finding the best feasible solution from a finite set of solutions

Finding the biggest diamond needle in a haystack

Scheduling a production while minimizing costs

Maximizing serviced customers during a day

Difficulty of combinatorial problems



In practice: generally a huge amount of possible solutions!

In theory: interesting combinatorial problems are NP-complete or NP-hard

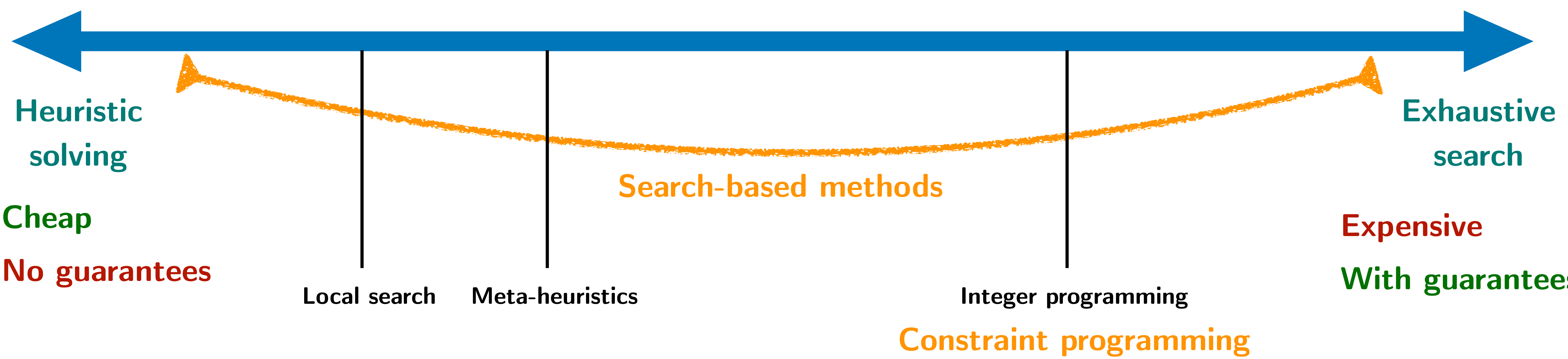
Consequence: there is no poly-time algorithms to solve them exactly

? How can we solve them ?

Idea 1: enumerate all the solutions and keep the best one (exhaustive search)

Idea 2: use a kind of intuition to build a solution (heuristic solving or greedy algorithm)

Idea 3: build or enumerate solutions in a clever way (search-based methods)



Observation: there are many search-based methods, with a specific dependency to a heuristic

Search-based methods

Great challenge: the efficiency of a method is often tightly linked with the quality of the heuristic

- **Greedy algorithm and local search:** huge dependency
- **Constraint programming:** high dependency for good performances (define how the search is directed)
- **Integer programming:** less dependent - but the approach is limited to specific problems

Consequence: a bad heuristic can give very poor performances to most solving approaches

? How to build an efficient heuristic ?

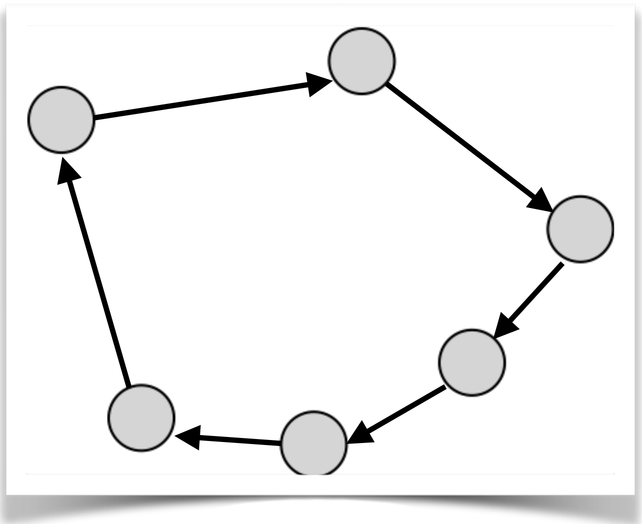
Option 1: hand-crafting the heuristic

Idea: design manually a heuristic, thanks to expert knowledge

Exemple (TSP): always visiting the closest available city

Difficulty 1: require a good understanding about the problem (e.g., LKH)

Difficulty 2: must be designed specifically for each problem



Search-based methods

Great challenge: the efficiency of a method is often tightly linked with the quality of the heuristic

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? How to build an efficient heuristic ?

Option 2: learning the heuristic

Observation: we do not leverage the fact that similar problems may be solved many times (e.g., routing)

Consequence: for each problem, the solving process repeatedly restart from scratch with no knowledge

Idea: use past experiments or historical data for learning a heuristic

This idea is actually quite old...

Back to the past...

A Hybrid Approach to Vehicle Routing using Neural Networks and Genetic Algorithms

Jean-Yves Potvin
Danny Dubé
Christian Robillard

Centre de recherche sur les transports
Université de Montréal
C.P. 6128, Succ. Centre-Ville,
Montréal (Québec),
Canada H3C 3J7

Using artificial neural networks to solve the orienteering problem

Qiwen Wang[a)], Xiaoyun Sun[b)], Bruce L. Golden[b)] and Jiyou Jia[a)]
[a)] *College of Business and Management, Beijing University, Beijing 100871, PR China*
[b)] *College of Business and Management, University of Maryland, College Park, MD 20742, USA*

Neural Networks for Automated Vehicle Dispatching

Yu Shen
Jean-Yves Potvin
Jean-Marc Rousseau

Centre de Recherche sur les Transports
Université de Montréal
C.P. 6128, Succ. "A"
Montréal (Québec)
Canada H3C 3J7

? When such papers were written and published ?

Answer: In the nineties !

Fun-fact 1: papers with similar names are still published :-)

Artificial Intelligence
Volume 313, December 2022, 103786

Neural large neighborhood search for routing problems ☆

André Hottung, Kevin Tierney

Neurocomputing
Volume 508, 7 October 2022, Pages 79-98
Go to table of contents for this volume/issue

Solve routing problems with a residual edge-graph attention neural network

Kun Lei [a], Peng Guo [a b], Yi Wang [c], Xiao Wu [a b], Wenchao Zhao [a]

Fun-fact 2: you may not know who is Jean-Marc Rousseau but you may know his son :-)

Observation: learning heuristics (with neural networks) is an old and still open research question!

Search-based methods

How learning can be used to solve a combinatorial problem ?

European Journal of Operational Research
Volume 290, Issue 2, 16 April 2021, Pages 405-421

Invited Review

Machine learning for combinatorial optimization: A methodological tour d'horizon

Yoshua Bengio [c b], Andrea Lodi [a b], Antoine Prouvost [a b]

Three integrations have been identified in this survey

(1) End-to-end learning

(2) Learning to configure algorithms

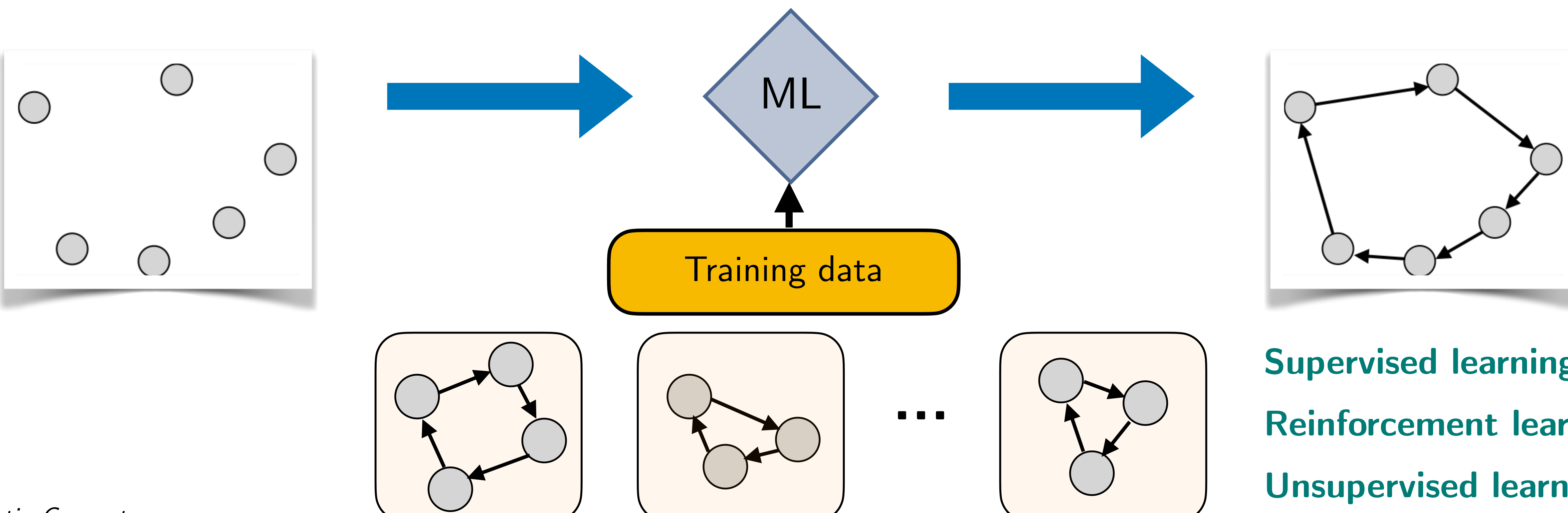
(3) Machine learning within combinatorial solvers

Examples for each of them were proposed this week :-)

Related fields: learning to model & tackling uncertainty (predict-and-optimize, constraint acquisition, etc.)

End-to-end learning

Idea: the problem is directly solved using machine learning



Supervised learning

Reinforcement learning

Unsupervised learning

Limitation of end-to-end learning

Fundamental limitation

paperswithcode.com/sota/
image-classification-on-mnist

Machine learning: set of tools dedicated to predict an output

Observation: machine learning can make mistakes! (100% accuracy is not achievable on test set)

Even in a very simple dataset (MNIST - standard dataset in ML)

Best accuracy reported: 99.87%

Difficulty: it can be an important bottleneck for combinatorial optimization!

Reason: we do not want solutions that are infeasible (or to lose optimality)

Challenge: how to handle arbitrary combinatorial constraints?

Related works on end-to-end learning (and analyses)

Learning combinatorial optimization algorithms over graphs [Khalil et al., NeurIPS-2017]

Neural combinatorial optimization with reinforcement learning [Bello et al., Arxived-2016]

Reinforcement Learning for solving the vehicle routing problem [Nazari et al., NeurIPS-2018]

Attention, learn to solve routing problems! [Kool et al., ICLR-2019]

Learning a SAT solver from single-bit supervision [Selsam et al., ICLR-2019]

End-to-end constrained Optimization learning: A survey [Kotary et al., IJCAI-2021]

Learning the TSP requires rethinking generalization [Joshi et al., Constraints-2022]

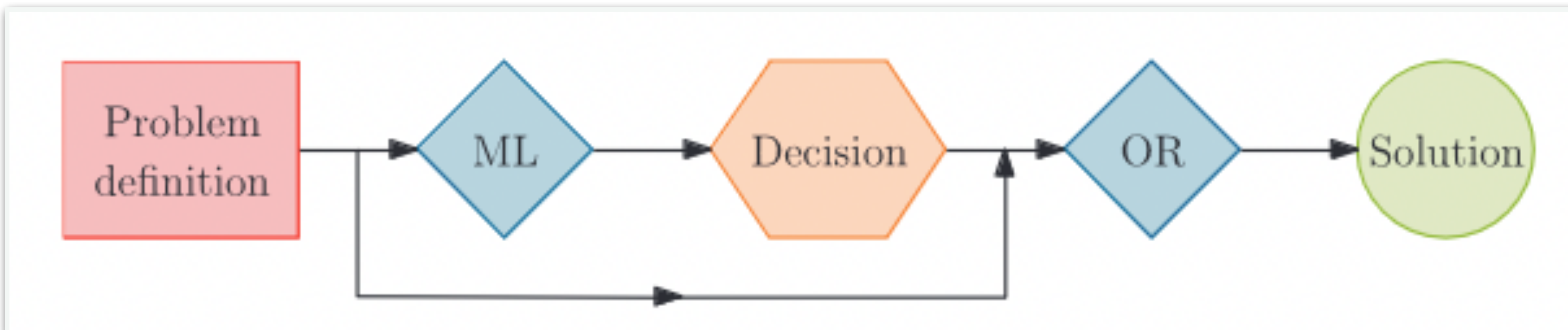
Ferdinando Fioretto
Syracuse University

End-to-end Constrained Optimization Learning

And many more!

Learning to configure algorithms

Learning to configure algorithms



Idea: machine learning is used to augment a solver with valuable information

Exemple 1: selecting appropriate parameters for the solver (e.g., CPLEX has more than 70 parameters)

Exemple 2: selecting a specific configuration (e.g., simplex or interior-point method for a linear relaxation)

Exemple 3: deciding if a pre-processing step must be carried out before calling the solver

Related names: algorithm configuration, automated tuning, portfolio selector

Comment: these approaches are often complementary with other learning approaches

Related works

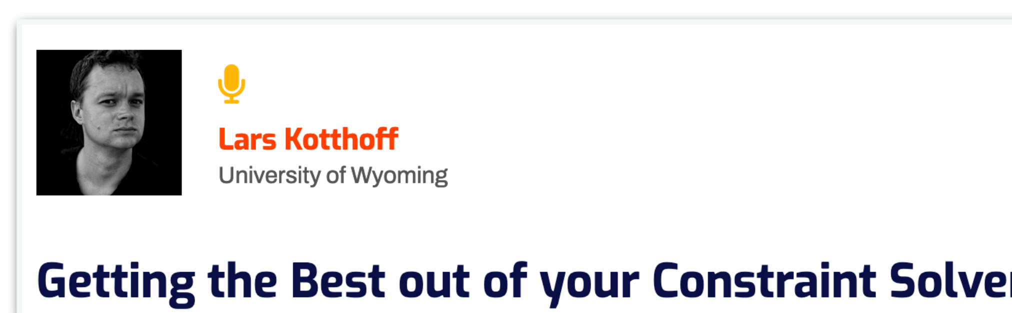
Sequential Model-Based Optimization for General Algorithm Configuration [Hutter et al., LION-2011]

The irace package: Iterated racing for automatic algorithm configuration [Lopez-Ibanez et al., ORP-2016]

Algorithm Selection for Combinatorial Search Problems: A Survey [Kotthoff, 2016]

Learning to schedule heuristics in branch and bound [Chmiela et al., NeurIPS-2021]

Automated dynamic algorithm configuration [Adriaensen et al., JAIR-2022]



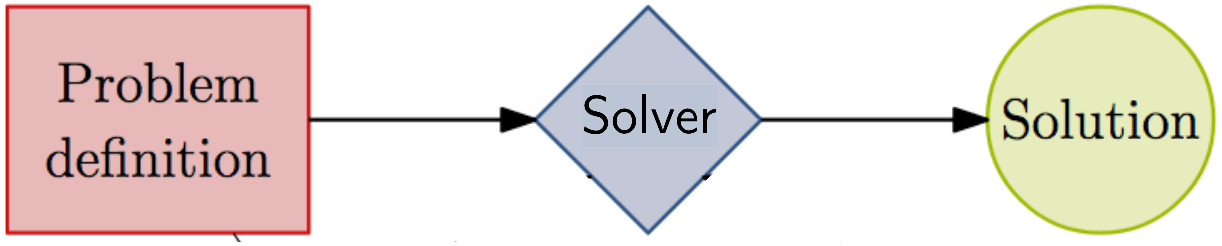
Machine learning alongside combinatorial solvers

Machine learning alongside combinatorial solvers

Traditional solver: can provide guarantee, but sometimes hard to make it efficient

Only learning: struggle to get guarantees, but easier to use (once trained)

Idea: use machine learning to speed-up the solving process inside the solver



Exemples: learning branching decisions or optimization bounds

Learning to search in branch and bound algorithms [He et al., 2014, NeurIPS]

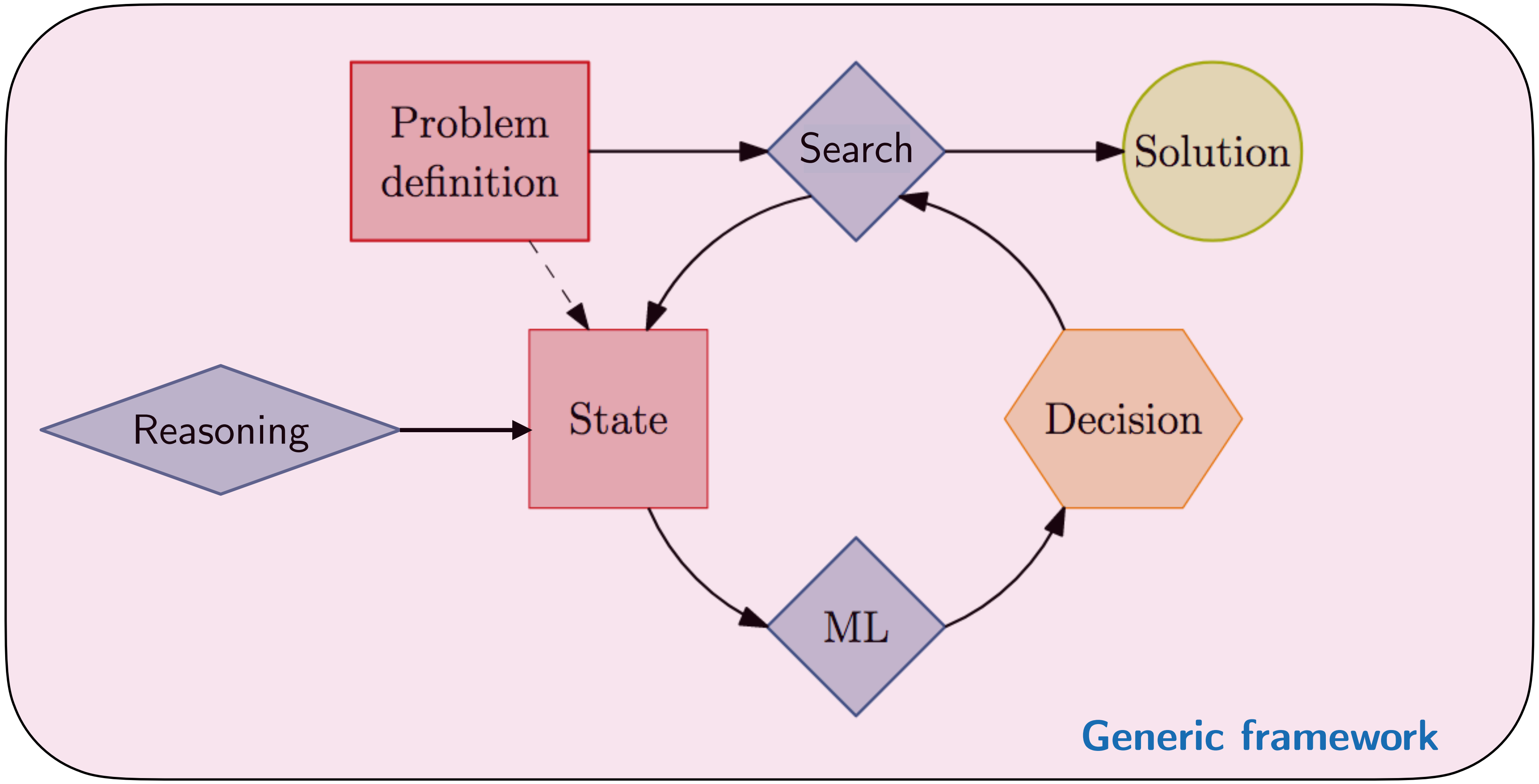
Learning to branch in mixed integer programming [Khalil et al., 2016, AAAI]

Exact combinatorial optimization with graph convolutional neural networks [Gasse et al., 2019, NeurIPS]

Improving variable orderings of approximate decisions diagrams using reinforcement learning [Cappart et al., 2022, IJOC]

Towards a multimodal artificial intelligence

? Can we integrate other aspects of artificial intelligence ?



Search: intelligence by intuition (heuristic with trials-and-errors)

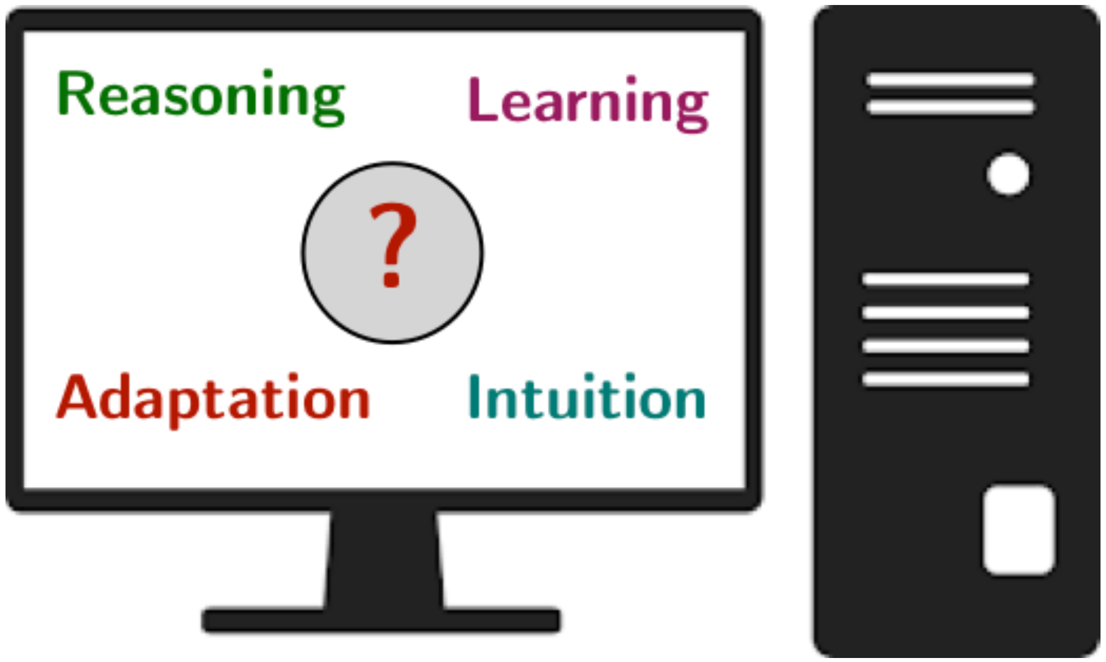
Machine learning: intelligence to learn from experiments

Reasoning: intelligence by logical reasoning

Generic: intelligence to adapt (or generalize) to new situations

Holy grail: making it easy to use (and efficient) for non-experts

Constraint programming as a unifying framework



Our research hypothesis

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

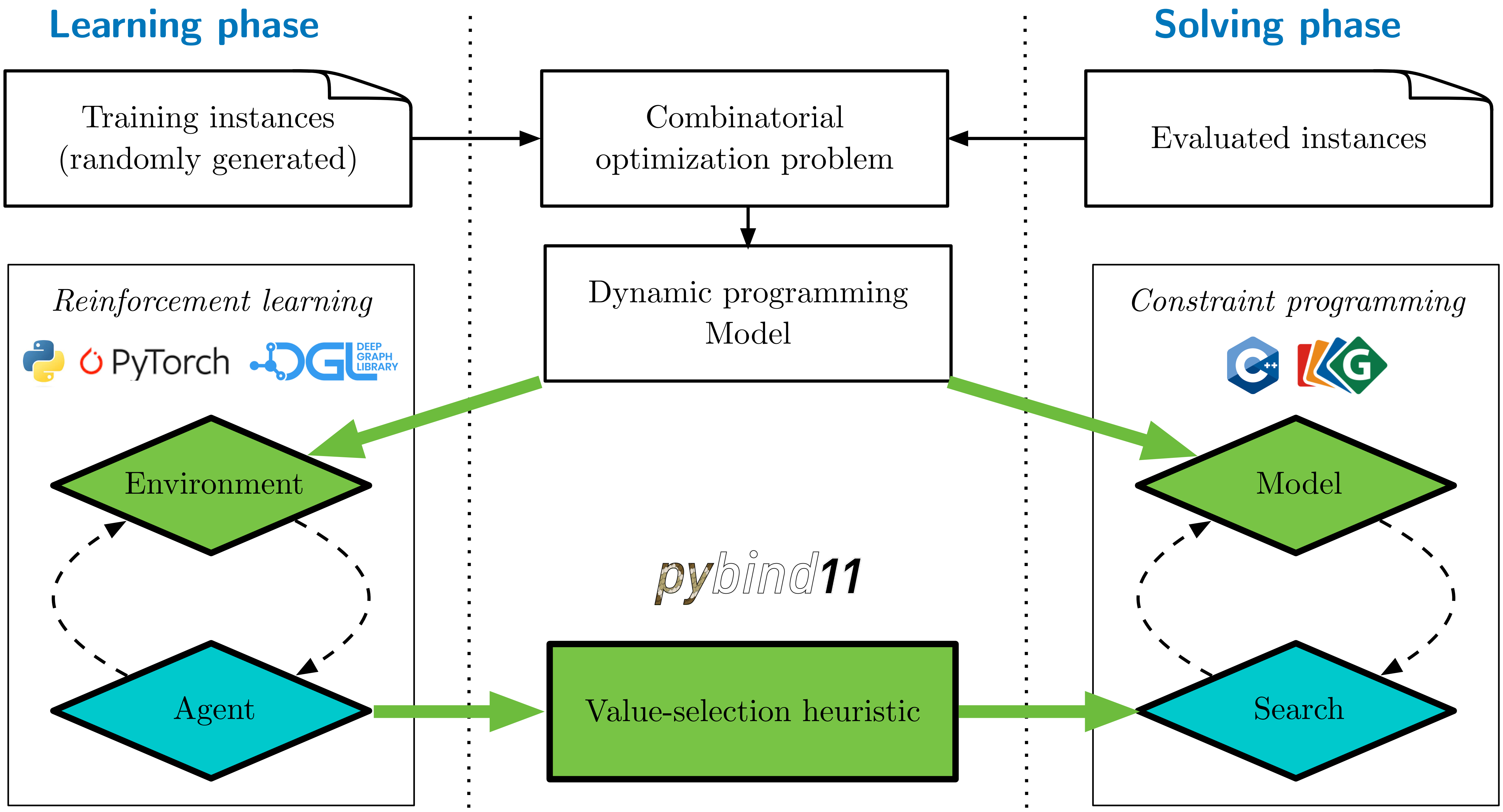
$$\text{CP} = \text{model} + \text{propagation} + \text{search}$$

Observation 1: model, propagation and search are present in most standard CP solvers

Observation 2: the *only* new part is the integration of learning

? Is it really difficult to achieve ?

A first proof of concept



Deep Q-learning (DQN)

Proximal policy optimization (PPO)

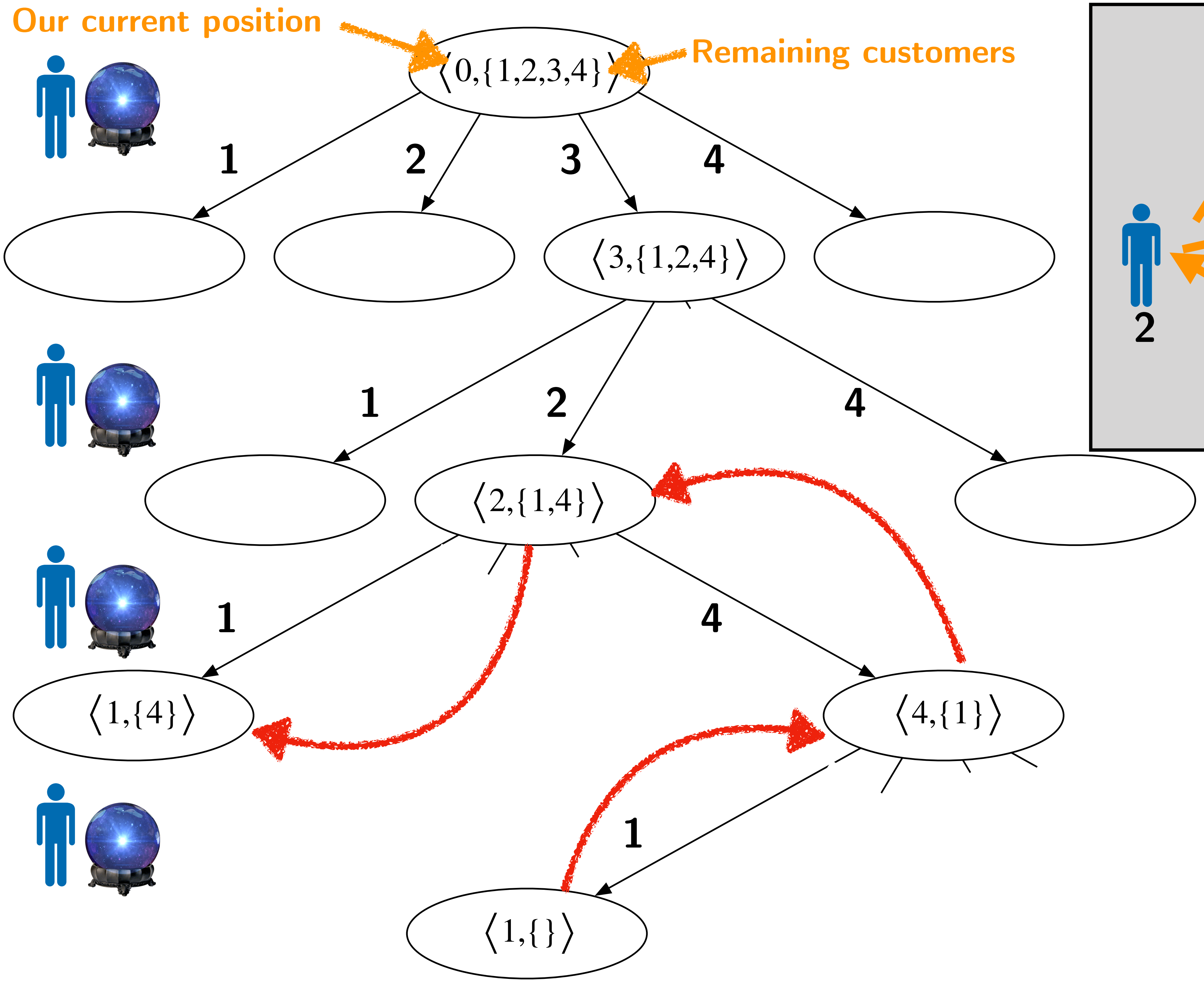
Depth-first search

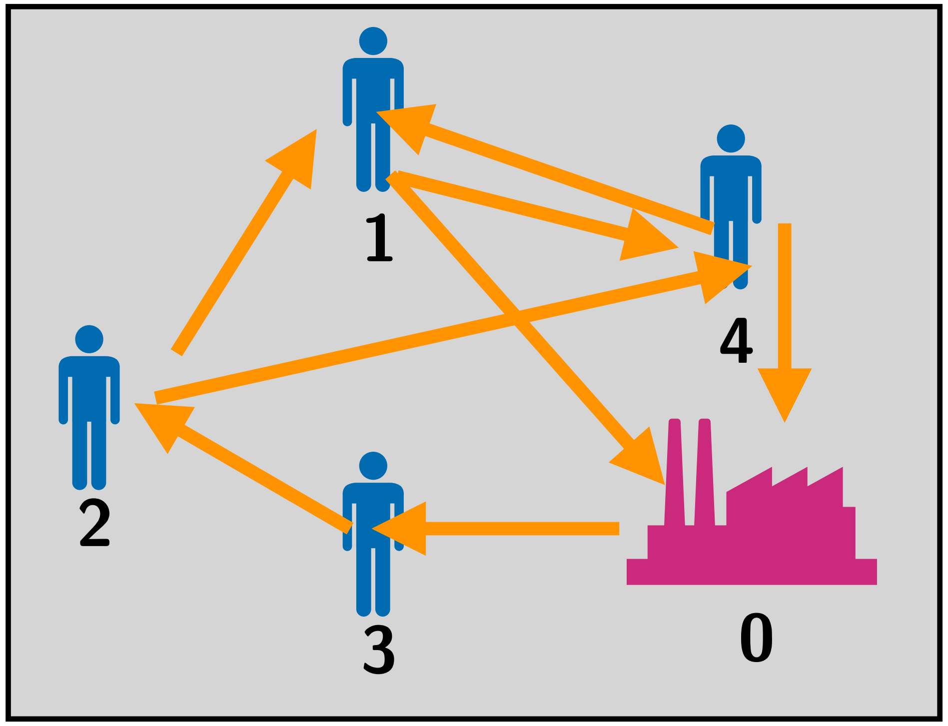
Restart-based search

Limited discrepancy search

Combining reinforcement learning and constraint programming for combinatorial optimization [Cappart et al. 2021, AAAI]

CP search with a learned heuristic on TSP





A first proof of concept

Algorithm 1: BaB−DQN Search Procedure.

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

Build the CP model from the recursive formalization

Initialize a standard CP search

Encode the current solving stage into an RL state

Use caching if the prediction was already done

Branch on the value predicted by the trained model

? Ok! It seems to be a good idea, but does it work ?

Additional improvement: caching to avoid unnecessary call to the trained model

Additional improvement: leveraging dominance to prune the search space (redundant constraints)

Good news: signals of learning were observed and good branching decisions could be obtained

Main assumption: we need to cast the combinatorial problem into a dynamic program

Limitation: learning is disconnected with the CP solver (loss of relevant information - e.g., propagation)

Difficulty: we need to build a specific model for each problem (e.g., a neural network)

Difficulty: loss of performances with the back-and-forth between C++ and python

Motivation a new CP solver

? There are a lot of drawbacks! Can we do something ?

Idea: embed the learning directly inside the CP solver

Difficulty: there is no available solver allowing us to do that easily (and efficiently)

Reason: friction between the need of an efficient language, and the ML support mostly available in Python

Technical contribution

Introducing and building a new CP solver, making easy to integrate learning inside

? Ok! but which programming language do you plan to consider ?

julia

(1) Simple to get on-board, yet fast and clean

(2) Active community in optimization and machine learning

(3) Quite young language (both a benefit and a drawback)

(4) No CP solver available (excepting one that seems no longer developed)

Moto of Julia: « *Looks like Python... runs like C* »

SeaPearl (Cee-Pee-Air-El) - CP with RL

SeaPearl.jl

CP = model + propagation + search + learning

Philosophy: minimalist CP solver dedicated to ease the integration of learning

Open-source project, available on Github (still under active development)

Solver: https://github.com/corail-research/SeaPearl.jl

Zoo of models: https://github.com/corail-research/SeaPearlZoo.jl

Next topics in this talk

(1) Describing the architecture behind SeaPearl

(2) Presenting few experiments on its performance

(3) Identifying current challenges and possible future research directions in this field

We have a lot of research ideas if you would like to contribute :-)

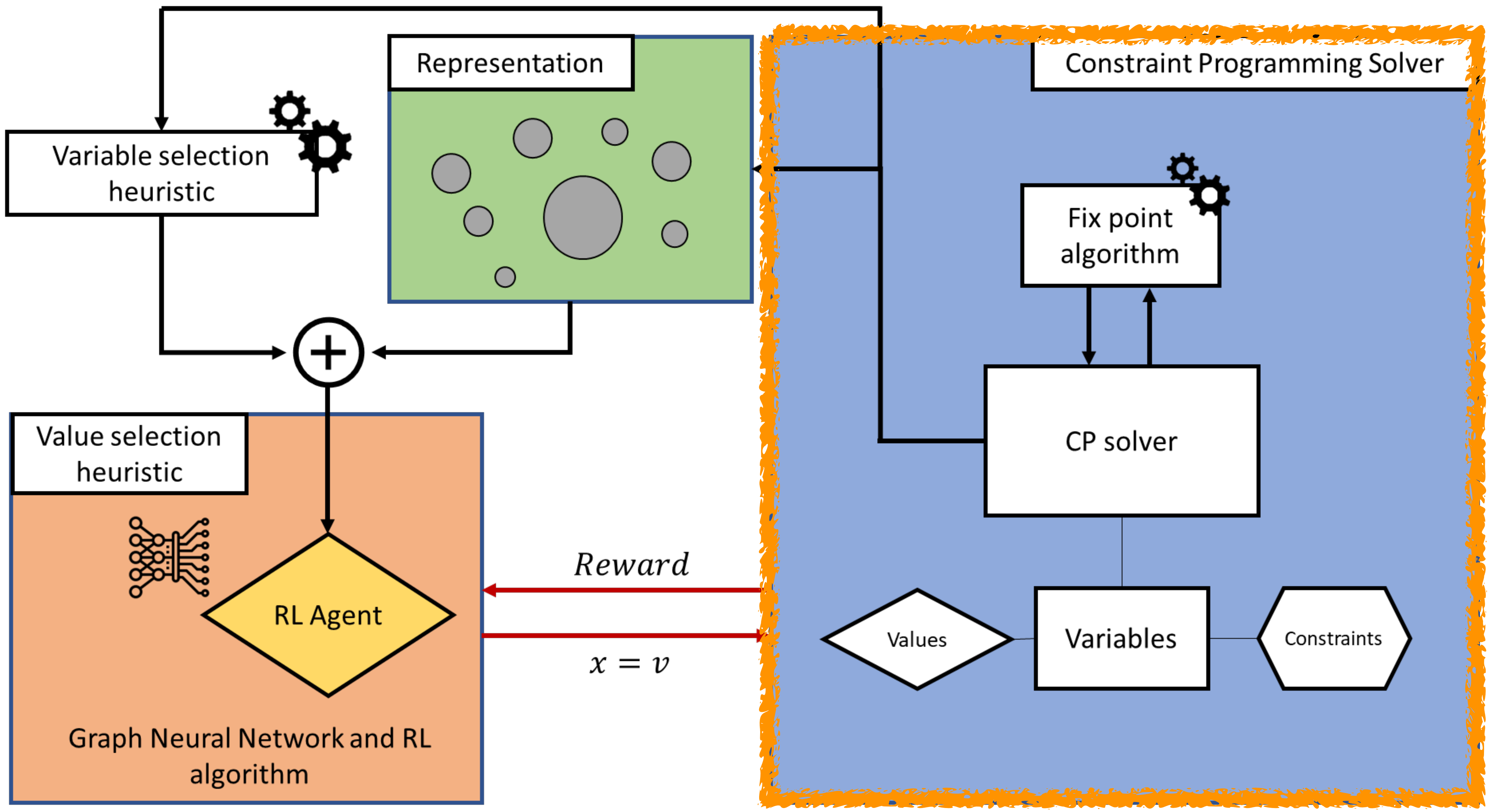
Lab session: a tutorial has been prepared in order to build a first CP model and train a model inside it

Hackathon: give you the opportunity to try other design choices

Seapearl: A constraint programming solver guided by reinforcement learning [Chalumeau, Coulon, Cappart and Rousseau, 2021, CPAIOR]

Learning a generic value-selection heuristic inside a constraint programming solver [Marty, Cappart et al., to appear at CP 2023]

Architecture behind SeaPearl



Main components of SeaPearl

Module 1: a constraint programming solver

Module 2: a generic representation function

Module 3: a learning agent, based on reinforcement learning and graph neural network

Constraint programming solver


Tias Guns
KU Leuven
10/07/2023
VHI 00.10 AULA GASTON EYCKENS
Welcome and Intro to Constraint Programming
Prof. Guns will welcome all to the summer school with a general motivation of why machine learning is increasingly used with constraint solving. This will be followed by an overview of the interactions between constraint solving and machine learning and how the program of the summer school highlights many of these

General characteristics

Inspiration: MiniCP solver (in Java)

Data structure: trail-based solver

Modeling: an interface with JuMP is planned

Search strategies

Search 1: depth-first search with branch-and-bound (default strategy)

Search 2: iterated limited discrepancy search (allow to leverage good heuristics)

Search 3: restart-based search (allow to leverage probabilistic heuristics)

Propagation engine

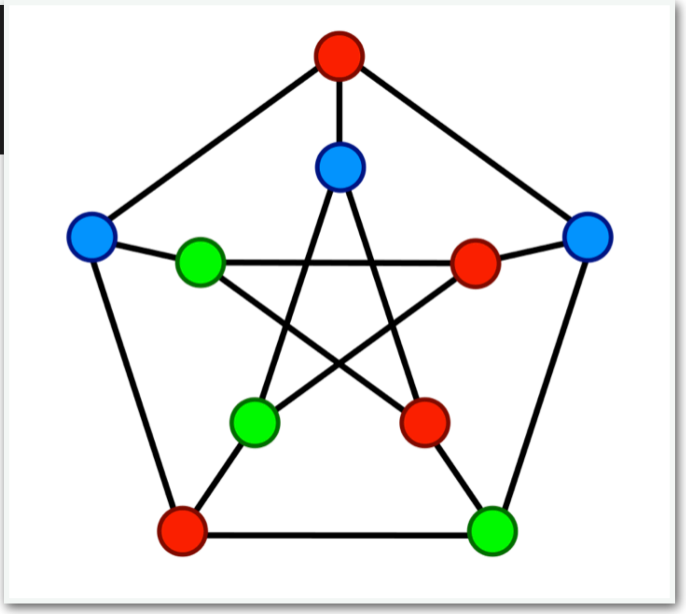
Filtering: constraint propagation at each node with fix-point execution

Constraints: intension, extension, allDifferent, sum, element (+ few others)

The solver is currently compatible for XCSP3 mini-track competition (but not the learning)

Modeling example: graph-coloring

```
trailer = SeaPearl.Trailer()
model = SeaPearl.CPModel(trailer)
```

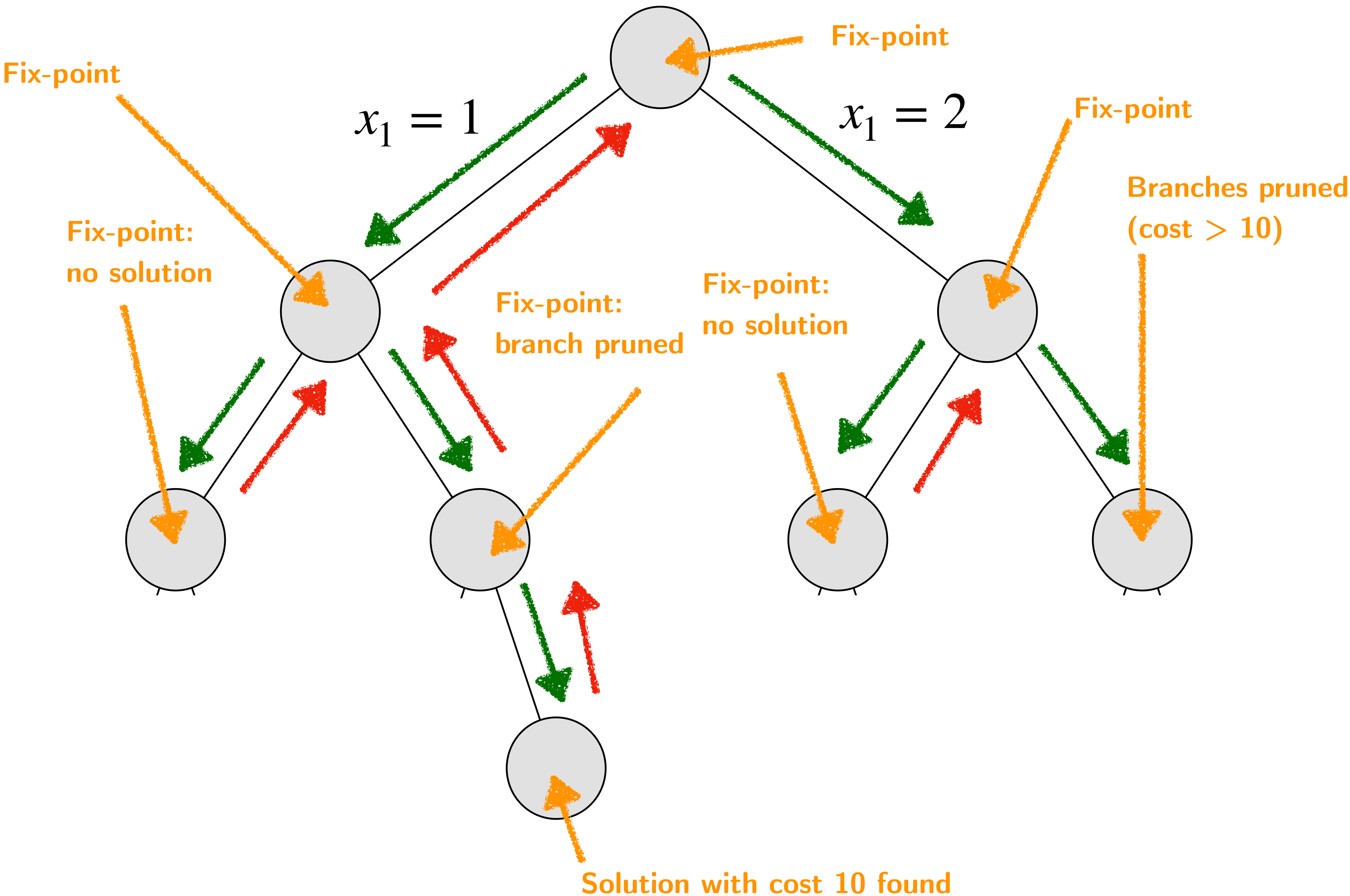


Goal: keeping the philosophy of CP and the ease in modeling

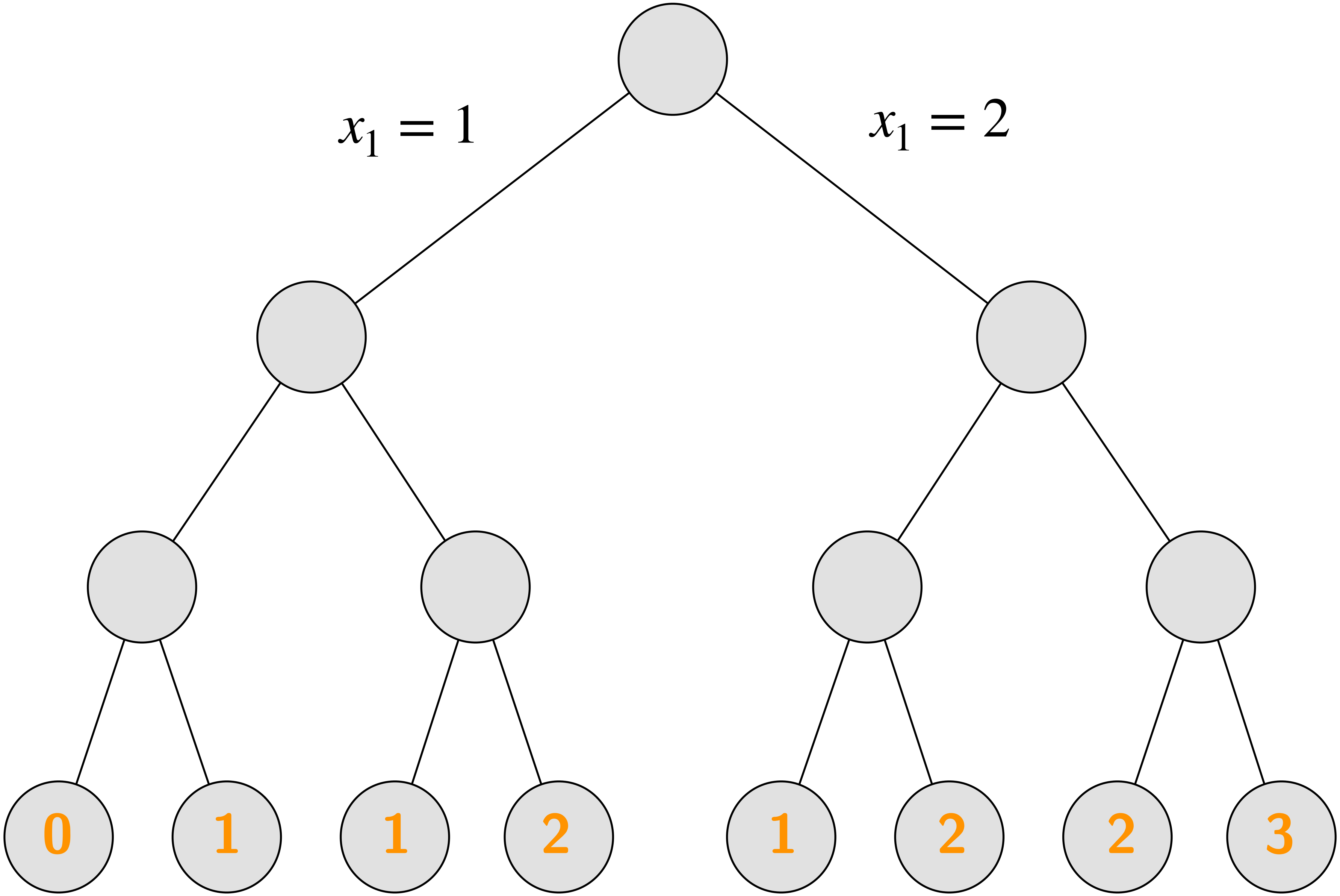
Prototyping: possible to write model directly in a jupyter notebook

https://github.com/corail-research/SeaPearlZoo.jl/blob/master/src/classic_cp/graph_coloring/graph_coloring.ipynb

Standard CP depth-first search (DFS)



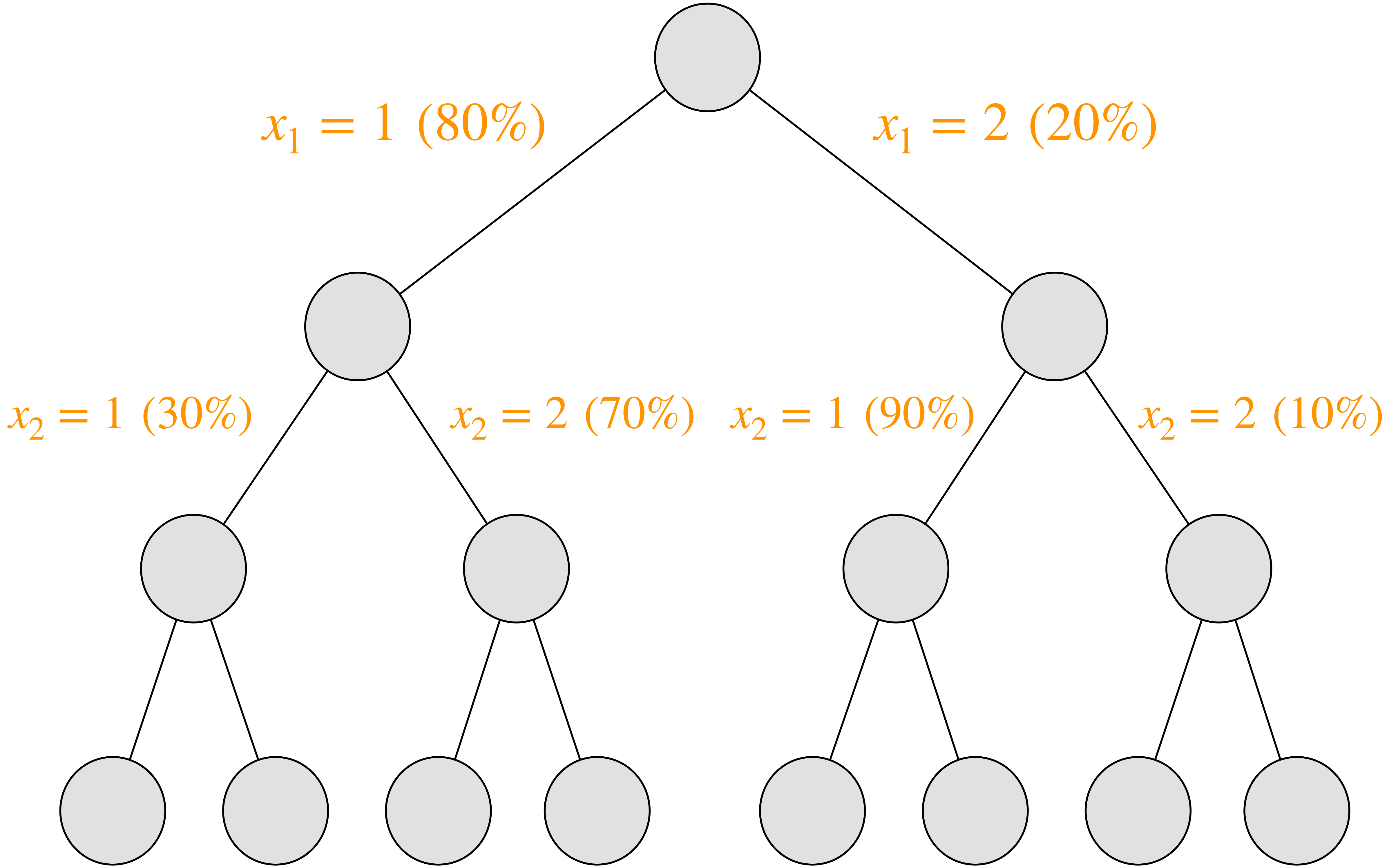
Iterated limited discrepancy search (ILDS)



Principle: explore the tree with no deviation from the left branch, then allow 1 deviation, then allow 2, etc.

Convention: the left branch is what is explored first (value recommended by the heuristic)

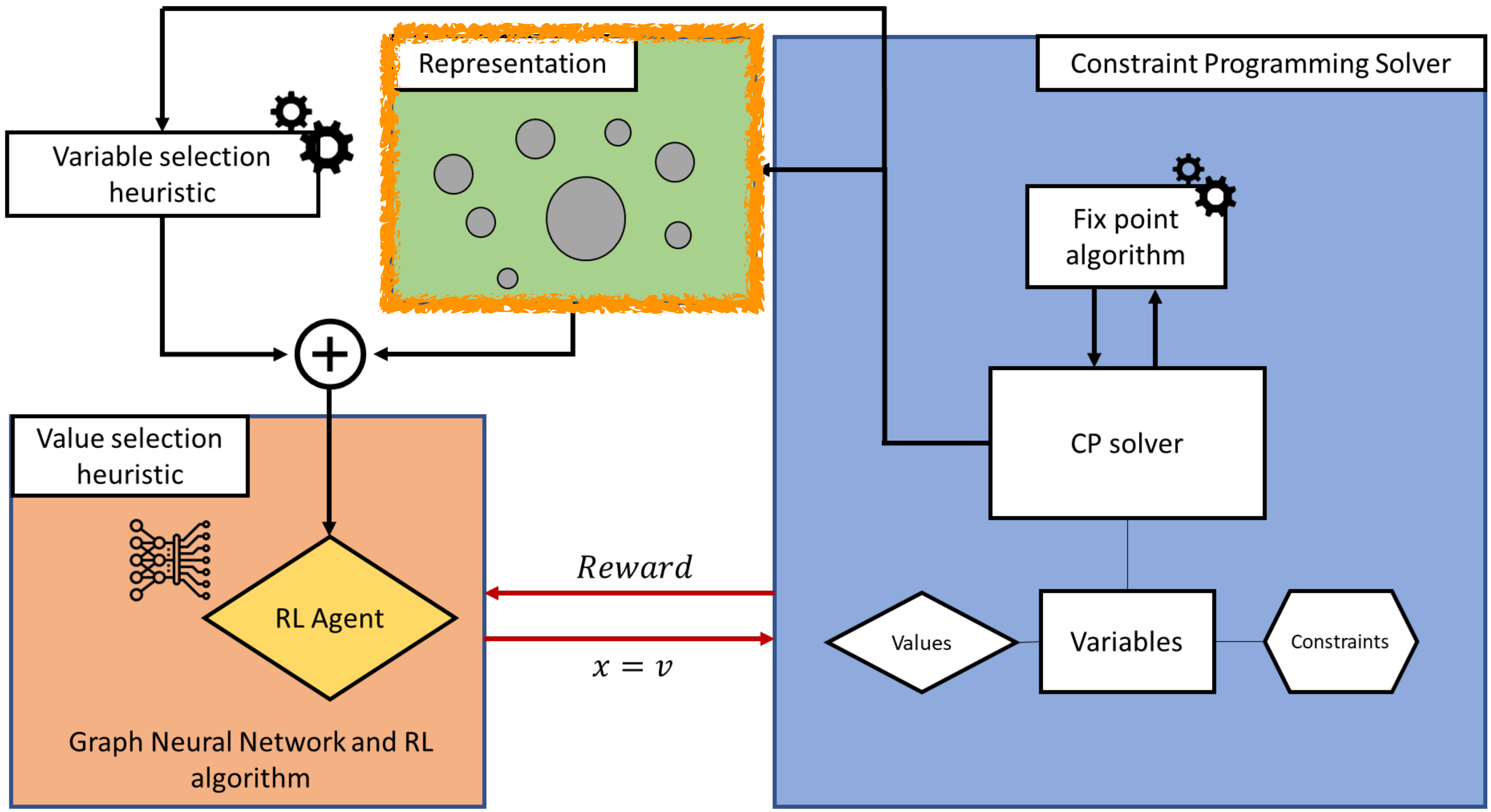
Restart-based search



Principle: follow the branch based on a weighted probability, and periodically restart

Restart schedule: Luby sequence in terms of number of failures (1, 1,2, 1,1,2,4, 1,1,2,1,1,2,4,8,...)

Architecture behind SeaPearl



Main components of SeaPearl

Module 1: a constraint programming solver

Module 2: a generic representation function

Module 3: a learning agent, based on reinforcement learning and graph neural network

Generic representation function

It is now going different than other CP solvers !

Our goal: leverage learning algorithms to speed-up the solving process (e.g., value-selection heuristic)

Observation: CP solvers can handle many combinatorial problems (routing, scheduling, assignment, etc.)

Practical use: the learning component should work for any problem given as input

Idea: build a function able to encode any combinatorial problem into a structure suited for learning

? What are the requirements of such a function ?

Requirement 1: able to encode variables with different domains

Requirement 2: able to encode any kind of constraint

Requirement 3: able to handle problems regardless of the number of variables

Requirement 4: able to handle problems regardless of the number of constraints

Requirement 5: preserving the combinatorial structure of the problem

Requirement 6: the function must be bijective (1-to-1 mapping with a CSP and the encoding)

? How can we build such a function ?

Generic representation function

Current proposition: encoding as a labeled tripartite heterogeneous graph

Heterogeneous graph: graph where the vertices and edges can have a different meaning

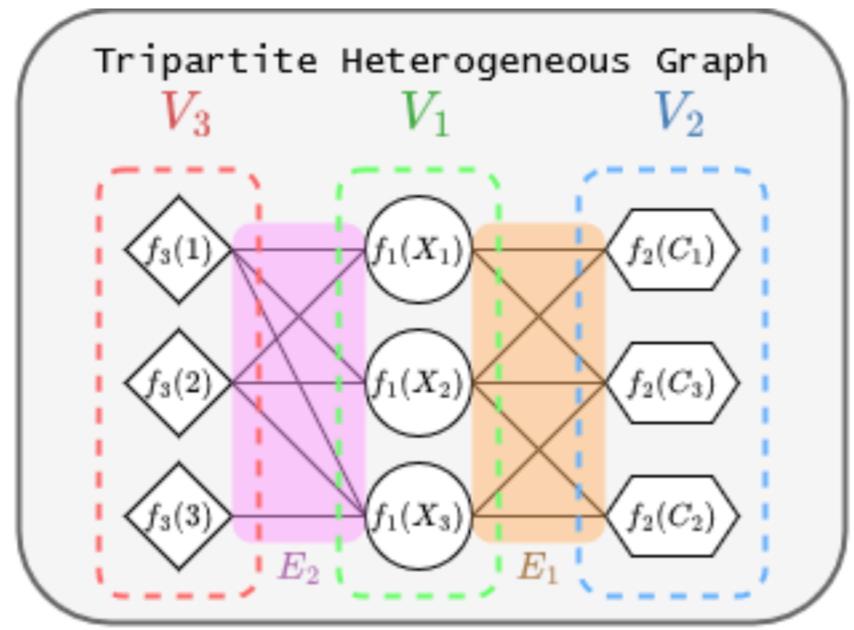
Tripartite: there are three kinds of vertices

Labeled: each vertex is decorated with additional information (i.e., features)

$X_1 \in \{1,2\},\ X_2 \in \{1,2\},\ X_3 \in \{1,2,3\}$

- $C_1 = X_1 \leq X_2$
- $C_2 = X_2 \leq X_3$
- $C_3 = AllDifferent(X_1, X_2, X_3)$

Encoding function



(1) One vertex per variable

(2) One vertex per constraint

(3) One vertex per value

(4) One edge if a variable is involved in a constraint

(5) One edge if a value is on the domain of a variable

V_1 : set of vertices for variables

V_2 : set of vertices for constraints

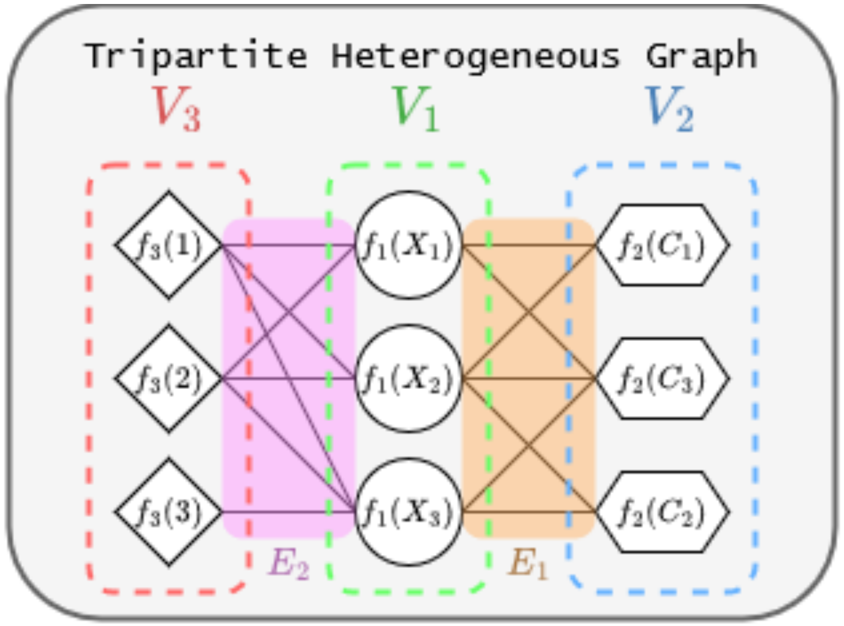
V_3 : set of vertices for values

E_1 : set of variable/constraint edges

E_2 : set of value/variable edges

Generic representation function

? What about the features on vertices ?



Features for variables

(1) Current domain size (integer)

(2) Initial domain size (integer)

(3) Is already assigned (binary)

(4) Is the objective to optimize (binary)

Features for constraints

(1) Constraint type (one-hot)

(2) Has reduced domains with propagation (integer)

Features for values

(1) Its numerical value (integer)

Conclusion

Goal: encoding any combinatorial problem in a generic way

Inspiration: bipartite encoding proposed by Gasse et al. for MIP

Extension: other information can be easily added as new features

Disclaimer: this representation is not perfect and has some drawbacks (discussed later)

V_1 : set of vertices for variables

V_2 : set of vertices for constraints

V_3 : set of vertices for values

E_1 : set of variable/constraint edges

E_2 : set of value/variable edges

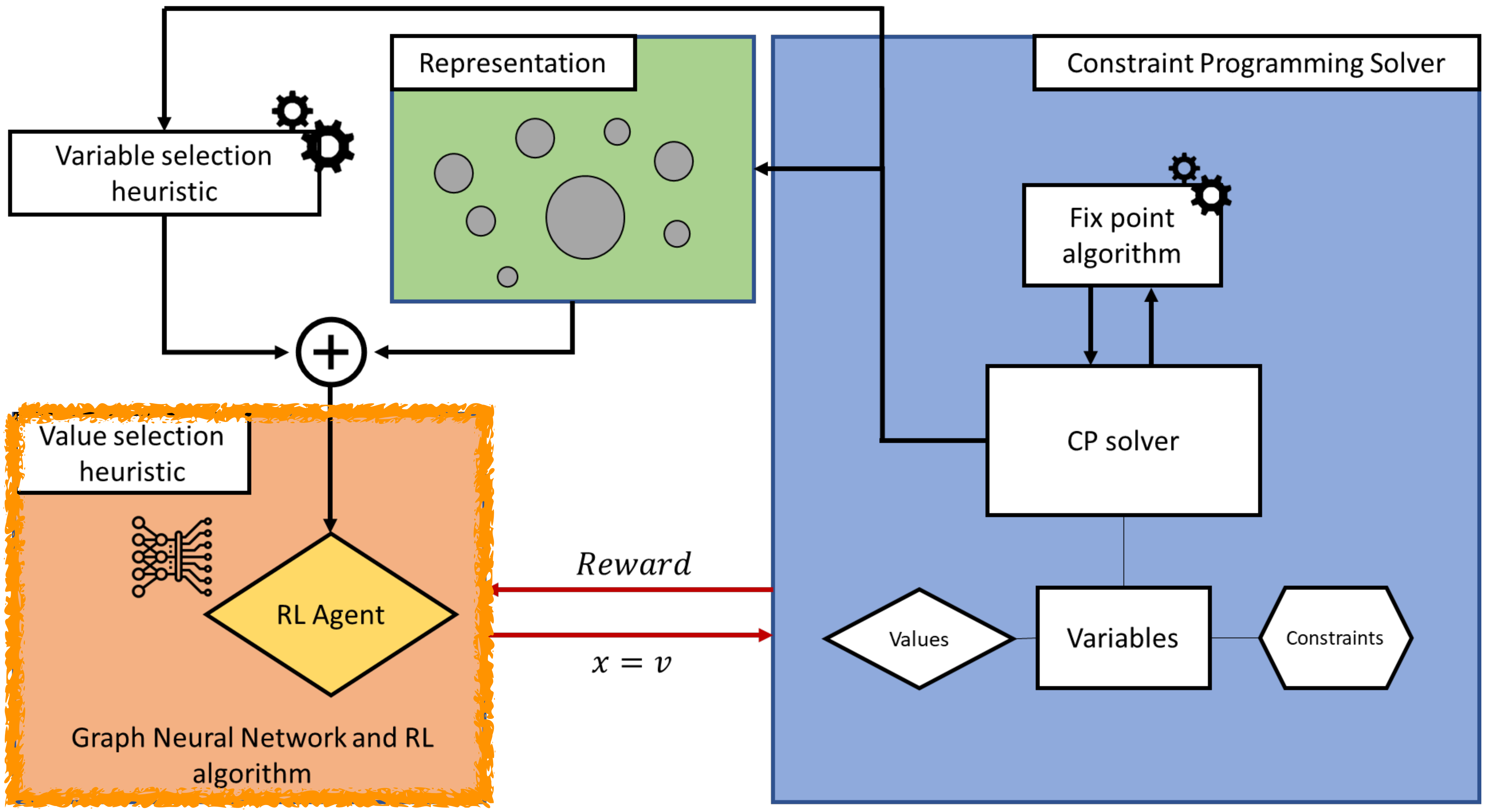
f_1 : features for variables

f_2 : features for constraints

f_3 : features for values

Exact combinatorial optimization with graph convolutional neural networks [Gasse et al., 2019, NeurIPS]

Architecture behind SeaPearl



Main components of SeaPearl

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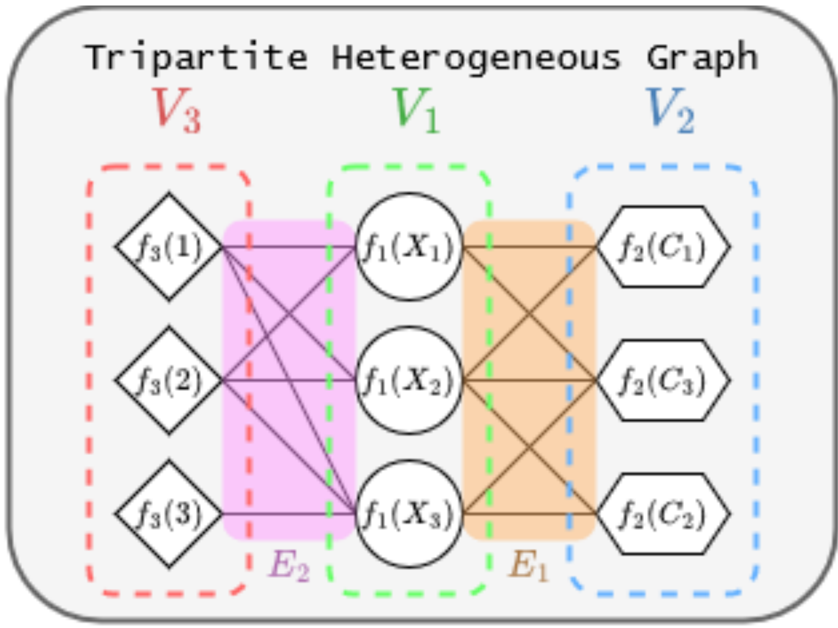
Learning a value-selection heuristic

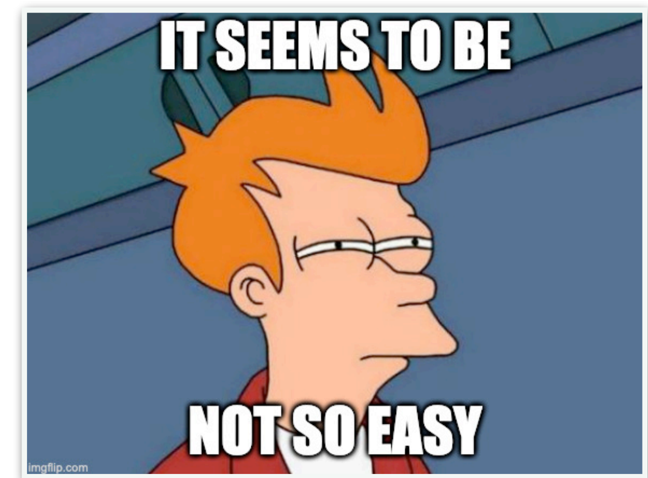


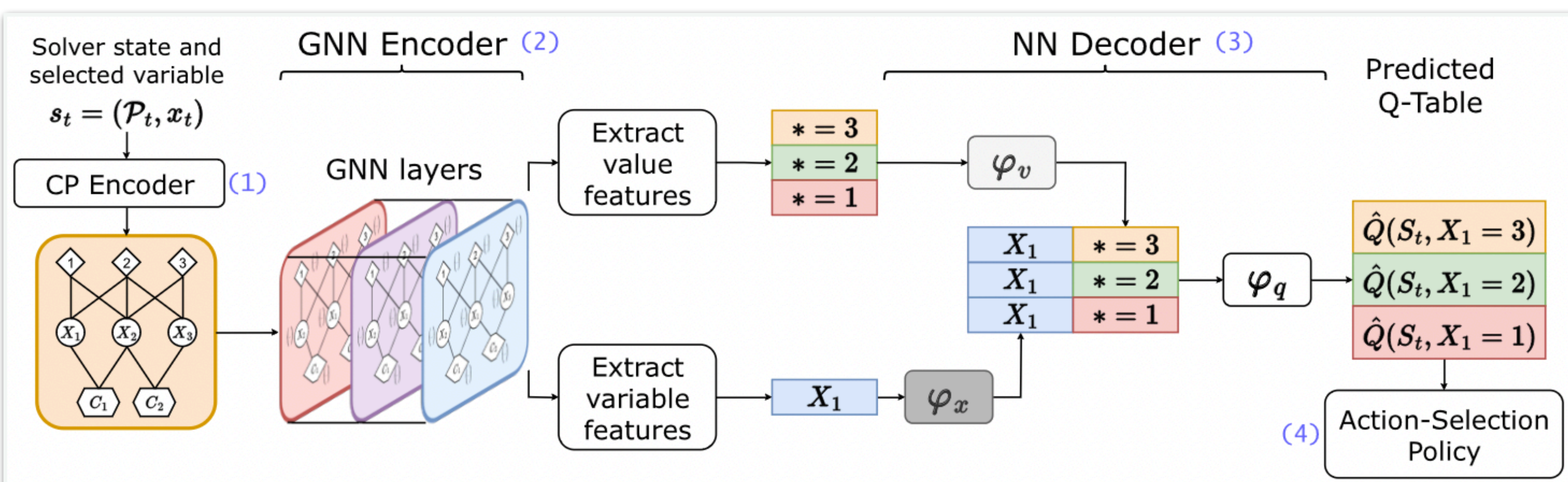
Branching on x1 **(e.g., first-fail)**

Trained Model

Training data

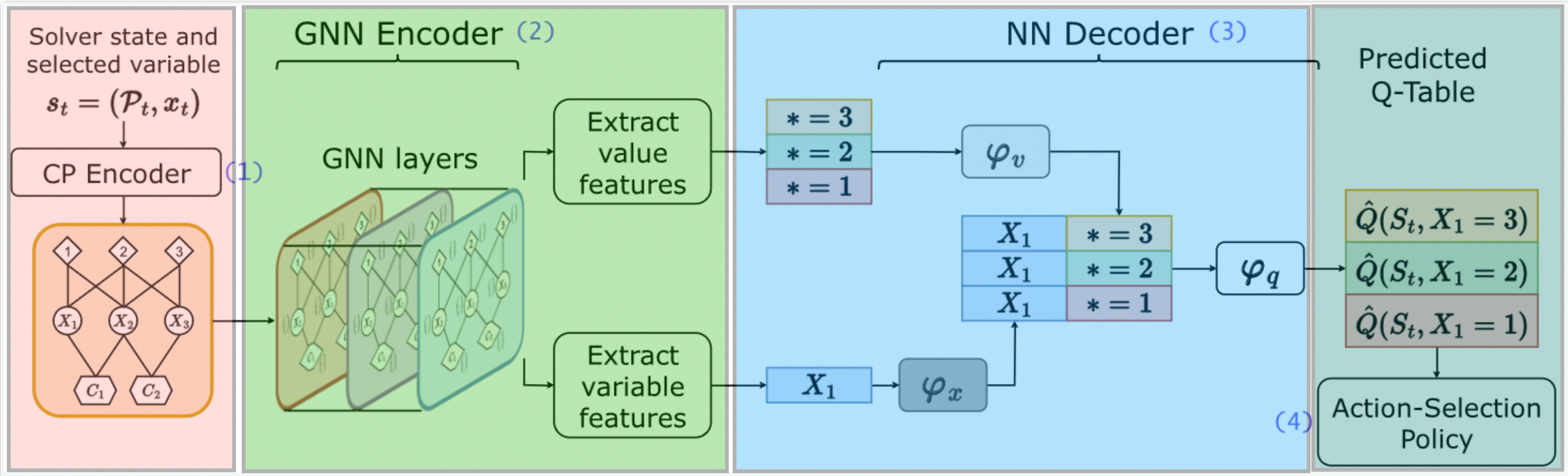
Branching on x1=2





With a training carried out by deep reinforcement learning

Learning a value-selection heuristic



Neural architecture

Step 1: encoding the current solving process as a labeled tripartite heterogeneous graph (previous slides)

Step 2: leveraging this graph thanks to a graph neural network and obtain an embedding for each node

Step 3: estimating the most promising value thanks to fully-connected neural networks

Step 4: selecting the branching value based on the estimated score of each value

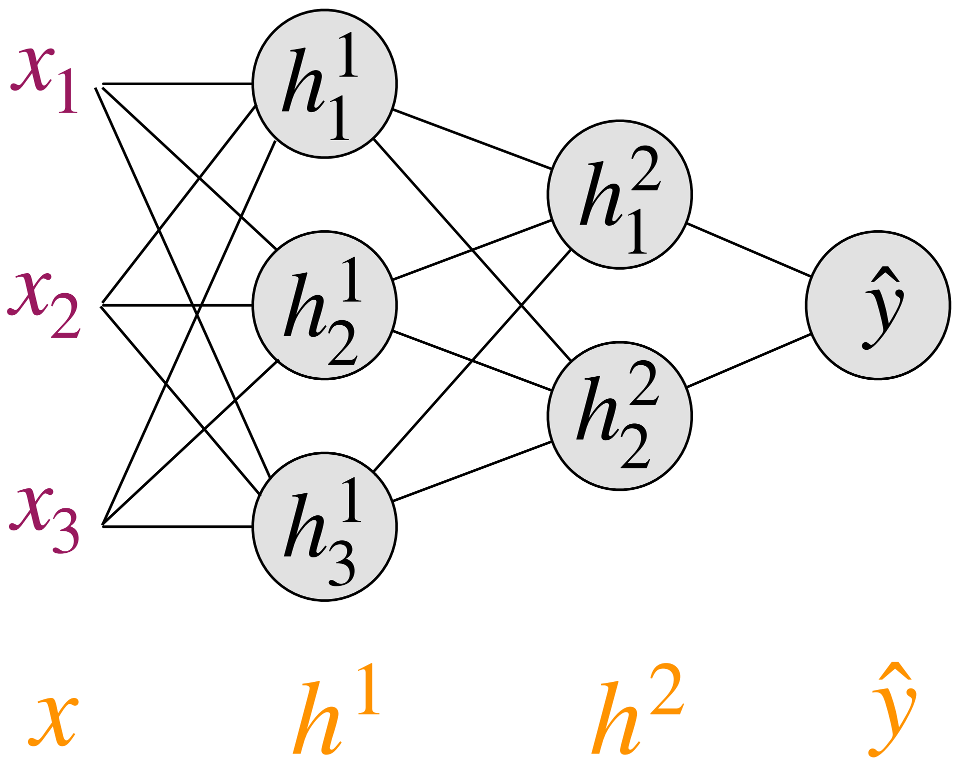
Learning algorithm

Paradigm: training based on deep reinforcement learning

Data: require historical or synthetic data (i.e., other combinatorial problems) to train the model

Benefit: there is no need to solve the historical problems a priori (can be very costly)

Primer on fully-connected neural network (FCNN)



Input: vector of features (x)

Layer 1: $h^1 = g\left(\theta^1 x + b^1\right)$

g : non-linear function (e.g., ReLU)

θ^1, b^1 : weights learned through backpropagation

Layer 2: $h^2 = g\left(\theta^2 h^1 + b^2\right)$

Layer 3: $\hat{y} = \theta^3 h^2 + b^3$

Output: real value (prediction)

Principle: each neuron computes a linear combination of the previous layer followed by a non-linearity

$$\boxed{\textbf{Fondamental equation of FCNN: } h^{k+1} = g\left(\theta^{k+1} h^k + b^{k+1}\right)}$$

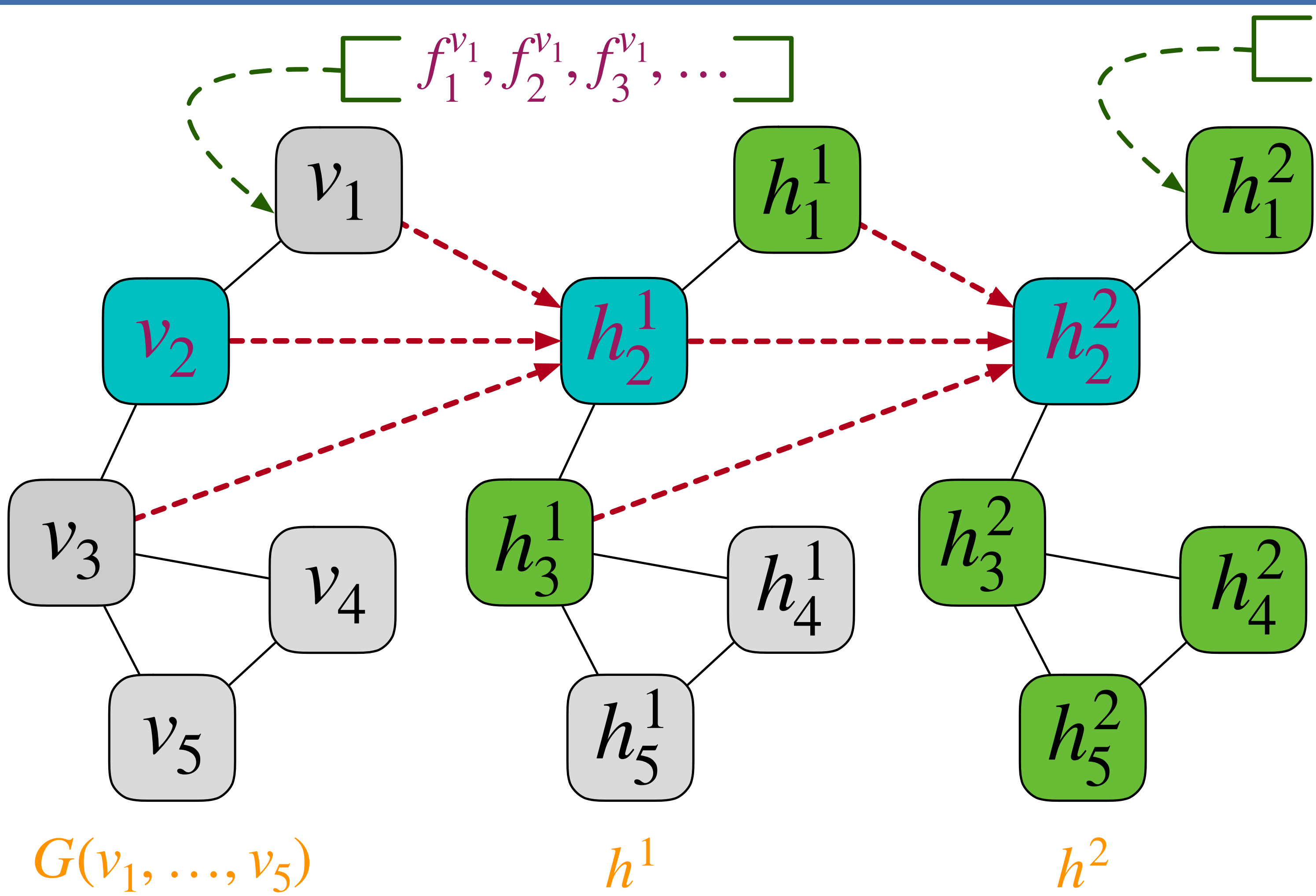
Learning aspect: trainable weights are involved at each layer

Main characteristic: the network is differentiable and can be trained by gradient descent algorithms

In practice: many variants exist (classification tasks, other activations, regularization mechanisms, etc.)

? What about graph neural networks ?

Primer on graph neural networks



Input: graph with node features (G)

Layer 1: $h_2^1 = g\big(\theta_1^1 v_2 \parallel (\theta_2^1 v_1 \oplus \theta_2^1 v_3)\big)$

$\oplus$: aggregation operation

$\parallel$: merging operation

Idem for each vertex at layer 1

Layer 2: $h_2^2 = g\big(\theta_1^2 h_2^1 \parallel (\theta_2^1 h_1^1 \oplus \theta_2^1 h_3^1)\big)$

Idem for each vertex at layer 2

Output: embedding for each node (e)

Principle: at each layer, each node aggregates information from its neighbours (message passing)

Learning aspect: trainable weights are involved at each layer (biases b have been omitted for clarity)

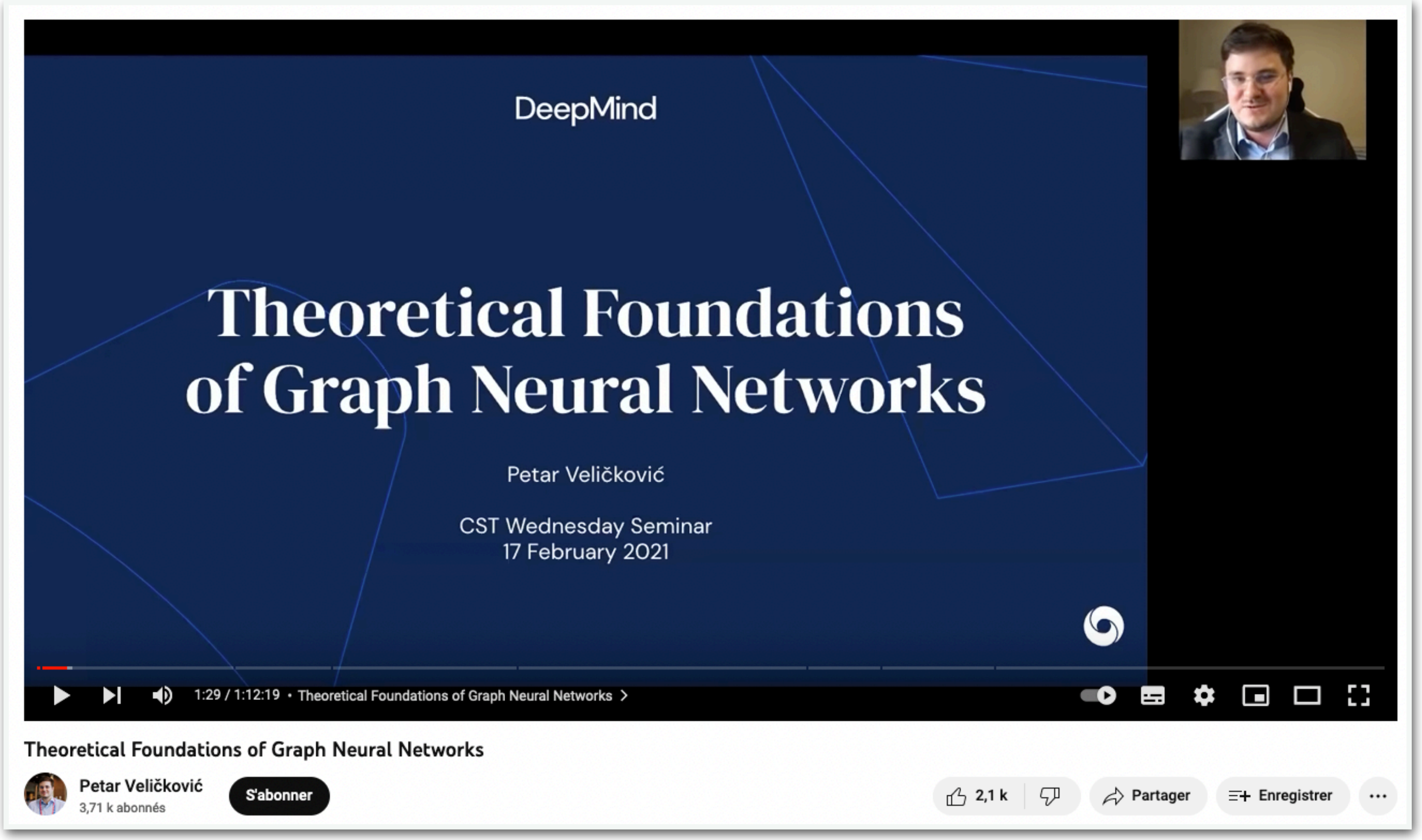
After few iterations: the nodes have information from more distant node

In practice: many architectures are existing (with attention, other aggregations, etc.)

Fondamental equation of GNNs: $h_u^{k+1} = g\Big(\theta_1^{k+1} h_u^k \parallel \bigoplus_{v \in N(u)} \theta_2^{k+1} h_v^k\Big)$

Primer on graph neural networks

? What are the benefits of graph neural networks?



Combinatorial Optimization and Reasoning with Graph Neural Networks

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Link: https://www.youtube.com/watch?v=uF53xsT7mjc

In practice: many architectures are existing (with attention, other aggregations, etc.)

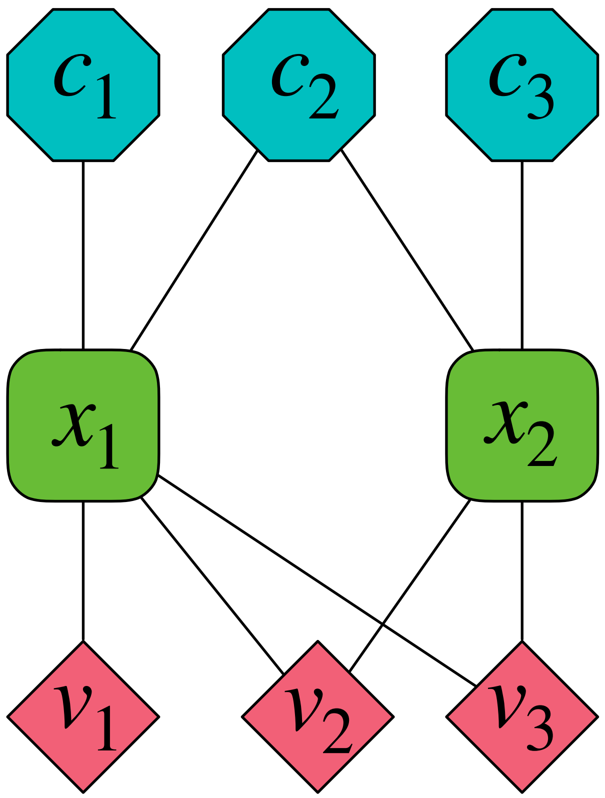
Last comment: architecture increasingly used in combinatorial optimization and worth to study

Content: survey on how GNNs can be used in combinatorial optimization and related challenges

Our GNN module

? But your graph is heterogeneous! How do you handle this?

Idea: having specific parameters for each type of nodes



Constraint nodes

Variable nodes

Value nodes

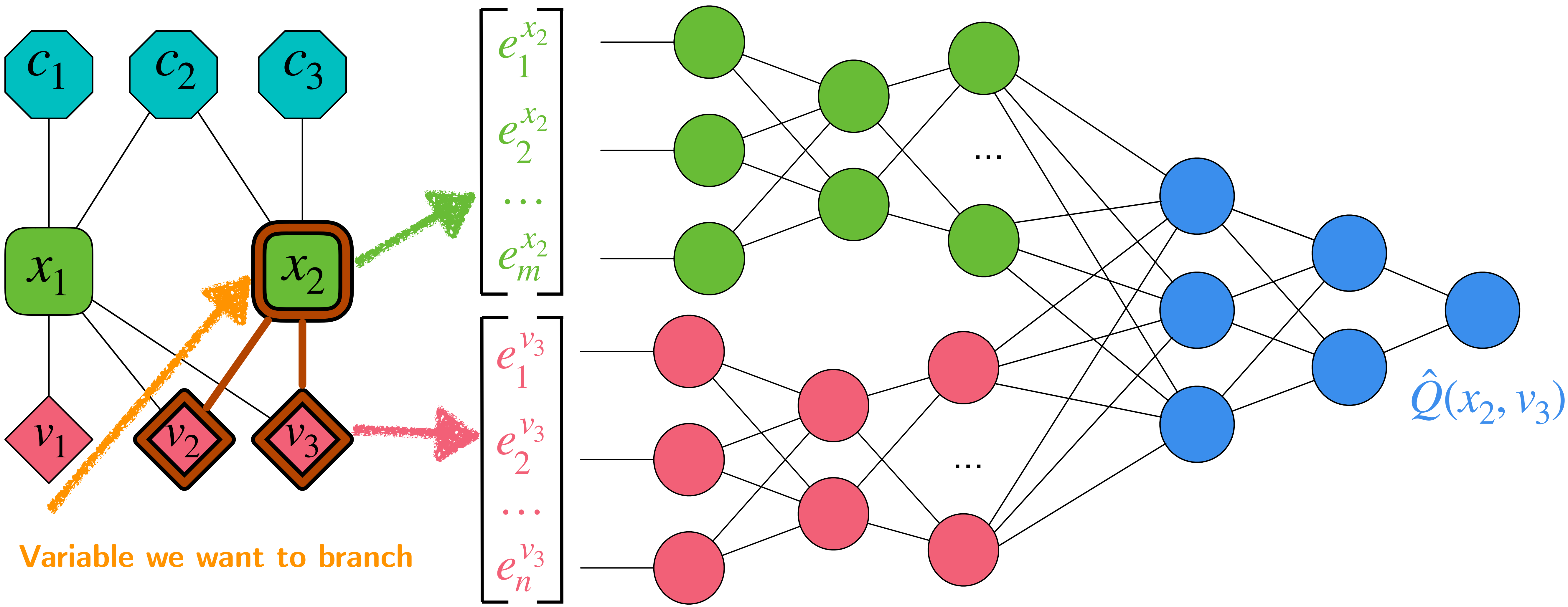
Keeping the initial features at each layer (skip connection as in ResNet)

Equation for variable nodes: $h_x^{k+1} = g\Big(\theta_1^k h_x^0 \parallel \theta_2^k h_x^k \parallel \big(\bigoplus_{c \in N_c(x)} \theta_3^k h_c^k\big) \parallel \big(\bigoplus_{v \in N_v(x)} \theta_4^k h_v^k\big)\Big)$

Equation for constraint nodes: $h_c^{k+1} = g\Big(\theta_5^k h_c^0 \parallel \theta_6^k h_c^k \parallel \big(\bigoplus_{x \in N_x(v)} \theta_7^k h_x^k\big)\Big)$

Equation for value nodes: $h_v^{k+1} = g\Big(\theta_8^k h_v^0 \parallel \theta_9^k h_v^k \parallel \big(\bigoplus_{x \in N_x(v)} \theta_{10}^k h_x^k\big)\Big)$

Our FCNN module



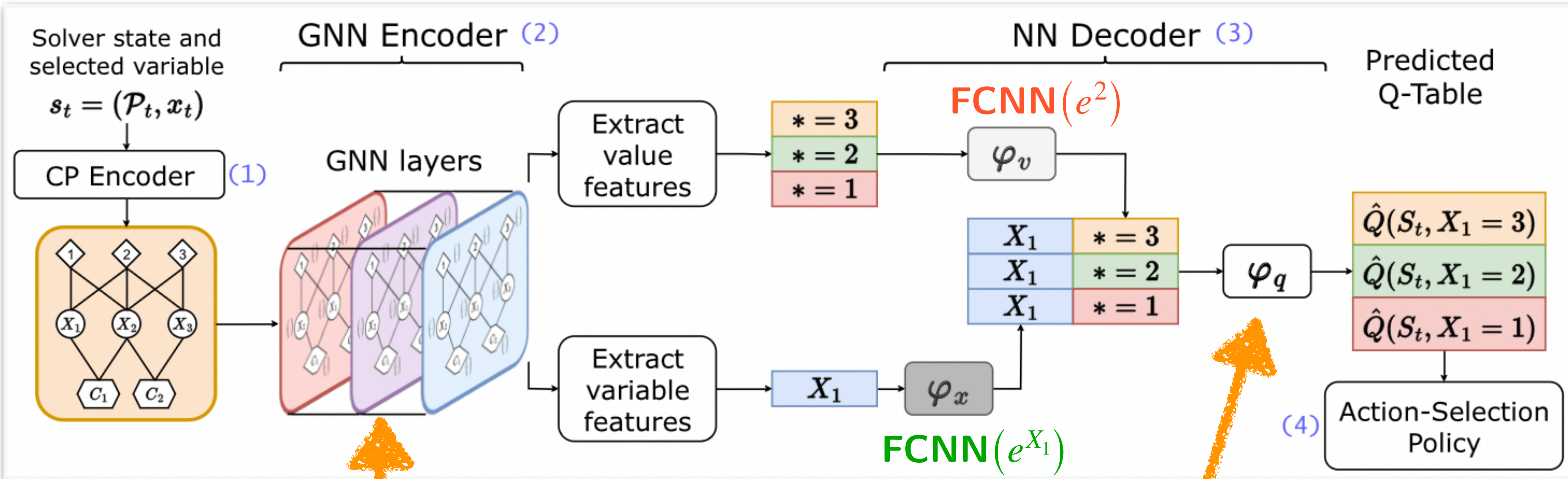
Embedding e^{x_2} : **vectorized representation of variable** x_2 **after GNN inference**

Embedding e^{v_3} : **vectorized representation of value** v_3 **after GNN inference**

$\hat{Q}(x_2, v_3)$: **prediction of how good** v_3 **is for variable** x_2 **(Q-value)**

Final inference: $\hat{Q}(x_2, v_3) = \mathrm{FCNN}\Big(\mathrm{FCNN}\big(e^{x_2}\big) \parallel \mathrm{FCNN}\big(e^{v_3}\big)\Big)$

Summary of the architecture



$$h_x^{k+1} = g\Big(\theta_1^k h_x^0 \,\|\, \theta_2^k h_x^k \,\|\big(\bigoplus_{c \in N_c(x)} \theta_3^k h_c^k\big) \,\|\big(\bigoplus_{v \in N_v(x)} \theta_4^k h_v^k\big)\Big)$$

$$h_c^{k+1} = g\Big(\theta_5^k h_c^0 \,\|\, \theta_6^k h_c^k \,\|\, \big(\bigoplus_{x \in N_x(v)} \theta_7^k h_x^k\big)\Big)$$

$$h_v^{k+1} = g\Big(\theta_8^k h_v^0 \,\|\, \theta_9^k h_v^k \,\|\, \big(\bigoplus_{x \in N_x(v)} \theta_{10}^k h_x^k\big)\Big)$$

$$\hat{Q}(X_1, 2) = \text{FCNN}\Big(\text{FCNN}(e^{X_1}) \,\|\, \text{FCNN}(e^2)\Big)$$

Branching value for x : argmax$_{v \in D(x)} \hat{Q}(x, v)$

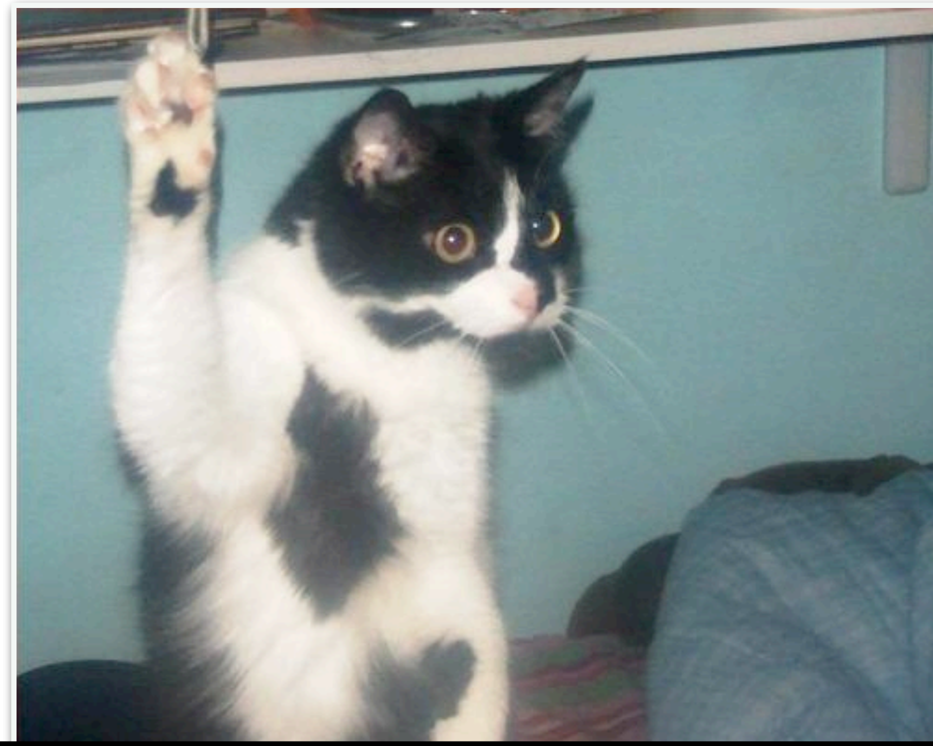
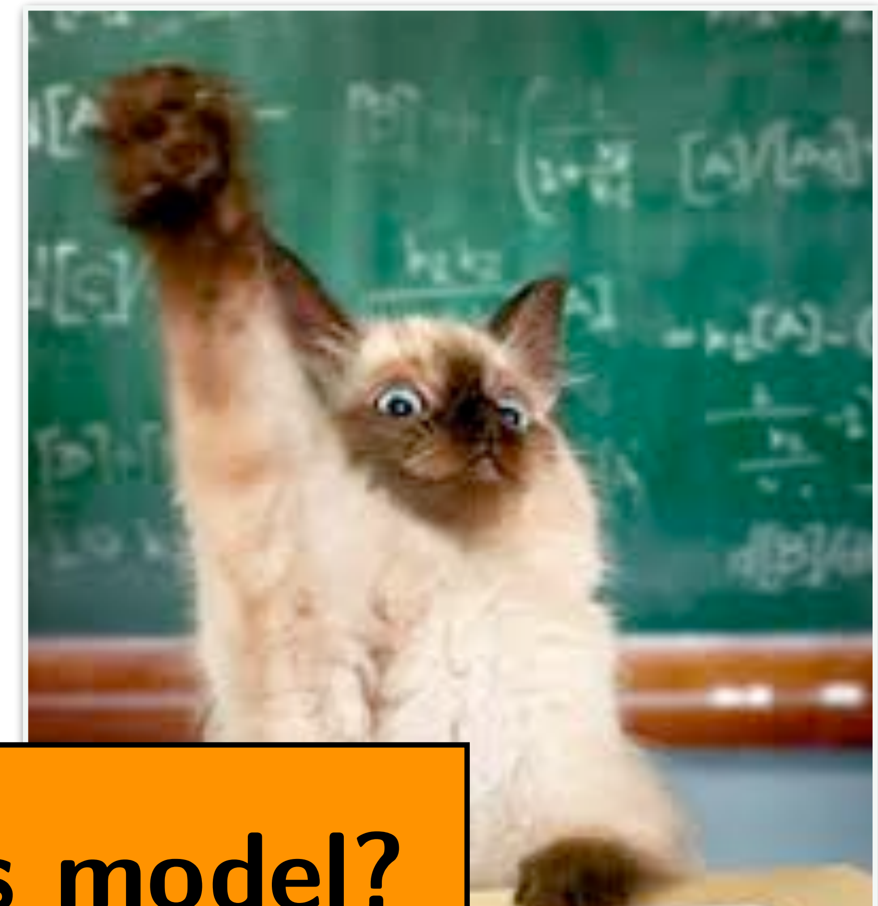
GNN step: leveraging the labeled tripartite heterogeneous graph and obtain an embedding for each node

FCNN step: estimating the most promising value thanks to fully-connected neural networks

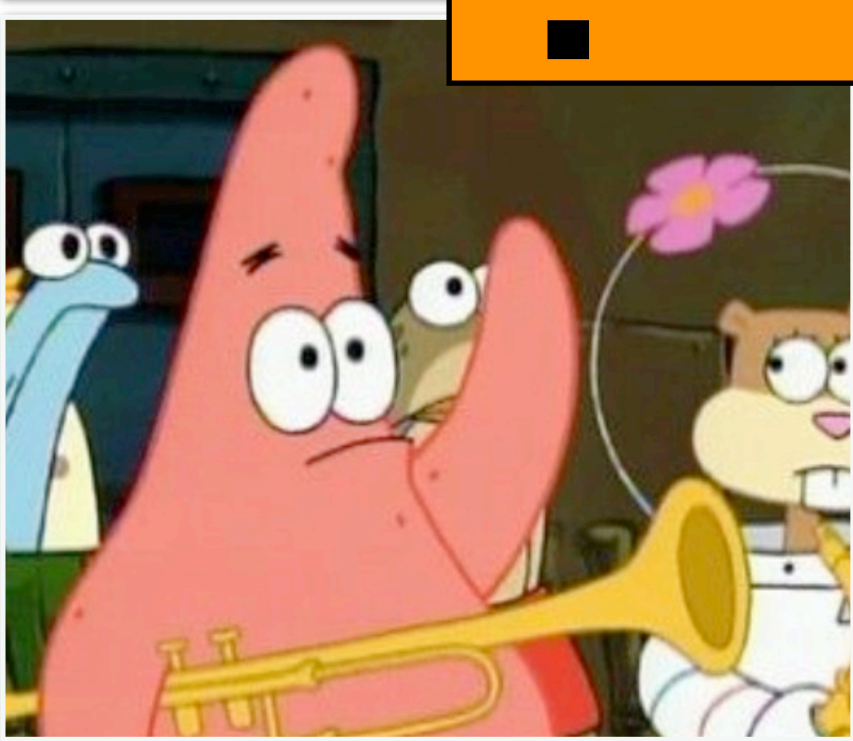
? **How do we select the final value to branch on a variable x ?**

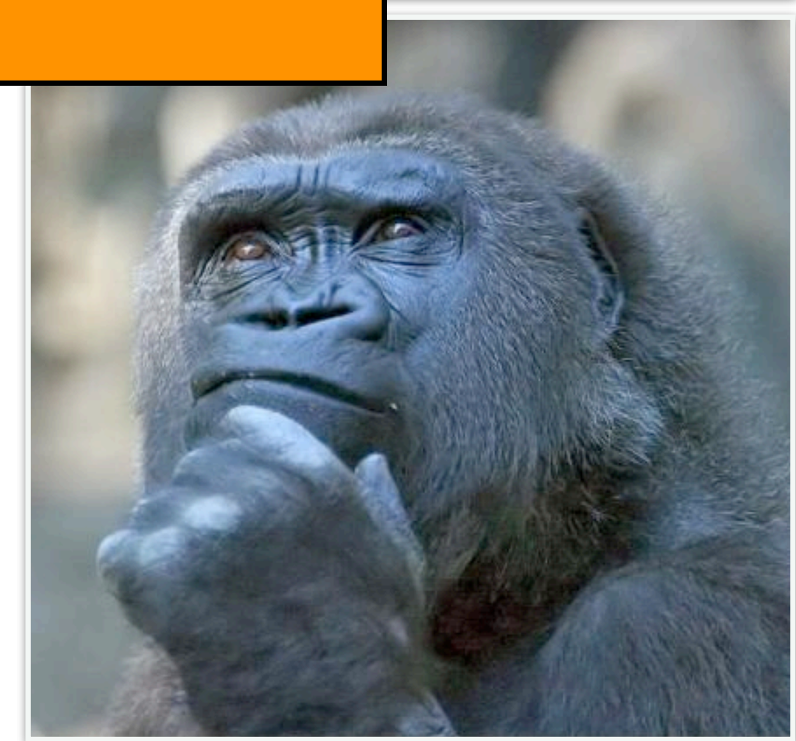
Final selection: taking the value inside the domain of x with the highest score

There is something missing...

? But how to train this model?





Learning phase

Hendrik Blockeel
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10/07/2023
VHI 00.10 AULA GASTON EYCKENS

Introduction to Machine Learning

General characteristics

Paradigm: training based on reinforcement learning

Data: require historical or synthetic data to train the model

Benefit: there is no need to solve the historical problems a priori

Training algorithm: deep Q-learning (support for proximal policy optimization -PPO- is on development)

Implementation

Reinforcement learning algorithm: based on *ReinforcementLearning.jl* package

Neural network architecture: based on *Flux.jl* package

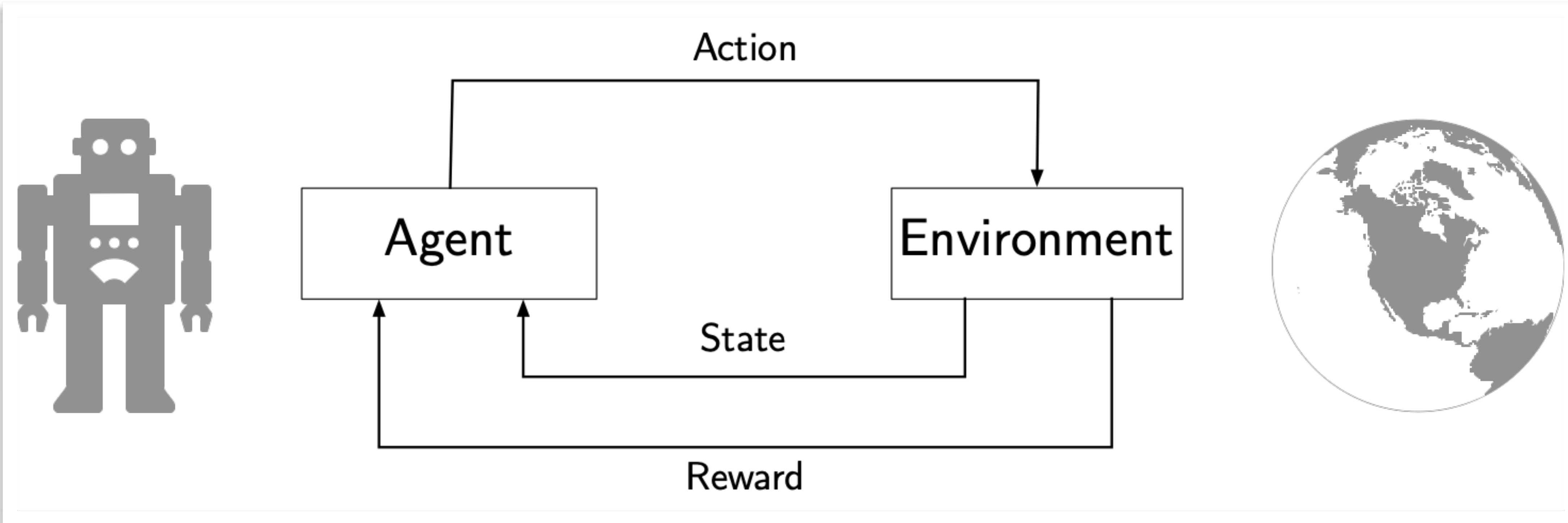
Note: some modifications have been done from the initial implementation to fulfill our specific needs

Novelty: on the reinforcement learning environment (and not so much on the training algorithm)

https://fluxml.ai/Flux.jl/stable/

https://juliareinforcementlearning.org/

Reinforcement learning environment



Reinforcement learning in a nutshell

Goal of the agent: obtain the most reward as possible during an episode

Episode: sequence of states from an initial state to a final state

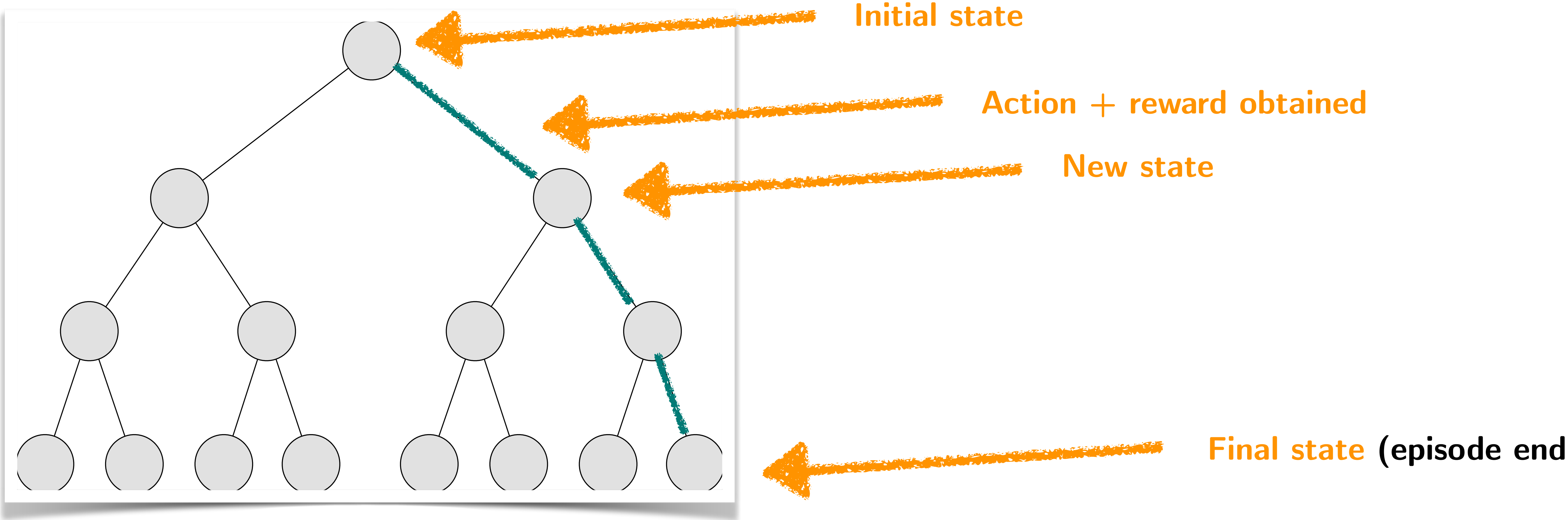
Action: move the agent in a new state (and update it through the transition)

Reward: score obtained after each action

Environment: formal definition of the set of states, possible actions, transition, and reward function

> **Solving a problem with RL require to define the environment (modeling step)**

Reinforcement learning environment



Environment

Agent to train: a value-selection heuristic inside a CP solver for a specific problem

Episode: a path from in the tree search without backtracks

Initial state: the root node (unsolved combinatorial problem)

Final state: a leaf node (either a feasible or unfeasible solution)

Action: selecting the value to branch on the current variable (agent choice)

Transition: branching and executing all the related CP solver stuff (fix-point, propagation, etc.)

Reward function: not trivial! Explanation on the next slide :-)

Reward function

Main principles

Goal: finding good solutions (and not to prove optimality)

Intuitive idea: use the final objective cost as reward signal

? What do you think about this reward ?

Difficulty: this information is only often available at the end of an episode (sparse reward issue)

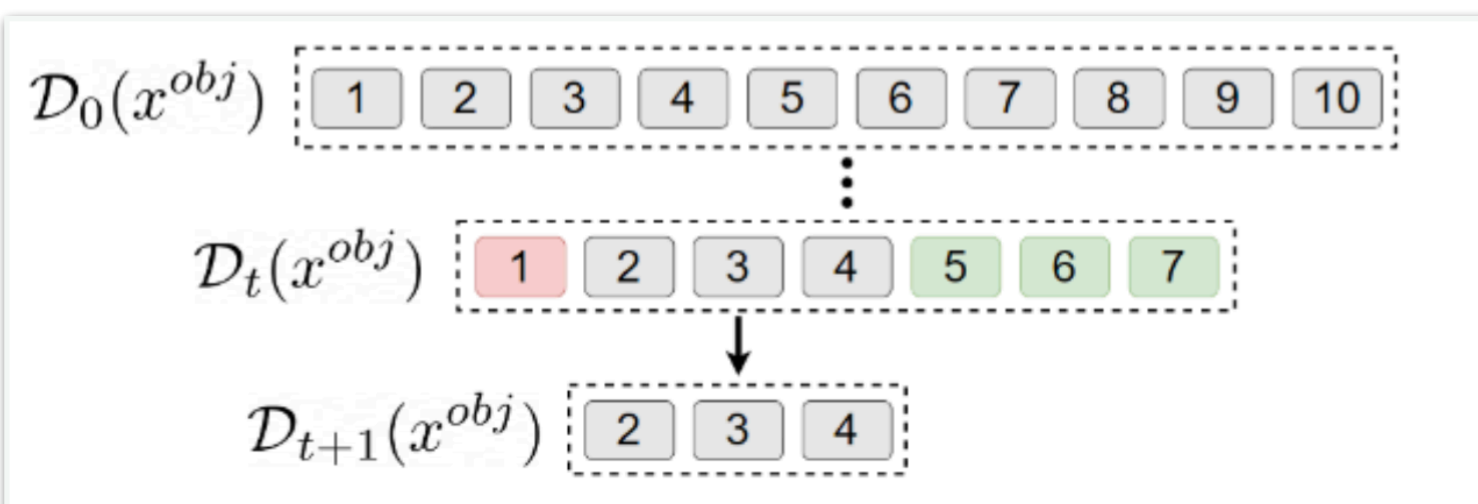
Proposition: rewarding scheme based on the domain reduction of the objective variable at each node

Propagation-based reward

Propagation scope: on the variable corresponding to the objective function (to minimize)

Principle 1: rewarding the propagation of largest values of the domain

Principle 2: penalizing the propagation of lowest values of the domain



10 values (initial domain)

3 highest values pruned at state $t+1$

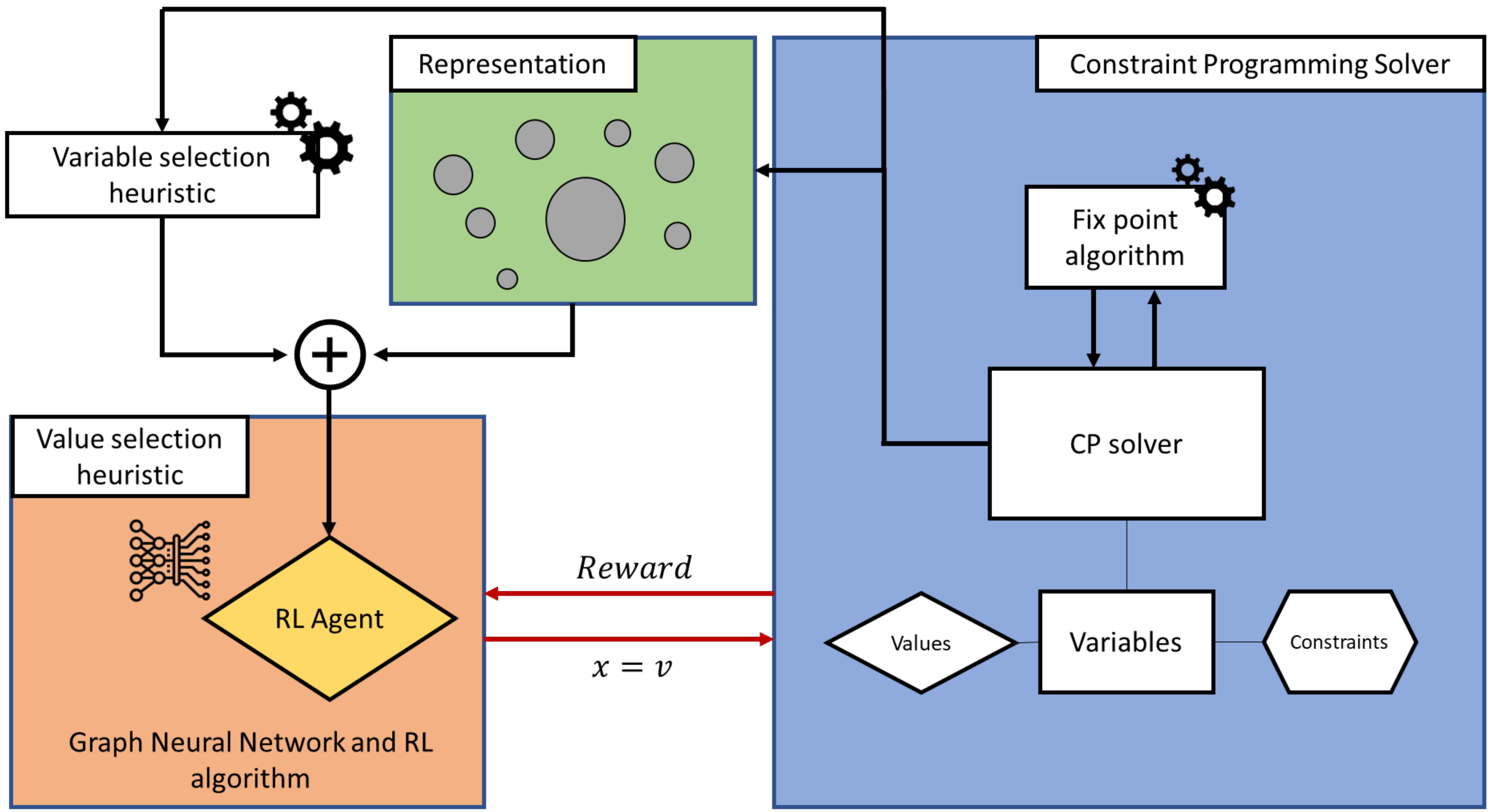
1 lowest value pruned at state $t+1$

Reward at state $t+1 = \frac{3-1}{10} = \frac{2}{10}$

Principle 3: penalizing episodes reaching an unfeasible solution

Final reward: accumulated reward from each transition

Architecture behind SeaPearl



Main components of SeaPearl

Module 1: a constraint programming solver

Module 2: a generic representation function

Module 3: a learning agent, based on reinforcement learning and graph neural network

Architecture behind SeaPearl

Main compon

Module 1: a const

Module 2: a gener

Module 3: a learni

Experimental setup

Experimental protocol

Combinatorial problems: graph coloring, maximum independent set, maximum cut

Instance sizes: graphs from 20 to 100 nodes

Models trained: one per configuration (problem/size pair)

Training phase: 72 hours on Nvidia Tesla V100 32Go GPU for the most difficult cases

Baselines: random selection, impact-based search, and activity-based search

Implementation: everything on SeaPearl (no comparisons yet with other solvers)

Metrics: optimality gap and execution time to reach a specific solution

> ***Question explored: what is the best solutions obtained given a limited budget of explored nodes ?***

			Learned				Activity-Based			Impact-Based			Random			
			1st dive	ILDS			DFS			DFS			DFS			
	Size	OPT	Gap	Gap	Node	Time	Gap	Node	Time	Gap	Node	Time	Gap	Node	Time	Budget
COL	20	5.05	0.06	0	27	< 1	0	378	< 1	0	374	< 1	0	378	< 1	10^3
	40	7.90	0.08	0	104	< 1	0	1,664	< 1	0	1732	< 1	0	1735	< 1	10^4
	80	8.75	0.06	0	120	1	0	7,051	2	0	7,057	2	0	7,211	2	10^5
MIS	30	9.90	0.08	0	88	< 1	0	215	< 1	0	297	< 1	0	293	< 1	10^3
	50	15.00	0.09	0	539	1	0	5,807	1	0	7,474	1	0	8,942	1	10^4
	100	21.70	0.20	0.02	28,392	253	0.09	35,536	7	0.10	38,154	8	0.10	41,774	9	10^5
MAXCUT	20	46.70	0.15	0.03	3,714	5	0.04	4,635	1	0.03	5,959	2	0.04	4877	1	10^4
	50	222.00	0.16	0.09	38,744	130	0.17	44,664	14	0.17	47,970	17	0.17	53,110	19	10^5

Performances of the approach

	Size	OPT	1st dive Gap	Learned ILDS Gap	Learned ILDS Node	Learned ILDS Time	Activity-Based DFS Gap	Activity-Based DFS Node	Activity-Based DFS Time	Impact-Based DFS Gap	Impact-Based DFS Node	Impact-Based DFS Time	Random DFS Gap	Random DFS Node	Random DFS Time	Budget
COL	20	5.05	0.06	0	27	< 1	0	378	< 1	0	374	< 1	0	378	< 1	10^3
	40	7.90	0.08	0	104	< 1	0	1,664	< 1	0	1732	< 1	0	1735	< 1	10^4
	80	8.75	0.06	0	120	1	0	7,051	2	0	7,057	2	0	7,211	2	10^5
MIS	30	9.90	0.08	0	88	< 1	0	215	< 1	0	297	< 1	0	293	< 1	10^3
	50	15.00	0.09	0	539	1	0	5,807	1	0	7,474	1	0	8,942	1	10^4
	100	21.70	0.20	0.02	28,392	253	0.09	35,536	7	0.10	38,154	8	0.10	41,774	9	10^5
MAXCUT	20	46.70	0.15	0.03	3,714	5	0.04	4,635	1	0.03	5,959	2	0.04	4877	1	10^4
	50	222.00	0.16	0.09	38,744	130	0.17	44,664	14	0.17	47,970	17	0.17	53,110	19	10^5

Number of explored nodes to obtain a given gap (capped at 100,000)

Optimality gap obtained with a single dive (no backtrack)

Average value of the optimal cost

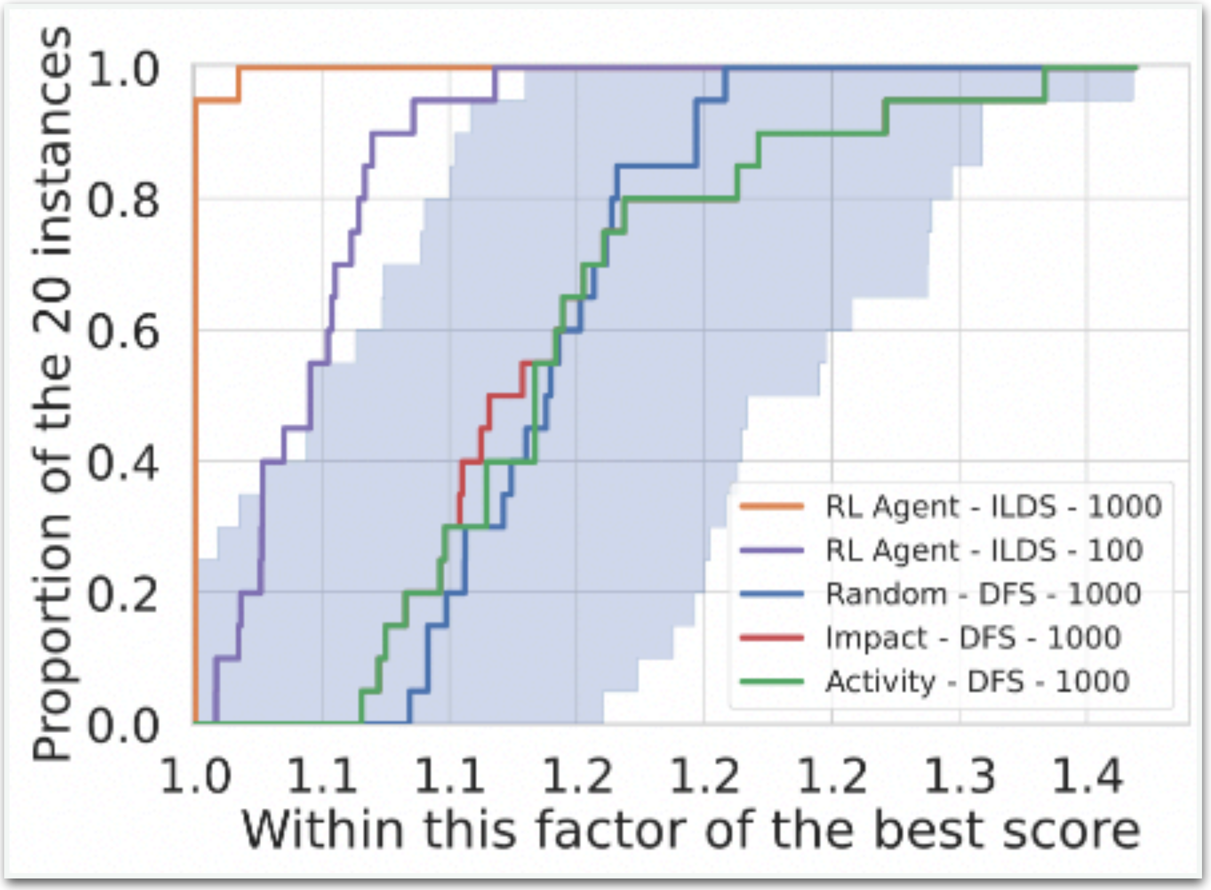
Configurations tested (20 instances per scenario)

Observation 1: a gap of 0.16 is obtained in a single dive while it 44,664 nodes for baselines to have 0.17

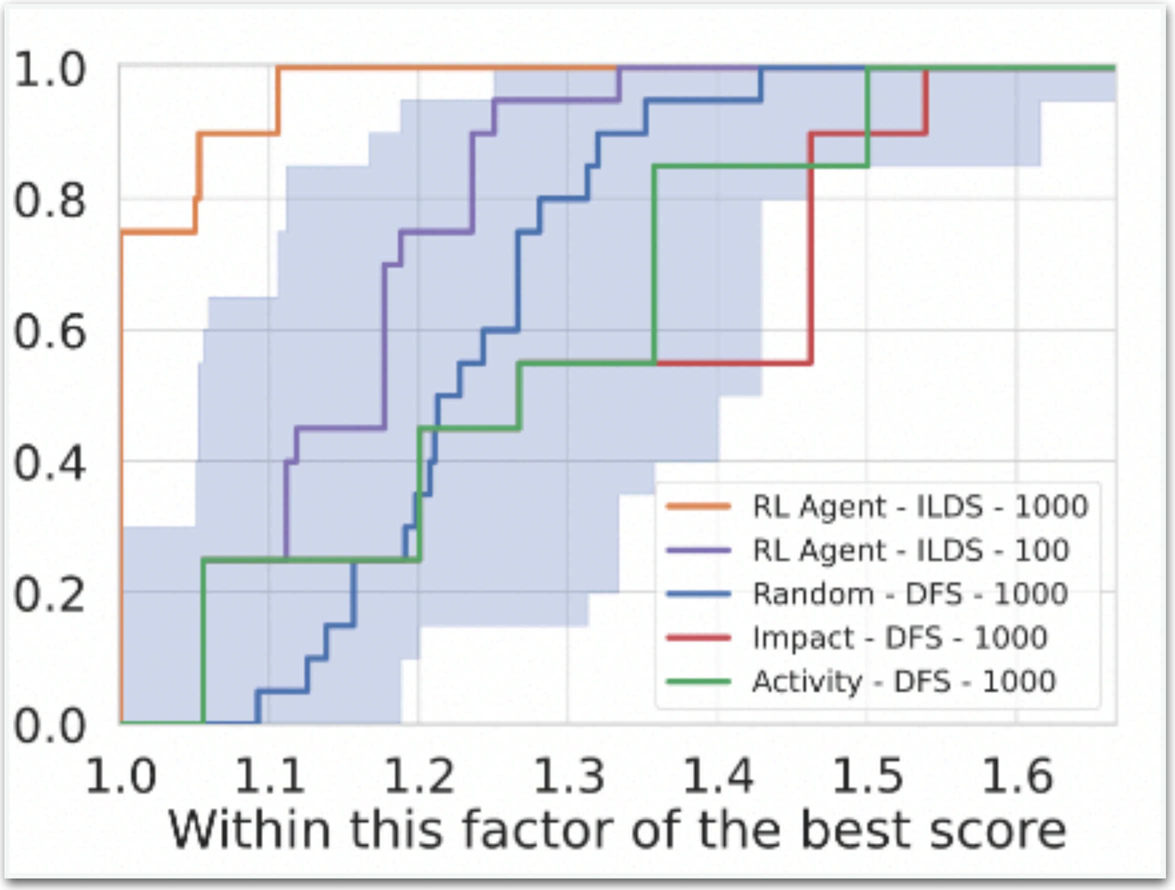
Observation 2: we are able to obtain good solutions in less explored nodes compared to baselines

Observation 3: the execution time of calling the NN is important

Zoom on the hardest scenarios - performance profiles



Maximum-cut with 50 nodes



Maximum independent set with 100 nodes

Baselines: each curve corresponds to a method

Metric: optimality gap

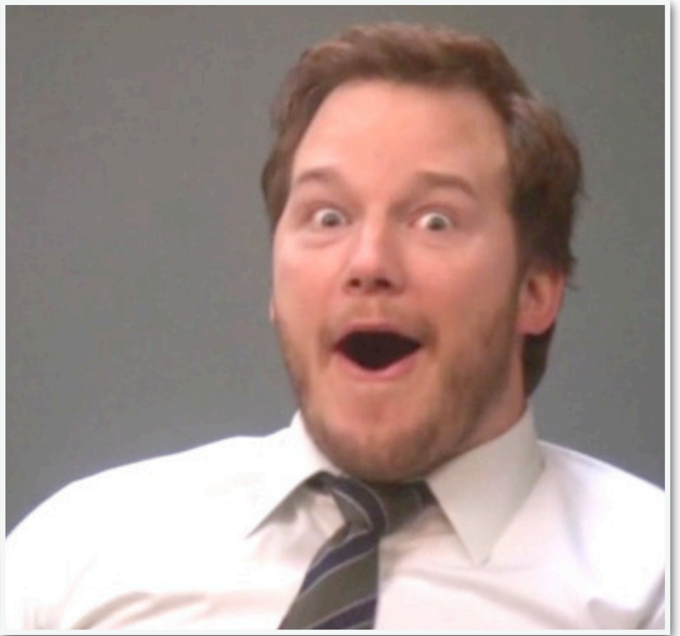
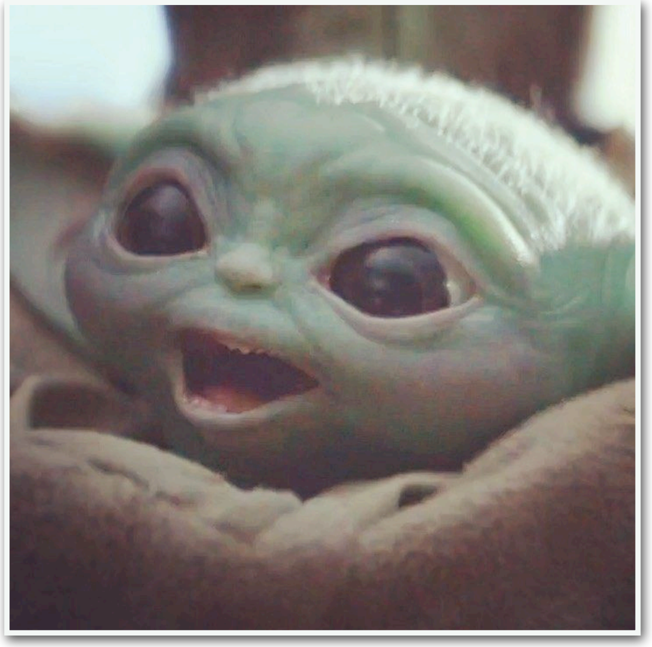
Performance profiles: each tick gives the proportion of instances able to achieve a given optimality gap

Interpretation: the upper is the curve, the better is the method

Observation: results obtained by the learned approach is robust among all the instances tested

Conclusion of the experiments: it seems that we are able to learn interesting branching decisions!

Second conclusion

? It seems great! Should I use this for solving my problems and get competitive results?

No!!!!

Explanation: I believe it is a promising research direction, but not mature yet to get competitive results

Getting quickly competitive results: currently better to use problem-specific heuristics

Take-home message: see this work as first building blocks to unlock new avenues in the mid-term

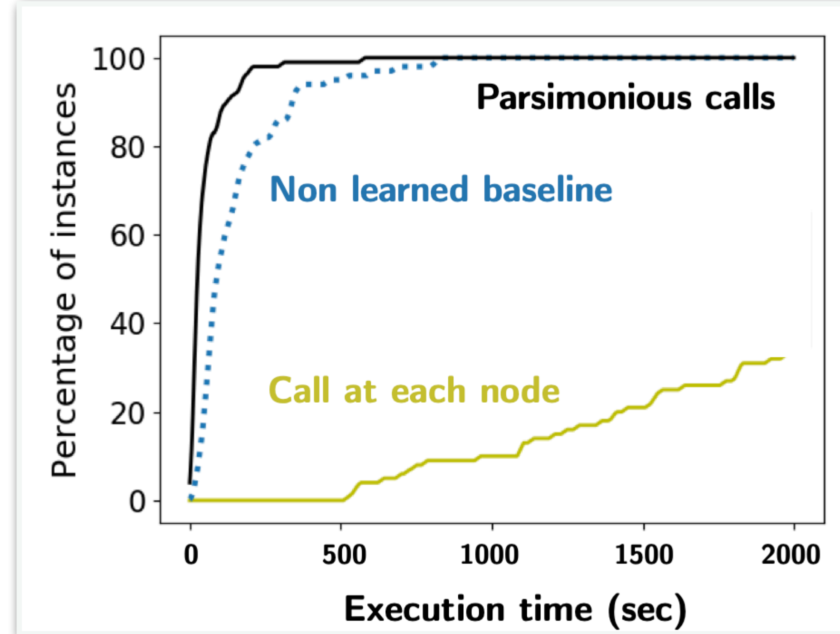
Personal note: I have the same opinion for many works using ML for combinatorial optimization :-)

? I also like this idea of a hybrid paradigm! What kind of research can I carry out in this field ?

Next slides: I will propose and discuss few challenges and related research questions

Research idea: reducing the inference time

			Learned				Random		
			1st dive	ILDS			DFS		
	Size	OPT	Gap	Gap	Node	Time	Gap	Node	Time
COL	20	5.05	0.06	0	27	< 1	0	378	< 1
	40	7.90	0.08	0	104	< 1	0	1735	< 1
	80	8.75	0.06	0	120	1	0	7,211	2
MIS	30	9.90	0.08	0	88	< 1	0	293	< 1
	50	15.00	0.09	0	539	1	0	8,942	1
	100	21.70	0.20	0.02	28,392	253	0.10	41,774	9
MAXCUT	20	46.70	0.15	0.03	3,714	5	0.04	4877	1
	50	222.00	0.16	0.09	38,744	130	0.17	53,110	19



Learned heuristic: 130 seconds to explore 38,744 nodes (298 nodes/second)

Random selection: 19 seconds to explore 53,110 nodes (2795 nodes/second)

Ratio: roughly an exploration rate 10 times slower!

Explanation: calling the model (GNN + FCNN) is much more costly than simple branching heuristics

? What can we do ?

Idea 1: caching Q-values and use them in similar states

Idea 2: reducing the inference time of the model (transfer learning, network pruning, etc.)

Idea 3: calling the model only in few nodes of the search tree (gave good results in another project)

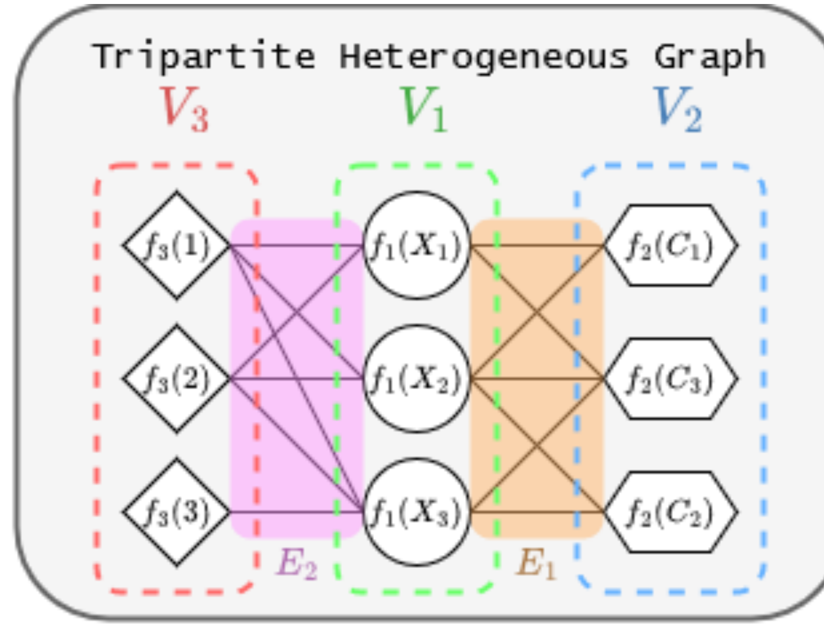
Improving Variable Orderings of Approximate Decisions Diagrams using Reinforcement Learning [Cappart, Rousseau et al., IJOC-2022]

Research idea: rethinking the representation

$X_1 \in \{1,2\},\ X_2 \in \{1,2\},\ X_3 \in \{1,2,3\}$

- $C_1 = X_1 \leq X_2$
- $C_2 = X_2 \leq X_3$
- $C_3 = AllDifferent(X_1, X_2, X_3)$

Encoding function



Challenge 1: scalability

Difficulty: the size of the representation is growing fast

Consequence: the training phase is harder and more costly

Idea: curriculum learning from small instances

5 vertices: 18 nodes (graph coloring)

20 vertices: 117 nodes

100 vertices: 1477 nodes

200 vertices: 4002 nodes

Challenge 2: expressivity

Difficulty: we may miss important relationships in the model

Exemple: inequalities with different constant values

$c_1 : x \leq y + 3$

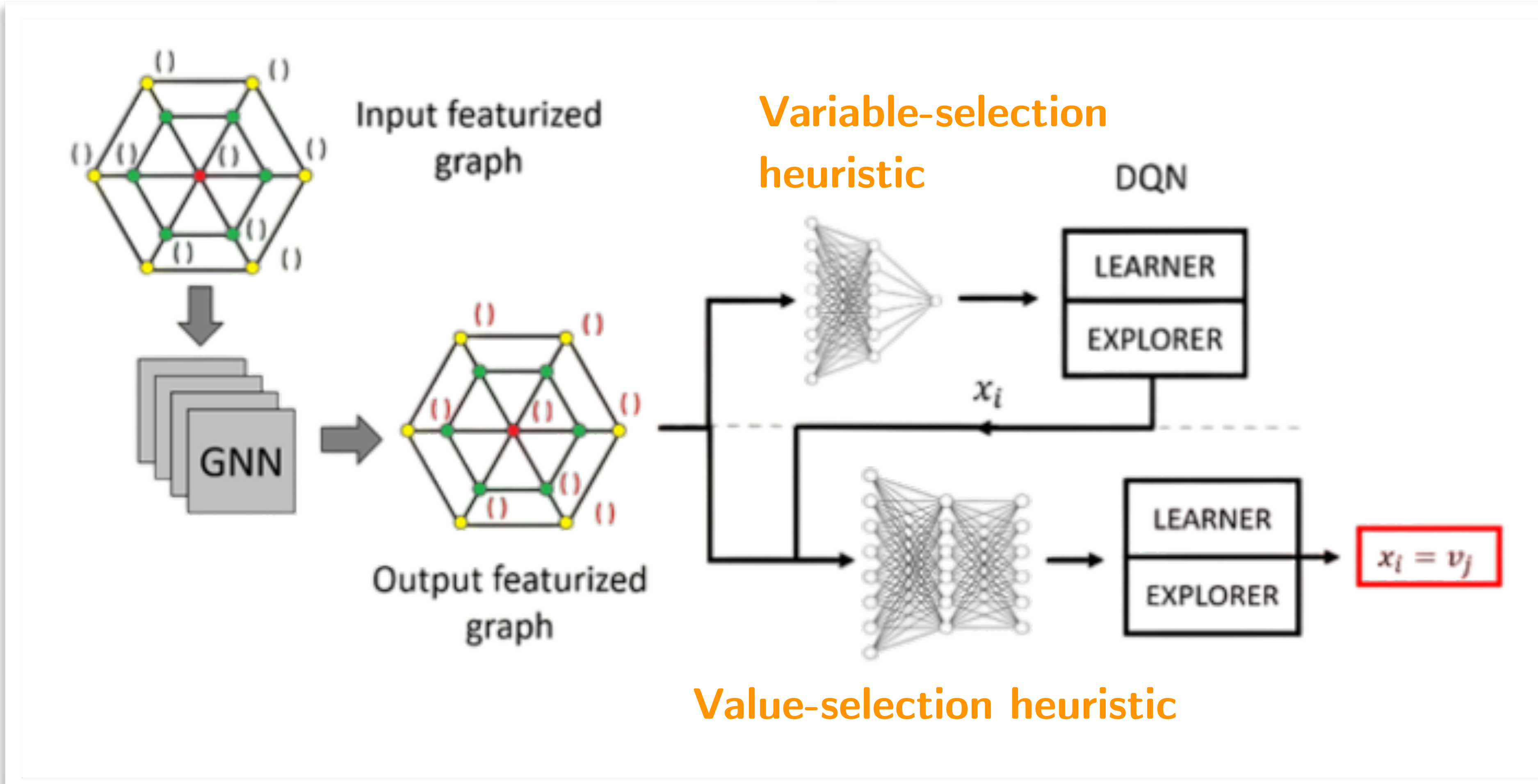
$c_2 : x \leq y + 6$

$c_3 : x \leq y^2$

Consequence: we either lose information on the constant, or that the constraint is similar

Idea: expend the representation with new information (as in an abstract syntactic tree)

Research idea: learning a double heuristic



Motivation: selecting the variable to branch on is also challenging

Idea: expend the architecture to learn a variable-selection heuristic at the same time

Possible option 1: adopting a methodology similar to cooperative multi-agent reinforcement learning

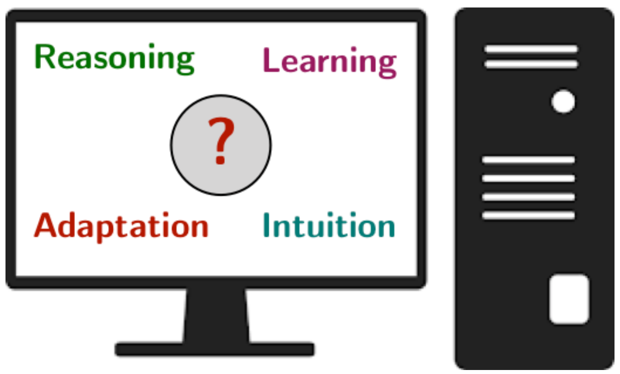
Possible option 2: allowing the agents to share information (a good value selection depends on the variable)

And many other ideas can also be leveraged and tested !

Conclusion

Our research hypothesis

Constraint programming can be used as a hosting technology for building an hybrid AI



CP = model + propagation + search + learning

SeaPearl.jl

Solver: https://github.com/corail-research/SeaPearl.jl

Zoo of models: https://github.com/corail-research/SeaPearl.jl

Paper: https://arxiv.org/abs/2102.09193 (updated version to appear at CP23)

Other related projects: https://corail-research.github.io/publications/

Contact: quentin.cappart@polymtl.ca

Combining reinforcement learning and constraint programming for combinatorial optimization [Cappart et al., AAAI 2021]

Seapearl: A constraint programming solver guided by reinforcement learning [Chalumeau, Cappart et al., CPAIOR 2021]

Learning a generic value-selection heuristic inside a constraint programming solver [Marty, Cappart et al., CP 2023]

Contributors

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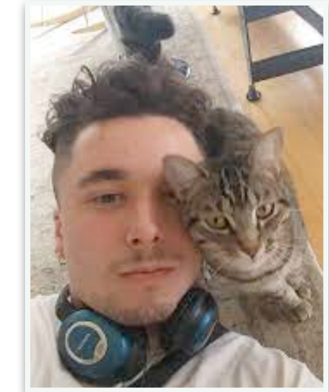



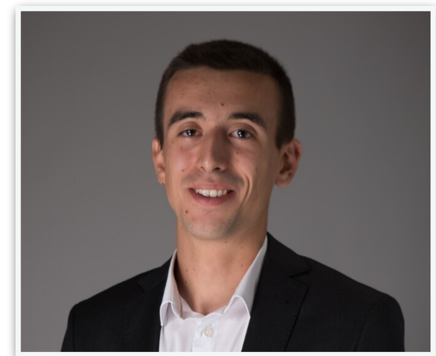
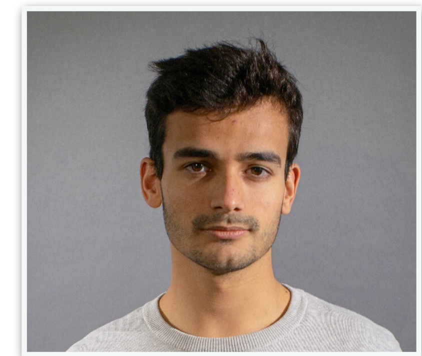

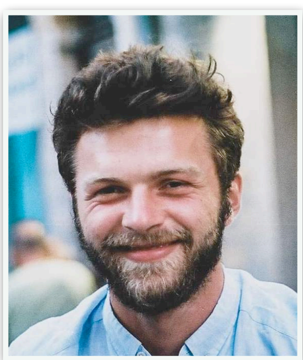
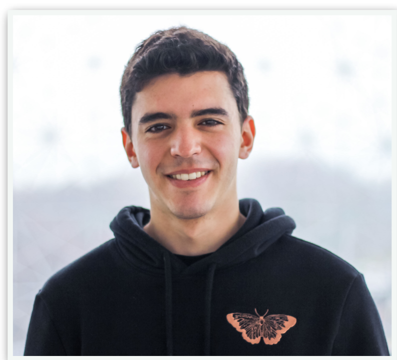
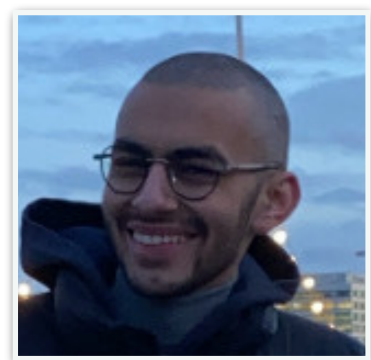

We are always open for new contributions :-)

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Learning a value-selection heuristic inside a constraint programming solver

ACP Summer School 2023 - Leuven

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Combinatorial Optimization and Reasoning in Artificial Intelligence Laboratory

Quentin Cappart