Boosting optimization via machine learning

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Tutorial overview: part 1

- Optimization for boosting Machine Learning: few details
- Machine Learning for boosting optimization: an overview
  - ✓ Supporting the modeling activity:
    - Machine Learning to detect constraints (e.g. Constraint Acquisition, Model Seeker)
    - Machine Learning models as constraints (e.g. Empirical Model Learning, partially dened constraints)
    - Objective function learning
  - ✓ Boosting Search
    - No good learning and recording
    - Reinforcement learning for search
    - Approximating branching heuristics
  - ✓ Algorithm selection and tuning
    - Using ML to predict the run time
    - Using ML to select the best approach
  - ✓ Similar approaches
    - Surrogate based optimization
    - Black box optimization
    - LION (Learning and Intelligent OptimizatioN) approach, metaheuristics
    - Model predictive control
- Concluding remarks and future research directions

Tutorial overview: part 2

- Hands on session (about Empirical Model Learning)
  - ✓ Overview of the target problem (Off-line/on-line optimization)
  - ✓ Overview of the tools
  - ✓ Sampling the on-line input space to build a training set
  - ✓ Approximating the on-line behavior via ML
  - ✓ Embedding the ML model in a combinatorial model

We are very grateful to….

- Nicolas Beldiceanu
- Bistra Dilkina
- Gene Freuder
- Arnaud Gotlieb
- Tias Guns
- Lars Kotthoff
- Arnaud Lallouet
- Nadjib Lazaar

for providing material used to prepare this tutorial

Machine learning and optimization

- A lot of research activity going on in two directions:

- Helping ML algorithms through optimization techniques

- Boosting optimization via ML
  - this is what this tutorial is about

Improving ML algorithms via optimization

- Pattern mining:
  - Optimization methods such as SAT/CP/ILP enable to express complex constraints on patterns and combination thereof
- Itemset mining and extensions (cost constraints, closed itemset, max itemset)

L. De Raedt, T. Guns, S. Nijssen. Constraint programming for itemset mining. KDD 2008

S. Nijssen, T. Guns. Integrating constraint programming and itemset mining. ECML PKDD 2010.

M. Maamar, N. Lazaar, S. Loudni, Y. Lebbah. A global constraint for closed itemset mining. CP 2016.

P. Schaus, J. Aoga, T. Guns. CoverSize: A global constraint for frequence-based itemset mining. CP 2017.

I.O. Dlala, S. Jabbour, L. Sais, B.B. Yaghlane. A Comparative Study of SAT-Based Itemsets Mining SGAI 2016.

Improving ML algorithms via optimization

- Pattern mining:
  - Optimization methods such as SAT/CP/ILP enable to express complex constraints on patterns and combination thereof
- Sequence mining with constraints on syntax, data covered, relationship

M. Gebser, T. Guyet, R.Quiniou, J.Romero, and T.Schaub. "Knowledge-based sequence mining with ASP." In IJCAI 2016

Aoga, John OR, Tias Guns, and Pierre Schaus. "An efficient algorithm for mining frequent sequence with constraint programming." ECMLPKDD 2016

Kemmar , Y. Lebbah, S. Loudni, P. Boizumault, and T. Charnois. "Prefix-projection global constraint and top-k approach for sequential pattern mining." Constraints 22, no. 2 (2017)

Improving ML algorithms via optimization

- Pattern mining:
  - Optimization methods such as SAT/CP/ILP enable to express complex constraints on patterns and combination thereof
- Pattern **set** mining

L. De Raedt, S. Nijssen, T. Guns. k-Pattern Set Mining under Constraints. IEEE TKDE, 2013.

A. Ouali, A. Zimmermann, S. Loudni, Y. Lebbah1 , B. Cremilleux, P. Boiiumault, L. Loukil. Integer Linear Programming for Patern Set Mining; with an Applicaton to Tiling. PAKDD 2017.

Improving ML algorithms via optimization

- Clustering:

Ouali, A., Loudni, S., Lebbah, Y., Boiiumault, P., Zimmermann, A., and Loukil, L. Efficiently finding conceptual clustering models with integer linear programming. IJCAI'16

Berg, Jeremias, and Matti Jarvisalo. "Optmal correlaton clustering via MaxSAT , AIJ Journal 2017

Bich Duong, Khanh-Chuong, and Christel Vrain. "A declaratve framework for constrained clustering". ECML, 2013. and AIJ 2017

Mueller, Marianne, and Stefan Kramer. "Integer Linear Programming Models for Constrained Clustering." Discovery science 2010. Vol. 6332. 2010.

Boosting optimization via ML

- Supporting the modeling activity:
  - Machine Learning is used to learn problem model components:
    - Constraints
    - Objective function
- Boosting Search/Solving
  - Machine Learning is used to speed up search:
    - Variable/value selection heuristics
    - New search strategies
    - Enabling specific algorithms during search
- Algorithm selection and tuning
  - Machine learning is used to select the best algorithm in a portfolio
  - Machine learning is used for parameter tuning

ML for supporting the modeling activity

M. Lombardi, M. Milano, Boosting Combinatorial Problem Modeling with Machine Learning, IJCAI2018

Supporting the modeling activity

- Use implicit information from a set of examples to obtain part of a combinatorial model
  - a constraint
  - an objective function.
- There are three main approaches:
  - extracting information using the native constraint language of the solver;
  - embedding a fully-fledged Machine Learning model in a combinatorial approach.
  - extreme case, the ML model makes up (almost) all of the combinatorial model.

Supporting the modeling activity

- Traditionally, combinatorial optimization problems are models from iterative interactions between a domain and an optimization expert.
- ML could replace (or support)
  - the optimization expert with a constraint acquisition algorithm,
  - the domain expert with an example generator.

- We need data:
  - Either historical data
  - Data from the expert
  - Data extracted from the real system or a simulator

Learning native constraint language components

Aimed at learning models in the general form:

$$\min z = x_0 \qquad (\mathbf{P1})$$
$$\text{subject to: } \pi_i(\vec{x}) \qquad \forall i \in I$$
$$\vec{x} \in D_{\vec{x}}$$

- where $\vec{x}$ are problem variables, $D_{\vec{x}}$ their domain and x_0 is the variable representing the objective value, $\pi_i(\vec{x})$ are problem constraints (predicates)

- Notably the predicates $\pi_i(\vec{x})$ are defined using the building blocks from the hosting approach

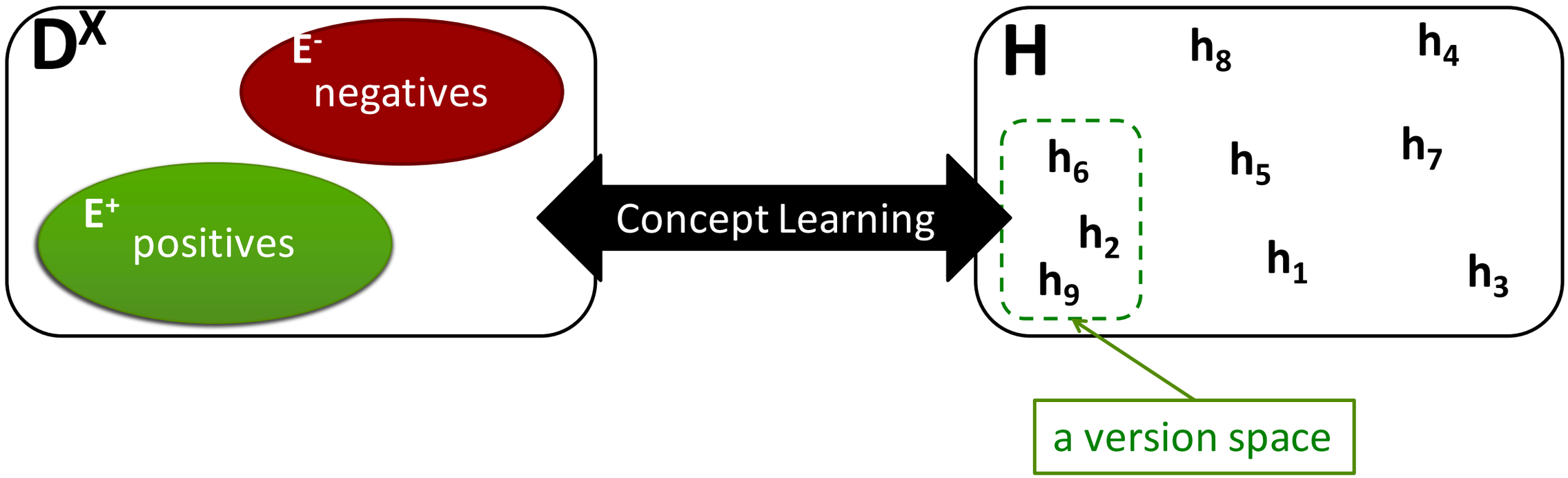
Learning native constraint language components

- Relevant approaches
  - Building over the constraint programming paradigm
    - CONACQ [Bessiere et al. , 2017a] (in its various versions),
    - QUACQ [Bessiere et al. , 2013],
    - Model seeker [Beldiceanu and Simonis, 2012]
  - Building over Inductive logic programming
    - [Lallouet et al. , 2010]

Version space learning [Mitchell82]

- Let $X=x_1,..,x_n$ a set of attributes of domains $D=D_1,..,D_n$
- A concept is a Boolean function
  - $f(x_i)=0$ => x_i is a negative instance
  - $f(x_j)=1$ => x_j is a positive instance
- Given a set of hypothesis **H**, any subset of **H** represents **a version space**
- A concept **to learn** is the set of **positive instances** that can be represented by **a version space**

Version space learning [Mitchell82]

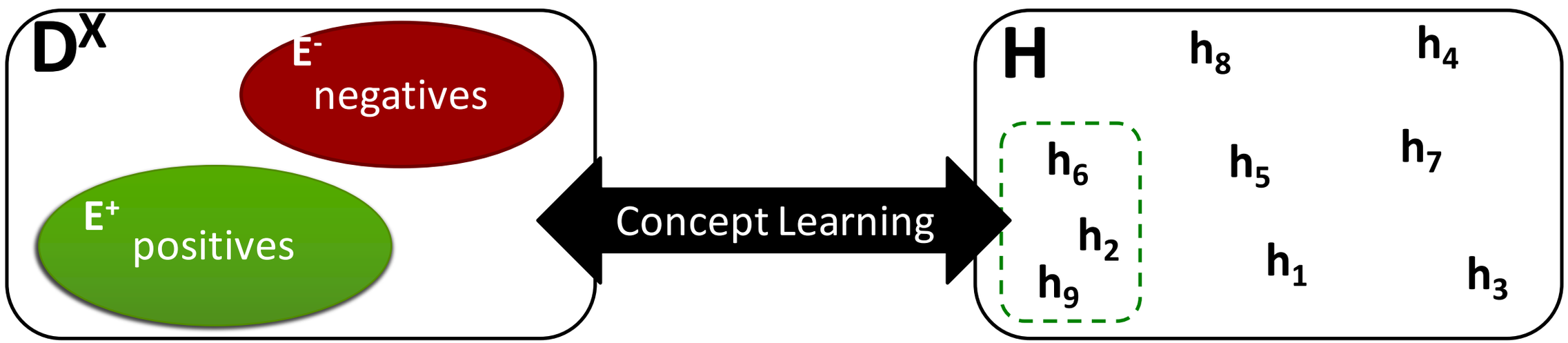


- Most specific concept to learn:

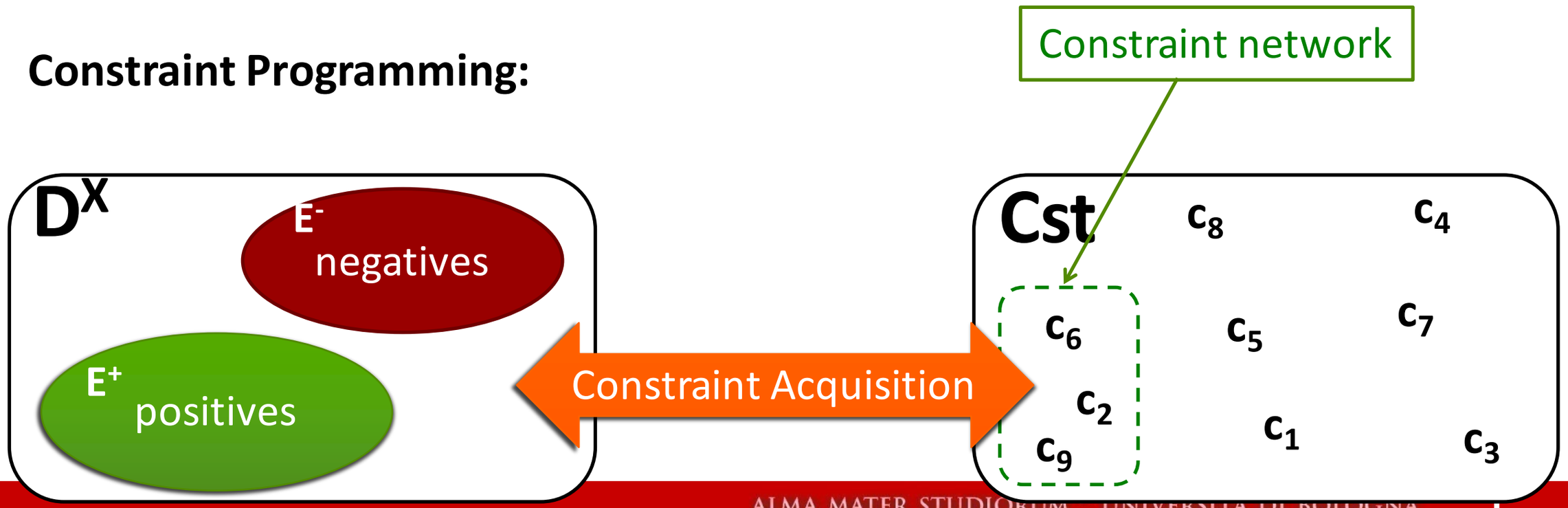
$$f: \quad (\forall x_i \in E^+ : f(x_i) = 1) \wedge (\forall x_i \in E^- : f(x_i) = 0)$$

$$f \equiv h_2 \wedge h_6 \wedge h_9$$

Constraint acquisition as version space learning

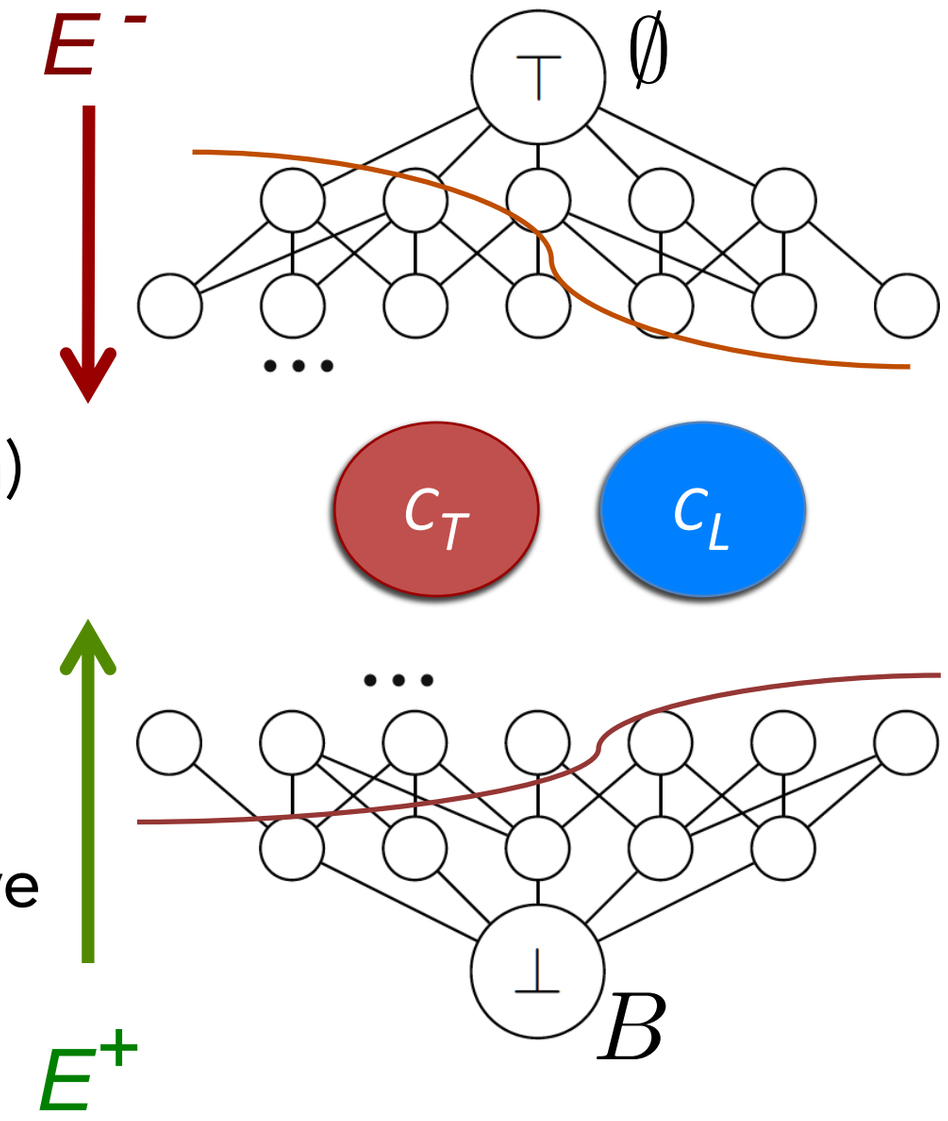


Constraint Programming:

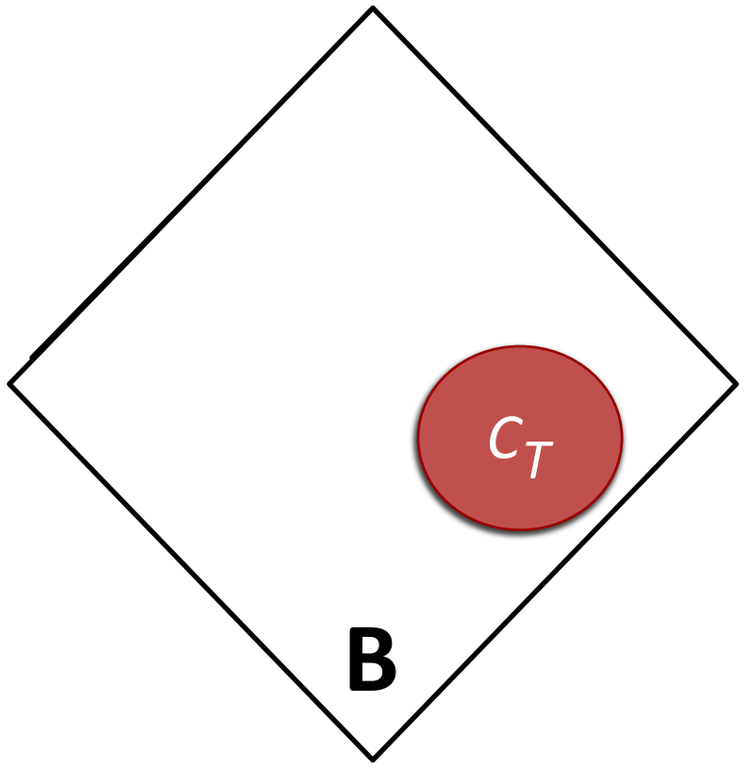


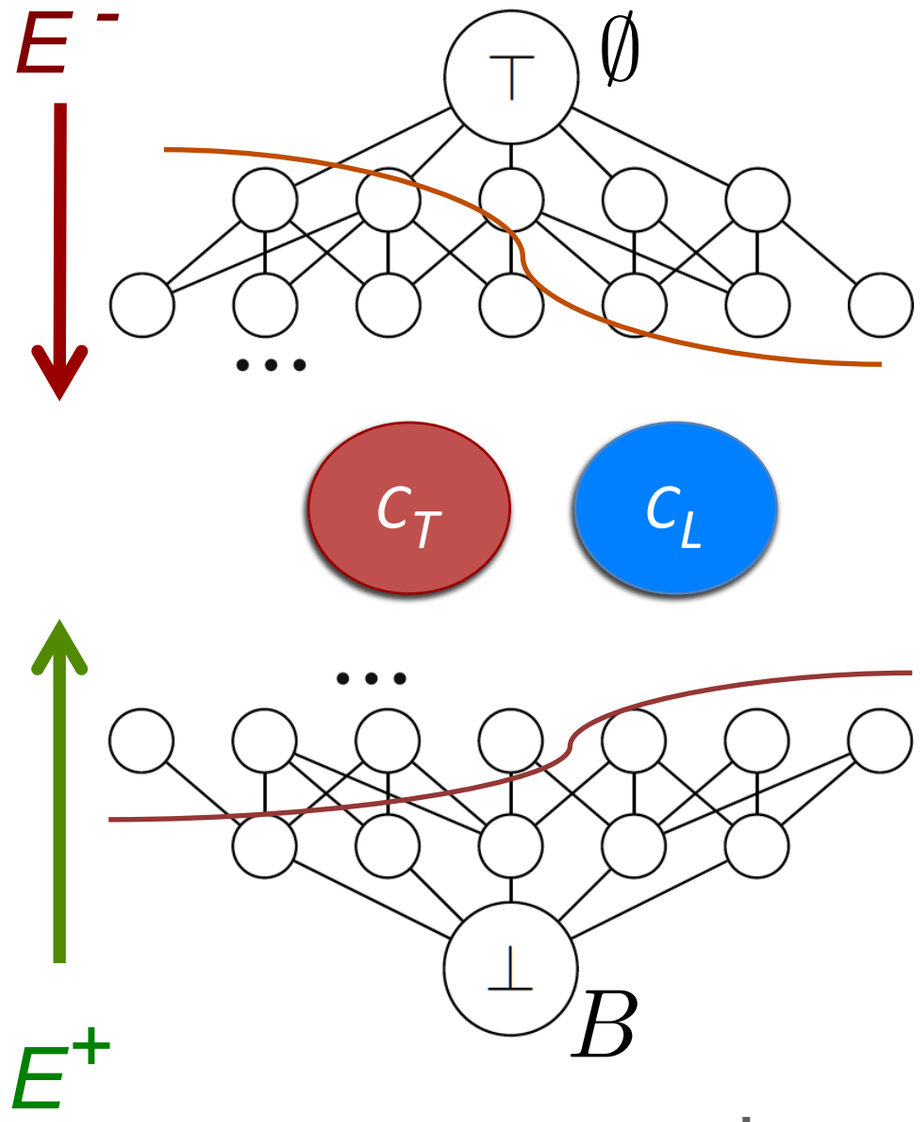
Constraint acquisition

- Inputs:
  - (X,D): Vocabulary
  - Γ: Constraint language
  - B: Bias (constraints/hypothesis)
  - C_T: Target Network (concept to learn)
  - (E^+,E^-): training set
- Output:
- C_L: Learned network such that: all positive and no negative example covered

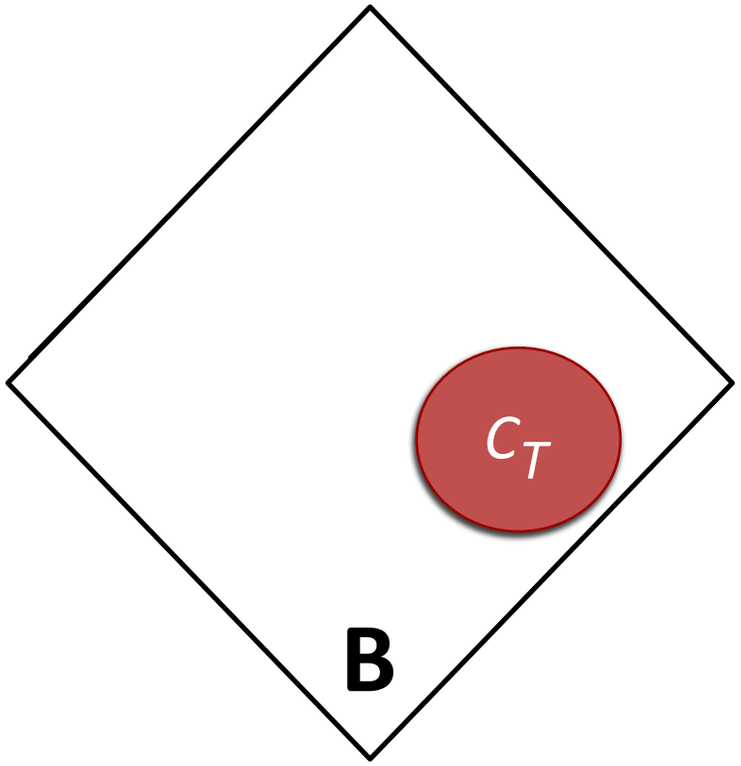


Convergence/collapse state

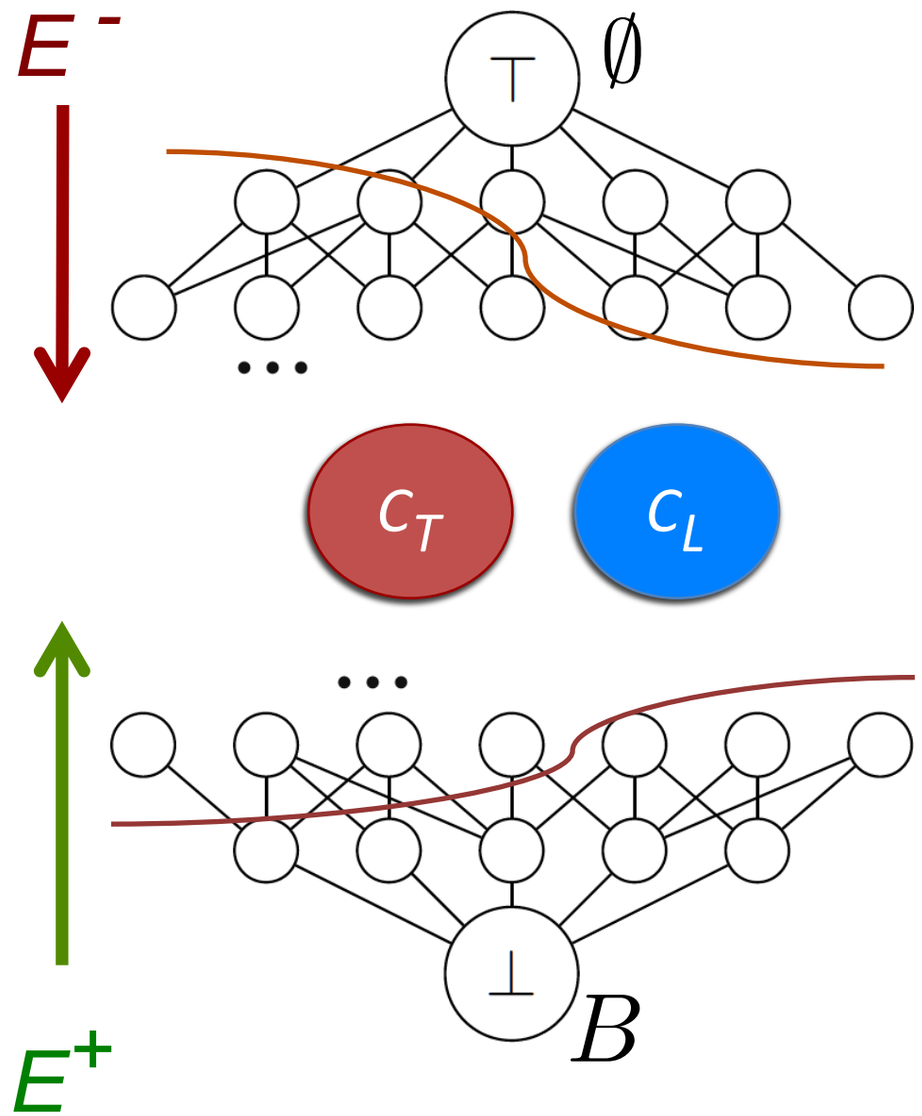




Convergence/collapse state



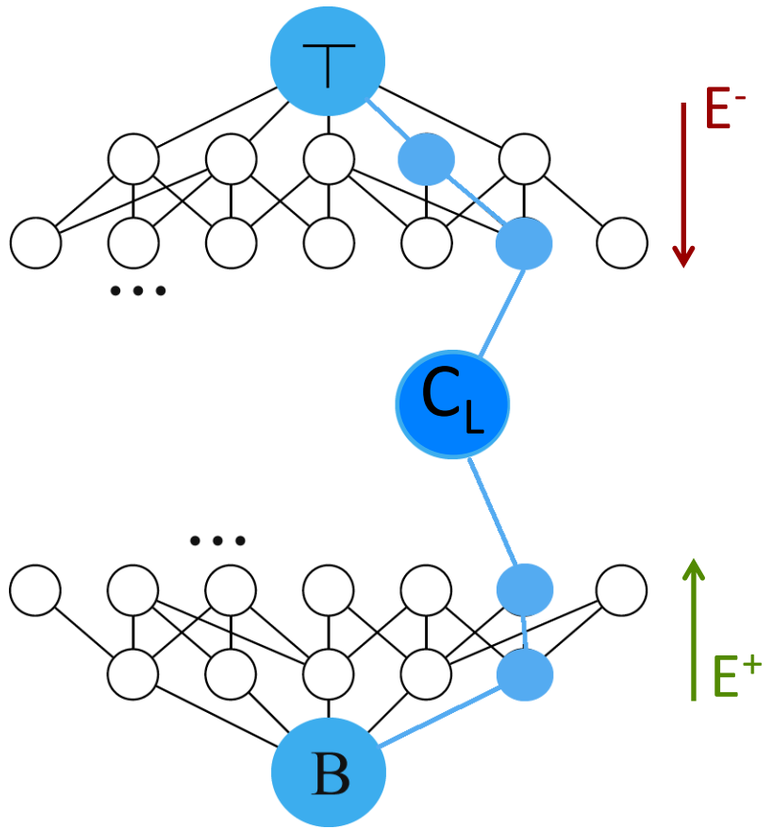
Collapse state



Acquisition via membership queries

- CONACQ [Bessiere et al. AIJ17]
  - SAT-Based constraint acquisition
  - Bidirectional search using Membership queries
  - Conacq1.0 (passive learning)
  - Conacq2.0 (active learning)

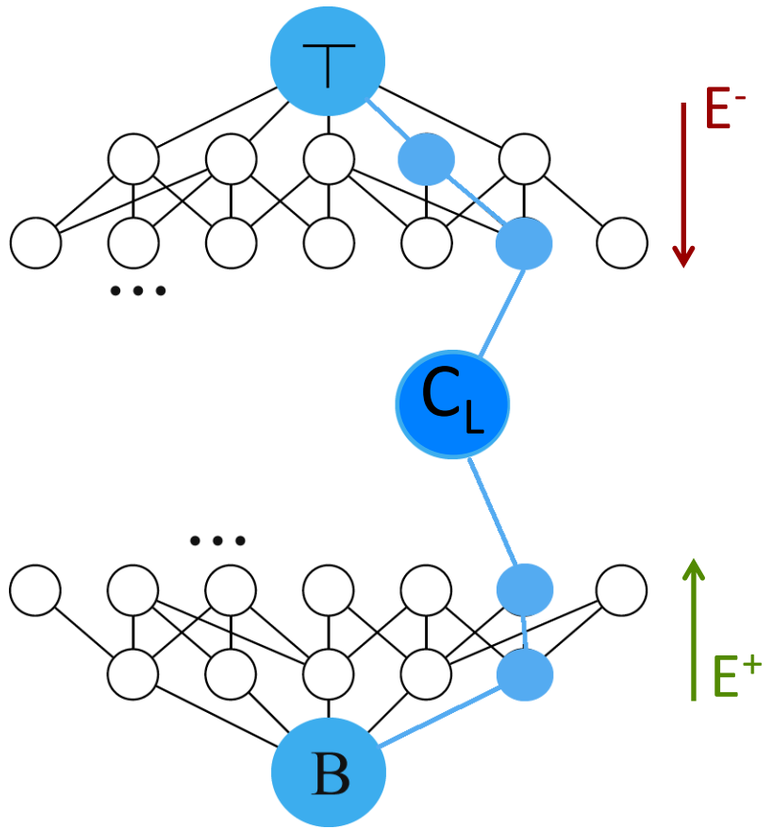
$$\mathcal{K} = \underbrace{(\neg x_1 \wedge \neg x_2 \wedge \neg x_3)}_{e^+} \bigwedge \underbrace{(x_4 \vee x_5 \vee x_6 \vee x_7)}_{e^-} \dots$$



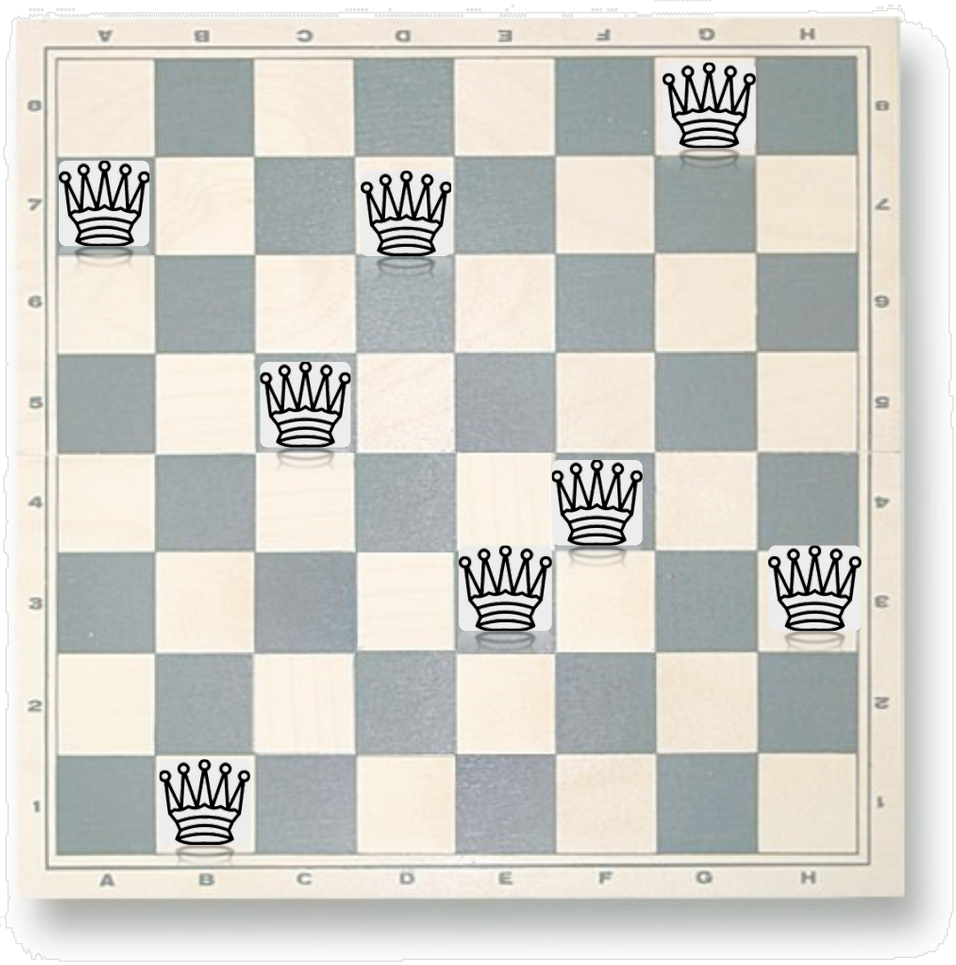
Non-learnability using Membership queries [Constraint Acquisition, AIJ17]

Quick acquisition

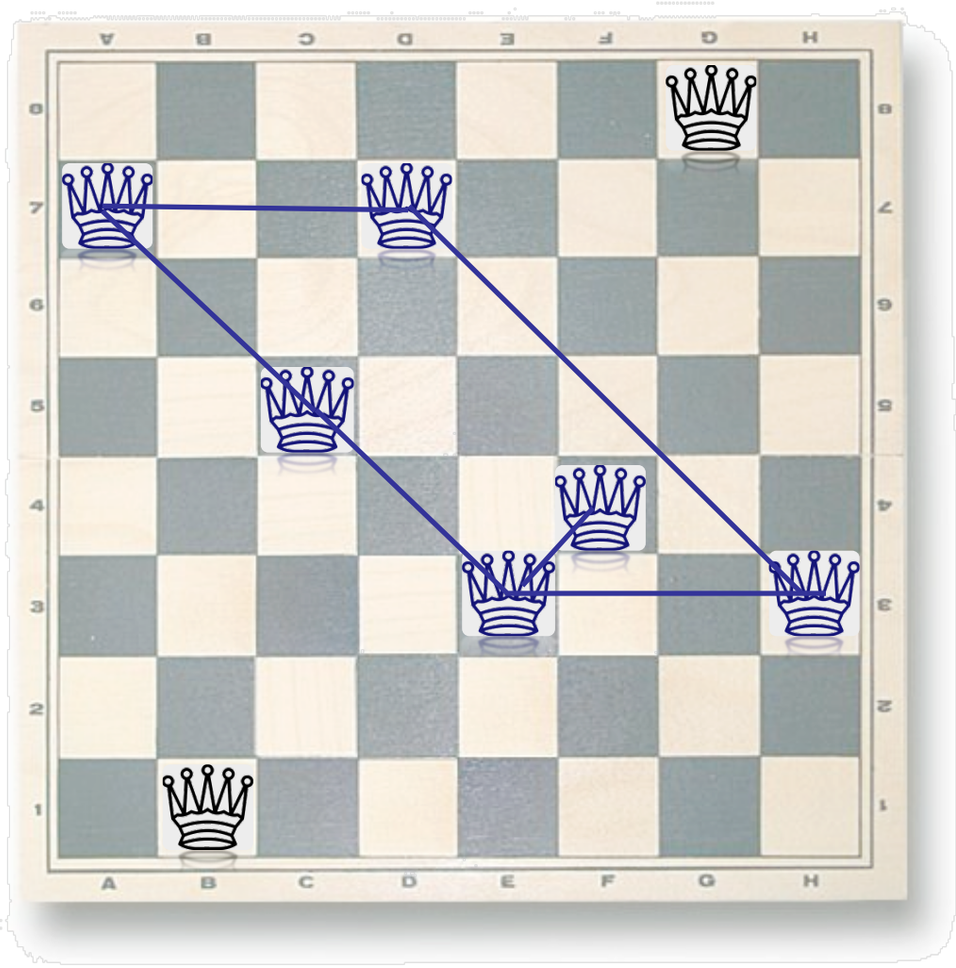
- QUACQ [Bessiere et al. IJCAI13]
  - Active learning approach
  - Bidirectional search
    - But it can be top-down search if no positive example
- Based on partial queries to elucidate the scope of the constraint to learn
- Learnability using partial queries



Membership queries

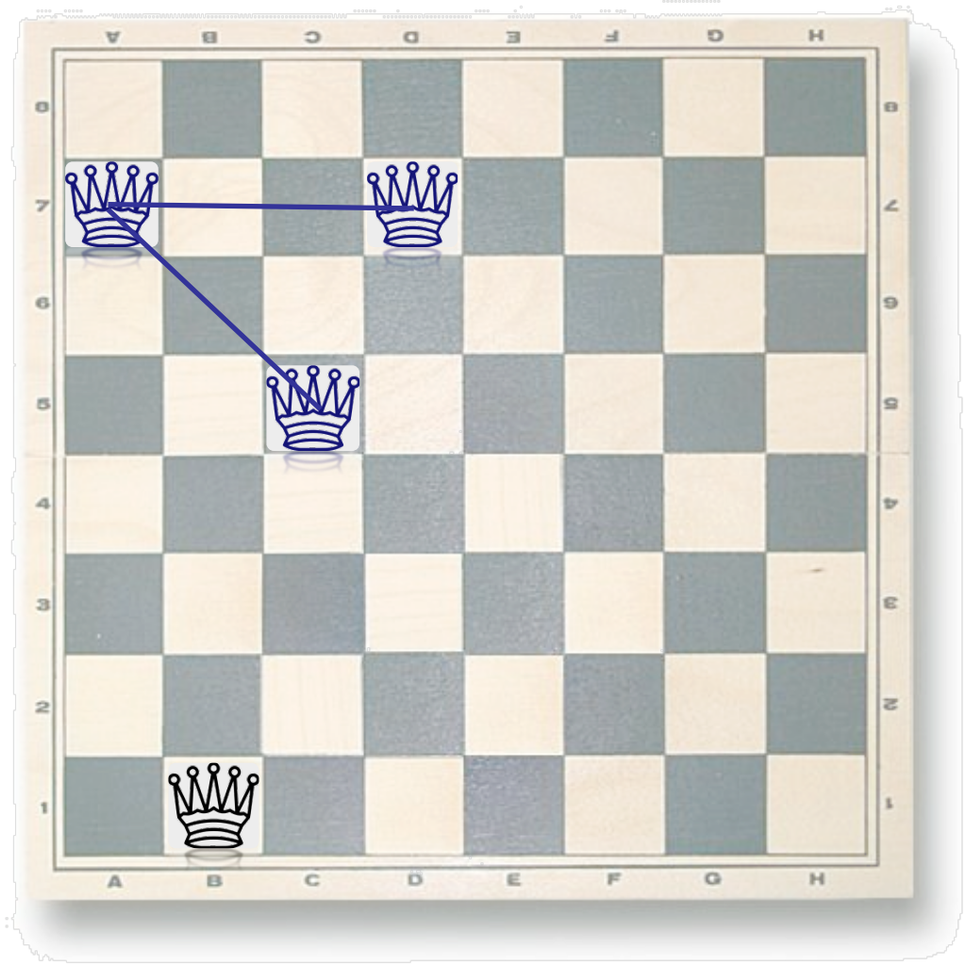


ask(2, 8, 4, 2, 6, 5, 1, 6)



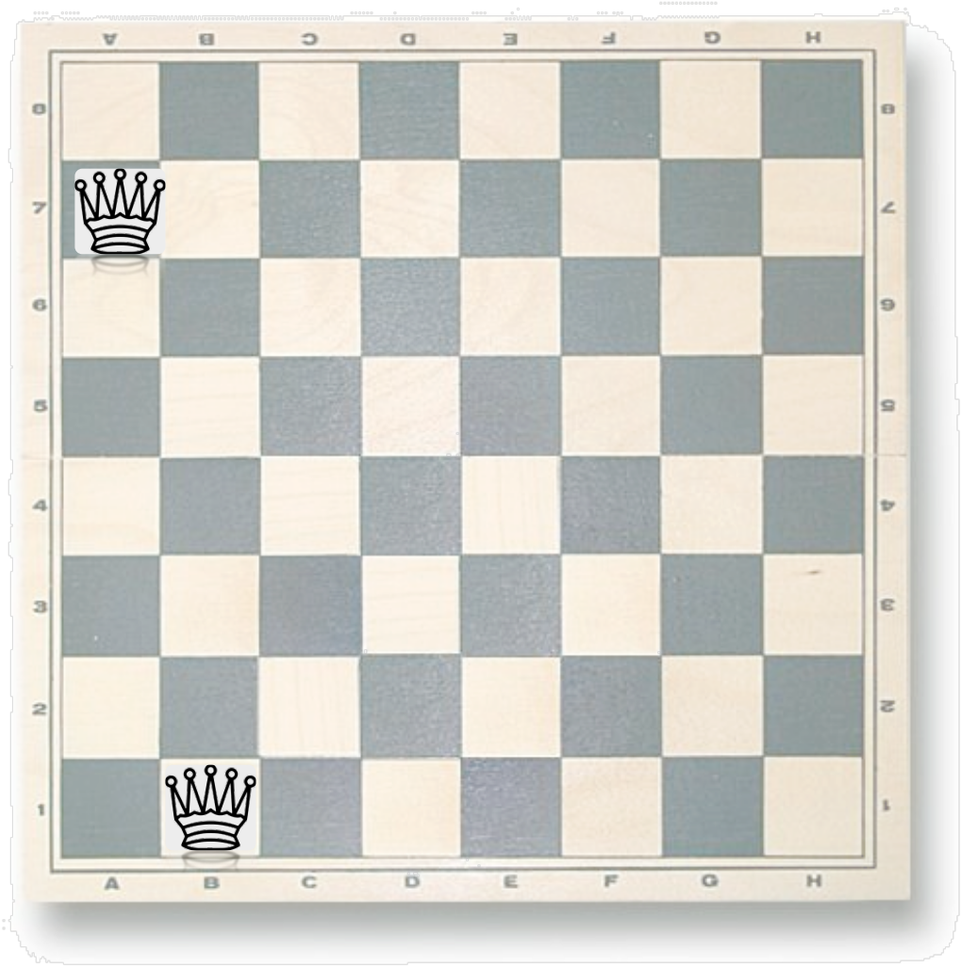
ask(2, 8, 4, 2, 6, 5, 1, 6) = No

Partial queries



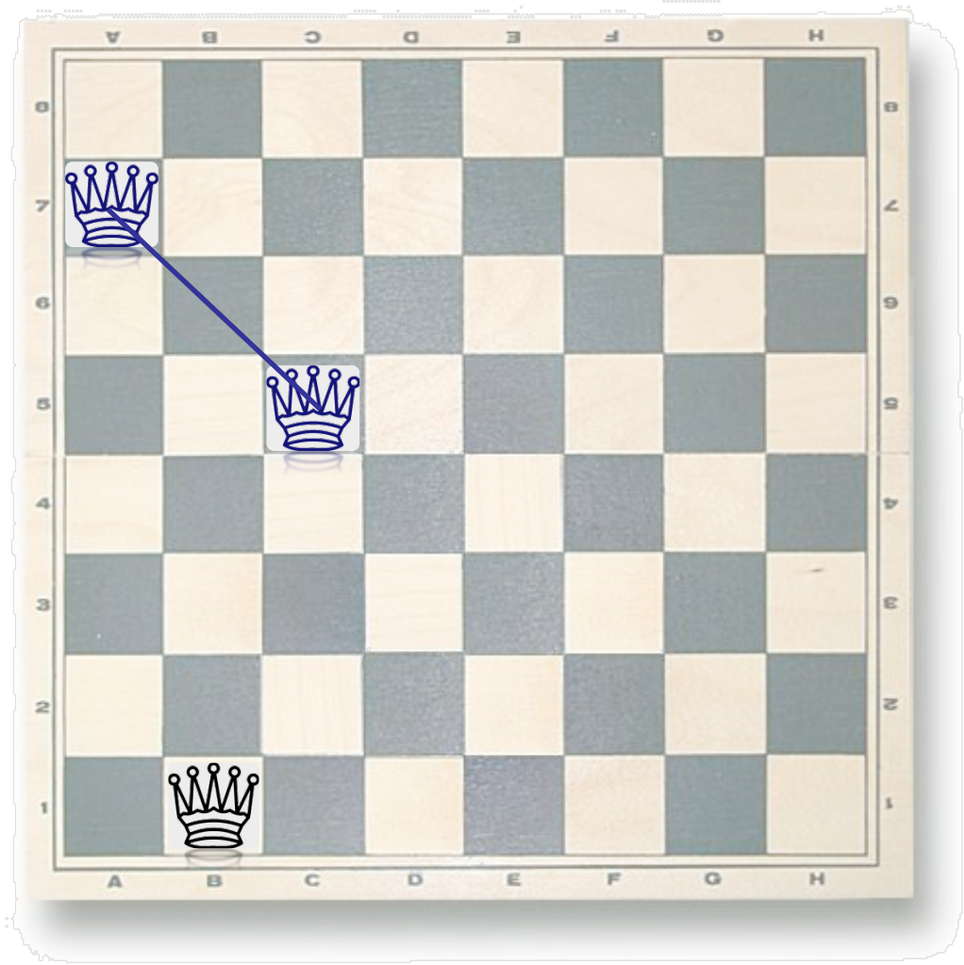
ask(2, 8, 4, 2, -, -, -, -) = No

Partial queries



ask(2, 8, -, -, -, -, -, -) = Yes

Partial queries



ask(2, 8, 4, -, -, -, -, -) = No

Partial queries

- The number of queries required to find the target concept is in:

$$O(|C_T| \cdot (\log |X| + |\Gamma|))$$

- The number of queries required to converge is in:

$$O(|B|)$$

QUACQ needs more than **8000** queries to learn the Sudoku model

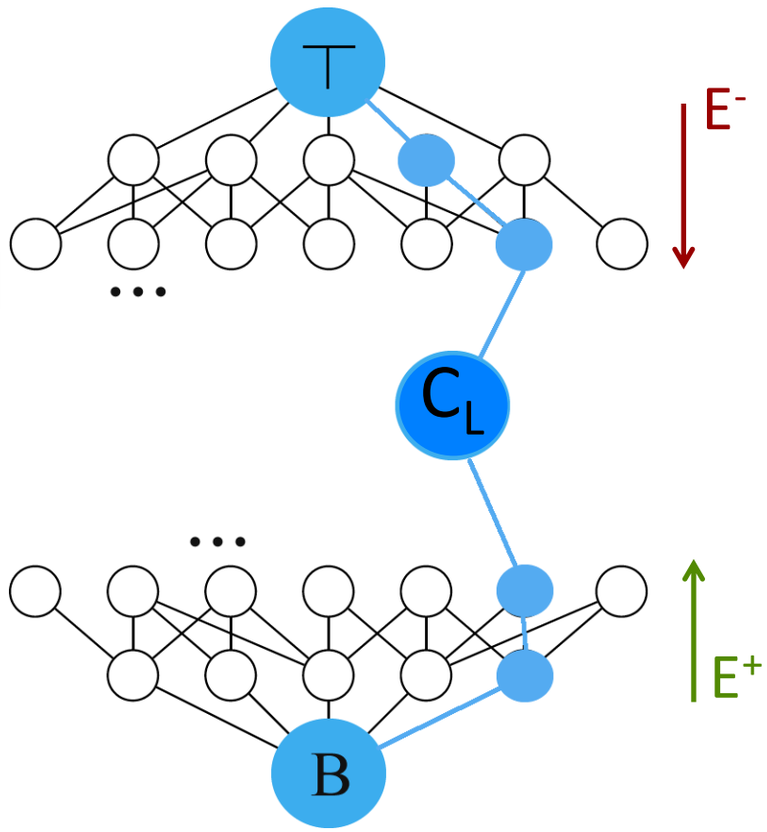
Limitations

- Too many queries to generate a model
  - More than 8000 queries for generating a SUDOKU model
- To overcome the limitation:
  - Either elicit more knowledge when asking queries to the user
  - Or learn structured problems

- Constraint acquisition works learning only binary constraints otherwise the bias would grow exponentially

Acquisition via more complex queries

- Matchmaker agents [Freuder and Wallace wAAAI97]
- Argument-Based CONACQ [Friedrich et al.09]
- ILP-Based Acquisition [Lallouet et al. 10]



Matchmaker agents

- Matchmaker agents are based on the Constraint Acquisition and Satisfaction Problem (CASP) paradigm

- Two agents: the solver and the customer
  - The customer knows the problem but not so explicitly that it can tell the solver outright
  - The solver suggests solutions based on the constraints it knows about
  - The customer then gives the solver the complete set of constraints violated by the last solution

Goal: limit the number of interactions

Matchmaker agents

Goal: limit the number of interactions

Two strategies:

SATISFACTION STRATEGIES

- Try to find solutions that satisfy additional constraints w.r.t. the ones known by the solver

VIOLATION STRATEGIES

- Try to find solutions that violate most the constraints

Eugene C. Freuder, Richard J. Wallace: Suggestion Strategies for Constraint-Based Matchmaker Agents. International Journal on Artificial Intelligence Tools 11(1): 3-18 (2002)

Argument-based acquisition

- Argumentation based learning generates a logical theory C based on a set of arguments ARC provided by an domain expert
- An argument *arg* is a set of constraints
- We have positive, negative, too strong, necessary, sufficient, too weak arguments
- Implementation based on
  - QUICKXPLAIN finding the minimal conflict set
  - HD-TREE: breadth first search to find all min conflict sets + hitting set

Argument-based acquisition

- The constraint acquisition algorithm continues to generate solutions until all the constraints in the given bias are fixed.
- Three stages:
  - generation of an example
  - validation of the solution by an expert
  - learning of the version space

K Schekotihin, G.Friedrich Argumentation Based Constraint Acquisition IEEE Int.Conf on Data Mining 2009

ILP-based acquisition

Use ILP to learn the model

- Search state = conjunction of litterals (clause)
- A rule r covers an example e if there exists σ such that σ(r) ⊆ e

- State evaluation = number of covered positive examples, number of negative examples rejected, size of the conjunction, etc.

- Search for a rule using classical ILP techniques (separate and conquer)
- Bidirectional search

ILP-based acquisition

$$
\begin{array}{rcl}
spec & ::= & rule \mid spec \wedge spec \\
rule & ::= & \forall\ variables:\ body \rightarrow head \\
variables & ::= & vs \in \texttt{DOMAIN} \mid variables, variables \\
vs & ::= & \texttt{VARIABLE} \mid vs, vs \\
body & ::= & \texttt{BODY\_ATOM} \mid body \wedge body \\
head & ::= & \texttt{HEAD\_ATOM} \mid \neg\texttt{HEAD\_ATOM} \mid head \vee head
\end{array}
$$

Arnaud Lallouet, Matthieu Lopez, Lionel Martin, Christel Vrain:
On Learning Constraint Problems. ICTAI (1) 2010: 45-52

ILP-based acquisition

$$\forall Q1, Q2 \in \mathit{Queens},\ \forall X1, X2, Y1, Y2 \in \mathit{Int}\ :$$
$$\mathit{position}(Q1, X1, Y1) \wedge \mathit{position}(Q2, X2, Y2)$$
$$\rightarrow Q1{=}Q2 \vee X1{\neq}X2$$
$$\bigwedge$$
$$\forall Q1, Q2 \in \mathit{Queens},\ \forall X1, X2, Y1, Y2 \in \mathit{Int}\ :$$
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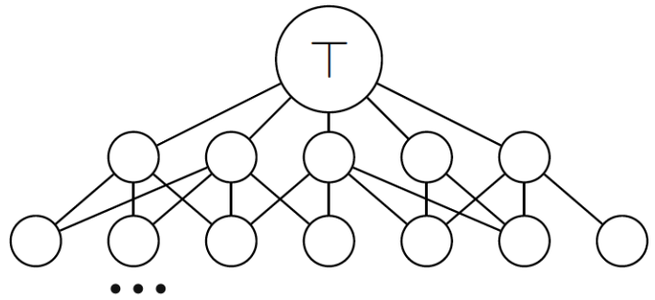
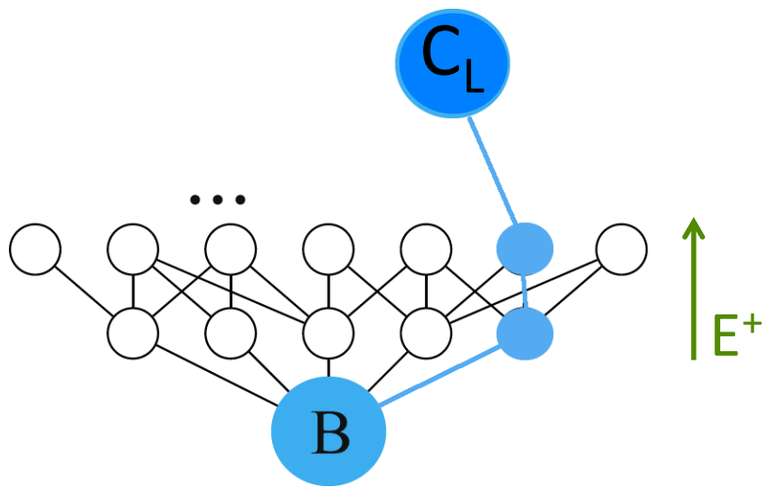
$$\mathit{position}(Q1, X1, Y1) \wedge \mathit{position}(Q2, X2, Y2)$$
$$\mathit{ecart}(X1, X2, L1) \wedge \mathit{ecart}(Y1, Y2, L2) \rightarrow Q1{=}Q2 \vee L1{\neq}L2$$

Structured problem acquisition: ModelSeeker

- ModelSeeker [Beldiceanu and Simonis, CP11'12]
  - Generates constraint models for structured problems from positive examples
  - Based on global constraint catalogue (≈1000)
  - Buttom-up search
  - ModelSeeker learns constraints underlying the scheduling of the Bundesliga (the German Football Liga) from a single example schedule.

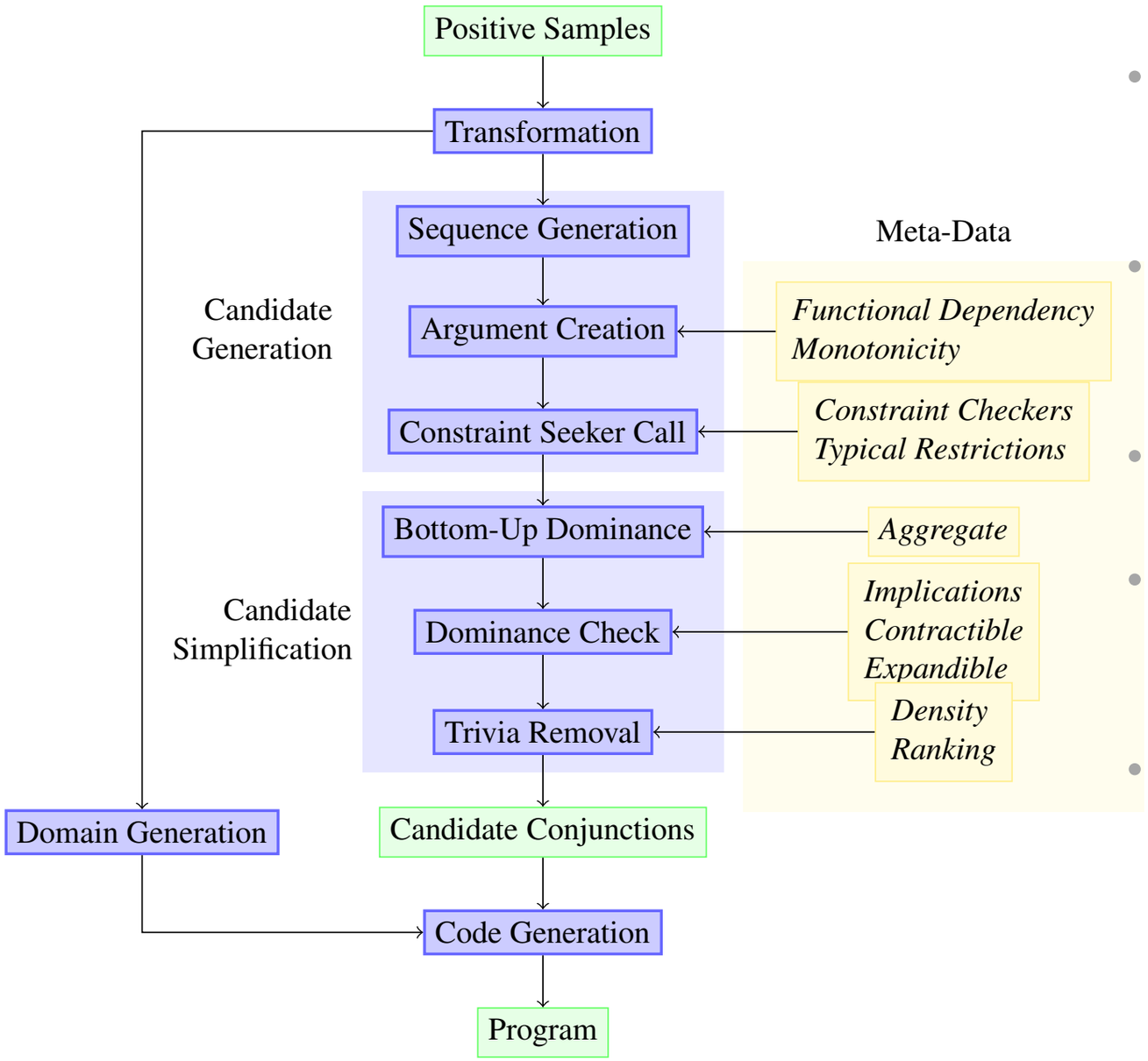




1						5	2	
				7	8			
						6		
	9			4				
			5			1		
	7							
		6	2					
	4						7	8
								3

2	4	9			3			
	8			1	2	4		
						9		
						7	2	4
	1						3	
3	9	4						
		8						
		6	4	5			9	
			1			8	6	5

Structured problem acquisition: ModelSeeker



- Transformation: transforms inputs in suitable representations
- Sequence generation: transforms vars in regular sets
- Argument creation: creates patterns
- Constraint Seeker: finds matching constraints using the catalogue
- The following three steps reduce the set of constraints that are output of the previous step

Embedding an ML model into a combinatorial model

Aimed at learning models in the general form:

$$\begin{aligned} \min z = x_0 \qquad & (\mathbf{P2}) \\ \text{subject to: } \pi_i(\vec{x}) \qquad & \forall i \in I \\ \nu_m(\vec{x}_{m,in}, \vec{x}_{m,out}) \qquad & \forall m \in M \\ \vec{x} \in D_{\vec{x}} \end{aligned}$$

- where $\vec{x}$ are problem variables, $D_{\vec{x}}$ their domain and x_0 is the variable representing the objective value, $\pi_i(\vec{x})$ are problem constraints (predicates) and $\nu_m(\vec{x}_{m,in}, \vec{x}_{m,out})$ is a proper encoding of a machine learning model in the hosting language

Motivating example problem: traffic light placement

- Add/remove traffic light over a whole city
- Traffic lights can be connected (green wave)
- Every operation has a cost (and there is a budget)
- Probably other constraints (not considered)
- Improve traffic figures

HP: we want to solve it! What is the toughest obstacle?

An example problem: traffic light placement

- Add/remove traffic light over a whole city
- Traffic lights can be connected (green wave)
- Every operation has a cost (and there is a budget)
- Probably other constraints (not considered)
- Improve traffic figures

HP: we want to solve it! What is the toughest obstacle?

Assessing the effect of traffic light placement on the traffic levels:

Impossible via expert-designed declarative models

Human behaviour – complex system

Assessing the effect of traffic light placement on the traffic levels

Traffic light placement: decidables

Traffic levels: observables

WE WANT TO LEARN THE IMPACT OF DECIDABLES ON OBSERVABLES

and

CAST THIS INTO AN OPTIMIZATION MODEL

A second example: policies for PV adoption

- Given a target of PV adoption to be achieved
- Decide which incentives to give
- Every incentive has a cost (and there is a budget)
- Probably other constraints (not considered)

HP: we want to solve it! What is the toughest obstacle?

A second example: policies for PV adoption

- Given a target of PV adoption to be achieved
- Decide which incentives to give
- Every incentive has a cost (and there is a budget)
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HP: we want to solve it! What is the toughest obstacle?

Assessing the effect of incentives on PV adoption:

Impossible via expert-designed declarative models

Human behaviour – Social Dynamics

Assessing the effect of incentives on PV adoption

Incentives: decidables

PV adoption levels: observables

WE WANT TO LEARN THE IMPACT OF DECIDABLES ON OBSERVABLES

and

CAST THIS INTO AN OPTIMIZATION MODEL

A third example: thermal-aware workload dispatching

- Given a target heterogeneous platform and a workload
- Decide workload (tasks) dispatching
- Every task has a thermal dynamics (and there is a thermal controller)
- Load balancing constraints
- **With thermal limits**

A third example: thermal-aware workload dispatching

- Given a target heterogeneous embedded platform and a workload
- Decide task allocation and scheduing
- Every task has a thermal dynamics (and there is a thermal controller)
- Probably other constraints (not considered)

HP: we want to solve it! What is the toughest obstacle?

A third example: thermal-aware workload dispatching

- Given a target heterogeneous embedded platform and a workload
- Decide task allocation and scheduing
- Every task has a thermal dynamics (and there is a thermal controller)
- Probably other constraints (not considered)

HP: we want to solve it! What is the toughest obstacle?

Assessing the effect of workload allocation on thermal dynamics:

Possible with simulation based on differential equations of the thermal dynamics BUT not manageable by combinatorial optimization techniques

Assessing the effect of workload allocation on thermal dynamics:

Workload allocations: decidables

Core temperatures: observables

WE WANT TO LEARN THE IMPACT OF DECIDABLES ON OBSERVABLES

and

CAST THIS INTO AN OPTIMIZATION MODEL

What do these problems have in common?

A strong combinatorial structure

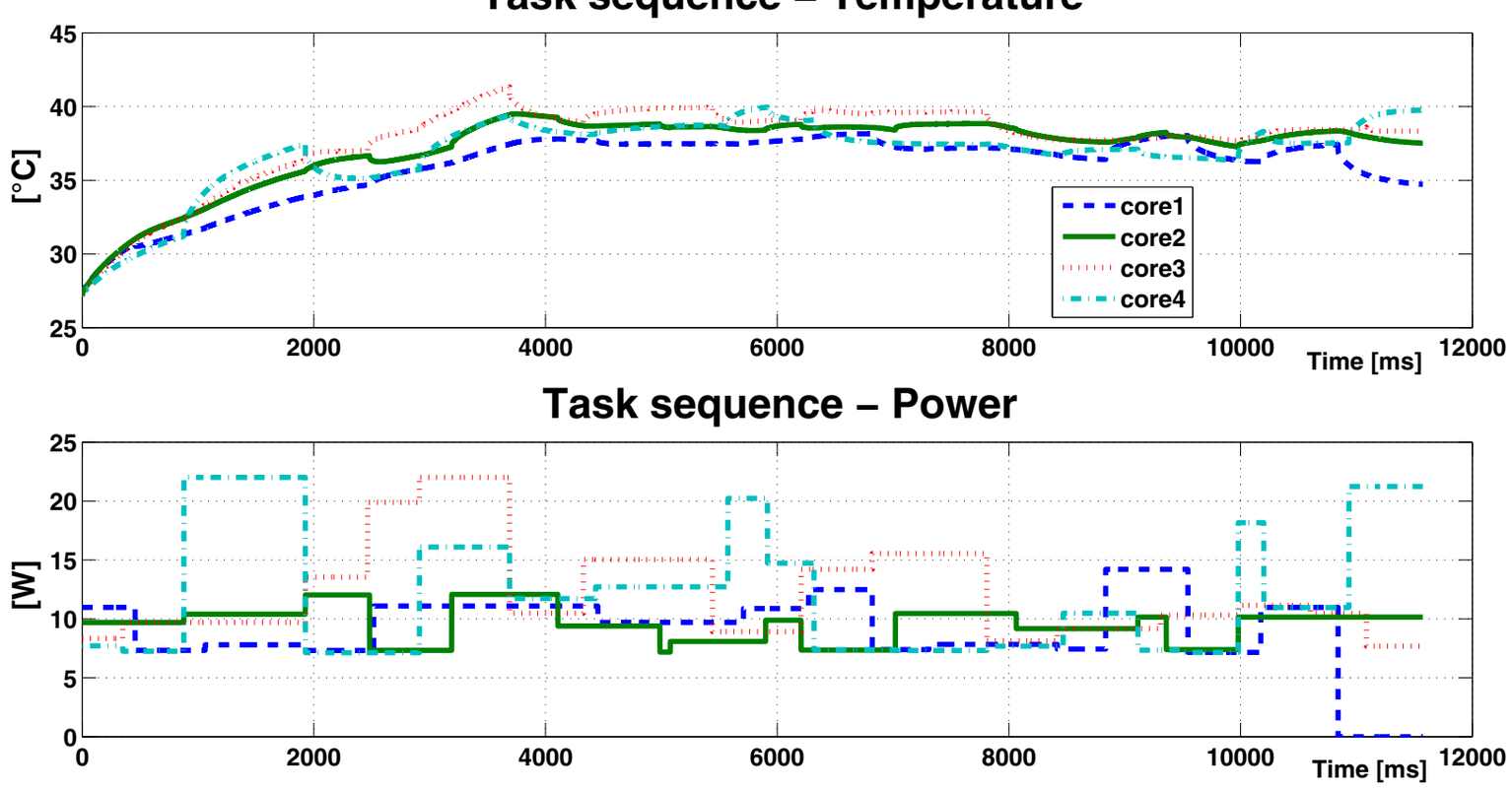
Part of the problem is not easily described through a manageable declarative model

Decisions influence predictions and vice versa

We have access to problem data (historical, simulated, real) to create a training set

Empirical Model Learning - EML

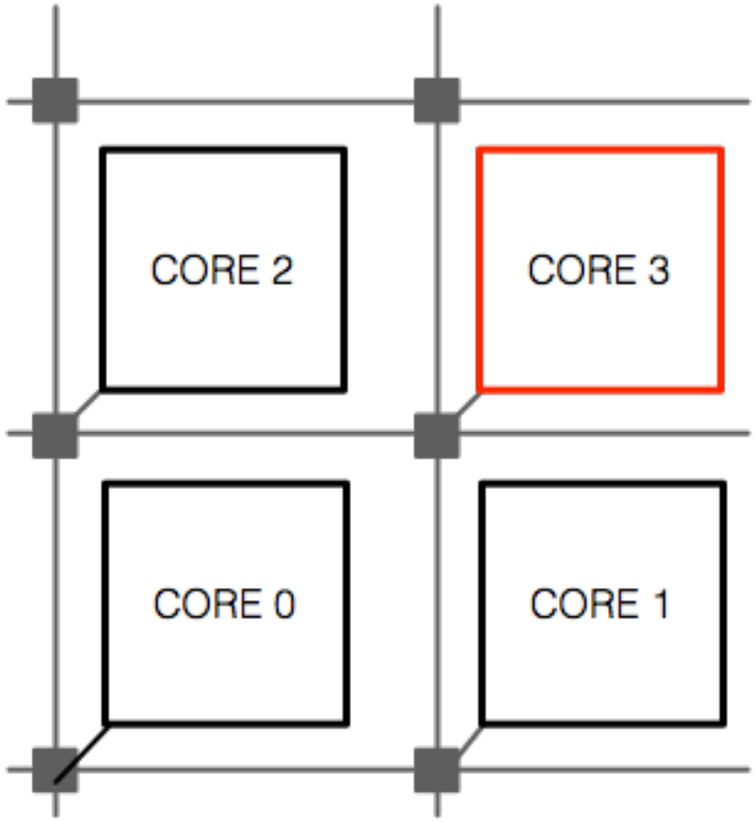
- Start from a set of observations extracted from runs on a real system
  - Sample the allocation space by running the system with different inputs of workload dispatching
  - Produce a training set

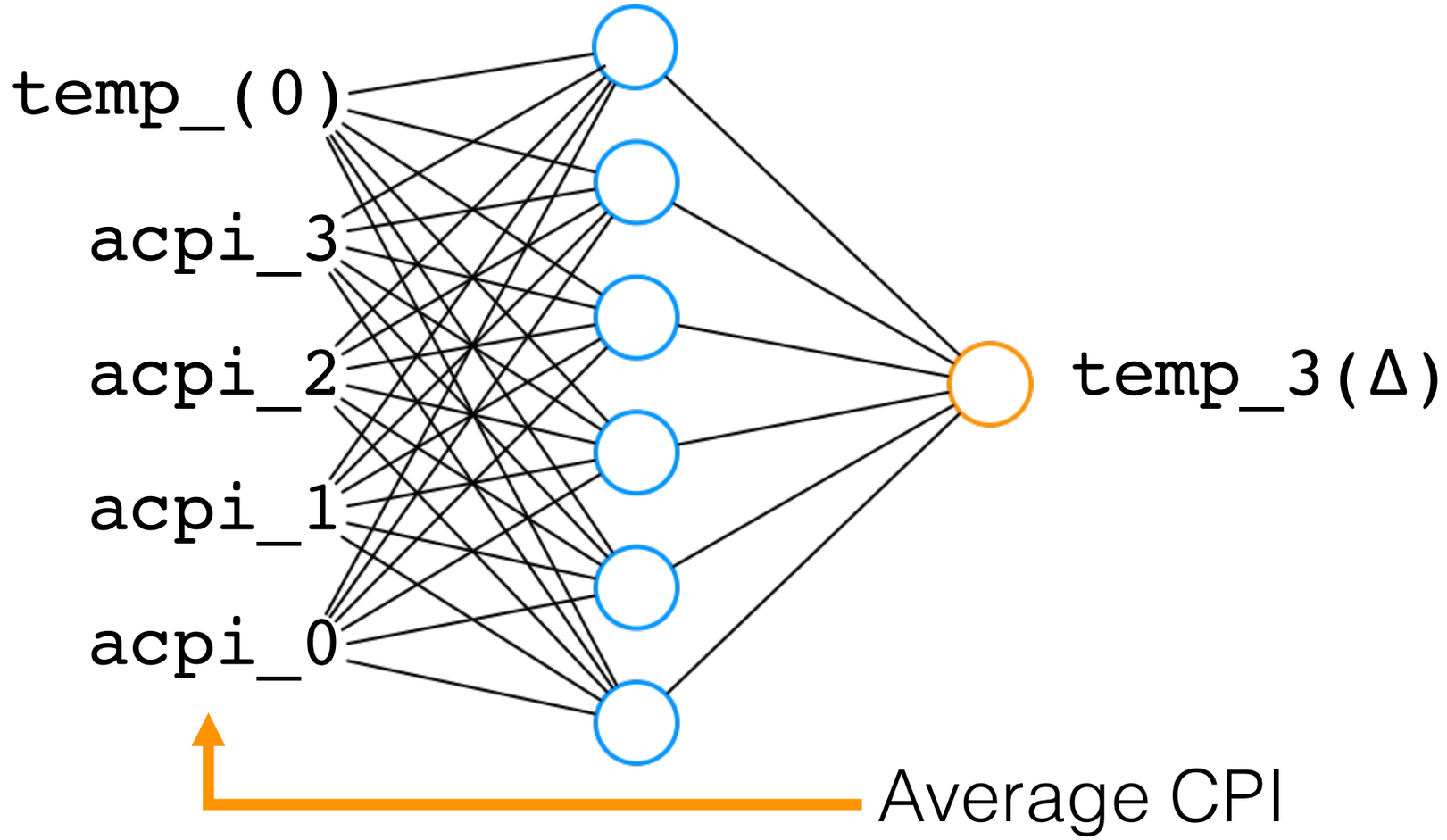


Empirical Model Learning - EML

- Start from a set of monitoring data from the real system:
- Learn an approximate function via Machine Learning

$$f\text{: dispatching} \longrightarrow \text{temperature}$$





Empirical Model Learning - EML

- Start from a set of observations
- Learn an approximate function via Machine Learning
- Embed this "empirical model" inside an optimization model

$$\min z = f(\vec{y})$$

subject to: $\vec{y} = g(\vec{x})$

all manner of complex constraints

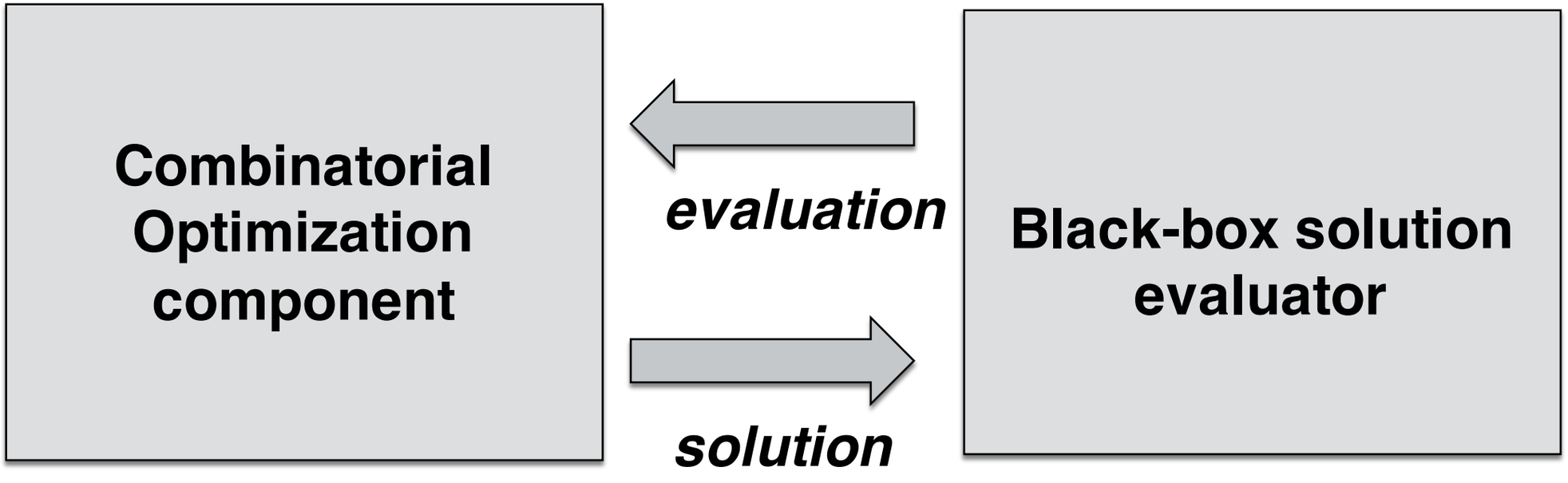
$$\vdots$$

In principle……

we can have a combinatorial problem solver

and a black box tool to test the solution

Can be very expensive



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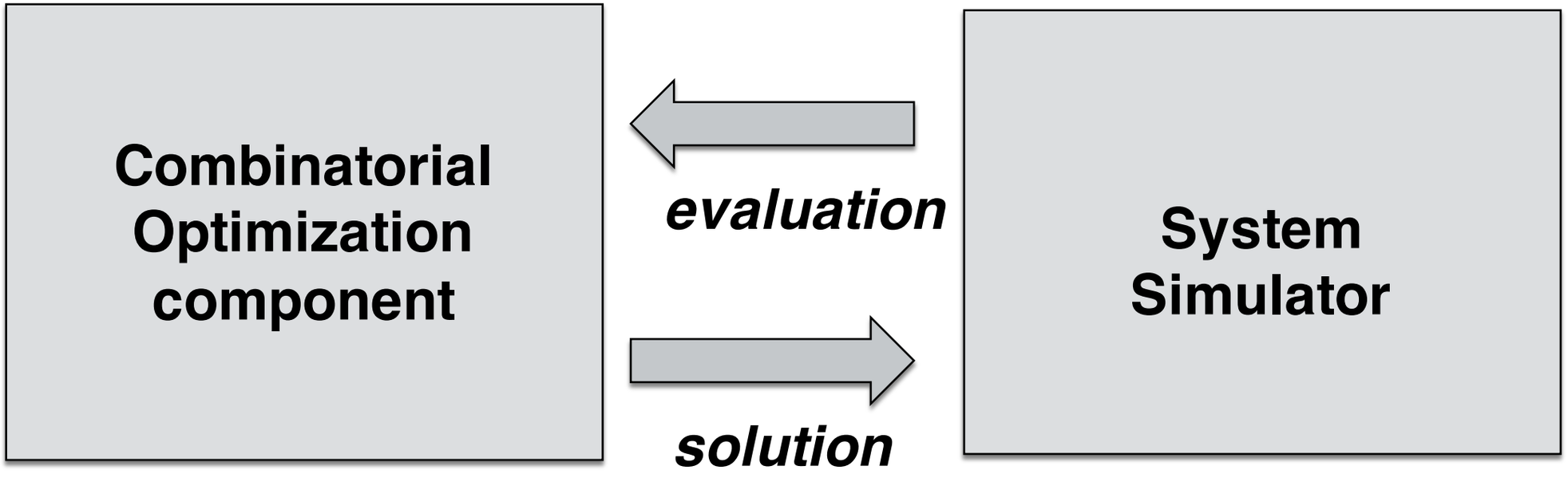

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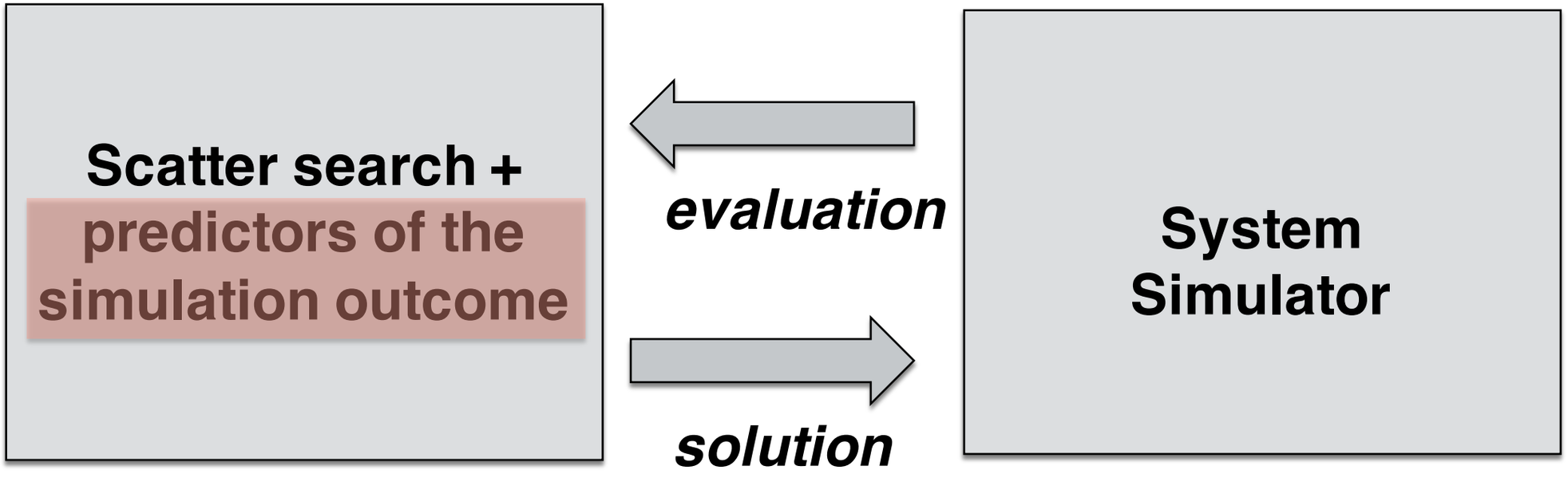


Note: these predictors enable a selection of solutions to be sent to the simulator

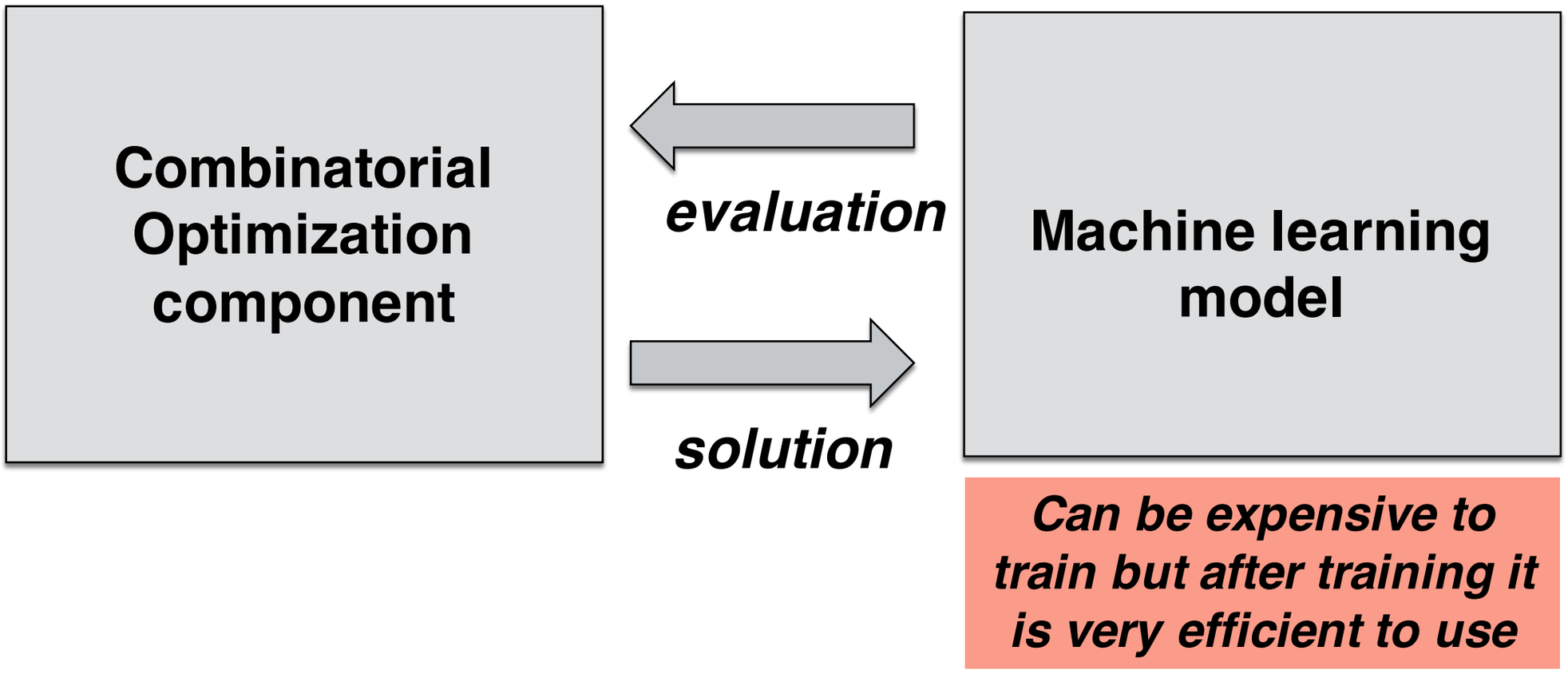
[OptQuest M. Laguna, 2011]

In principle……

we can have a combinatorial problem solver

and a black box tool to test the solution

What if the black box tool is a machine learning model?



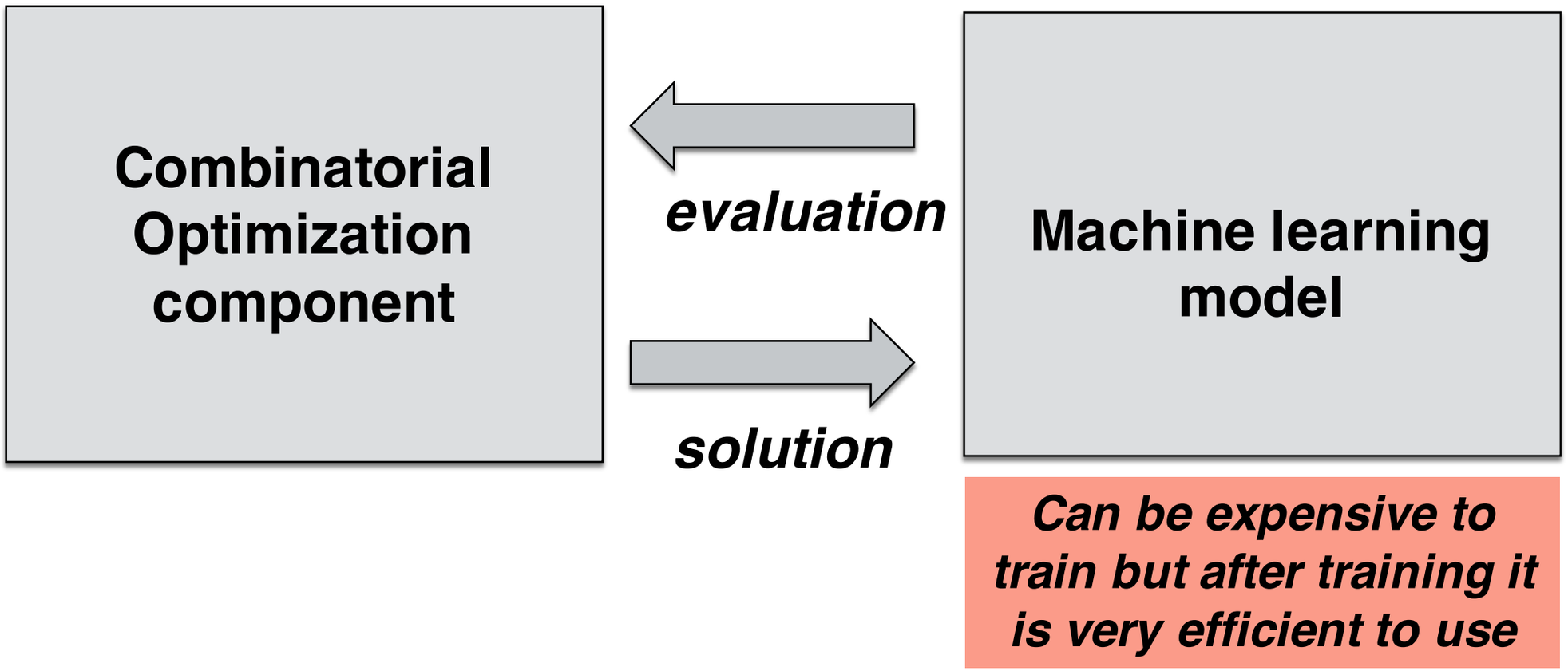
Surrogate models: [Henao, Maravelias, AIChE 2011], [Cozad, Sahinidis, Miller, 2014]

In principle……

we can have a combinatorial problem solver

and a black box tool to test the solution

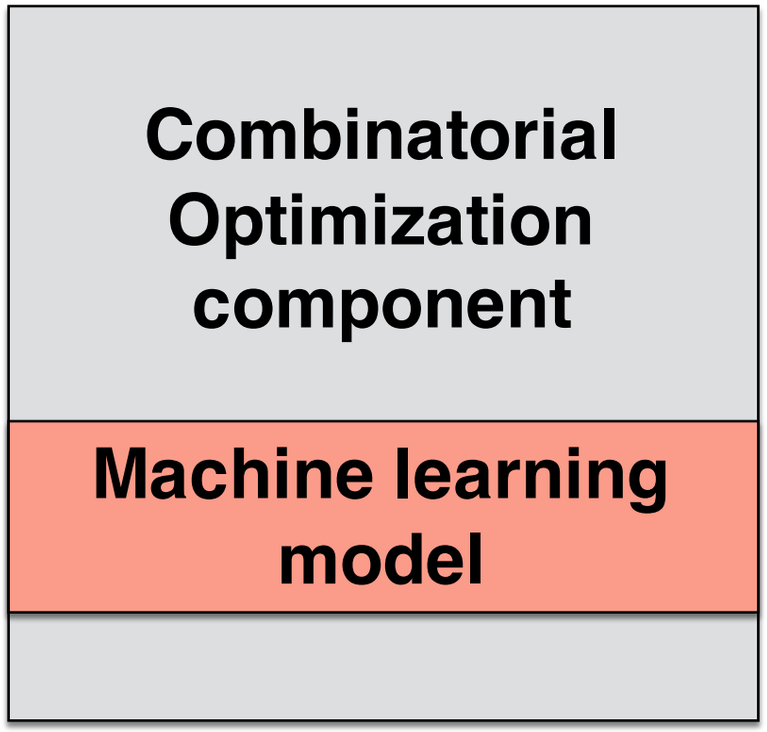
What if the black box tool is a machine learning model?



Still….. a generate and test mechanism

Empirical Model Learning – EML

In EML the learned model is embedded into the optimization component and used to actively reduce the search space during execution



Empirical Model Learning – EML

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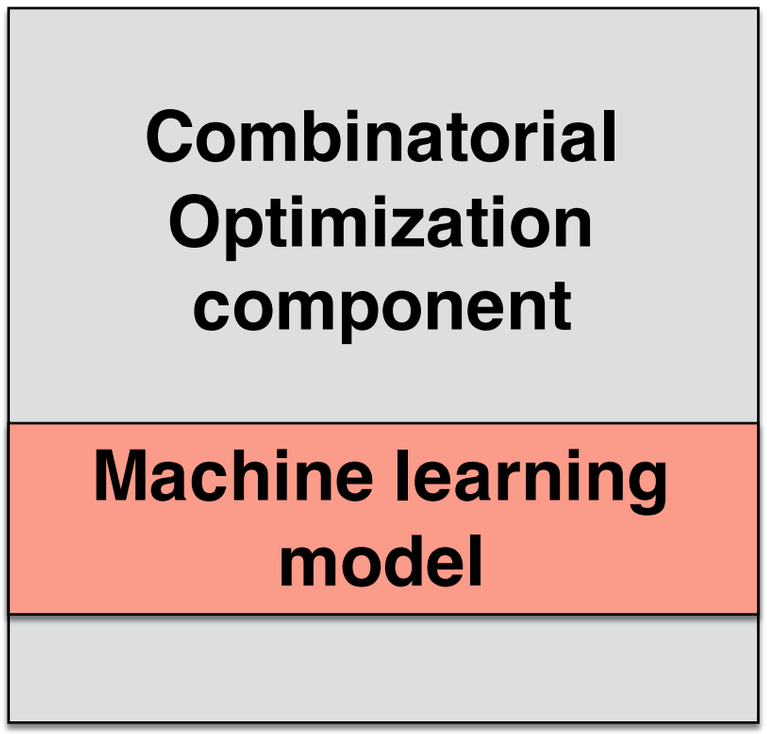


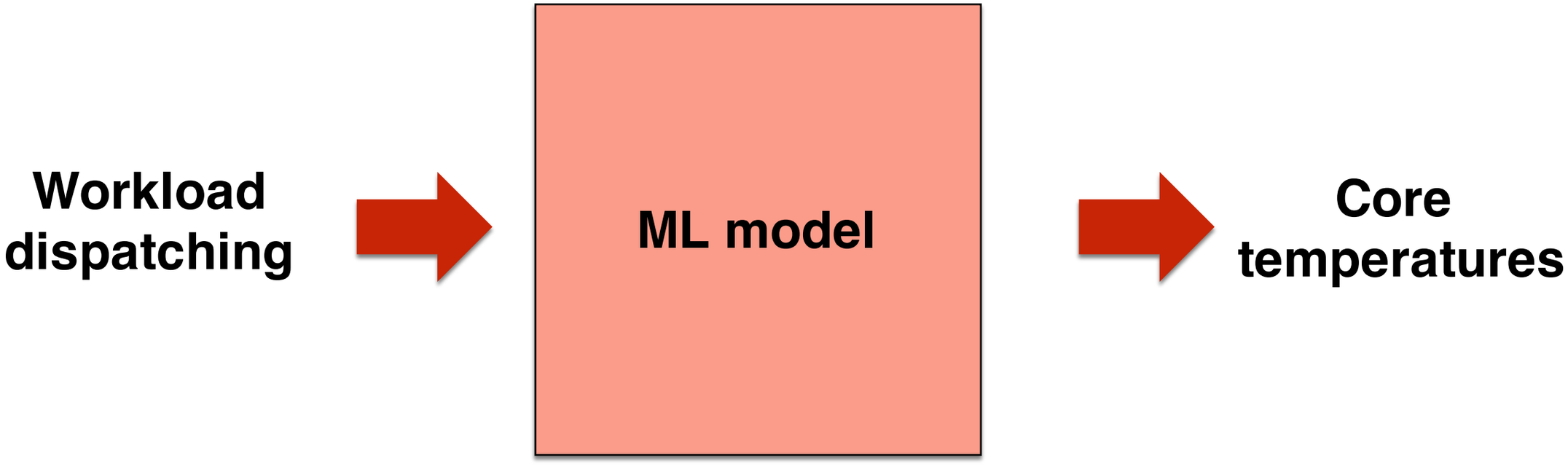
Not limited to objective functions, but also constraints and any relation between decidables and observables

Lombardi, Milano, Bartolini, Empirical Decision Model Learning, AIJ (244), 2017

Empirical Model Learning – EML

What is the difference between EML and the traditional use of ML models?

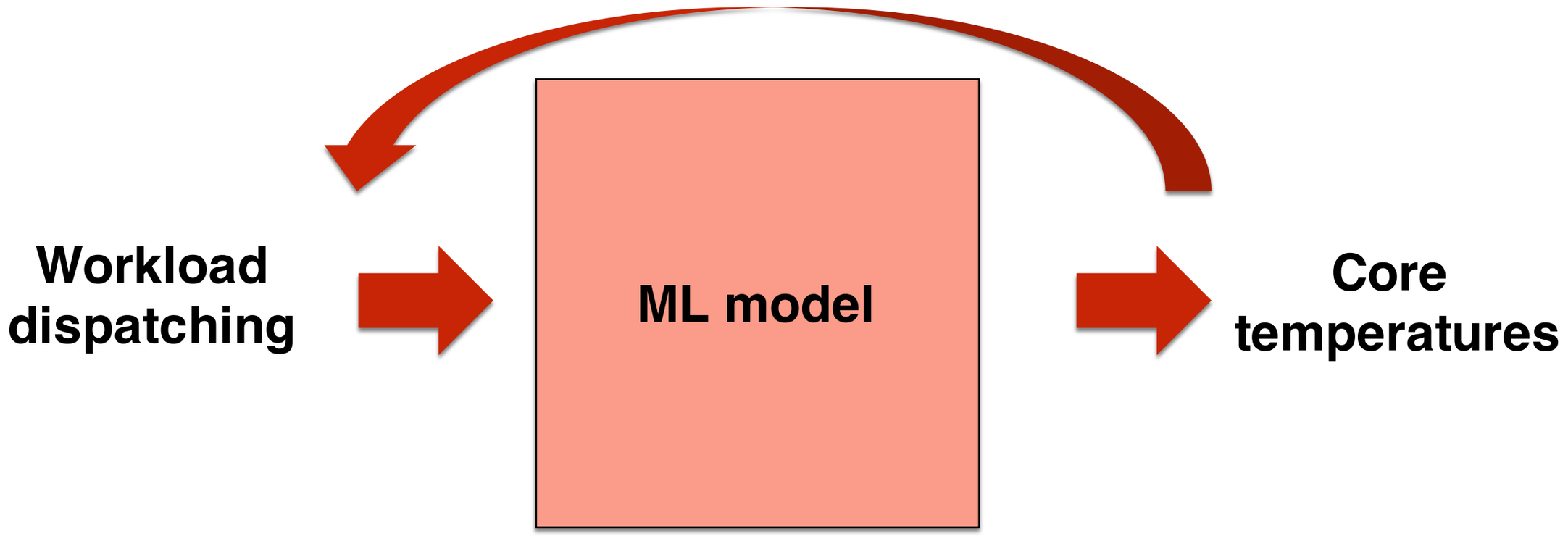
Traditional approaches work forward



Empirical Model Learning – EML

What is the difference between EML and the traditional use of ML models?

EML works forward and backward



The ML model becomes a constraint: given temperature limits we remove combinations of workload decisions that lead to inconsistent temperatures

Thermal-aware workload dispatching

COMBINATORIAL COMPONENT

Given n tasks m cores

$\sum_j \sum_i x_{ij} = 1$

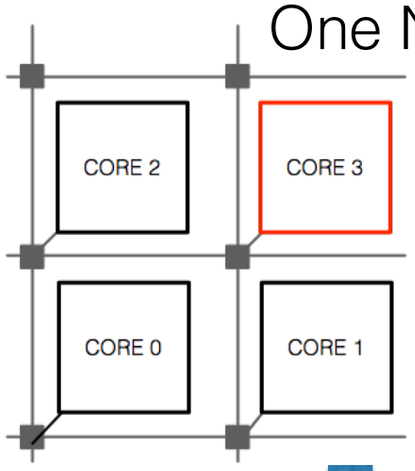
$\sum_i x_{ij} = n/m$ Load balancing

Other constraints (e.g. scheduling)

x_{ij} is 1 if task i is allocated on core j

MACHINE LEARNING MODEL

One NN per core



min (max $temp_j$)

$\sum_j \sum_i x_{ij} \leq 1$

$\sum_i x_{ij} = n/m$

EM(x, temp)

Other constraints (e.g. scheduling)

x_{ij} is 1 if task i is allocated on core j

Empirical Model Learning – EML

The questions are:

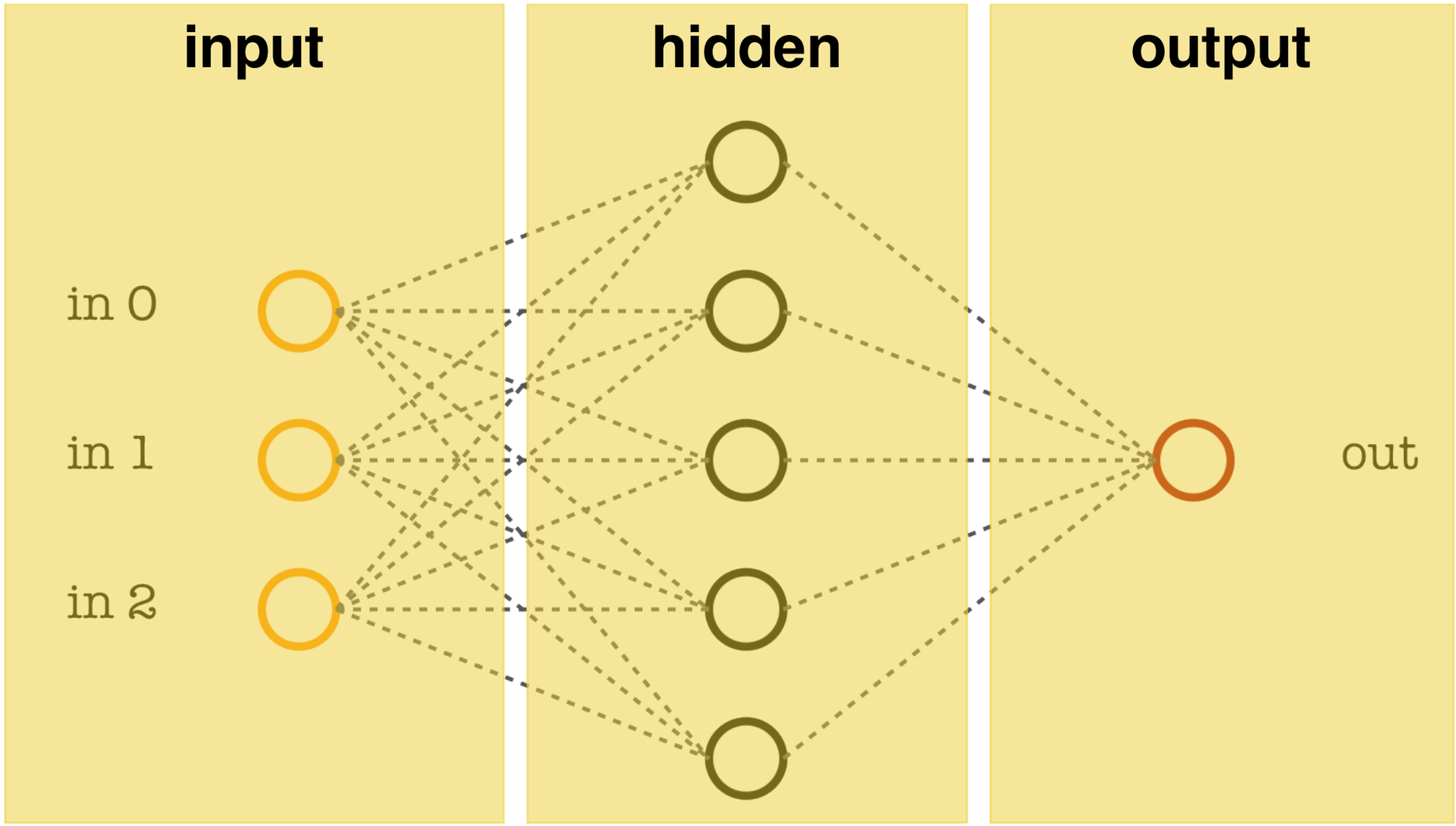
1) how do we embedded Machine learning models into a combinatorial model?
2) How do we provide operational semantics to these models so that they can actively prune the search space?

We will explore:

- Neural Networks
- Decision Trees

In different optimization techniques: CP in the talk, but also MINLP/ILP, SMT

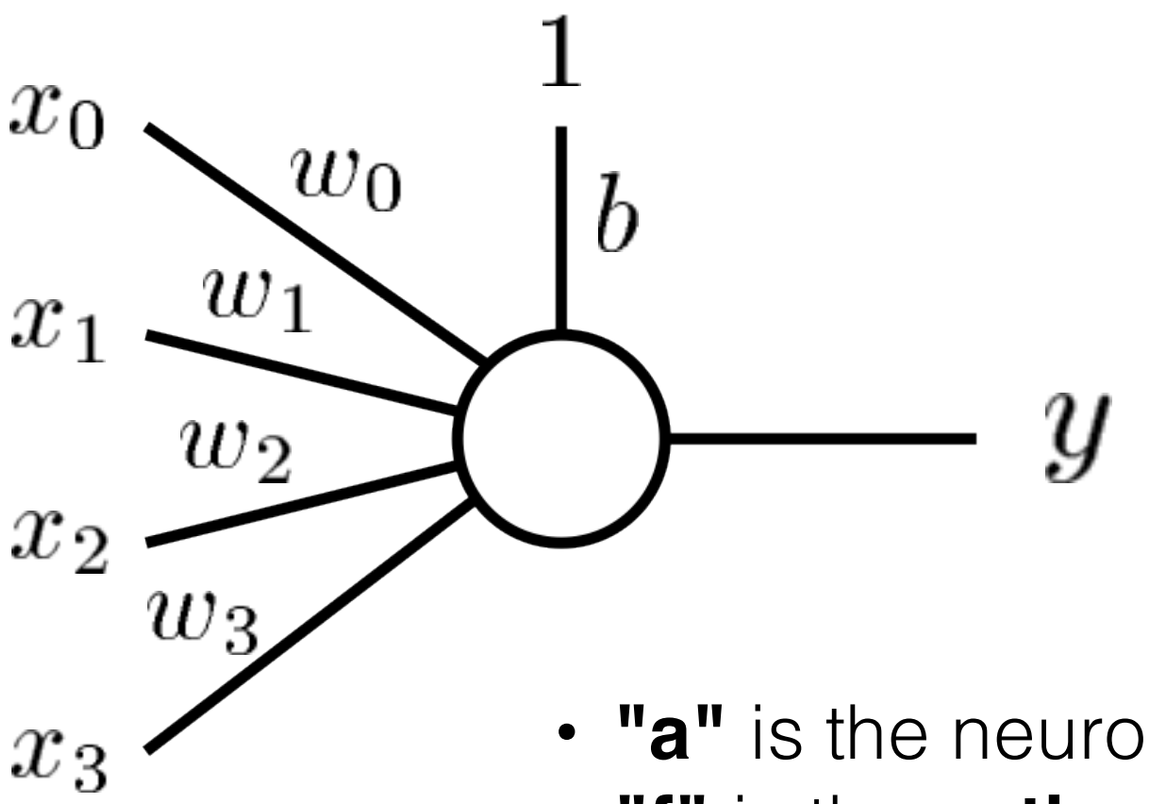
Artificial Neural Networks



- Computational model, consisting of parallel computation units (neurons) connected in a network structure
- Usually: no cycles (feed-forward) and multiple layers

Artificial Neural Networks

Artificial Neuron = scalar function with vector input



$$a = \sum_i w_i \cdot x_i + b$$

$$y = f(a)$$

- **"a"** is the neuron **activity**
- **"f"** is the **activation function**
- **weights** are obtained in the **learning phase**

The activation function is a **monotonic non-decreasing function** of the neuron activity

Bartolini, Lombardi, Milano, Benini, Neuron Constraints to Model Complex Real World Problems, CP2011.

Neural Networks in a Combinatorial Model

A Neural Network is a declarative (nonlinear) model

- Can be embedded in a MINLP model directly

1. We should insert variables for NN inputs and outputs in the model
2. Insert the NN non linear equations in the model

Neural Networks in a Combinatorial Model

A Neural Network is a declarative (nonlinear) model

- Can be embedded in a CP model via variables and constraints
- Here: **artificial neuron = a global "neuron constraint"**

```
act.function([X], Y, [W], b)
```

Input variables

Output variable

Weights

Bias

Structure of the Neuron Constraint

- An internal variable **A** for the neuron activity
- Bound consistency on the equality: $\mathtt{A} = \sum_i w_i \cdot \mathtt{X}_i + b$

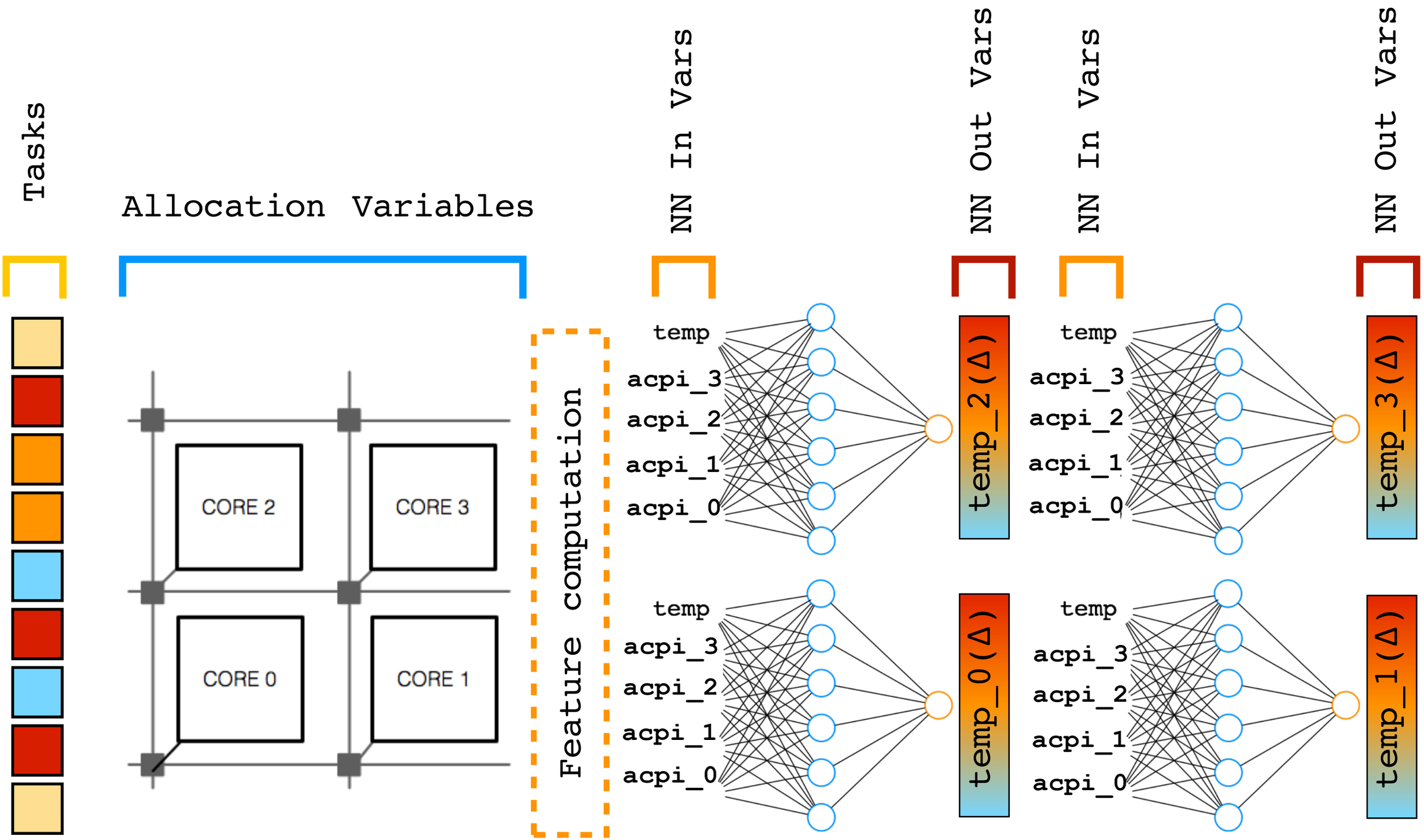
Filtering for the activation function:

1. $\max(\mathtt{A})$ updated $\Rightarrow \max(\mathtt{Y}) = f(max(\mathtt{A}))$
2. $\max(\mathtt{Y})$ updated $\Rightarrow \max(\mathtt{A}) = f^{-1}(\max(\mathtt{Y}))$

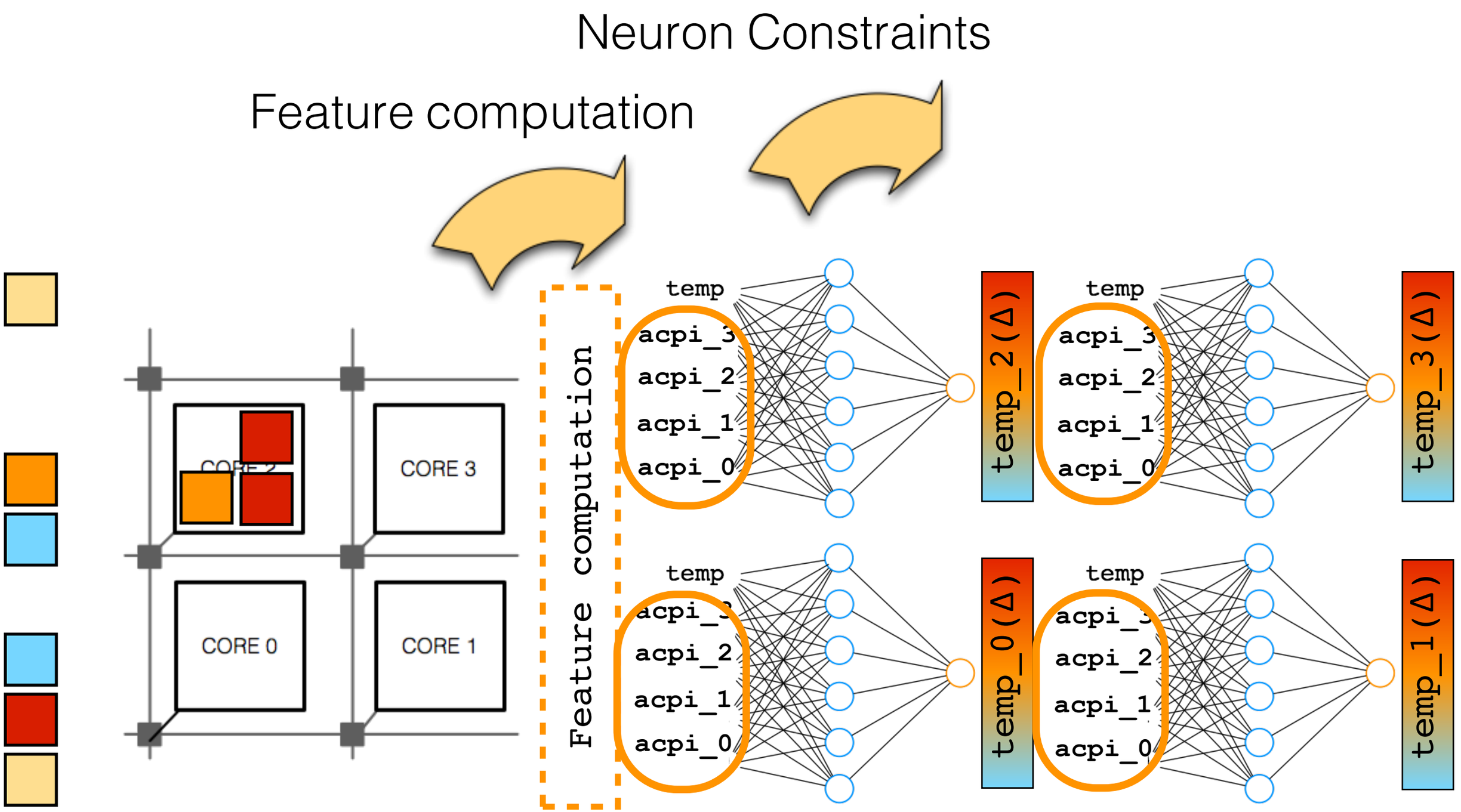
- Similar rules for minima
- The value $f^{-1}(max(\mathtt{Y}))$ is replaced by $\max\{a' \mid f(a') = \max(\mathtt{Y})\}$ to avoid precision errors
- Filtering from **Y** to **A** and from **A** to **Y**

We can combine many neuron constraints in a artificial neural network global constraint: **`ann(output, inputs)`**

How it works at search time



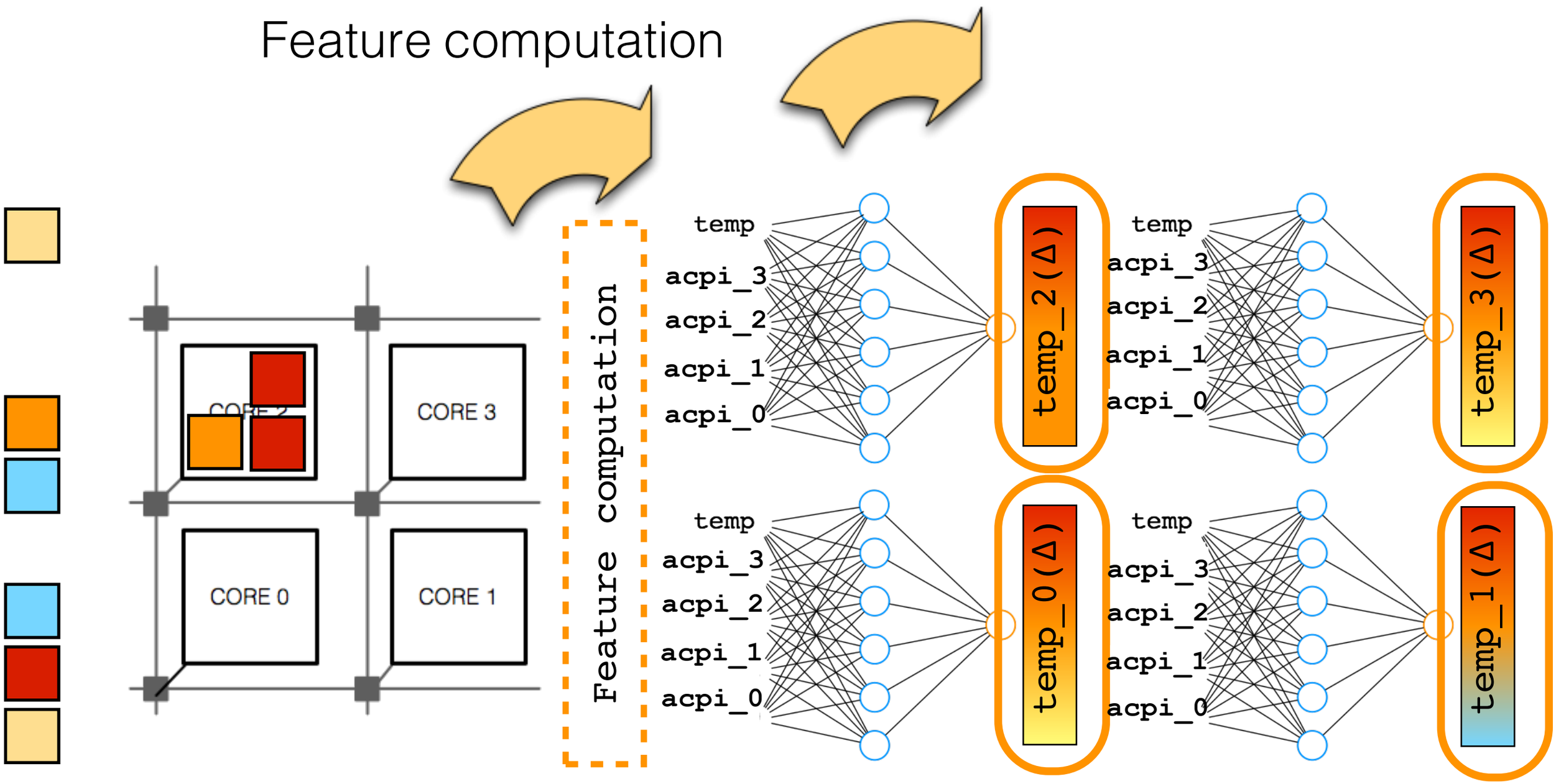
How it works at search time



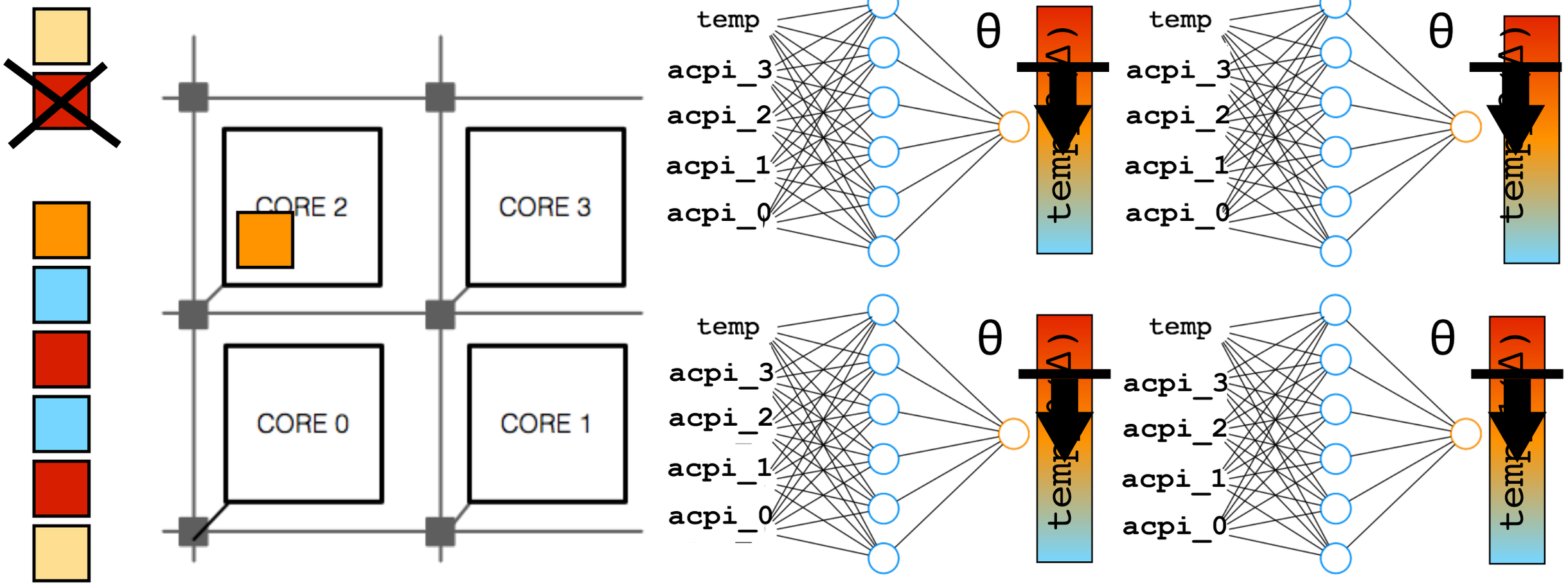
Forward Propagation

Neuron Constraints

Feature computation



Backward propagation



EML: CP model

Problem data:

- `n` tasks (with CPI values)
- Each task is assumed to run indefinitely
- `m` = 48 cores
- Room temperature

Decision variables:

$$\texttt{CORE}_\texttt{i} \in \{0..m-1\} \quad \forall t_i$$

Balancing constraints:

Roughly the same number of tasks per core

$$gcc([\texttt{CORE}_\texttt{i}], \{0..m-1\}, \lfloor {}^{n}/_{m} \rfloor, \lceil {}^{n}/_{m} \rceil)$$

EML: CP Model

Equivalent allocation variables:

$$\mathtt{X_{i,j}} = 1 \Leftrightarrow \mathtt{CORE_i} = j$$

Average CPI per core (FEATURE COMPUTATION):

$$average(\mathtt{ACPI_j}, [CPI_i], [\mathtt{X_{i,j}}|_{\mathtt{j=k}}]) \qquad \forall \text{ core } k$$

Neural Network: collection of act_function constraints

$$\mathtt{ann}_j(ctemp_j, ACPI_j, ACPI_{ngbr} \ldots, rtemp)$$

Objective:

$$\min \max_{j \in cores} ctemp_j$$

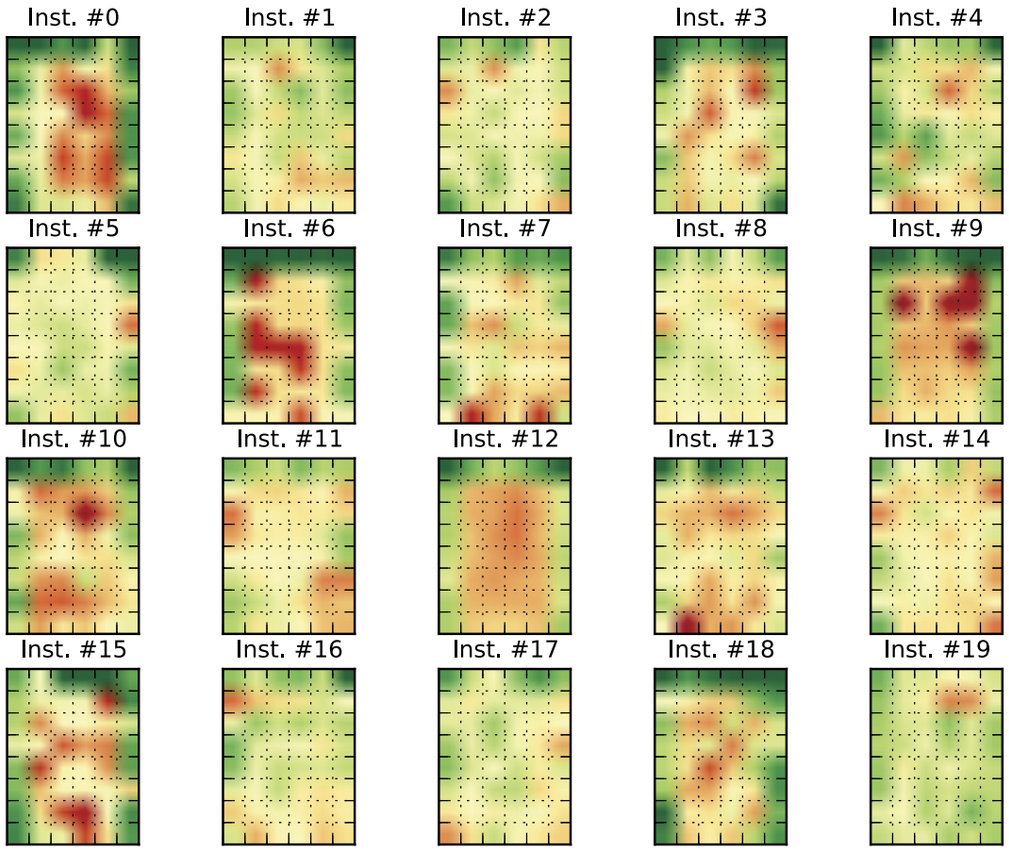
Bartolini, Lombardi, Milano, Benini, Optimization and Controlled Systems: A Case Study on Thermal Aware Workload Dispatching, AAAI 2012

Results

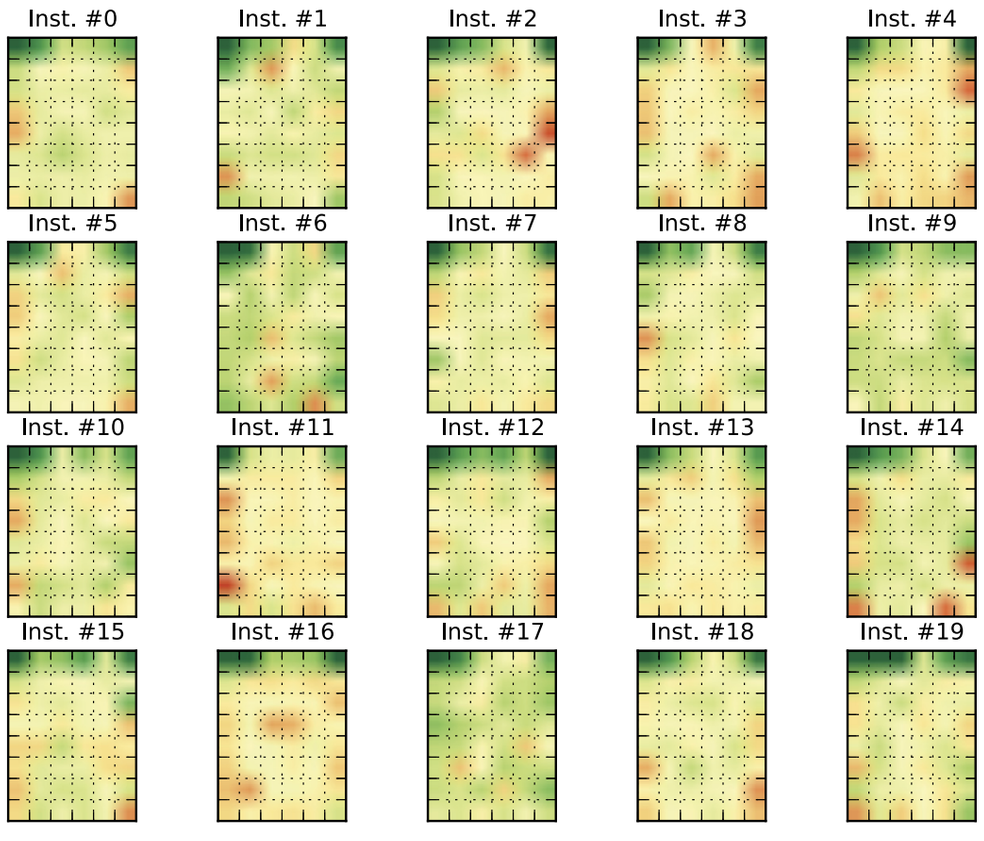
Solution Approach:

- Model solved via Large Neighborhood Search (LNS)
- First solution via a CPI balancing heuristic

Heat generated on the cores by MILP using an expert design model



Heat generated on the cores by the EML approach



How to cast a decision tree in a combinatorial model

Three encodings:

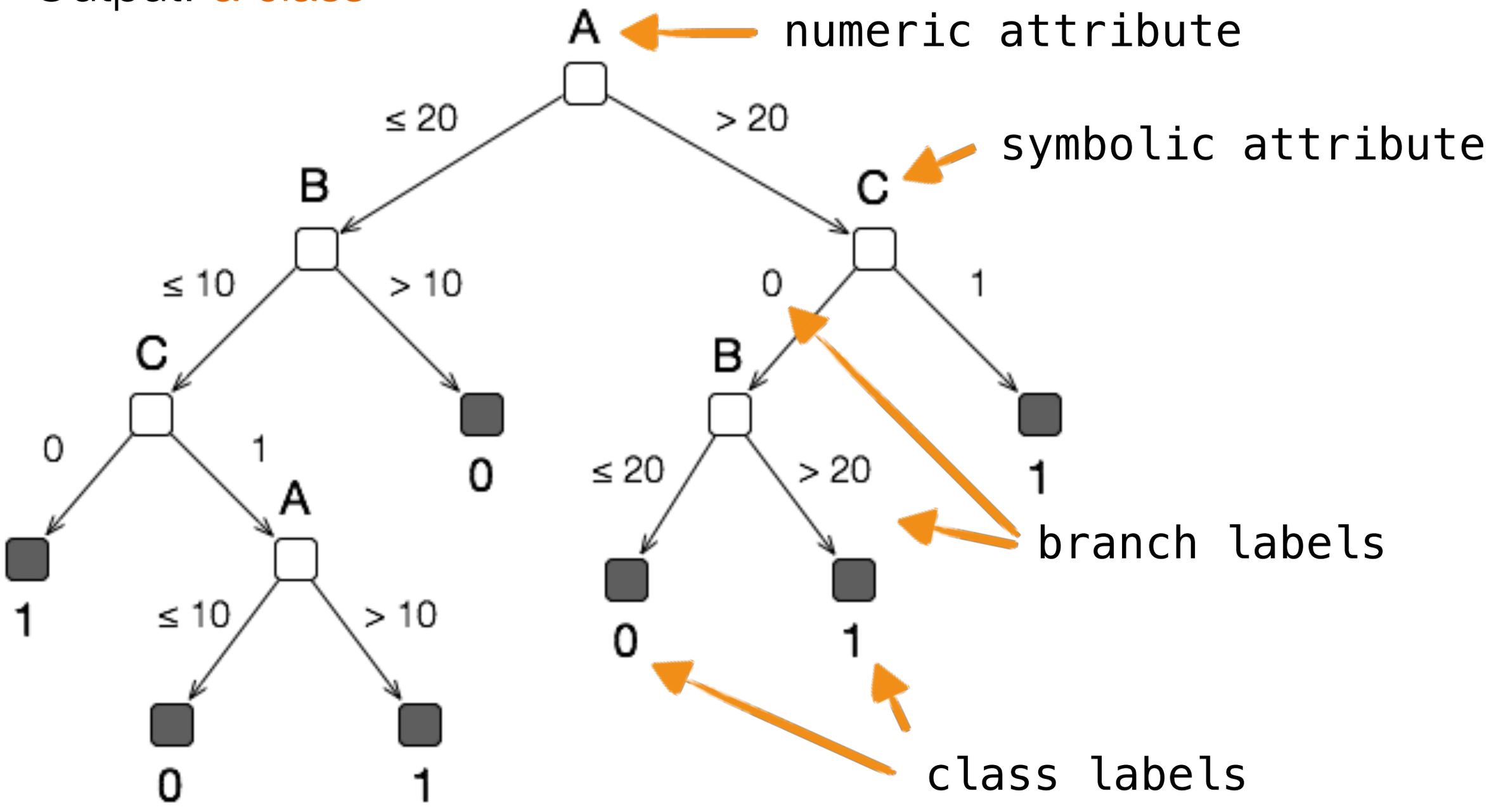
- Meta-constraints
- Table constraint
- Other encodings

Extension: Random Forests

Bonfietti, Lombardi, Milano: Embedding Decision Trees and Random Forests in CP, CPAIOR 2011

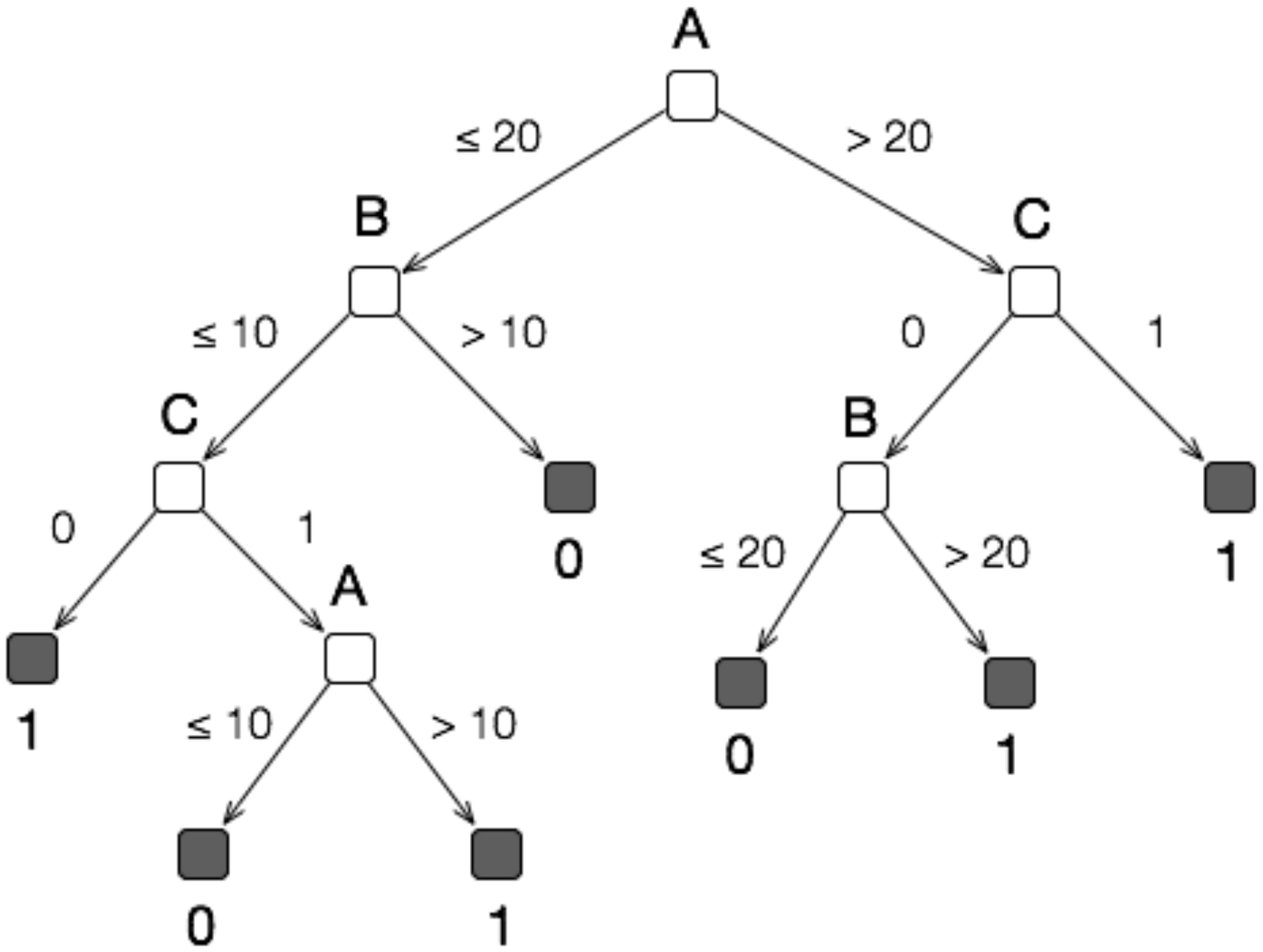
Decision Tree

- Input: tuple of attribute values
- Output: a class

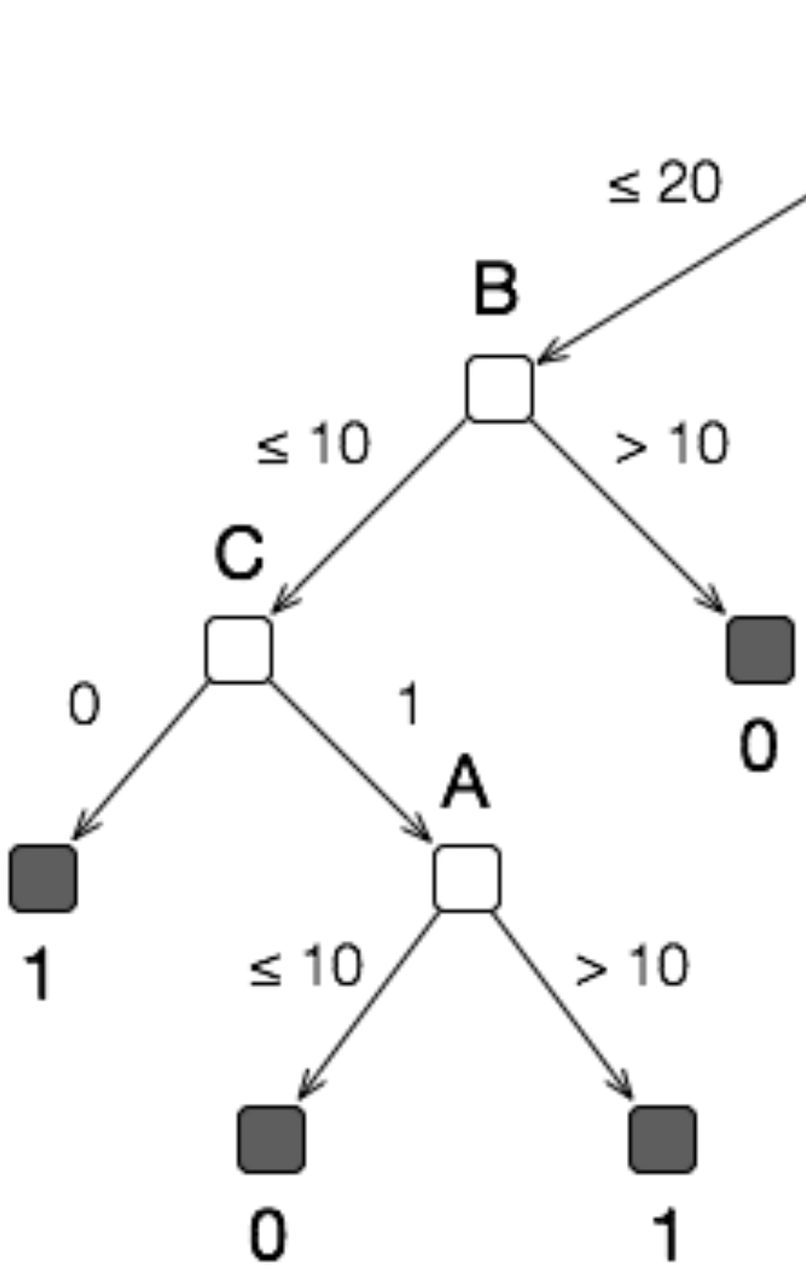


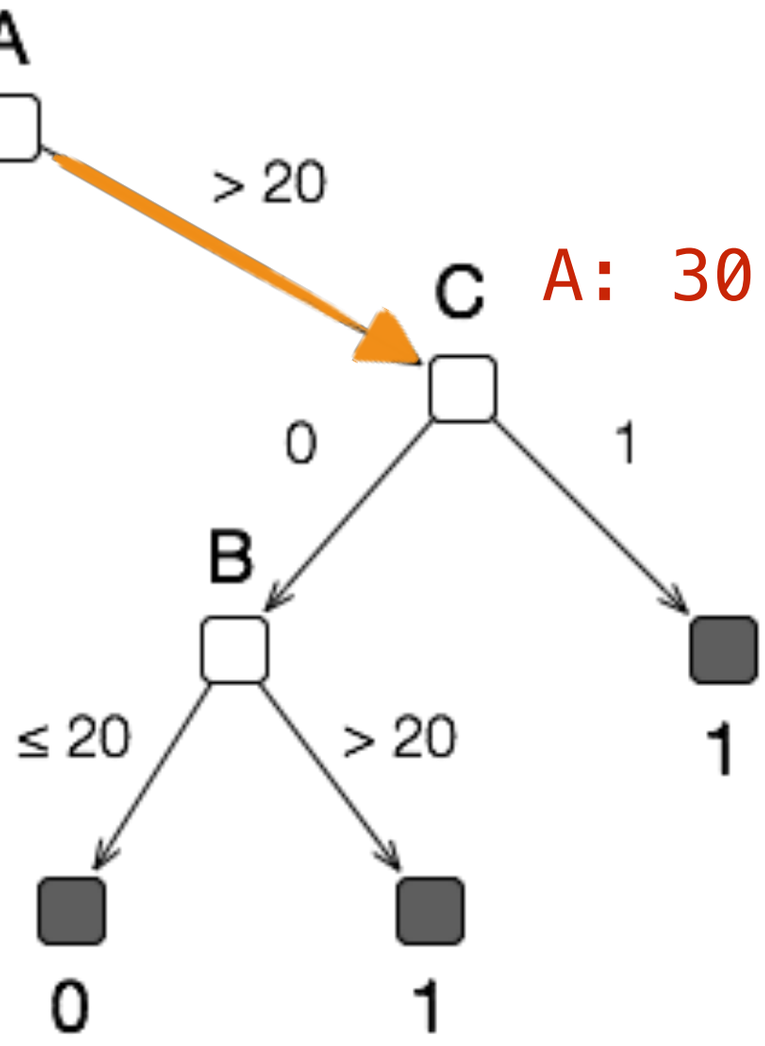
Classification example

A: 30, B: 20, C: 1

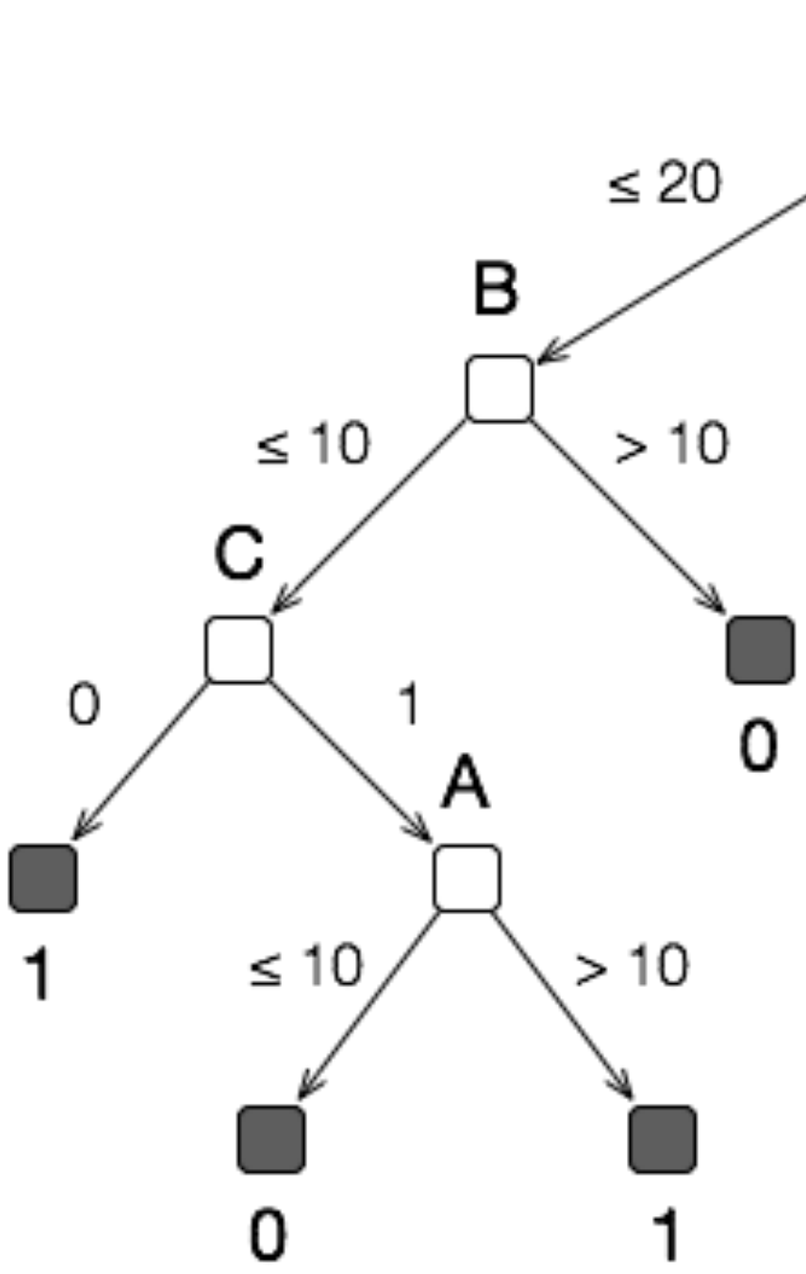


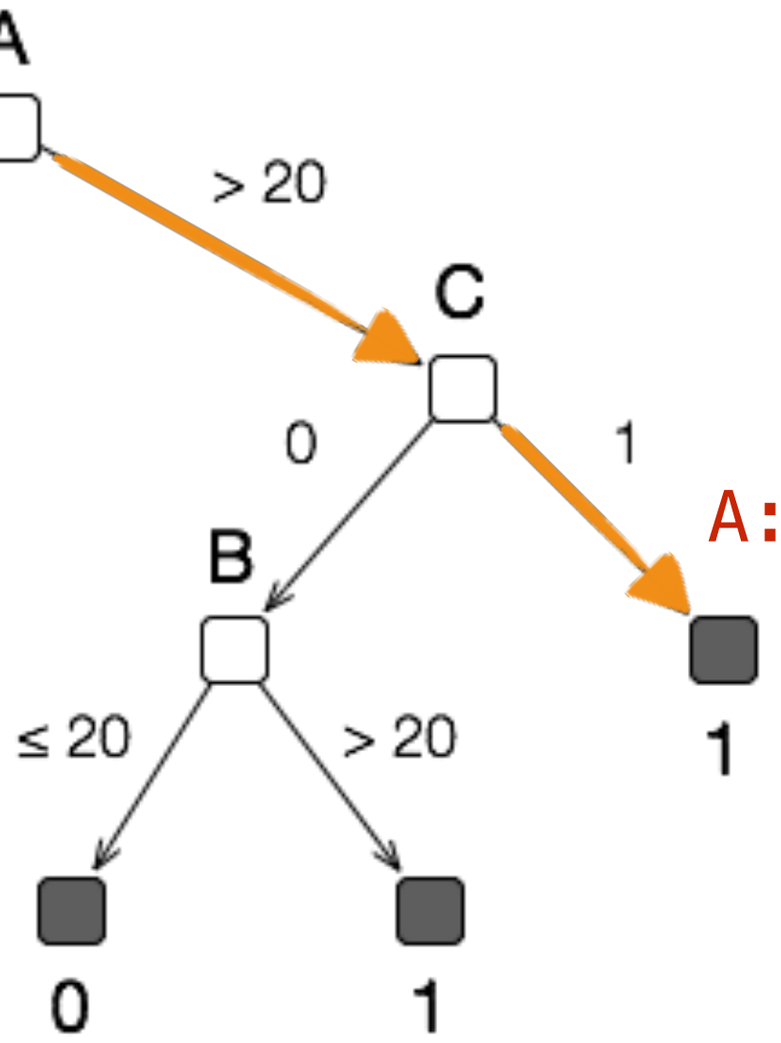
Classification example





Classification example





A: 30, B: 20, C: 1
class = 1

How do we embed a DT in CP?

- A decision variable for each attribute

```
A ∈ {-inf, inf}
B ∈ {-inf, inf}
C ∈ {0, 1}
```

- A decision variable for the class

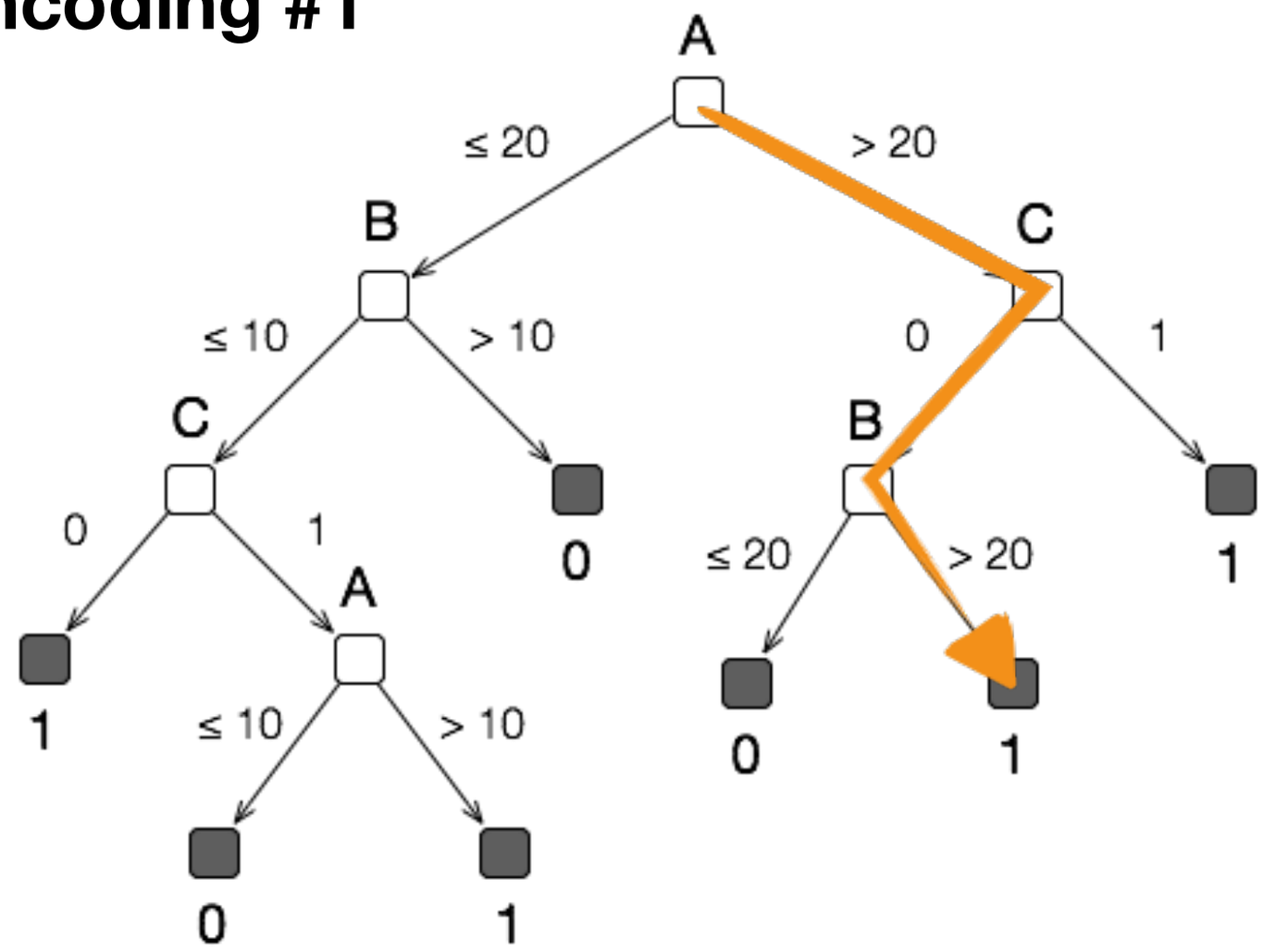
```
Y ∈ {0, 1}
```

- Enforce consistency on:

$$Y = DT(A, B, C)$$

This is the tricky part

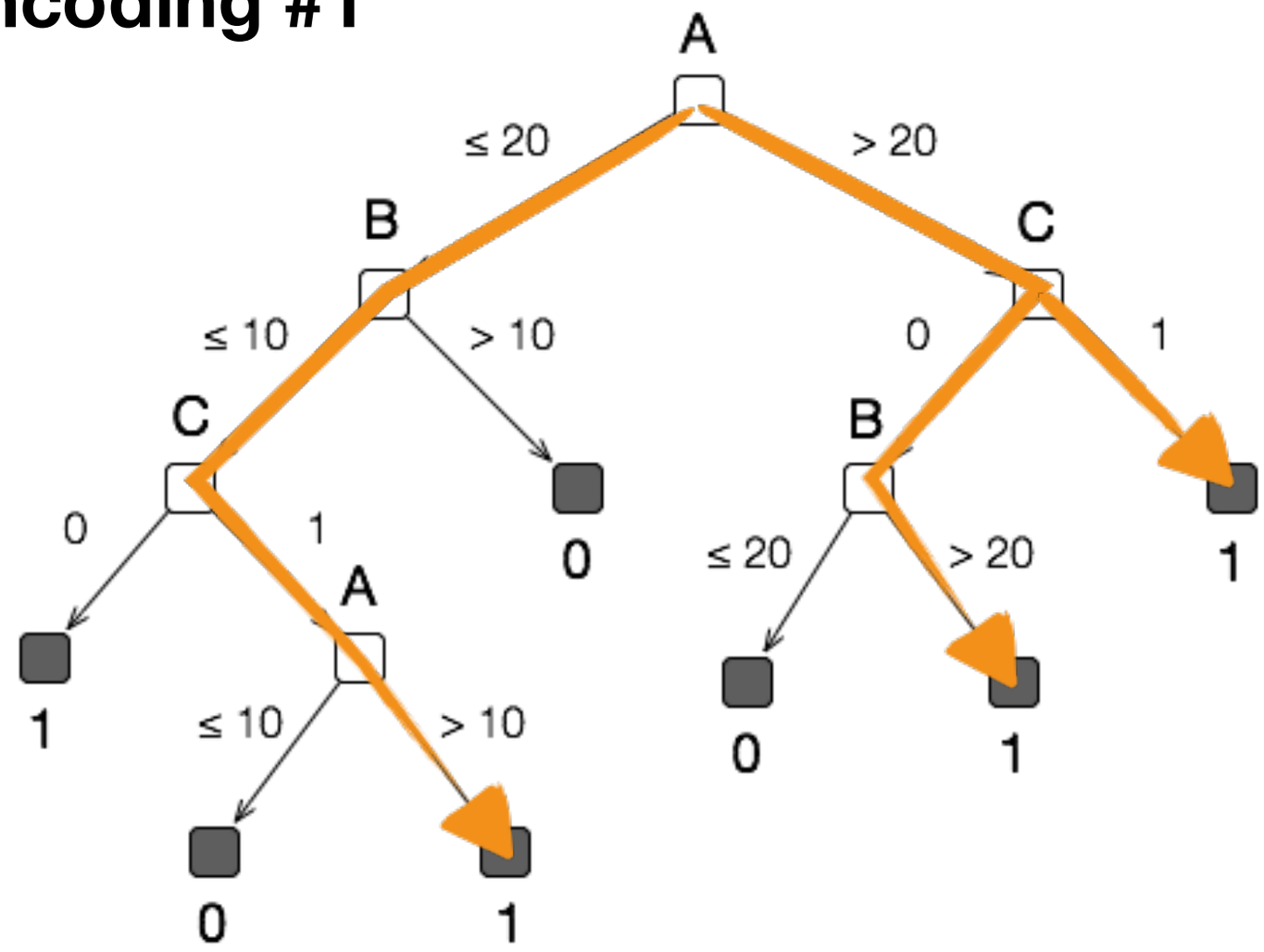
Encoding #1



A path is an implication

$$[A > 20] \wedge [C = 0] \wedge [B > 20] \Rightarrow [Y = 1]$$

Encoding #1

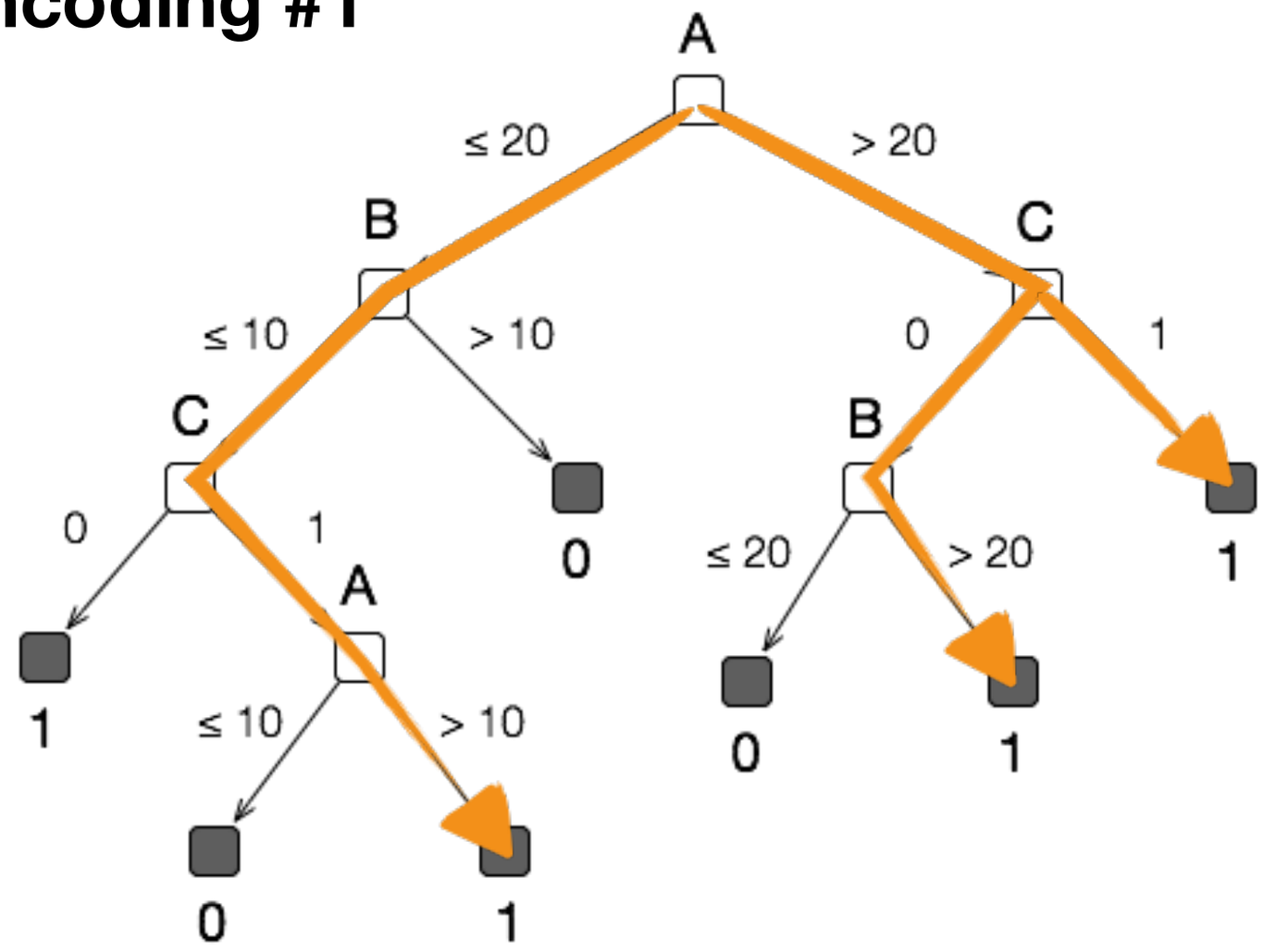


A path is an implication

The tree defines all the paths

$$
\begin{aligned}
& ([A > 20] \wedge [C = 0] \wedge [B > 20]) \vee \\
[Y = 1] \Leftrightarrow\ & ([A > 20] \wedge [C = 1]) \vee \\
& ([A \leq 20] \wedge [B \leq 10] \wedge [C = 1] \wedge [A > 10])
\end{aligned}
$$

Encoding #1



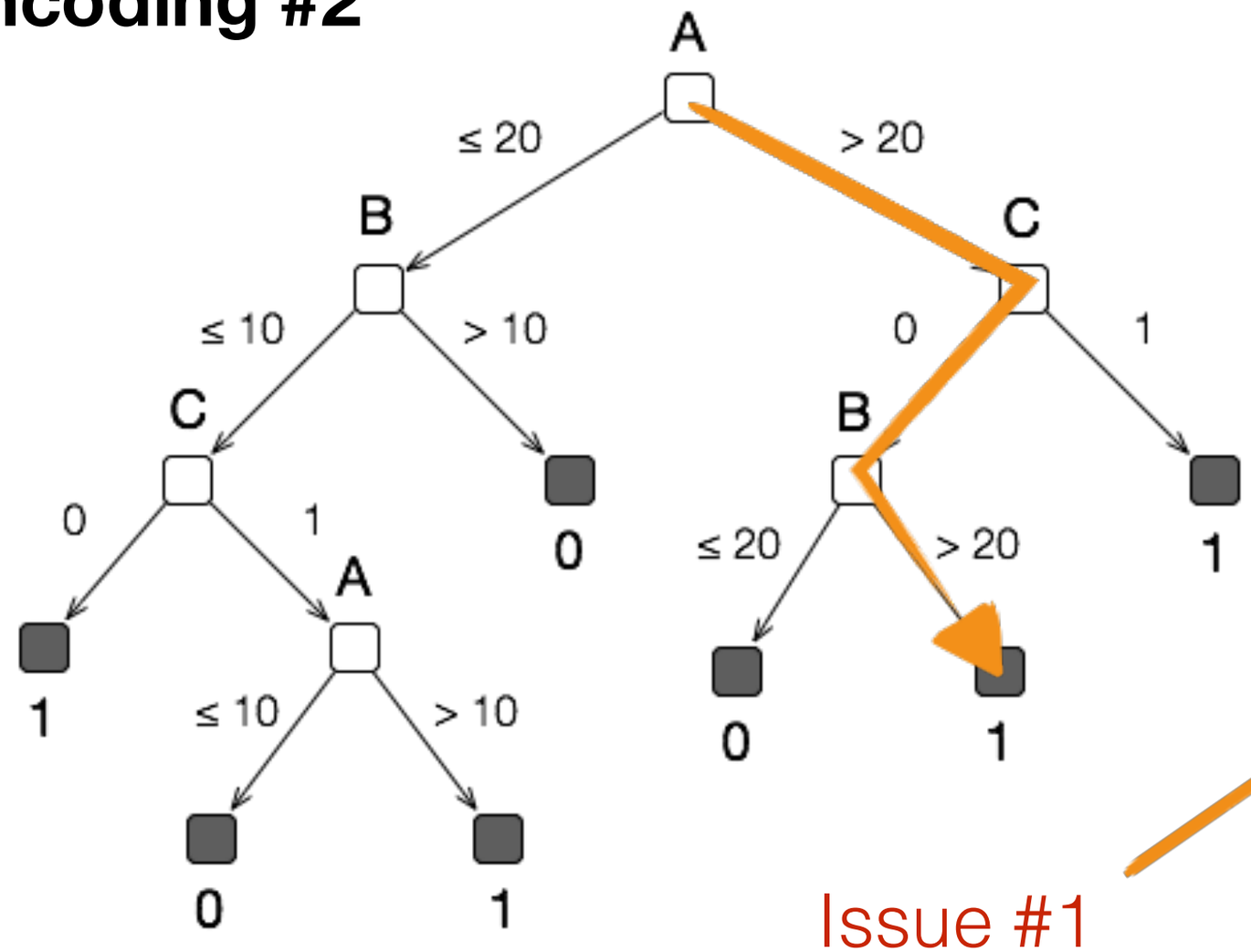
A path is an implication

The tree defines all the paths

- Polynomial size
- Polynomial time propagation
- Does not enforce GAC
- Very suitable for SMT

Can we do better?

Encoding #2



Path ↔ set of feasible assignments

A	B	C	Y
21	21	0	1
21	22	0	1
21	23	0	1
…	…	…	…

Issue #1

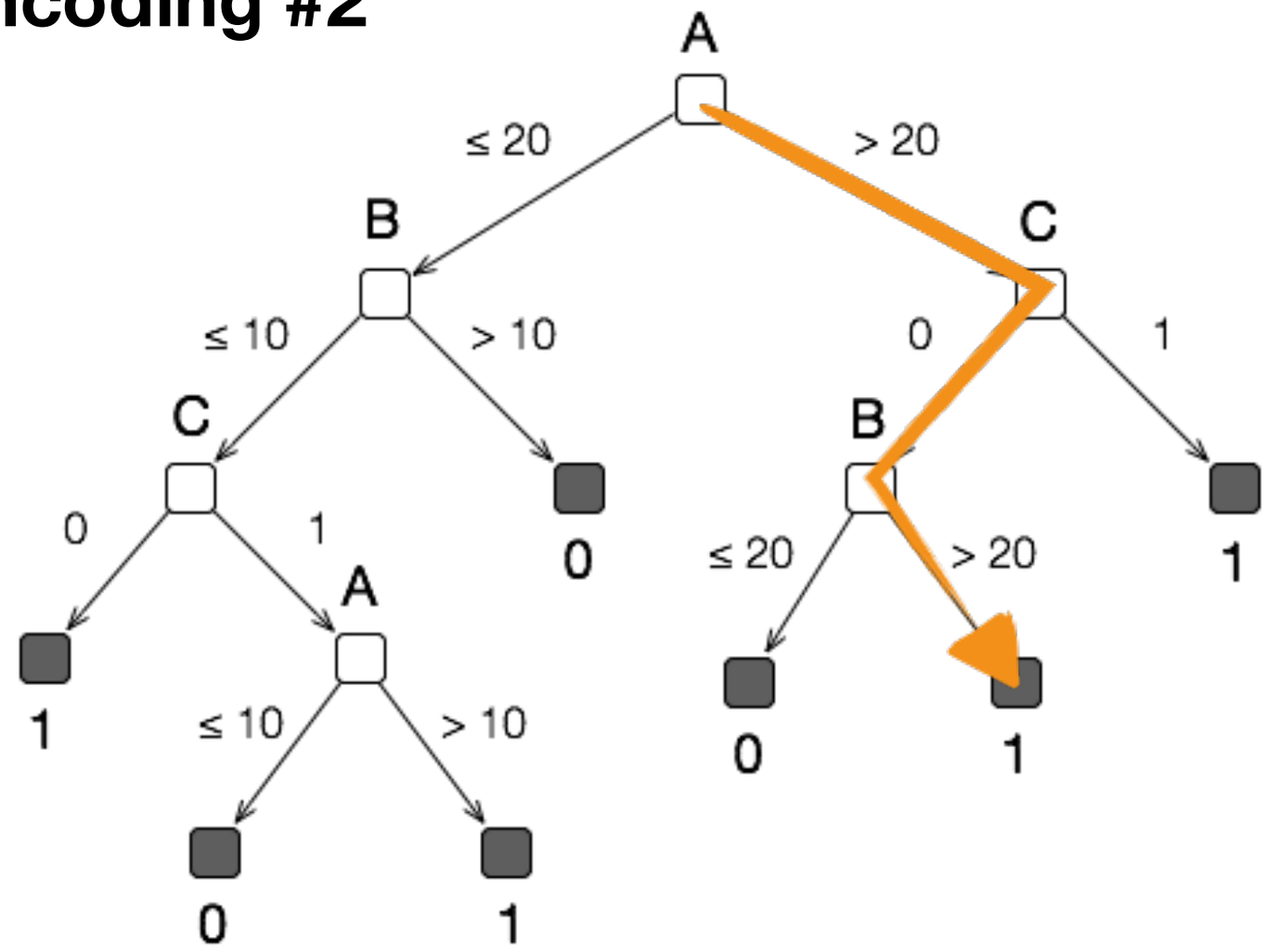
numeric attributes

use discretization

We can use a table constraint!

Bessiere, Regin, IJCAI 97

Encoding #2



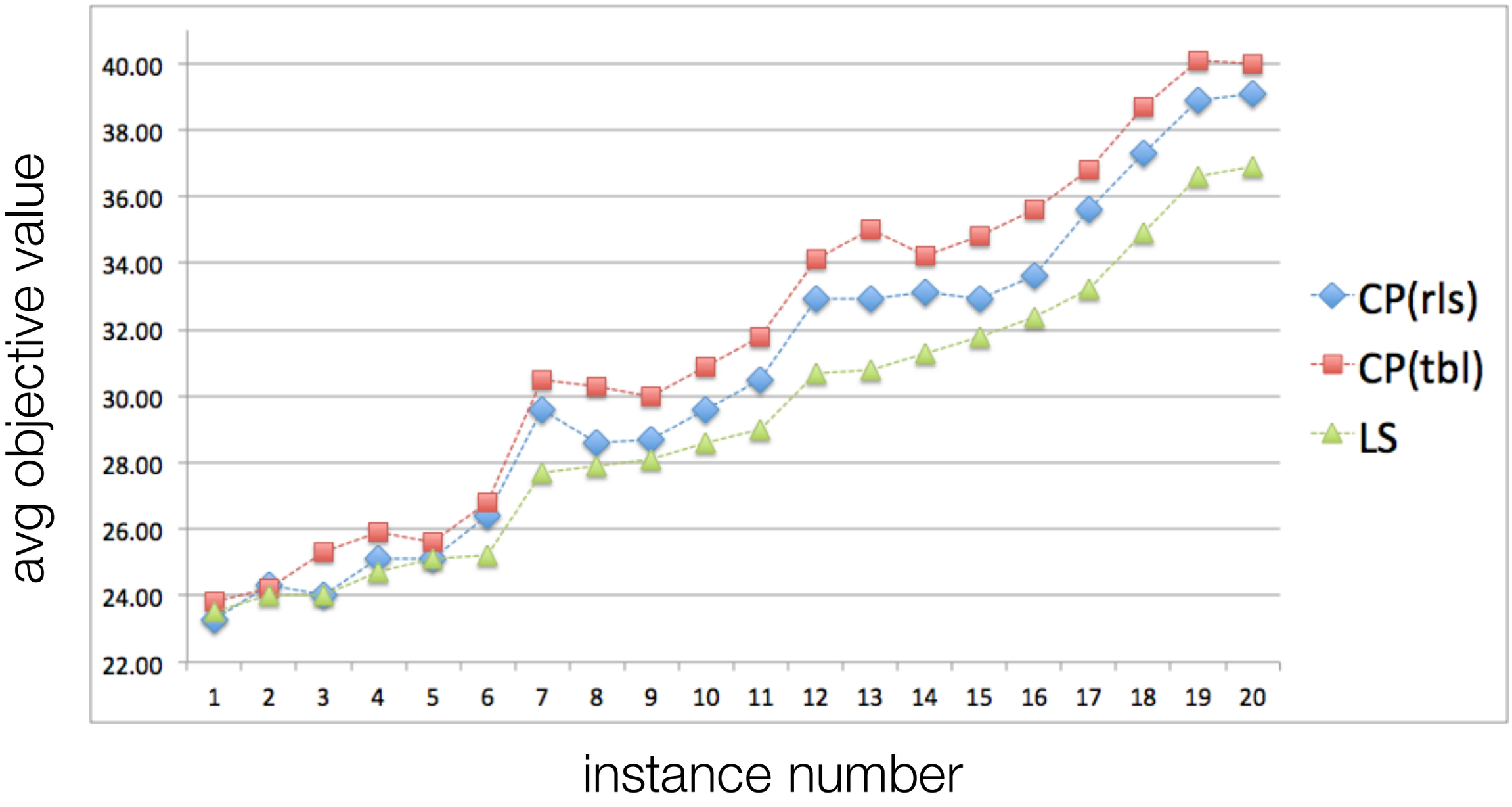
Path ↔ set of feasible assignments

A	B	C	Y
21	21	0	1
21	22	0	1
21	23	0	1
…	…	…	…

Continuous attributes can be discretised using the splitting thresholds appearing in the tree

Solution quality

- 20 instances, 48 cores, 288 jobs
- CP with LNS against Localsolver, 90 sec time limit



More compact encodings:

- **use an MDD**
- **use compressed tuples**
- **convert to a sNNF - sdNNF**
- **decomposition approaches**

Technical report

Variants

- **Random forests**
- **Regression trees**
- **Multi-output trees**

In a nutshell:

EML enables combinatorial optimization over complex real world systems

- It's not the only solution…
- …and it does not need to be about CP

But CP is very well suited for EML!

- Ease of embedding (a EM in a global constraint)
- Flexibility and modularity (the EM is "just a constraint")

In a nutshell:

EML enables combinatorial optimization over complex real world systems

- It's not the only solution…
- …and it does not need to be about CP

But CP is very well suited for EML!

- Ease of embedding (a Neural Network in a global constraint)
- Flexibility and modularity (the EM is "just a constraint")

Which issues shall we address to make it work?

Issue #1

- You can always embed a ML in (e.g.) Local Search
- Can CP work better?

Yes (we have data)! Mainly thanks to propagation

Issue #1

- You can always embed a ML in (e.g.) Local Search
- Can CP work better?

Yes (we have data)! Mainly thanks to propagation

We need inference methods for ML models

(e.g. bounds on the I/O of a Neural Network)

- Inference should be effective (tight bounds)
- Inference should be efficient

Issue #2

Complex ML models

more accurate

slow, weak propagation

Risk: poor quality solutions

Simple ML models

less accurate

effective propagation

Risk: apparently good solutions

Issue #2

Complex ML models

more accurate

slow, weak propagation

Risk: poor quality solutions

Simple ML models

less accurate

effective propagation

Risk: apparently good solutions

There is an accuracy/optimization trade-off

- How to characterize it?
- Can we find design rules?

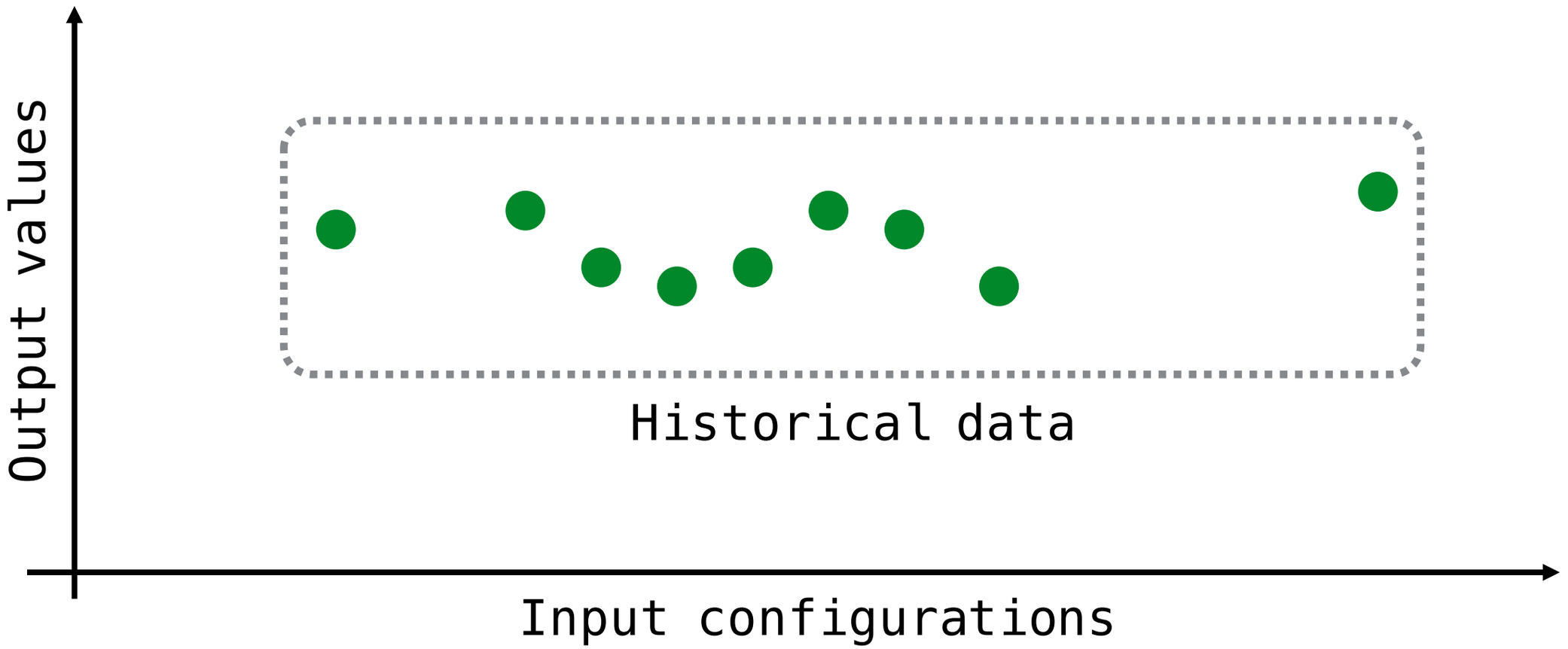
We are currently working on Deep NN with a Google Faculty Award

- Very interesting approach by Fischetti and Jo:
- They model a DNN with fixed weights in MIP
- They define upper bound tightening procedures as follows
  - They consider units layer by layer
  - For the current unit, remove from the model all the constraints and variables related to all other units in the same layer or in subsequent layers
  - Solve twice the resulting model for min and max the output

M. Fischetti, Jason Jo, Deep neural networks and mixed integer linear optimization, Constraints 23, 2018

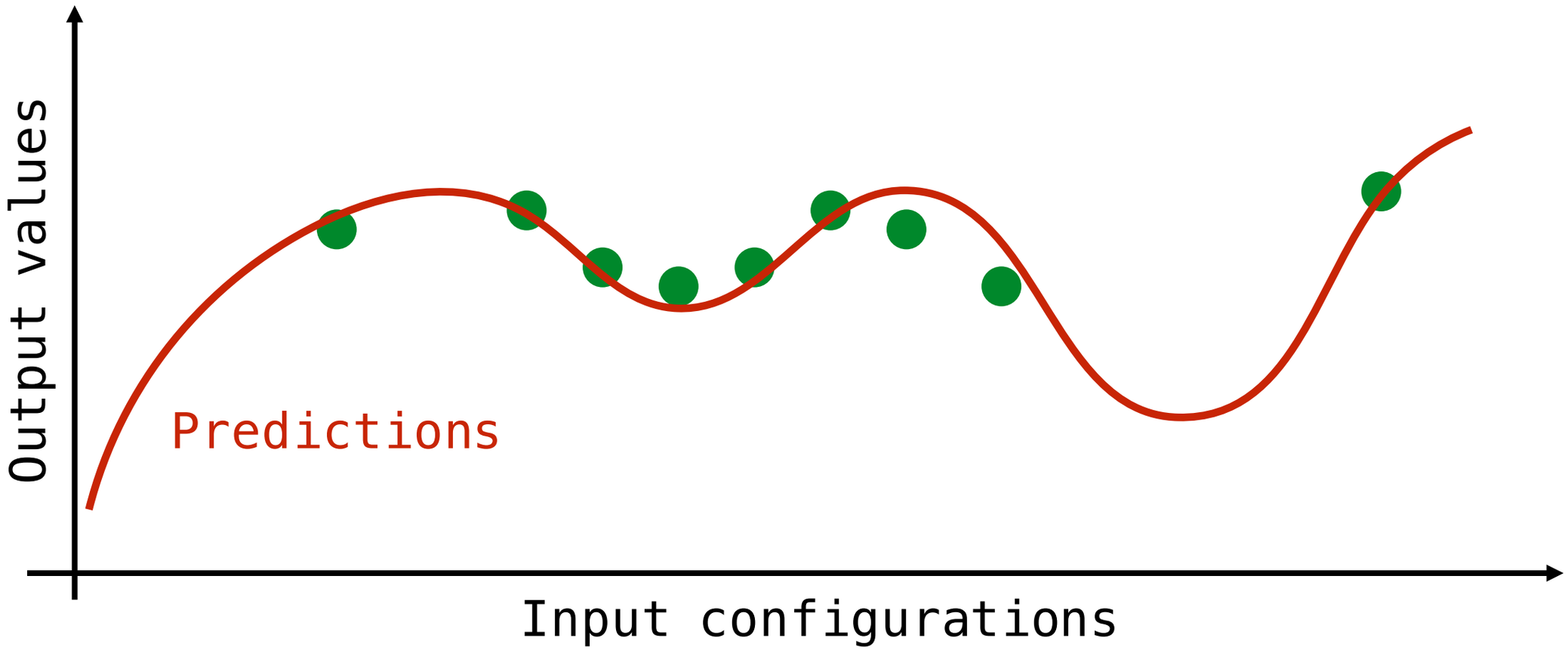
Issue #3

A typical training set in ML looks like this:



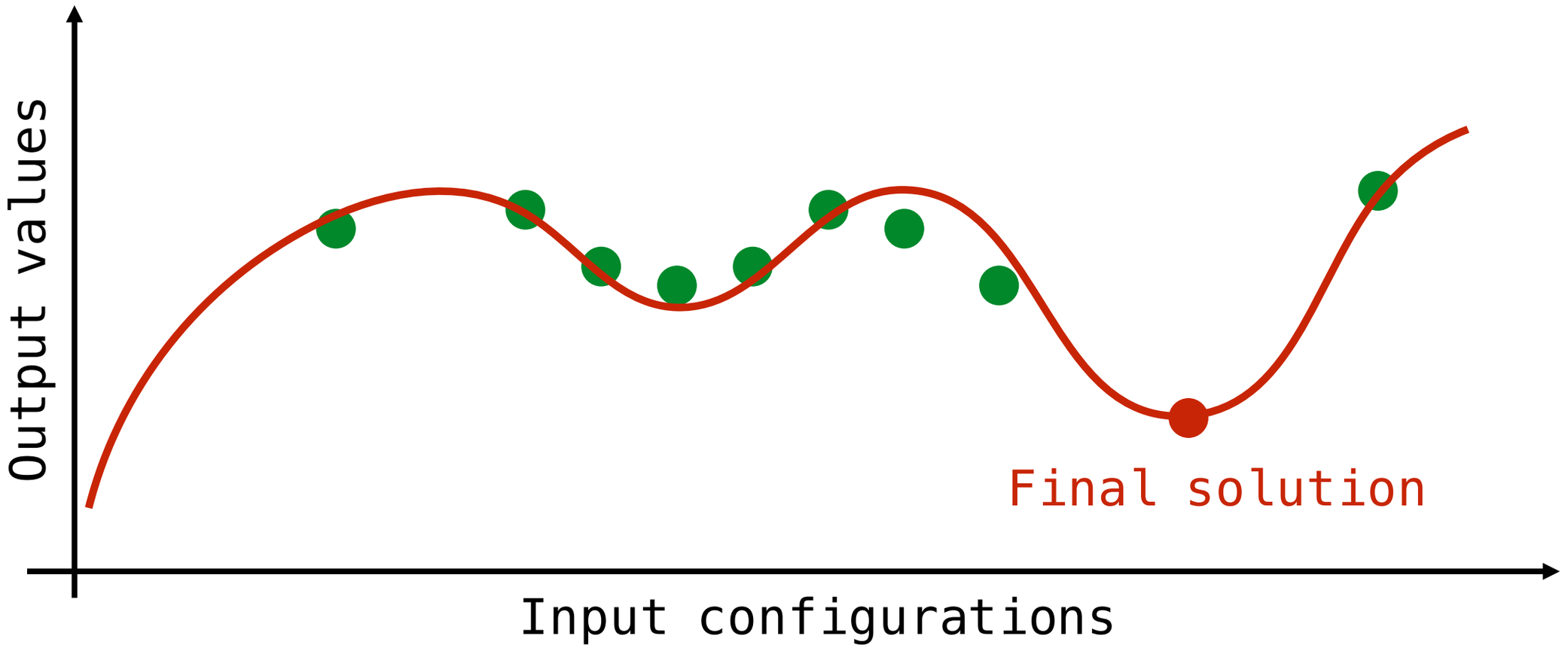
Issue #3

The ML model provides a prediction for every input value



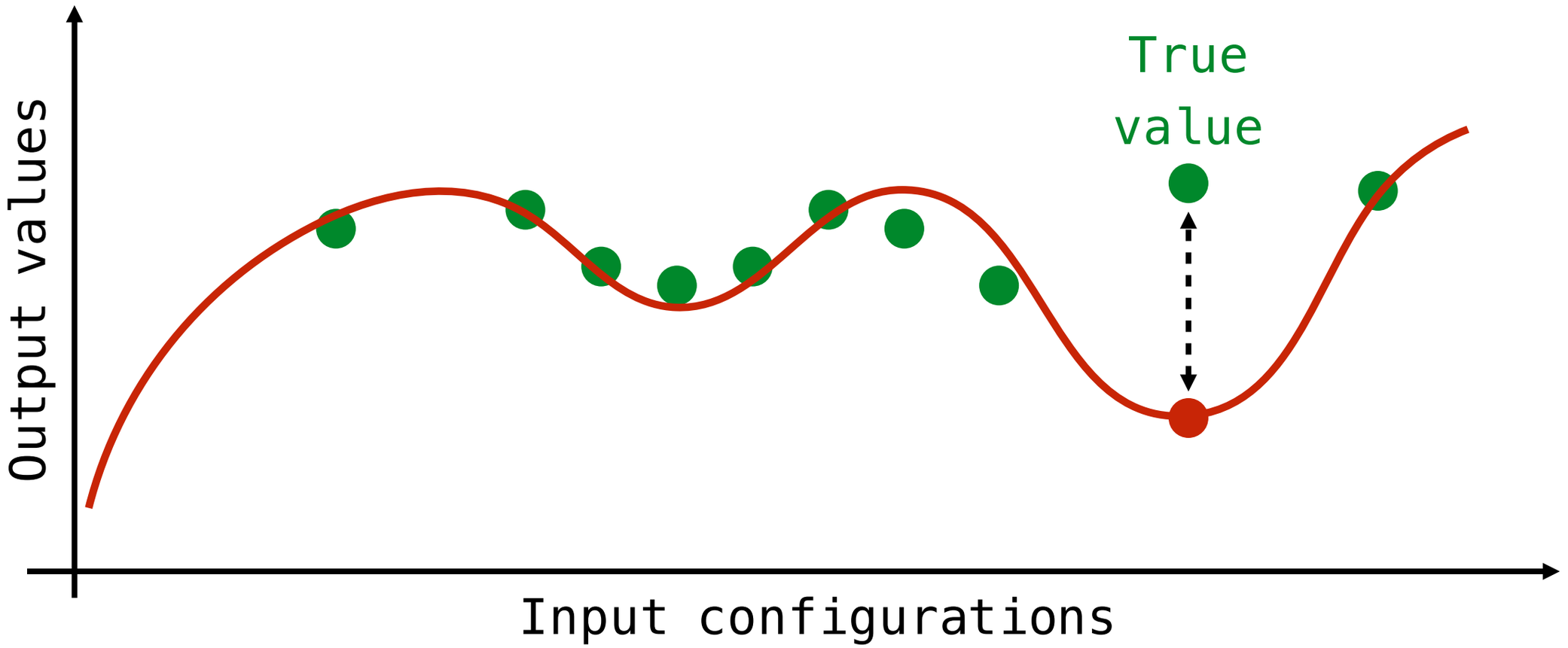
Issue #3

The optimizer will search for the best one (HP: prediction = cost)



Issue #3

If this is far from known examples, there may be a large error



Issue #3

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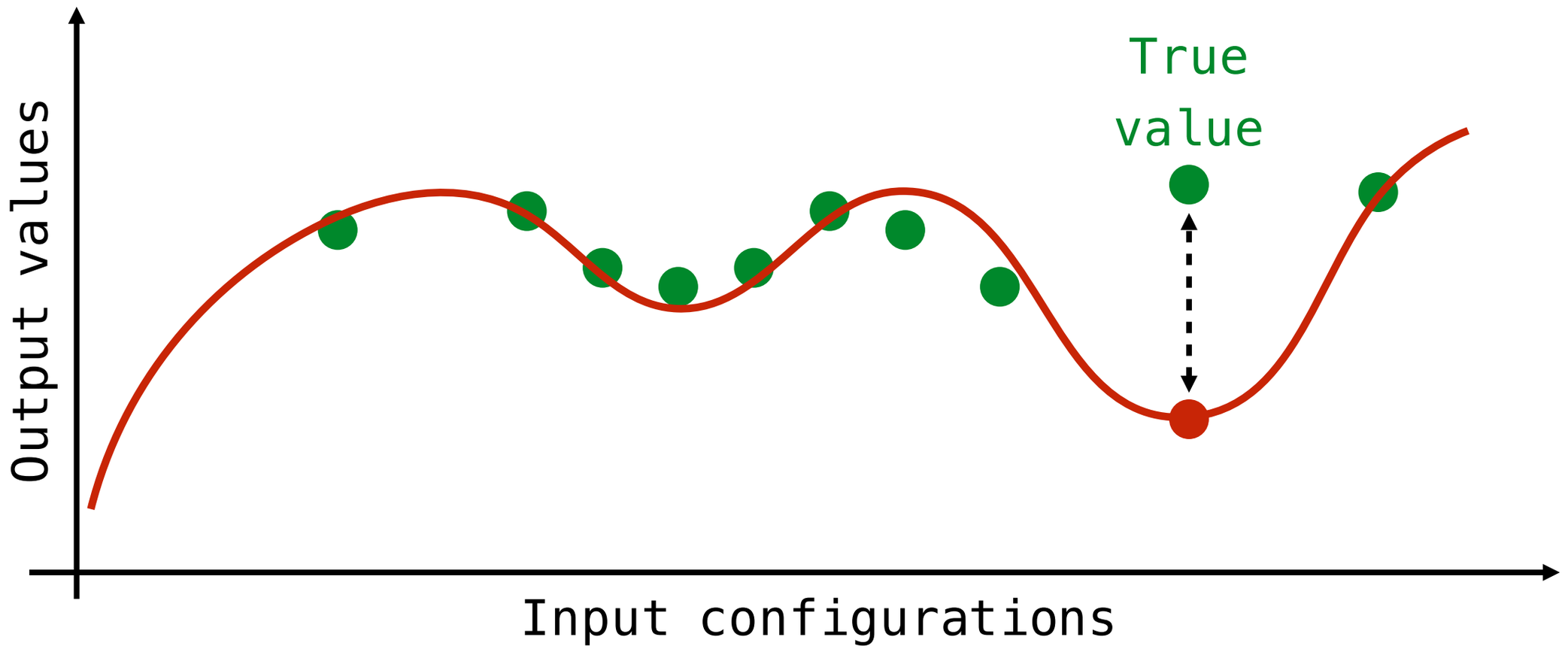


How do we choose representative observations?

Borrow concepts from black-box optimization, surrogate model construction by adaptive sampling

Issue #4

Many ML model provide estimated confidence levels

Can we take them into account when optimizing?

Issue #4

Many ML model provide estimated confidence levels

Can we take them into account when optimizing?

Some ML models can deal with uncertain inputs

Can we employ EML in stochastic optimization?

Some errors are more ***important*** than other

Using ML to solve the problem

Aimed at learning models in the general form:

$$\min z = x_0 \qquad (\mathbf{P3})$$
$$\text{subject to: } \nu_m(\vec{x}_{m,in}, \vec{x}_{m,out}) \qquad \forall m \in M$$
$$\vec{x} \in D_{\vec{x}}$$

- where $\vec{x}$ are problem variables, $D_{\vec{x}}$ their domain and x_0 is the variable representing the objective value,

  and $\nu_m(\vec{x}_{m,in}, \vec{x}_{m,out})$ is a proper encoding of a machine learning model in the hosting language

Galassi

Aimed at learning models in the general form:

Nuova citazione + Zico Kolter

Aimed at learning models in the general form:

ML for Search

A. Lodi and G.Zarpellon On learning and Branching: a survey, TOP 2017

Search strategies

- In tree-based search strategies: two foundamental steps
  - Variable selection: on which variable to branch
  - Node selection: which value to assign to the variable

  Some work on ML applied to MIP to guide these choices

- Heuristic search strategies are more diverse
  - Large neighborhood search
  - Heuristic search

ML in MIP search

- In MIP the heuristics for selecting a variable is sometimes based on Strong Branching and variants
  - ML can be used to approximate SB by means of supervised learning technique
  - Feature extraction to describe the branching variable
  - A regressor is learned to predict the estimated SB value
  - The regressor is used as a branching heuristics

- Features should be
  - Size independent
  - Invariant to changes within the instance
  - Scale-independent (if parameter change)

ML in MIP search

- Experimented on MIPLIB
  - 10^5 observations
  - On MIPLIB the new search strategy imitates full Strong Branching-modest improvement
- Learning within the same instance
- SB scores are only used to select the single best variable
- Learning to imitate the correct ranking of the candidate variables at each node

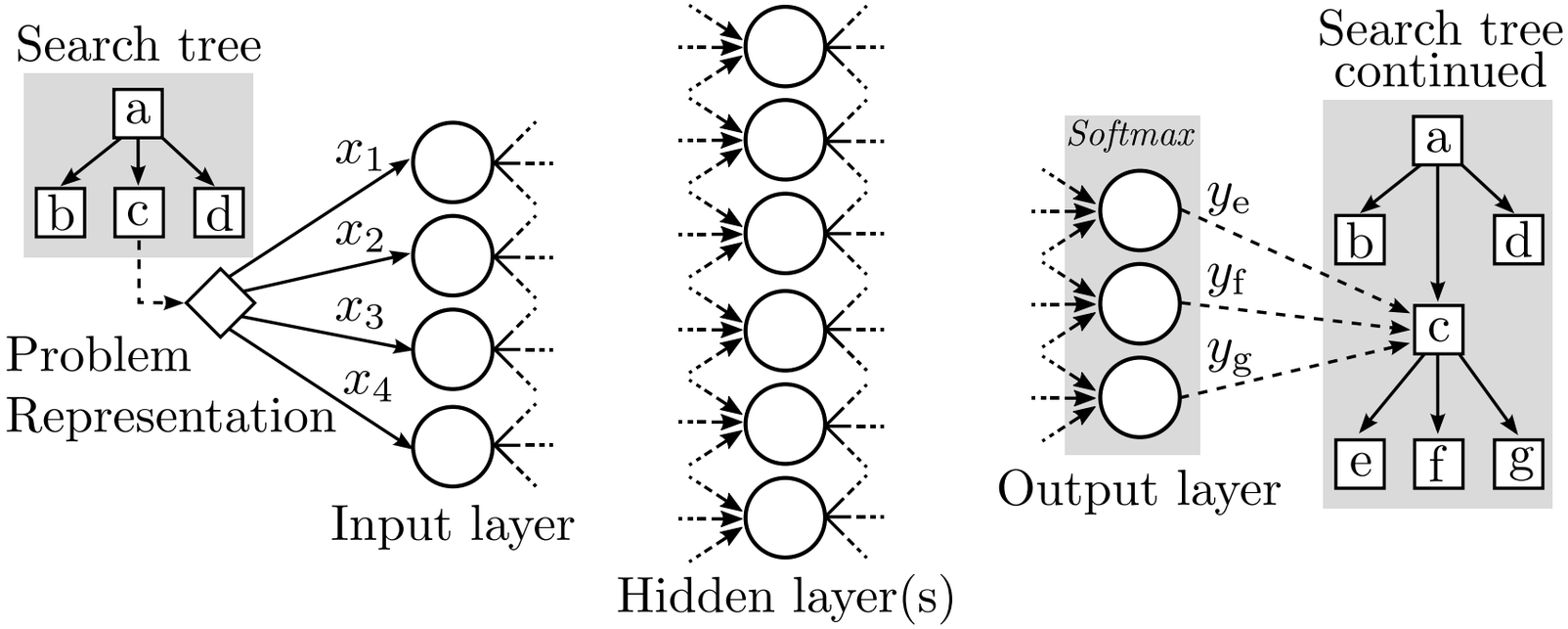
A. Marcos Alvarez, Q. Louveaux, L. Wehenkel "A machine learning_based approximation of strong branching" INFORMS J. of Computing 29(1), 2017

Deep networks assisted heuristic tree search

- DLTS is an incomplete tree search in which decisions about which branches to explore and how to bound nodes are made by a DNN
  - DFS, LDS, weighted Beem search
  - Plus aggressive pruning
- The DNN is problem specific
- Two networks:
  - a policy network to make predictions on the best branch
  - a value network to predict the cost of completing the solution

A.Hottung, S.Tanaka, K.Tierney
Deep Learning Assisted Heuristic Tree Search for the Container Pre-marshalling Problem
arXiv:1709.09972

Deep networks assisted heuristic tree search



The output is a probability distribution over the available branches

A.Hottung, S.Tanaka, K.Tierney
Deep Learning Assisted Heuristic Tree Search for the Container Pre-marshalling Problem
arXiv:1709.09972

ML in MIP search

- Instead of an off-line ML method, an online learning strategy could be employed
  - Data generated on-the-fly within the search process itself
  - Reliability: depending on the number of times a real SB score was computed for a given var one could deem the candidate reliable
  - Drawback: not adapting over time (after all var are reliable)
  - Perpetual version of the method

A. Marcos Alvarez, L. Wehenkel, Q. Louveaux "On-line learning of strong branching approximation in Branch and Bound" Tech. Rep. Univ. Liege, 2016

ML in MIP search

- Again on learning during search in MIP
- Two general branching strategies:
  - Strong Branching (SB) : simulate branching on multiple variables; select var. with max product of LP increase large computation time , small number of nodes
  - Pseudocost Branching (PC) : choose based on running averages of observed branching effect for each variable a lot of manual tuning , small time, reasonable number of nodes
- Can we get the best of both worlds (SB and PC)?
  - small number of nodes
  - small time
  - as little manual tuning as possible

E. Kalil, P. Le Bodic, L. Dong, G. Nemhauser, B. Dilkina “Learning to branch in Mixed Integer Programming” in AAAI2016

ML in MIP search

- Relaxed Binary Labels:
  - yij = 1; if SB score of xj is within α of max SB score at Ni
  - yij = 0; otherwise

  where α in (0,1) is small

- Goal: Learn a function of the features that ranks variables with better labels higher than other variables.

- Note that for data collection: run SB for some nodes, and use SB scores as labels for variables within each node; compute features describing each variable (dataset D)
- Also decide if run the primal heuristics or not.

E. Kalil, P. Le Bodic, L. Dong, G. Nemhauser, B. Dilkina "Learning to branch in Mixed Integer Programming" in AAAI2016

ML in MIP search

- Reinforcement learning:
  - Within a node selection stage the tree is traversed from root to leaf (best first)
  - Once the leaf is reached the tree is updated: computed for the leaf and propagated upward

– Score(N)= estimate(N) + Γ [visits(P)/100]/visits(N)

Measure of node quality

Exploration/exploitation balance

P: parent node
N: current node

A. Sabharwal, H. Samulowitz, H. Reddy, " Guiding combinatorial optimization with UCT". CPAIOR 2012

ML in MIP search

- The essential part of the reward measure consists of LP objective values combined with visit counters
- Good tradeoff between exploration and exploitation.

Design of heuristic algorithms on graphs

- Research question: Given a graph optimization problem G and a distribution of problem instances, can we learn better heuristics that generalise to unseen instances?
- Approach:
  - adopt a greedy meta-algorithm design
  - Use a graph embedding network (deep network) to represent the policy in the greedy algorithm
    - The network *featurizes* nodes capturing their properties
    - Parametrises the evaluation function
  - Q-learning to learn a greedy policy

H. Dai, E. Khalil, Y. Zhang, B. Dilkina, L. Song, "Learning Combinatorial Optimization Algorithms over Graphs, NIPS 2017

Design of heuristic algorithms on graphs

- To estimate the quality of the partial solution S' resulting from adding a node to S, we use an evaluation function Q which is learned using a collection of problem instances

$$\widehat{Q}(h(S), v; \Theta)$$

- Q is based on an estimation of the state S, adding node v and based on parameters Θ

- Parameters are tuned via a deep network

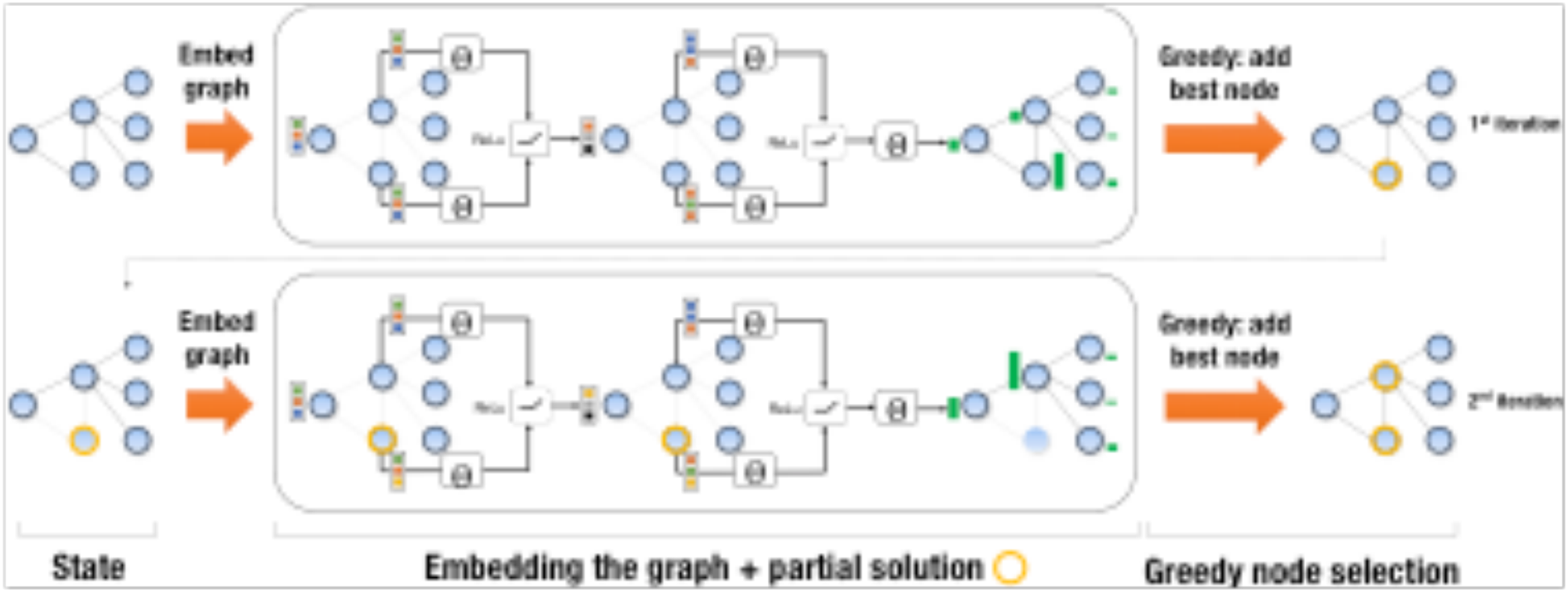
H. Dai, E. Khalil, Y. Zhang, B. Dilkina, L. Song, "Learning Combinatorial Optimization Algorithms over Graphs, NIPS 2017

Graph embedding

- The graph embedding network provides a p-dimensional feature embedding for each node, **given the current partial solution S**
- Updated at each node of the search tree
- **After few steps of recursion the network will produce a new embedding for each node considering**
  - **Node characteristics**
  - **Long range interactions between node features**
- **Use node embedding to update the evaluation function Q of the partial solution**

H. Dai, E. Khalil, Y. Zhang, B. Dilkina, L. Song, "Learning Combinatorial Optimization Algorithms over Graphs, NIPS 2017

Graph embedding



H. Dai, E. Khalil, Y. Zhang, B. Dilkina, L. Song, "Learning Combinatorial Optimization Algorithms over Graphs, NIPS 2017

Q-learning

- We would like to learn an evaluation function Q across a set of m graphs from distribution D (different size)
- Reinforcement learning formulation
  - State: sequence of nodes
  - Transition: tagging a node selected by the last action
  - Action: an action is a node that is not part of the current state
  - Rewards: r(S,v) is the change in the cost function after taking action v and transitioning to S'

$$r(S, v) = c(h(S'), G) - c(h(S), G),$$

  - Policy: deterministic greedy policy

$$\pi(v|S) := \operatorname{argmax}_{v' \in \overline{S}} \widehat{Q}(h(S), v')$$

H. Dai, E. Khalil, Y. Zhang, B. Dilkina, L. Song, "Learning Combinatorial Optimization Algorithms over Graphs, NIPS 2017

Q-learning

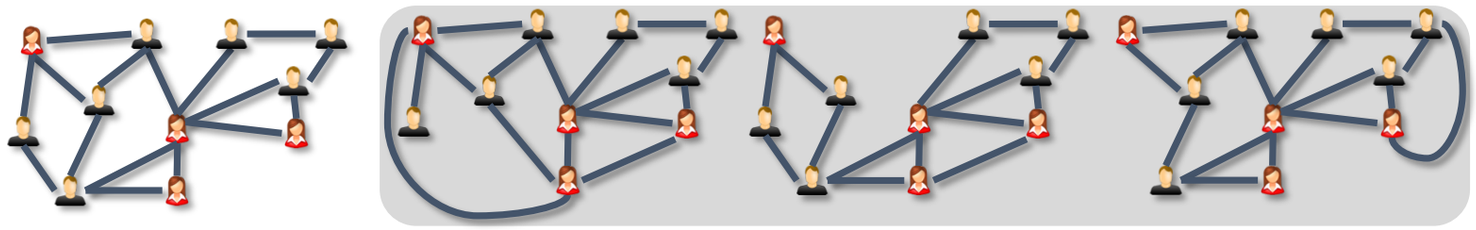
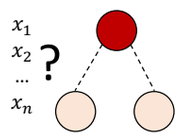
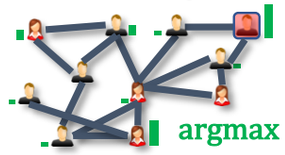
- The update of the Q function is in general performed when a full solution has been built (delayed reward)
- Updating it at every step too miopic
- Tradeoff: update after n steps

- Overall very interesting performances.

H. Dai, E. Khalil, Y. Zhang, B. Dilkina, L. Song, "Learning Combinatorial Optimization Algorithms over Graphs, NIPS 2017

General view: by E.Khalil and B.Dilkina

Goal: Generality of MIP + Flexibility of Feature Learning

Single instance v/s Distribution			
Formulation	$\min \boldsymbol{c}^T \boldsymbol{x}$ s.t. $\boldsymbol{Ax} = \boldsymbol{b}$, x_I integers		
Representation	Feature **Engineering**		Feature **Learning**
Learning task	Ranking	Classification	Reinforcement Learning
Final task	**Branching** 	**Heuristics** feasibility pump neighborhood search diving	**Greedy** 

ML for Portfolio Selection and Algorithm configuration

Material extracted by the presentation of Lars Kotthoff at the ACP Summer School, Jackson, 05 June 2018

Kotthoff, Lars. "Algorithm Selection for Combinatorial Search Problems: A Survey." AI Magazine 35, no. 3 (2014): 48–60.

Algorithm selection

- Different algorithms have different performances on different problems
- .....even on different instances of the same problem
- often no clear winner among different approaches

we need an algorithm performance estimator

Algorithm selection

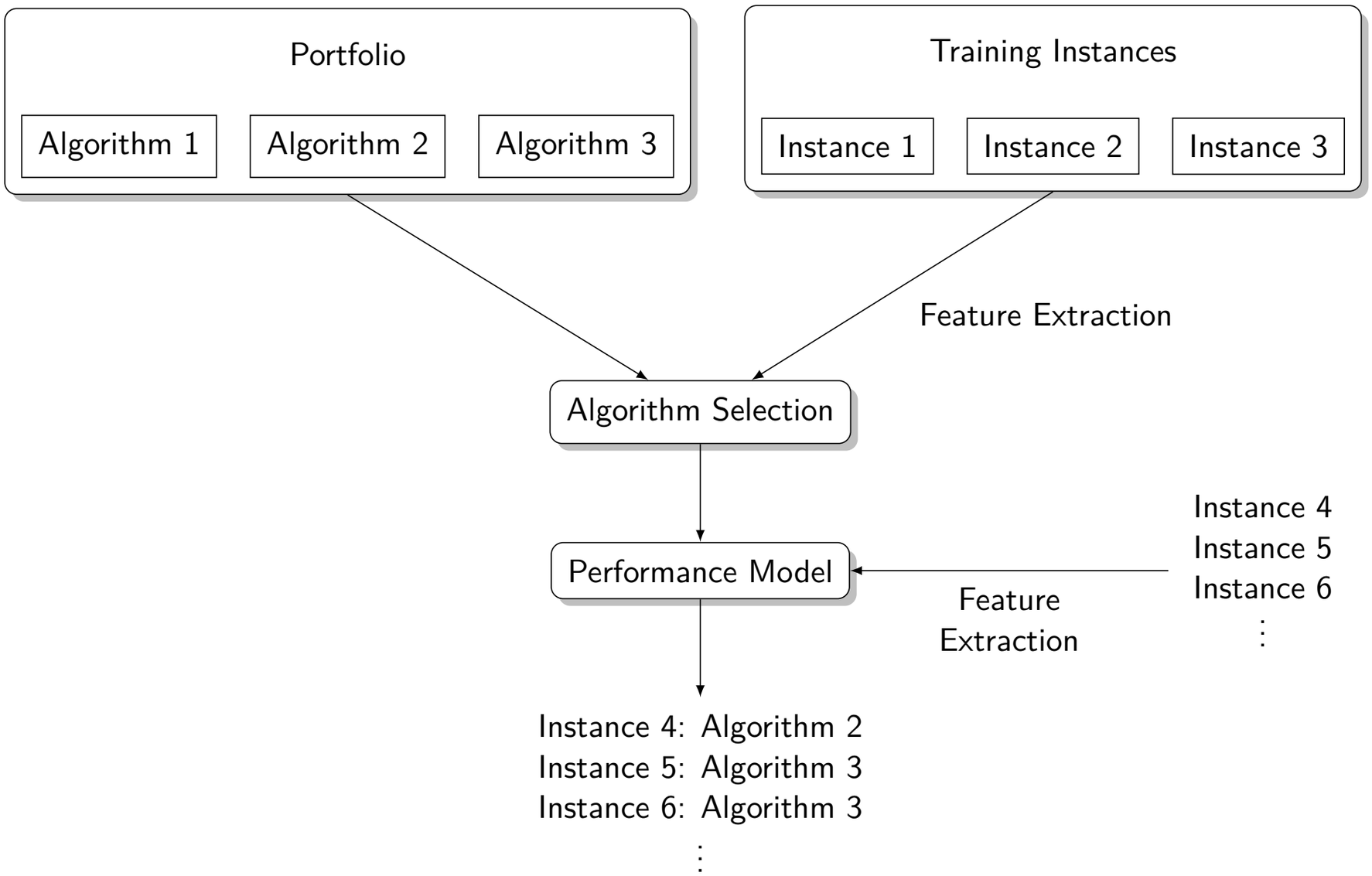
- Different algorithms have different performances on different problems
- .....even on different instances of the same problem
- often no clear winner among different approaches

we need an algorithm performance estimator

Performance models

- Performance models of black-box processes
- also called surrogate models
- Replace expensive underlying process with cheap approximate model
- Build the approximation on the basis of real evalution via machine learning techniques
- No knowledge about the underlying process

Algorithm selection



Algorithm portfolios

- Instead of a single algorithm use several complementary algorithms
- Idea from Economics – minimize the risk by spreading it out across several securities
- For computational problems – minimize the risk of algorithm performing poorly
- Algorithm used in a loose sense (constraint solvers, search strategies, modeling choices, different propagation algos)

Algorithm portfolios

- Most approaches rely on machine learning
- Train with representative data (training set) – performance for all algorithms in a portfolio
- Evaluate performance on a test set (unseen instances)
- Need to balance easy/hard instances on both sets
- May need hundreds/thousands of instances

Algorithm selection ingredients

- Feature extraction
- Performance evaluator
- Prediction based selector/scheduler

Feature extraction

- Syntactic features: analyse instance description
  - Number of vars/constraints/clauses
  - Ratios
  - Graph properties (node degree, connectivity)
- Probing features: run algorithms for short time
  - Number of nodes/propagation within time limit
  - Estimated search space size
- Dynamic features: instance changes while algo running
  - Number of constraint propagation
  - Change in var domains

Feature extraction

- Syntactic features: analyse instance description
  - Number of vars/constraints/clauses
  - Ratios
  - Estimated search space size
- Dynamic features: instance changes while algo running
  - Number of constraint propagation
  - Change in var domains

Which features?
Mix of complex/simple features
In the end…..whatever works best

Performance evaluator

- Model for entire portfolios
  - Predict the best algorithm in the portfolio (classification)
  - Clustering and assign algorithms to clusters
  - Important to assign a weight during learning (difference best-worst time) to focus on important instances

Gent, Ian P., Christopher A. Jefferson, Lars Kotthoff, Ian Miguel, Neil Moore, Peter Nightingale, and Karen E. Petrie. "Learning When to Use Lazy Learning in Constraint Solving." In ECAI2010.

Kadioglu, Serdar, Yuri Malitsky, Meinolf Sellmann, and Kevin Tierney. "ISAC – Instance-Specific Algorithm Configuration." In ECAI2010.

Performance evaluator

- Model for individual algorithms
  - Predict the performance of each algorithm
  - Compare predictions and chose the best

Xu, Lin, Frank Hutter, Holger H. Hoos, and Kevin Leyton-Brown. "SATzilla: Portfolio-Based Algorithm Selection for SAT." J. Artif. Intell. Res. (JAIR) 32 (2008)

- Hybrid methods, e.g. pairwise comparisons

Xu, Lin, Frank Hutter, Holger H. Hoos, and Kevin Leyton-Brown. "Hydra-MIP: Automated Algorithm Configuration and Selection for Mixed Integer Programming." In RCRA@IJCAI11

Kotthoff, Lars. "Hybrid Regression-Classification Models for Algorithm Selection." In 20th European Conference on Artificial Intelligence, 480–85, 2012.

Prediction selector

- Best algo
- N best algorithms ranked
- Allocation of resources to algorithms
- Change the current one?

Kotthoff, Lars. “Ranking Algorithms by Performance.” In LION 8, 2014.

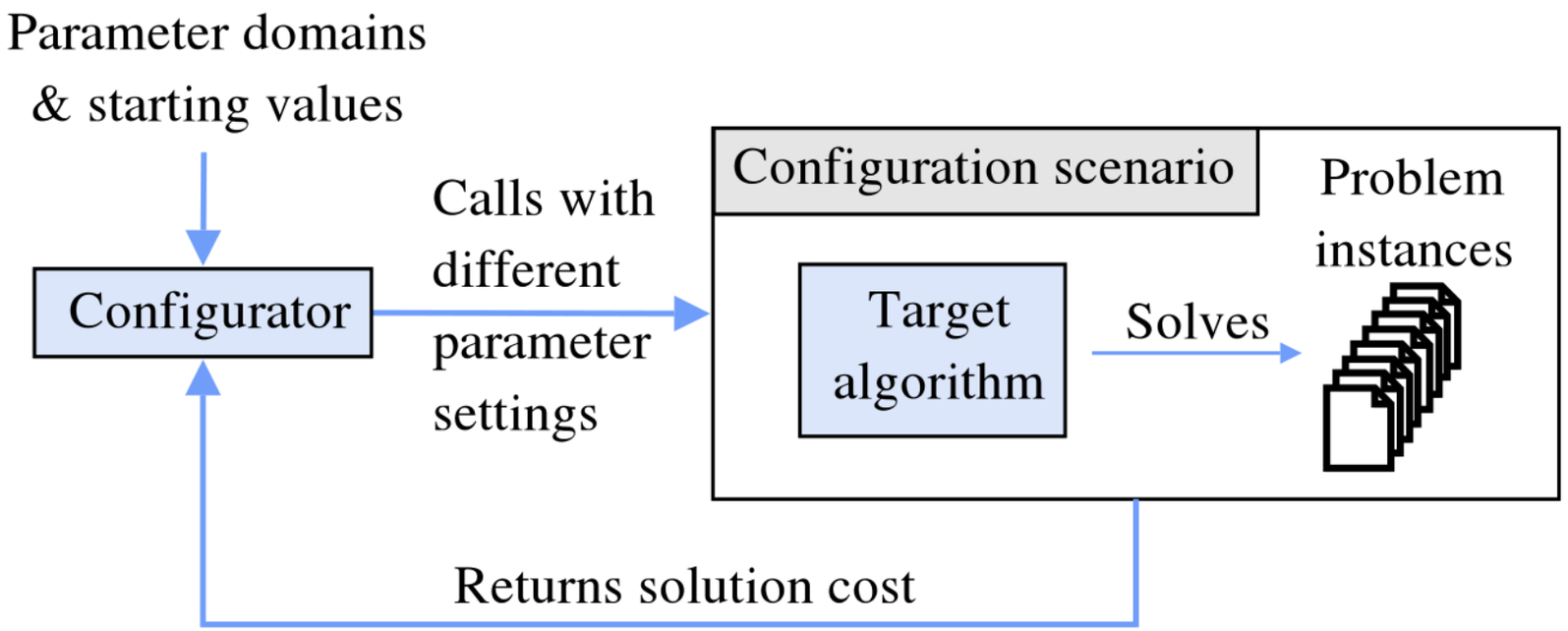
Kadioglu, Serdar, Yuri Malitsky, Ashish Sabharwal, Horst Samulowitz, and Meinolf Sellmann. “Algorithm Selection and Scheduling.” In CP2011.

Stergiou, Kostas. “Heuristics for Dynamically Adapting Propagation in Constraint Satisfaction Problems.” AI Commun. 22, no. 3 (2009): 125–41.

Algorithm configuration

- Given a set of problems, find the best algorithm parameter configuration
- Parameters:
  - Anything you can change
    - search heuristic, variable ordering ….
- Some will affect performances

Algorithm configuration



Frank Hutter and Marius Lindauer, "Algorithm Configuration: A Hands on Tutorial", AAAI 2016

Model based algorithm configuration

- Evaluate small number of configurations
- Build model of parameter-performance surface based on the results
- Use model to predict where to evaluate next
- Repeat
- Allows targeted exploration of new configurations
- Can take instance features into account like algorithm selection
- Risk of overtuning (similar to overfitting)

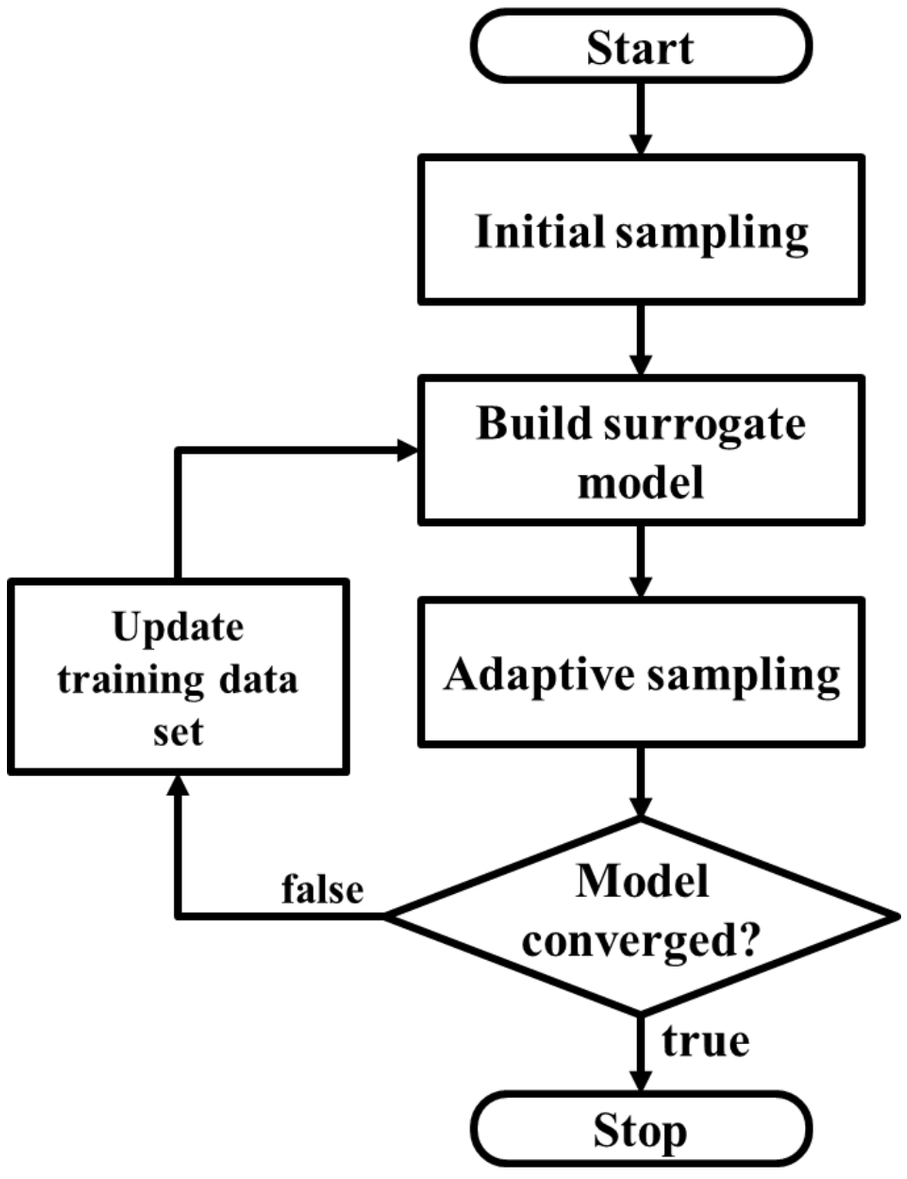
Xu, Lin, Holger H. Hoos, and Kevin Leyton-Brown. "Hydra: Automatically Configuring Algorithms for Portfolio-Based Selection." In AAAI2010.

To wrap up

Thanks for listening!

Questions?

Alamo – Sahinidis et al.



Alamo – Sahinidis et al. adaptive sampling