

Constraint Acquisition: Learning Constraint Models from Data

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Introduction

- Constraint programming (CP)
 - □ Solving combinatorial problems in Al

A1		B2			с	3		
B1	C1	D2	A2					
D1		C2		в3	A3			





Model + Solve paradigm





Introduction

Modelling is not always trivial

- Requires expertise
- Bottleneck for the wider use of CP



Constraint Acquisition

Structure Learning: learn the constraints of the problem, not parameters





Introduction (4/4)

Passive acquisition: Using existing data



(Inter)active acquisition: Interact with the user



Inputs and Outputs



Terminology

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X: Variables, $X = \{x_1, x_2, x_3, ..., x_{|X|}\}$

D^x: Domains

- **\Gamma:** Constraint Language, $\Gamma = \{r_1, r_2, r_3, \dots, r_{|\Gamma|}\}$
- **B**: Set of candidate constraints, $B = \{c_1, c_2, c_3, \dots, c_{|B|}\}$
- C_L: Learned constraint set

E: set of Examples,
$$E = \{e_1, e_2, e_3, ..., e_{|E|}\}$$

Goal:

 C_L is equivalent to the (unknown) target set C_T

Inputs and Outputs

Running Example: 4x4 Sudoku

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- X: Variables of the problem, $X = \{x_{1,1}, x_{1,2}, x_{1,3}, ..., x_{4,4}\}$
- **D**^x: Domains of the variables, $D^{X_i} = \{1, 2, 3, 4\}$
- *Γ*: Constraint Language, $\Gamma = \{=, \neq, \leq, \geq\}$ ←

The user may not know what constraint relations appear in the model

- **B**: Set of candidate constraints, $B = \{x_{1,1} \neq x_{1,2}, x_{1,1} = x_{1,2}, ...\}$
- C_L : learned constraints, ideally all the \neq constraints in rows, cols and blocks
- *E*: set of Examples, $E = \{e_1, e_2, e_3, ..., e_{|E|}\}$



Droblem Formulation

Inputs and Outputs

Alternative: Model with global constraints

X: Variables of the problem, $X = \{x_{1,1}, x_{1,2}, x_{1,3}, ..., x_{4,4}\}$

Evample

D^{*X*}: Domains of the variables, $D^{X_i} = \{1, 2, 3, 4\}$

- **\Gamma:** Constraint Language, $\Gamma = \{A | ID ifferent\}$
- **B:** Set of candidate constraints, $B = \{A | ID ifferent(x_{1,1}, x_{1,2}, \ldots), A | ID ifferent(x_{1,2}, x_{3,5}, \ldots), \}$

C_L: learned constraints, ideally all the AllDifferent constraints in rows, cols and blocks

E: set of Examples, $E = \{e_1, e_2, e_3, ..., e_{|E|}\}$

Pr		Formula	ation	_		Exam	pie e_1		
X _{1,1}	X _{1,2}	X _{1,3}	X _{1.4}		1	1	3	4	Create B candidate set Constraint Approximition system CL
X _{2,1}	X _{2,2}	X _{2,3}	X _{2,4}		3	2	1	1	Vocabulary (<i>X</i> , <i>D</i>)
X _{3,1}	X _{3,2}	X _{3,3}	X _{3,4}		2	2	3	1	O Examples E Or Answer8
X _{4.1}	X _{4,2}	X _{4.3}	X _{4.4}		2	з	4	3	Queries

- **B**: set of (remaining) candidate constraints
- C_T: target set of constraints

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 C_L: learned set of constraints





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Examples: Assignments to the variables of the problem

• Learning from **positive** examples (Solutions):

- Violated constraints cannot be part of the model
- Otherwise, it could not be a solution

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→ Shrinking the bias



Learning from *negative* examples (Non-solutions):

- One (or more) violated constraint is a constraint of the problem
- Otherwise, it would be a solution

Learning Constraints







We discussed:

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- Why Constraint Acquisition
- Passive and active acquisition
- Inputs and outputs of CA
- Candidate Elimination



Passive Acquisition





Assignment to all variables of the problem, labelled as:

- a solution
- or a non-solution



Passive Acquisition





A Model Seeker: Extracting Global Constraint Models from Positive Examples, N. Beldiceanu et al., CP, 2012



Statistical approaches – BayesAcq

Robust approach: Can handle noise in training set



Classifier-based constraint acquisition, S. Prestwich et al., AMAI, 2021

Statistical approaches – SeqAcq



Robust Constraint Acquisition by Sequential Analysis, S. Prestwich., ECAI, 2020

COUNT-CP: Learn using generate and aggregate



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Learning Constraint Programming Models from Data using Generate-and-Aggregate, M. Kumar et al., CP, 2022

KULEUVEN Passive Constraint Acquisition Small Summary



We discussed:

- Passive Constraint Acquisition
- Different approaches
- Learning global and fixed arity constraints
- Learning first-order constraints

Interactive Constraint Acquisition



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Learning Constraints through Partial Queries, C. Bessiere et al., AIJ, 2023



Challenges for interactive CA

Minimum number of queries

Minimum waiting time for the user





Interactive Constraint Acquisition



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Learning Constraints through Partial Queries, C. Bessiere et al., AIJ, 2023

Interactive Constraint Acquisition



Positive answer: Eliminate candidates

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Quer	٦y	: :	is this	а	solution?
[[3	4	1	2]		
[1	2	3	4]		
[4	1	2	3]		
[2	3	4	1]]		
Ansv	vei	r:	Yes		

Negative answer: Learn constraints

Quer	٠y	0	: is	this	а	solution?
[[1	3	2	2]			
[3	2	3	2]			
[1	1	1	1]			
[2	4	3	2]]			
Answ	/er	۰ :	No			



Query generation

Informative query

• Generate "informative" examples

Quality of query

• Get the maximum amount of information

Convergence





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Query generation

Find an Informative ("irredundant") query

- Not violating any learned constraint in C_L
- Violating at least one constraint from B

Find $e \in sol(C_L \land \bigvee_{c \in B} \sim c)$



Learning Constraints through Partial Queries, C. Bessiere et al., AIJ, 2023

KULEUVEN What we can learn from examples

•

Learning from *negative* examples (Non-solutions):

- One (or more) violated constraint is a constraint of the problem

- Otherwise, it would be a solution

Learning from *positive* examples (Solutions):

- Violated constraints cannot be part of the model
- Otherwise, it could not be a solution



• In both cases, we get information only about the violated candidates and not about the satisfied ones!



Query generation

Find an Informative ("irredundant") query

- Not violating any learned constraint in C_L
- Violating at least one constraint from B

Find $e \in sol(C_L \land \bigvee_{c \in B} \sim c)$



- We know that the violated constraints cannot be part of the model

- Otherwise, it could not be a solution



- We know that (at least) one of the violated constraints is a constraint of the problem

- Otherwise, it would be a solution



Query generation



Quality of query

• Get the maximum amount of information





Query generation

Quality of query

- Better generated examples lead to faster convergence
 - More information per query -> less queries needed





Query generation

Finding an Irredundant query

• Finding an informative query is not always easy...

B can be huge!!



B can contain indirectly implied constraints

Assume a simple 9x9 Sudoku puzzle.

- Combinations of ≠ constraints imply others
- 648 of them imply the rest 162

When the 648 constraints have been learned and must be satisfied, the rest cannot be violated!

Indirect implications are not detected with simple propagation!!

Query generation

Custom solvers

- Custom solvers are often employed to deal with this
 - Looking for $e_Y \in sol(C_L[Y] \land \bigvee_{c \in B[Y]} \sim c)$
 - Arbitrary $Y \subseteq X$

Projection-based query generation

- Project down to the relevant variables $Y = \bigcup_{c \in B} var(c)$
 - We can only get information on variables of constraints in B
 - Avoiding indirect implications
- Find $e_Y \in sol(C_L[Y] \land \bigvee_{c \in B[Y]} \sim c)$



Interactive Constraint Acquisition

What happens after query generation?





Learning a constraint



- 1. FindScope: exploit partial (sub)queries to find the problematic part of the assignment
- 2. FindC: Try different assignments to find the specific constraint in the scope

Learning Constraints through Partial Queries, C. Bessiere et al., AIJ, 2023



Learning Constraints through Partial Queries, C. Bessiere et al., AIJ, 2023
Finding the scope of a constraint



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Finding the scope of a constraint







Finding the relation of a constraint



We have found the scope: $\{x_{1,1}, x_{2,2}\}$ Assume that the candidate constraints for this scope are: $\{x_{1,1} \neq x_{2,2}, x_{1,1} > x_{2,2}, x_{1,1} < x_{2,2}\}$

What is the real conflict?



Try different assignments to find the specific constraint in the scope







Positive

Remove $x_{1,1} < x_{2,2}$

Only $x_{1,1} \neq x_{2,2}$ left as candidate: Learn it $\mathcal{C}_L \leftarrow \mathcal{C}_L \cup \{x_{1,1} \neq x_{2,2}\}$

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Learning Constraints through Partial Queries, C. Bessiere et al., AIJ, 2023

Interactive Constraint Acquisition QuAcq



- Learning one violated constraint per generated example
- Logarithmic number of queries for each constraint

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Interactive Constraint Acquisition Multiple Acquisition



Multiple Acquisition:

- Learn multiple constraints in each loop instance
- Don't generate a new example when a constraint is learnt
 - Instead, get an example in a subset of variables not violating the constraint found



- Can't store all of it at the same time??

- Too slow query generation??

GrowAcq: Growing Acquisition

Start with $Y_1 \leftarrow \emptyset$, or a small subset of X



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GrowAcq: Growing Acquisition

Start with $Y_1 \leftarrow \emptyset$, or a small subset of X

Bot Saves time during query generation! We can use more efficiently the time to guide better Constraint Acquisition



Guided Bottom-up Constraint Acquisition, D. Tsouros et al., CP, 2023



Interactive Constraint Acquisition Small summary



We discussed:

- How Interactive CA works
- Query generation
- Finding the scope of problem constraints
- Finding the relation of the constraints
- Growing Acquisition



Guiding Interactive Constraint Acquisition



Quality of query

- Better generated examples lead to faster convergence
 - More information per query -> less queries needed



Not fully aligning with the goal!!



Better generated examples lead to faster convergence





Better generated examples lead to faster convergence





- Positive answers: shrink *B* fast $\rightarrow max \sum_{c \in B} \llbracket e \notin sol(c) \rrbracket$
- Negative answers: Find the conflict fast $\rightarrow min \sum_{c \in B} \llbracket e \notin sol(c) \rrbracket$

What if we can predict if a candidate is a constraint of the problem or not?

Use of Oracle $O(c) = (c \in CT)$, to guide query generation based on the prediction of the constraint



1. Aim for positive answers first: $max \sum_{c \in B} \llbracket e \notin sol(c) \rrbracket$ 2. When a (probably true) constraint has to be violated, leading to a *negative answer* $min \sum_{c \in B} \llbracket e \notin sol(c) \rrbracket$

Guided Bottom-up Constraint Acquisition, D. Tsouros et al., CP, 2023

5()



Guided Bottom-up Constraint Acquisition, D. Tsouros et al., CP, 2023

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Guiding CA when finding the scope

Exploit partial (sub)queries to find the conflicting part

How are the removed variable assignments decided???

Follow the same logic

- But the new example is a sub-example of previous one
- Instead of deciding variable assignments, decide which variables to keep in the assignment

$$e_{Y} = \underset{e_{Y} \mid Y \subseteq var(e)}{\operatorname{argmax}} \sum_{c \in B} \llbracket e_{Y} \notin sol(c) \rrbracket \cdot (1 - |\Gamma| \cdot \llbracket O(c) \rrbracket)$$

$$Aim \text{ to violate}$$

$$O(c)$$

$$True$$

$$Aim \text{ to satisfy}$$

KULEUVEN Guiding CA when finding the relation

Try different assignments to find the specific constraint in the scope

How are the assignments decided???

Follow the same logic
But the new example has to be an assignment only to the scope S found

$$e_{S} = \underset{e_{S} \in Sol(C_{L}[S] \land B[S])}{\operatorname{argmax}} \sum_{c \in B} \llbracket e_{S} \notin sol(c) \rrbracket \cdot (1 - |\Gamma| \cdot \llbracket O(c) \rrbracket)$$

$$Aim \text{ to violate}$$

$$Aim \text{ to satisfy}$$

KULEUVEN Do we have an oracle O(c) to guide CA

The oracle O(c) "classifies" a candidate as a problem constraint or not



KULEUVEN Do we have an oracle O(c) to guide CA





Using Machine Learning for the prediction

Dataset: Constraint features and class (True or False)

- Constructing during the acquisition process
- Constraints that we know are part of the problem or not
- When a constraint is learned add a positive instance
- When a constraint is removed from *B* add a negative instance
- Use both relation and scope features

Relation-based features	Scope-based features
Relation name (string)	Dim[i] same_val (Bool)
Has constant (Bool)	Dim[i] avg (float)
Constant value (int)	Dim[i] distance (int)
Arity (int)	



Using Machine Learning for the prediction

Dataset: Constraint features and class (True or False)

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- Constraints that we know are part of the problem or not
- When a constraint is learned add a positive instance
- When a constraint is removed from *B* add a negative instance
- Use both relation and scope features

Example for constraint

 $\mathbf{x}_{1,1} \neq \mathbf{x}_{1,2}$ in Sudoku

Relation-based features		Scope-based features		For the 2 dimensions
Relation name (string)	≠	Dim[i] same_val (Bool)	True, False	
Has constant (Bool)	False	Dim[i] avg (float)	1, 1.5	
Constant value (int)	-1	Dim[i] distance (int)	0, 1	
Arity (int)	2			_

KULEUVEN Using Machine Learning in the Oracle

The oracle O(c) "classifies" a candidate as a problem constraint or not

Use of any classification technique to simulate the Oracle

$$O(c) = Class(c)$$

classifier.predict()

Use of probabilities?
$$O(c) = \frac{1}{\log(|Y|)} \le P(c)$$

 classifier.predict_proba()

Minimize the expected number of queries

Y: size of the example

log(|Y|): number of queries for each constraint when not guided

 $\frac{1}{\log(|Y|)}$: Percentage of queries resulting on a constraint learnt

KU LEUVEN Using Machine Learning in the Oracle

The oracle O(c) "classifies" a candidate as a problem constraint or not

Use of any classification technique to simulate the Oracle

Use of probabilities?	$O(c) = \frac{1}{\log(V)} \le P(c)$			
	- Using predicted probabilities instead of class works way better!!			
	- Assuming that a candidate is a constraint of the problem even if the probability is less than 50% (but above the threshold)			
Minimize the expected not - Threshold defined to minimize number of queries!				
Y : size of the example log(Y): number of queries for each constraint when not guided $\frac{1}{log(Y)}$: Percentage of queries resulting on a constraint learnt				



Open challenges





Number of queries

- Number of queries needed to converge is still large.
- Use also more expressive types of queries
- Generalize!







Specific classes of constraints

- Global constraints: Exploding the set of candidate constraints
- Linear inequalities with constants: Need to consider all possible constants -> Exploding the set of candidate constraints

COUNT	$x_1 + 5 < x_2$	
ALLDIFFERENT	$ x_1 + 12 > x_4$	
CUMULATIVE		
SUM	x ₁ - x ₂ != 238	
CIRCUIT		





Noisy data

- Unlike in machine learning, most constraint acquisition techniques still assume the user always (knows how to) answer correctly
- Tighter integration with modern machine learning techniques



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Conclusions



We discussed:

- How to guide constraint acquisition using probabilities for the candidates
- Guiding all layers of constraint acquisition
- How to use Machine Learning for guiding
- Open challenges



Holy grail 2.0

Acquire the model from text description!

Recent advances in LLMs and NL4OPT

Can we use this technology to acquire models directly from text description??



Holy grail 2.0



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Holy grail 2.0

I have only 10 hours to spend in Leuven. So I can only see a small number of attractions in the city. Visiting each attraction takes different amounts of time independent of the order in which it is visited, and they will give me different levels of happiness. Is it possible to come up with a list of attractions to visit to get maximum happiness in these 10 hours?

Parameters:

- in': the number of attractions
- " 't': a list of 'n' integers representing the time it takes to visit each attraction
- " 'h': a list of 'n' integers representing the happiness level of each attraction
- "max_time': the maximum time available to visit the attractions (in this case, 10 hours)

Variables:

x': a list of 'n' binary variables, where 'x[i] = 1' if attraction 'i' is visited, and 'x[i] = 0' otherwise.

Constraints:

- The total time spent visiting the attractions cannot exceed 'max_time': $\sum_{i=1}^{n} t_i x_i \leq max_time$
- We can only visit each attraction at most once: $\sum_{i=1}^{n} x_i \leq 1$

Objective function:

Maximize the total happiness level of the visited attractions: $\max \sum_{i=1}^{n} h_i x_i$

```
----- Model in CPMpy: -----
```

from cpmpy import *

Parameters n = 5 t = [2, 3, 1, 4, 2] h = [5, 7, 3, 8, 4] max_time = 10

Variables
x = boolvar(shape=n)

Constraints
constraints = [
 # Total time spent visiting the attractions cannot exceed max_time
 sum(t[i]*x[i] for i in range(n)) <= max_time,
 # We can only visit each attraction at most once
 sum(x[i] for i in range(n)) <= 1
1</pre>

Objective function
objective = maximize(sum(h[i]*x[i] for i in range(n)))

Solve the problem model = Model(constraints + [objective]) stats = model.solve()

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Conclusions



We discussed:

- Background on constraint acquisition
- Passive and interactive constraint acquisition
- Approaches for passive acquisition
- How interactive constraint acquisition works
- Using Machine Learning to guide interactive constraint acquisition
- Open challenges

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Thank you for your attention