Self-Supervised Transformers as Iterative Solution Improvers for Constraint Satisfaction

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Constraint Reasoning

Constraint Satisfaction Problems

Variables

$$X = \{X_{1,1}, X_{1,2}, \dots, X_{9,9}\}$$

represent cell assignments

Domains

$$D = \{D_1, D_2, \dots, D_{81}\}$$

$$D_i = \{1,2,3,4,5,6,7,8,9\}$$

Constraints

$$AllDifferent(X_{1,1}, X_{1,2}, \dots, X_{1,9})$$ each row has different values

...

$$AllDifferent(X_{1,1}, X_{2,1}, \dots, X_{9,1})$$ each column has different values

...

$$AllDifferent(X_{1,1}, X_{1,2}, \dots, X_{3,3})$$ each 3×3 square has different values

...

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

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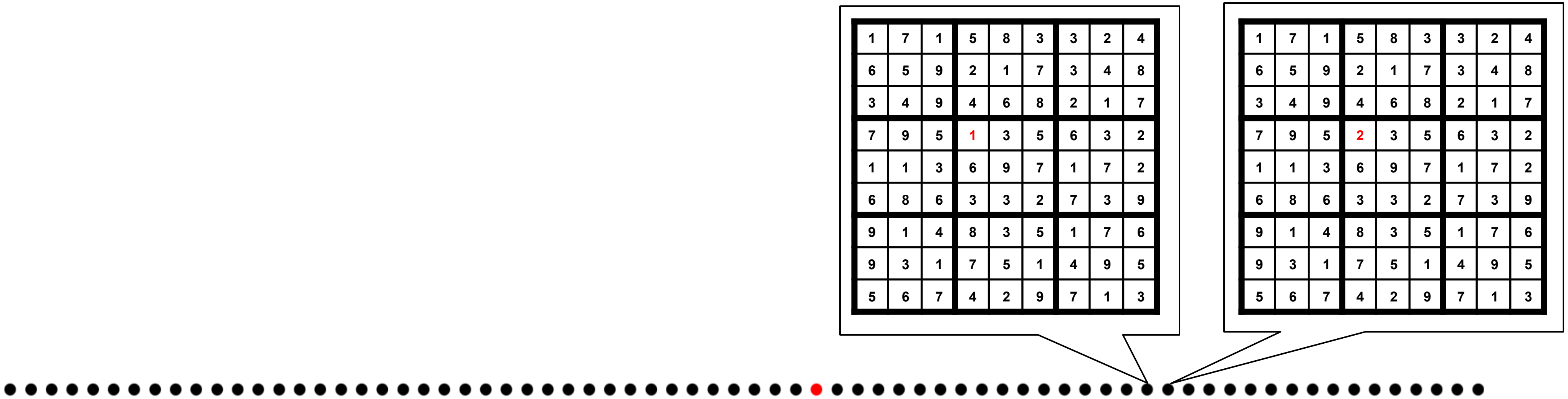
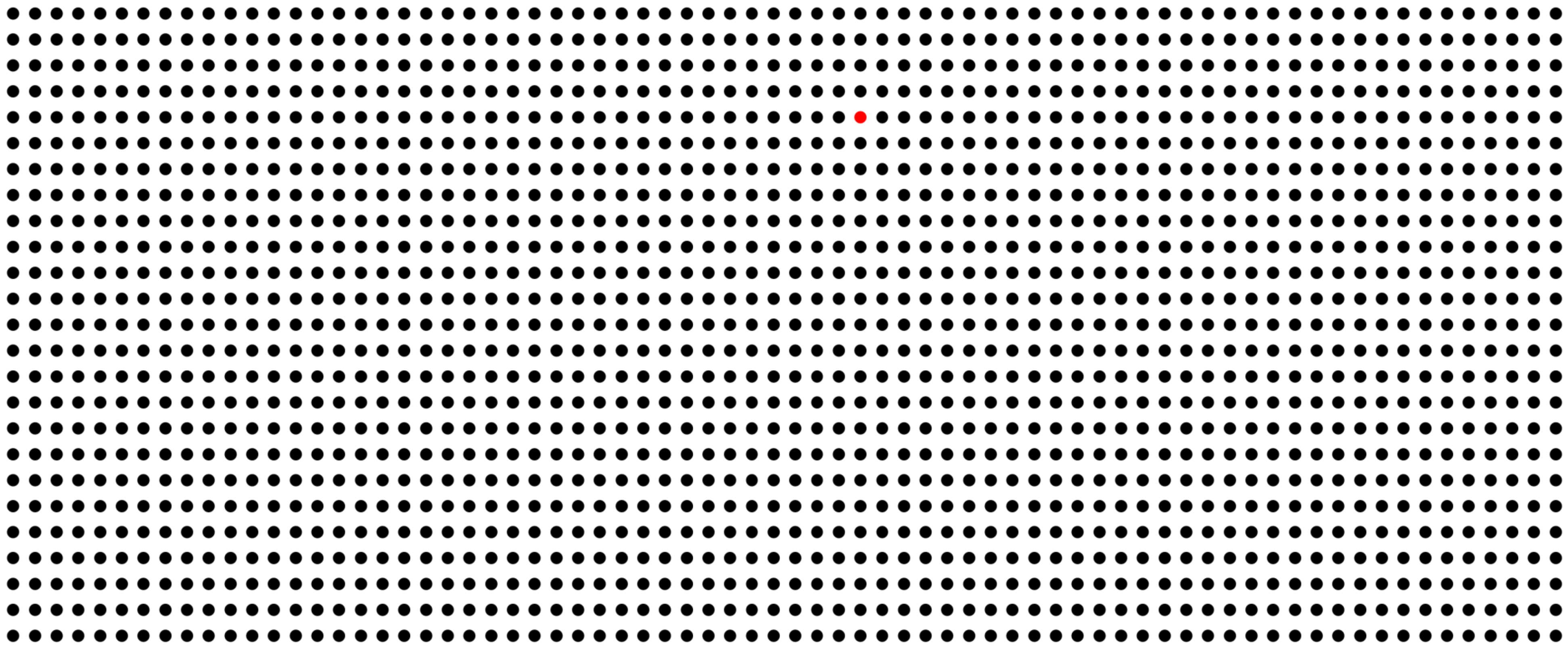
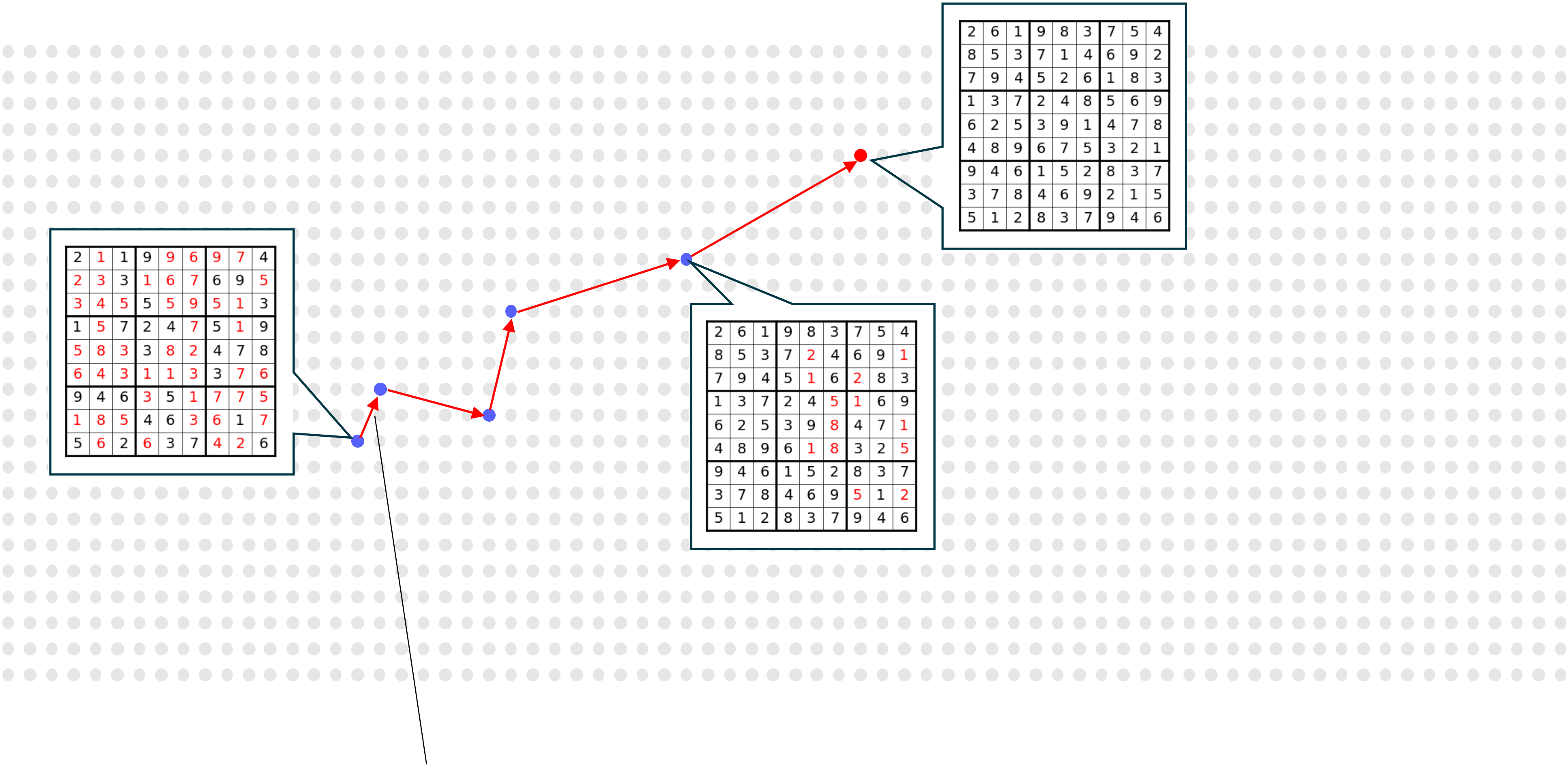
Traditional Technique: Stochastic Search



Traditional Technique: Stochastic Search



Traditional Technique: Stochastic Search



Can we learn to do a single step of stochastic search?

Our model: ConsFormer

ConsFormer: What is the input?

Variable assignments as a set of tokens

→ Token embedding for discrete domains

$$2 \Rightarrow \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \Rightarrow \begin{pmatrix} e(2) \end{pmatrix}$$

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

⇒

e(2)
e(1)
e(1)
e(9)
e(9)
e(6)
e(9)
e(7)
e(4)
e(2)
e(3)
e(3)
⋮

Need to also encode positional information!

ConsFormer: What is the input?

Variable assignments as a set of tokens

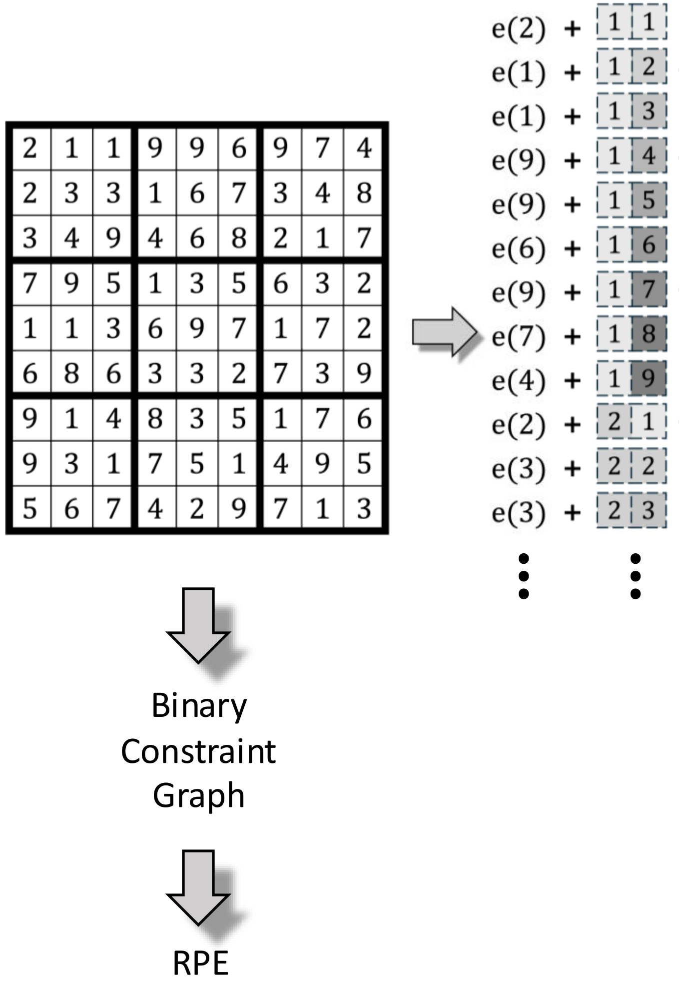
→ Token embedding for discrete domains

Variables indices

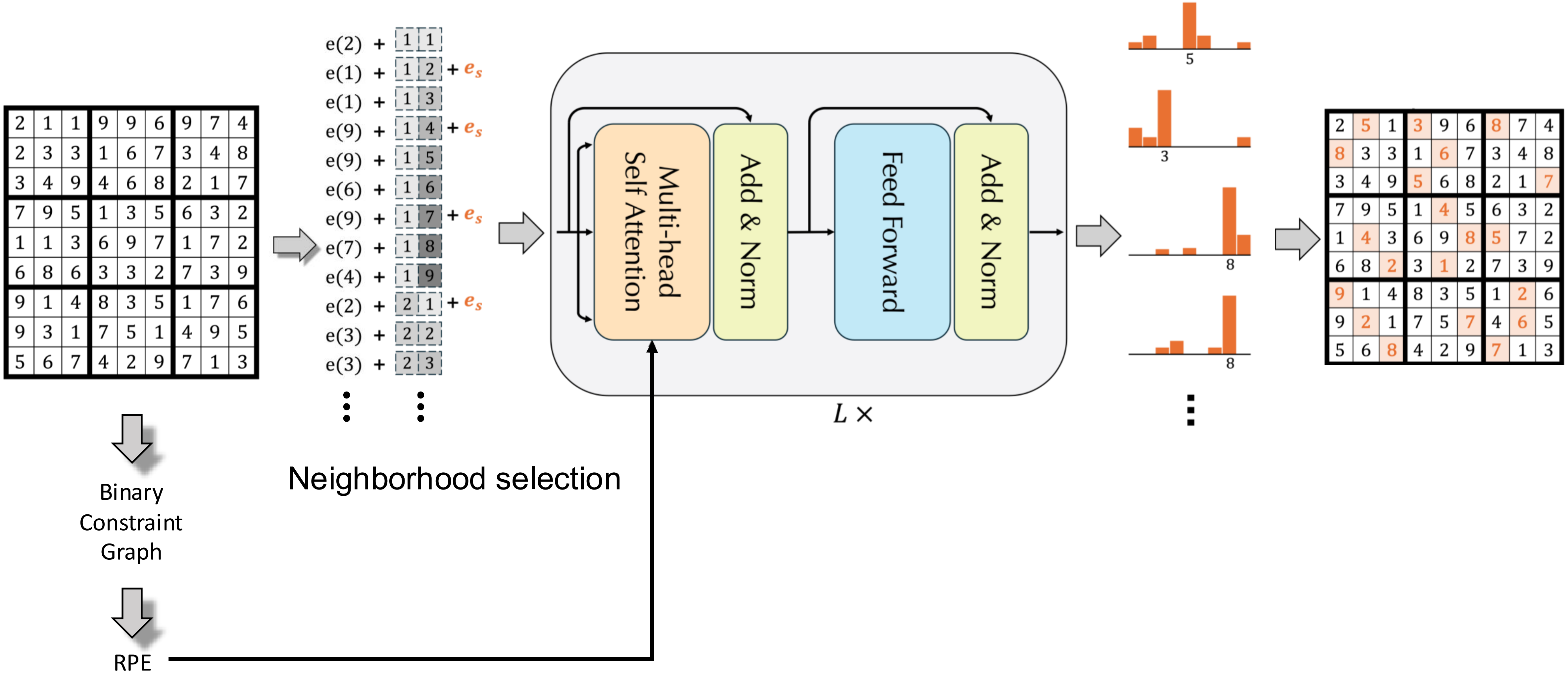
→ Absolute Positional Encodings

Variables under the scope of the same constraints

→ Relative Positional Encodings



ConsFormer: What is the architecture?



ConsFormer: How to learn?

Need a signal to guide model learning.
Existing work mostly fall into two categories.

- Supervised Learning →

Challenge:
- Labels are difficult to obtain for complex instances.
- Labels are ambiguous for instances with multiple correct solutions.

- Reinforcement Learning →

Challenge:
- Uses black-box reward function which are often sparse and overly complicated.

Our approach: Self-supervised Learning

ConsFormer: How to learn?

In traditional stochastic search, we can define *Violation Degree* to assess how badly constraints are violated.

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

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

$$AllDifferent(x_{14}, x_{15}, x_{16}, x_{24}, \dots x_{36})$$

$$\sum_{j \in [1,2,\dots,9]} \max\left(0, |\{x_i \in X \mid x_i = j\}| - 1\right)$$

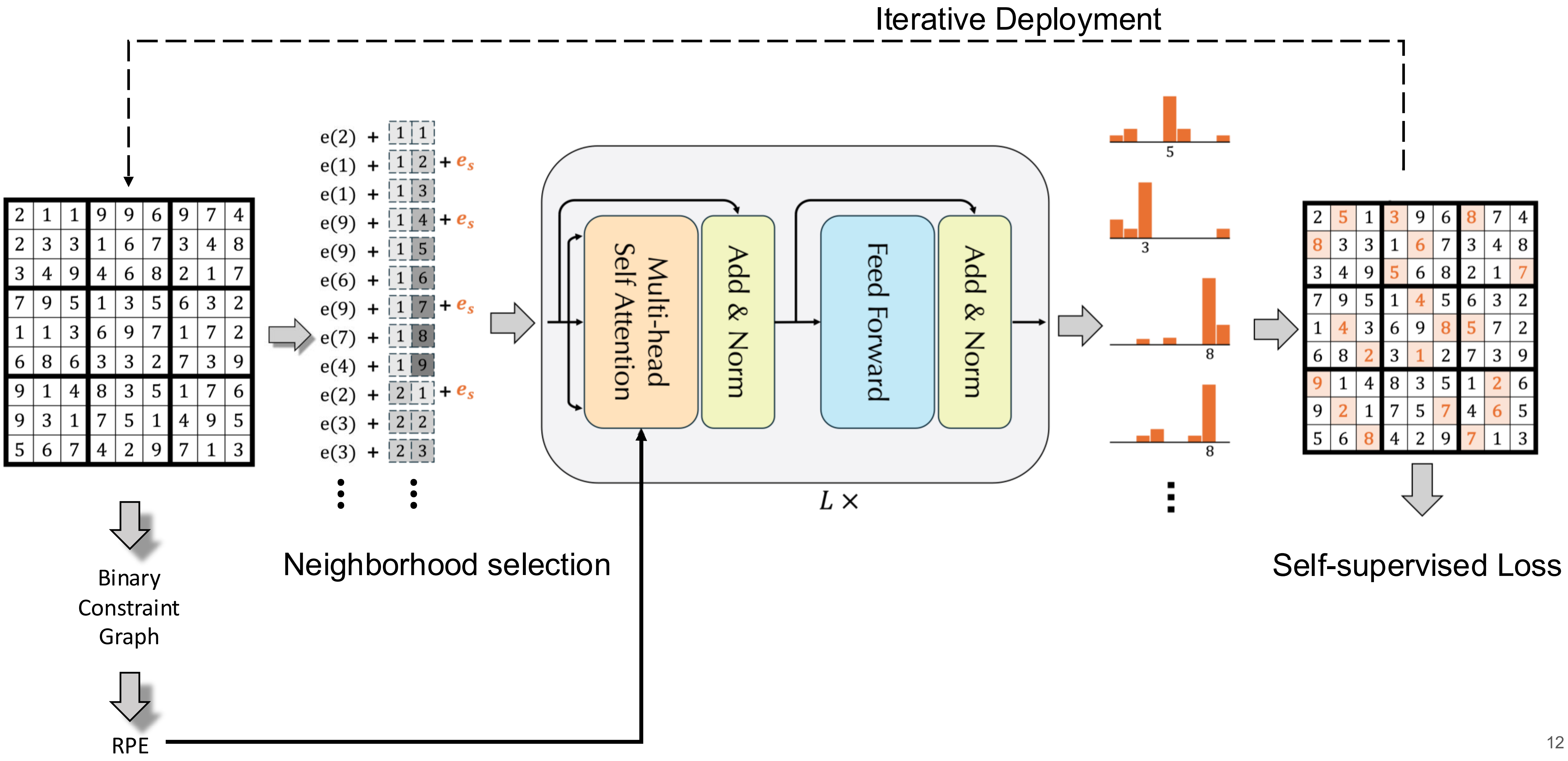
$$X = \{x_{14}, x_{15}, x_{16}, x_{24}, \dots, x_{36}\}$$

$1 + 1 + 2 = 4$

$1 + 2 = 3$

→We adapt this method and design differentiable penalty functions.

ConsFormer



Iterative Deployment
e(2) + 1 1
e(1) + 1 2 + e_s
e(1) + 1 3
e(9) + 1 4 + e_s
e(9) + 1 5
e(6) + 1 6
e(9) + 1 7 + e_s
e(7) + 1 8
e(4) + 1 9
e(2) + 2 1 + e_s
e(3) + 2 2
e(3) + 2 3
Multi-head Self Attention
Add & Norm
Feed Forward
Add & Norm
$L \times$
Binary Constraint Graph
RPE
Neighborhood selection
Self-supervised Loss

Results

Problem	Method	Test Instances	Harder OOD Instances
Sudoku	Z. Yang et al. (2023)	99.8	28.6
	ConsFormer	**100**	**77.74**
Graph-Coloring ($k = 5$)	OR-Tools	**83.08**	**57.16**
	ANYCSP	79.17	34.83
	ConsFormer	81.0	47.33
Graph-Coloring ($k = 10$)	OR-Tools	52.41	10.25
	ANYCSP	0.00	0.00
	ConsFormer	**52.60**	**11.92**
NurseRostering	OR-Tools	**100**	**100**
	ANYCSP	-	-
	ConsFormer	**100**	**100**
MAXCUT	OR-Tools	143.89 (1.84%)	378.62 (3.08%)
	ANYCSP	**1.22** (0.02%)	**51.63** (0.42%)
	ConsFormer	24.44 (0.31%)	155.88 (1.27%)

Thank you!

Read our paper here