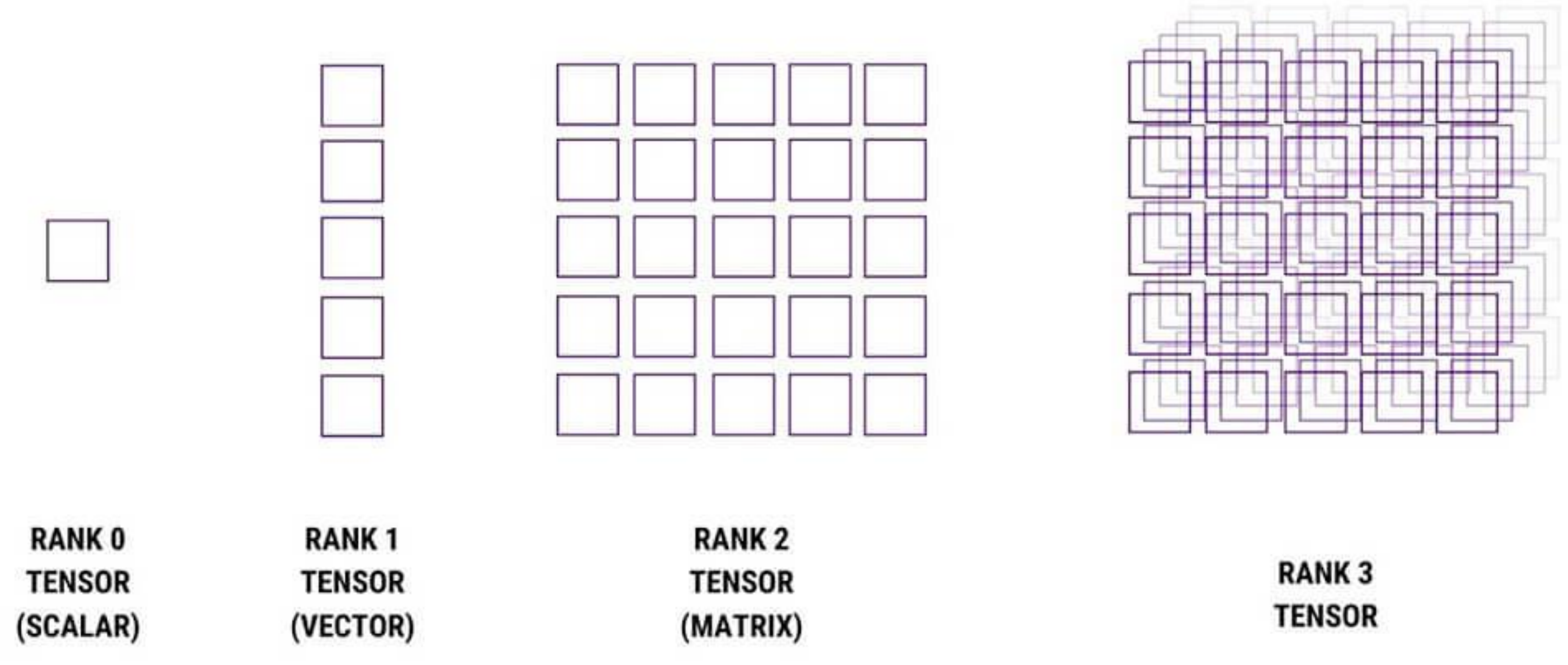
Learning with Graphs

Roger Wattenhofer

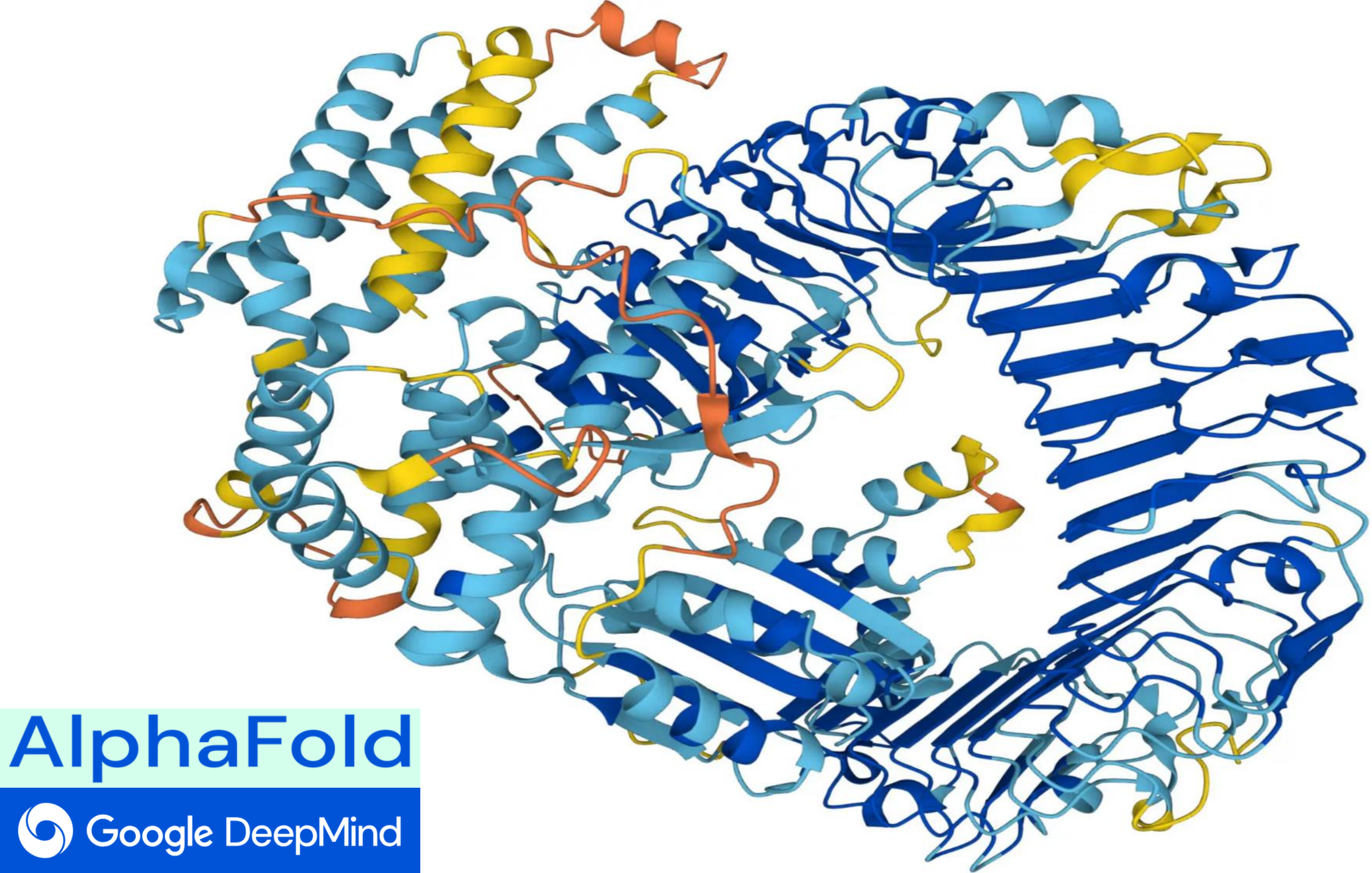

Midjourney

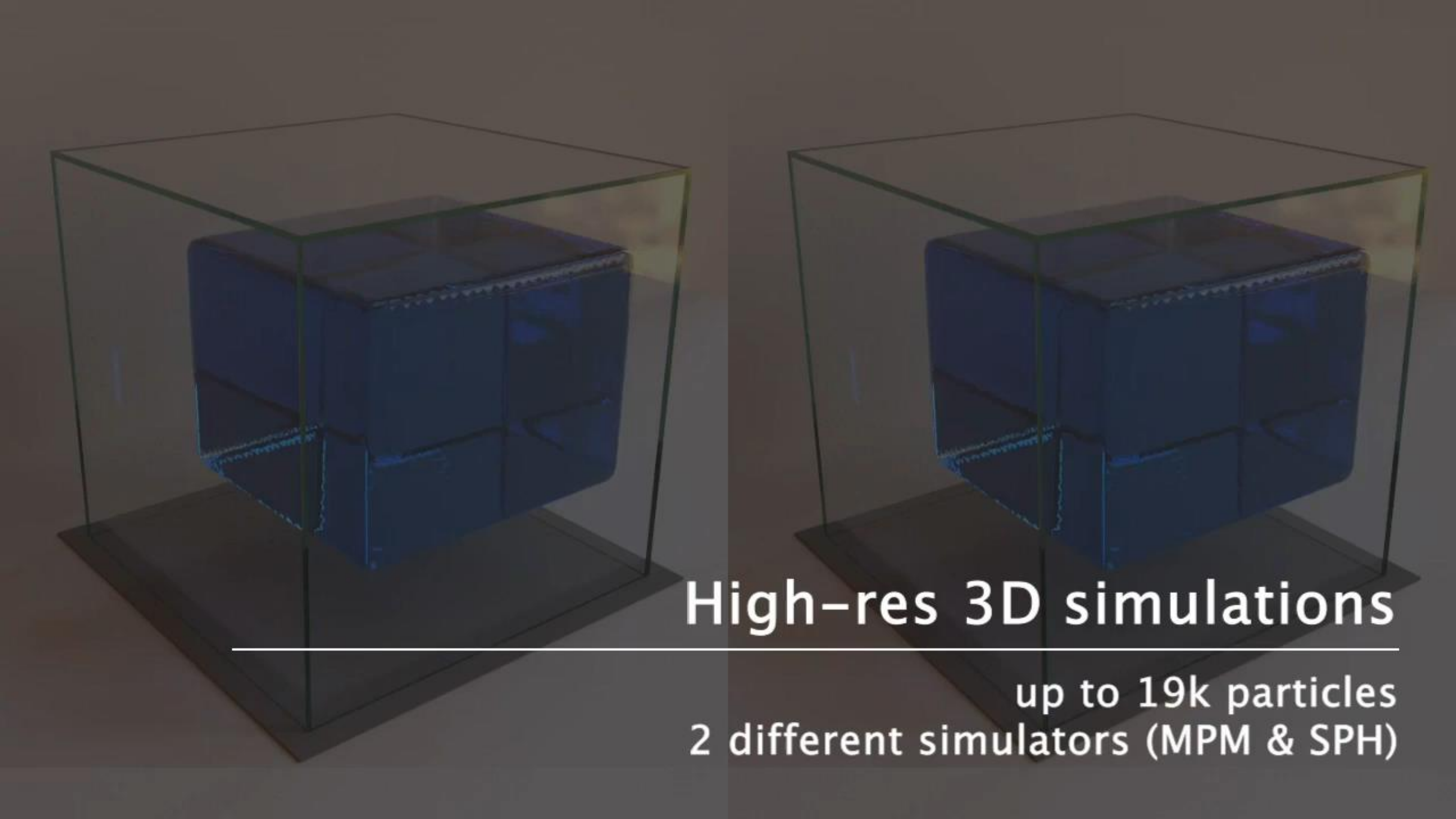

Boris Eldagsen

Machine Learning Deals with …

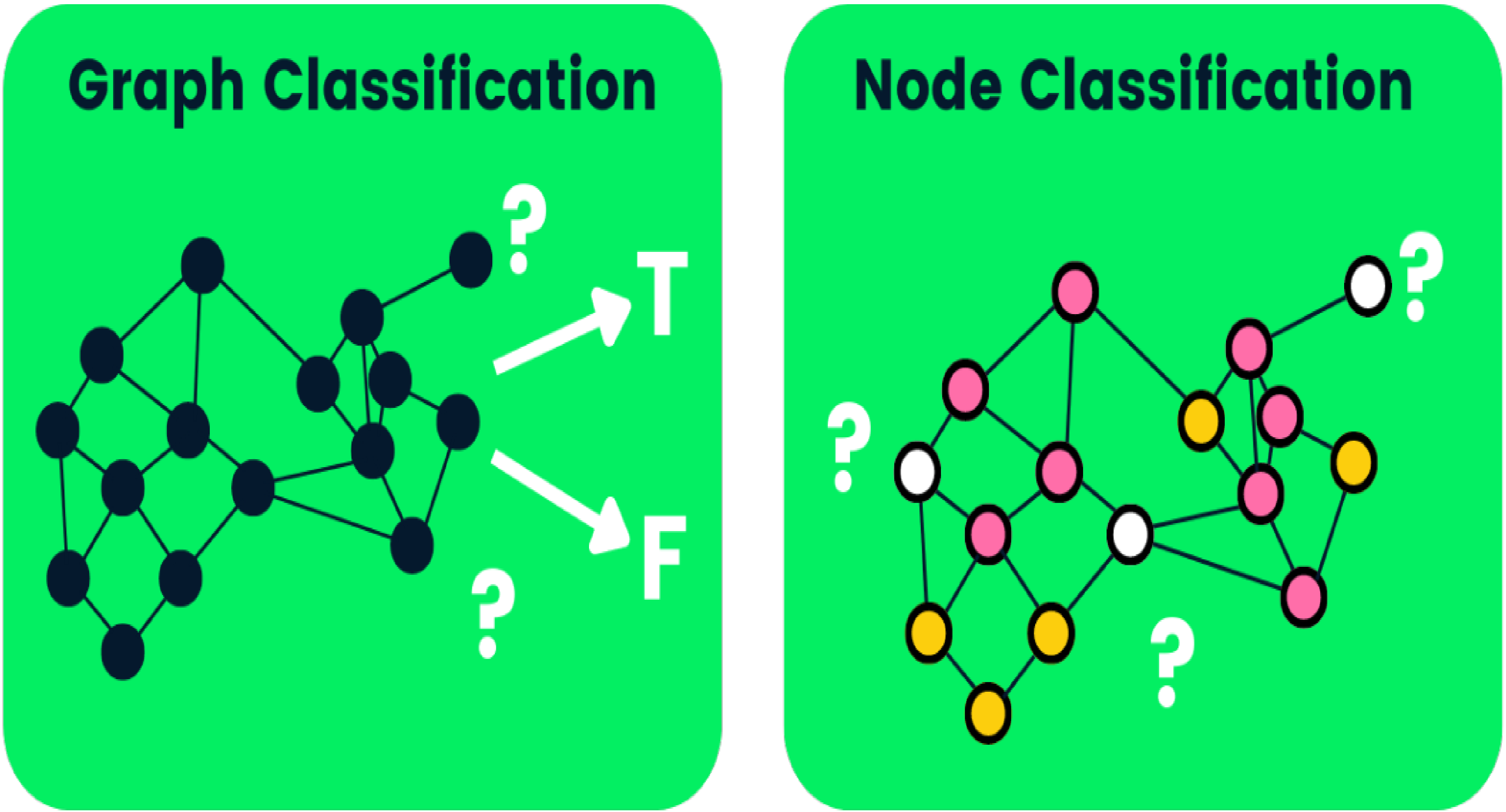


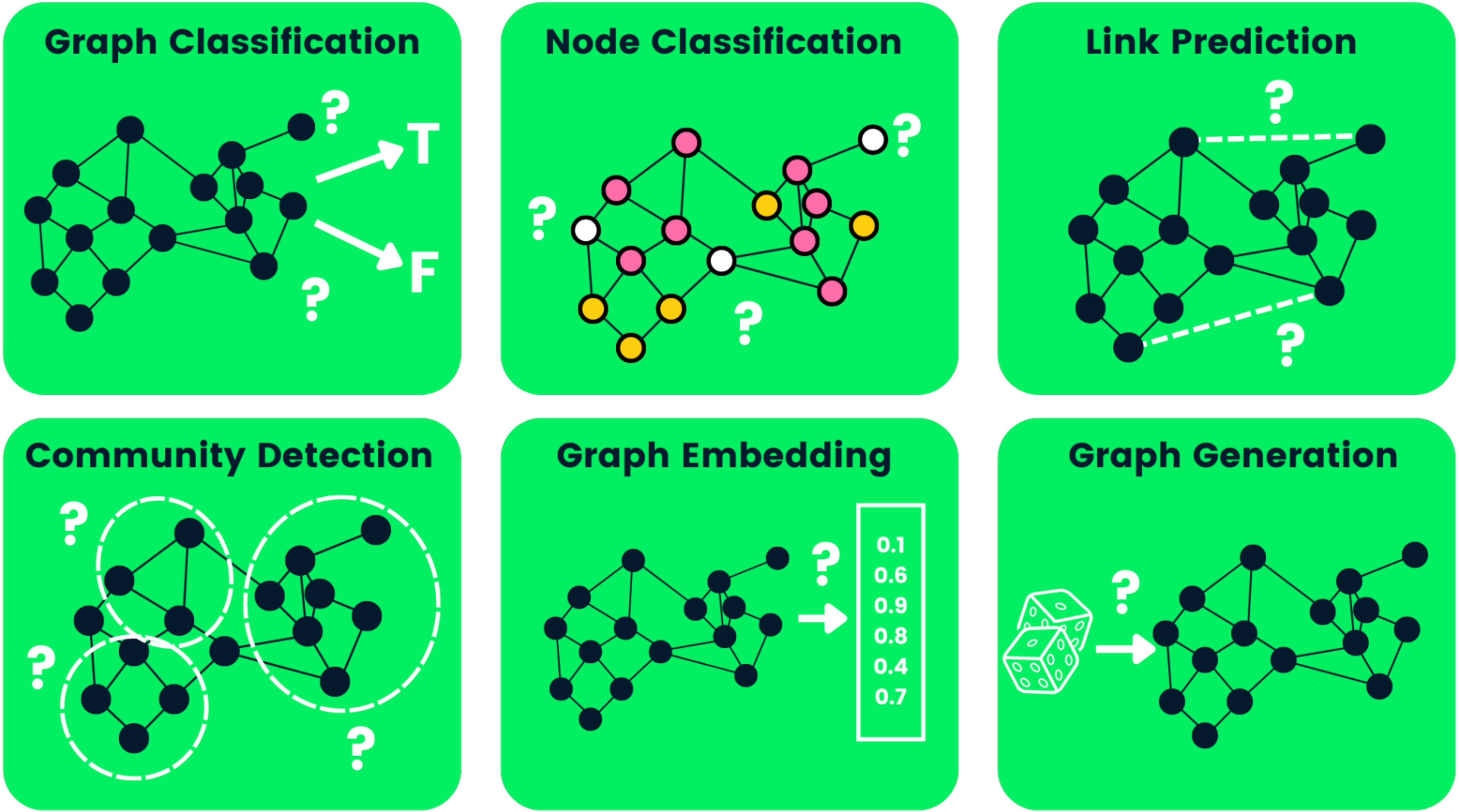
Networks
Social Networks
Neural Networks
Mobile Networks
Wireless Networks
Financial Networks
Economic Networks
Biological Networks
Computer Networks


AlphaFold
Google DeepMind


High-res 3D simulations
up to 19k particles
2 different simulators (MPM & SPH)

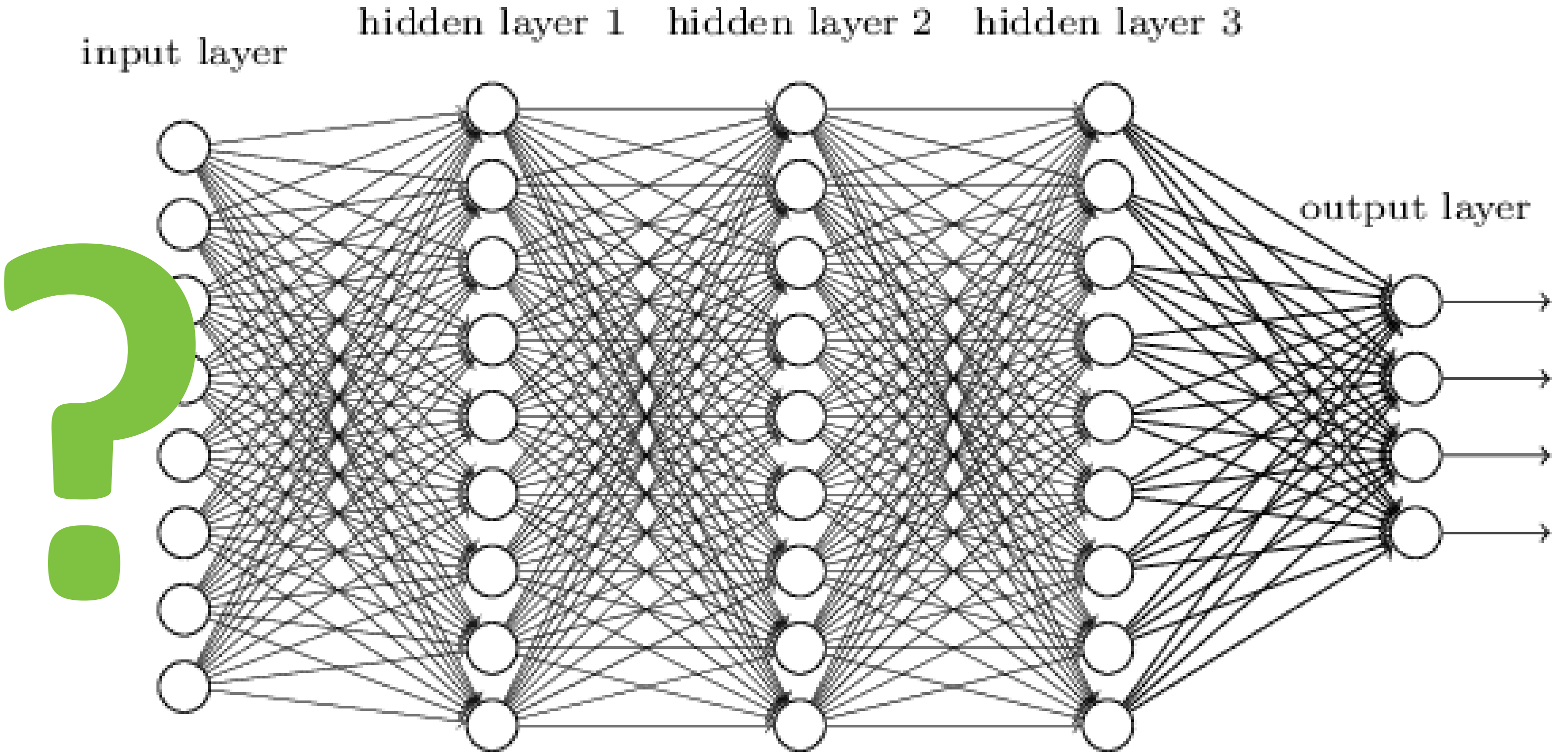
Refik Anadol, Unsupervised, MOMA


Graph Classification
?
T
F
?
Node Classification
?
?
?

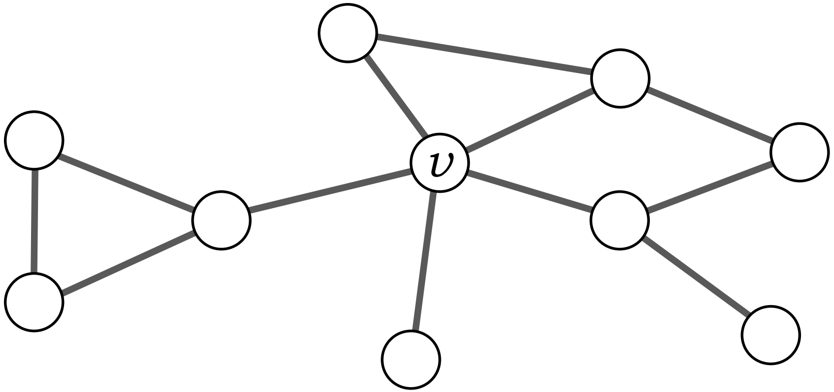

Graph Classification
T
F
Node Classification
Link Prediction
Community Detection
Graph Embedding
0.1
0.6
0.9
0.8
0.4
0.7
Graph Generation

Graph Neural Networks

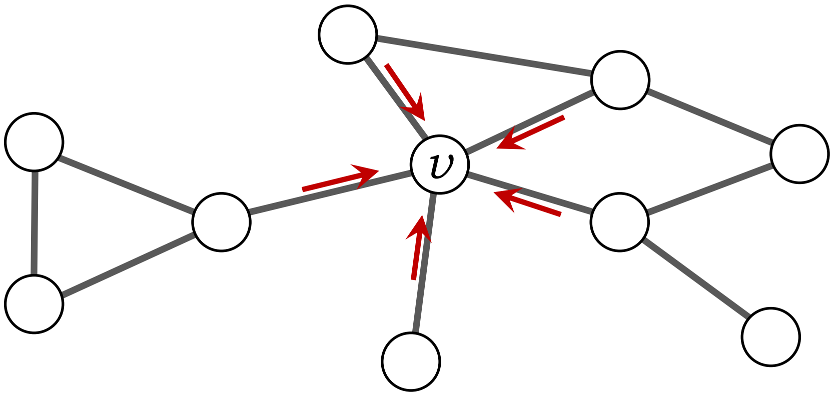
Roger Wattenhofer


input layer
hidden layer 1
hidden layer 2
hidden layer 3
output layer

Graph Neural Networks

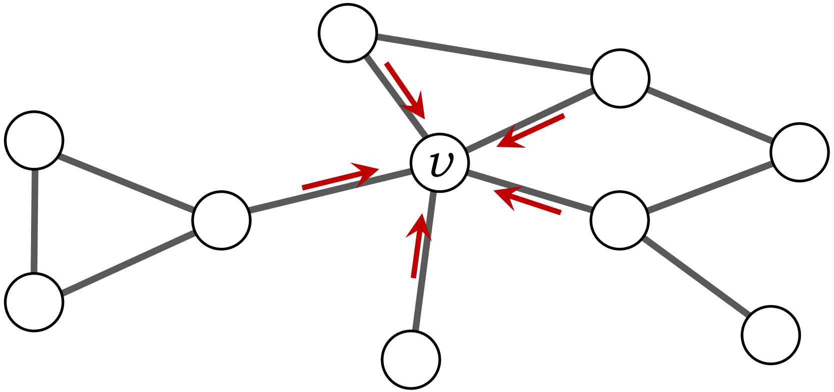


Graph Neural Networks



$a_v = \textsc{Aggregate}\left(\{\{ h_u \mid u \in N(v) \}\} \right)$ (Min, Max, Mean, Sum)

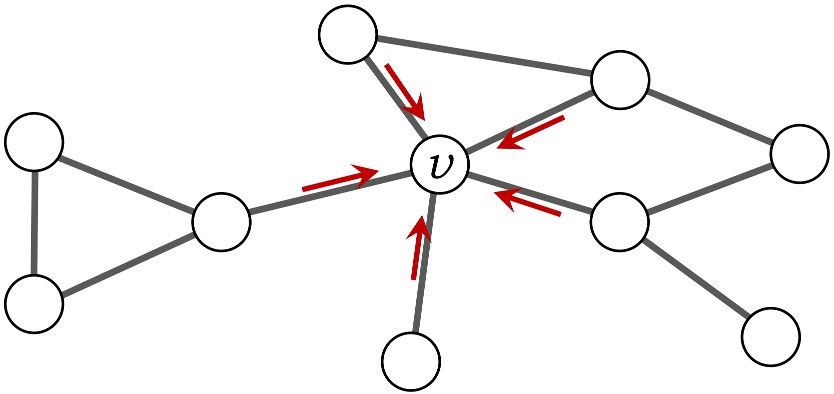
Graph Neural Networks



a_v = AGGREGATE ({{ h_u | $u \in N(v)$ }}) (Min, Max, Mean, Sum)

$h_v^{(t+1)}$ = UPDATE (h_v, a_v)

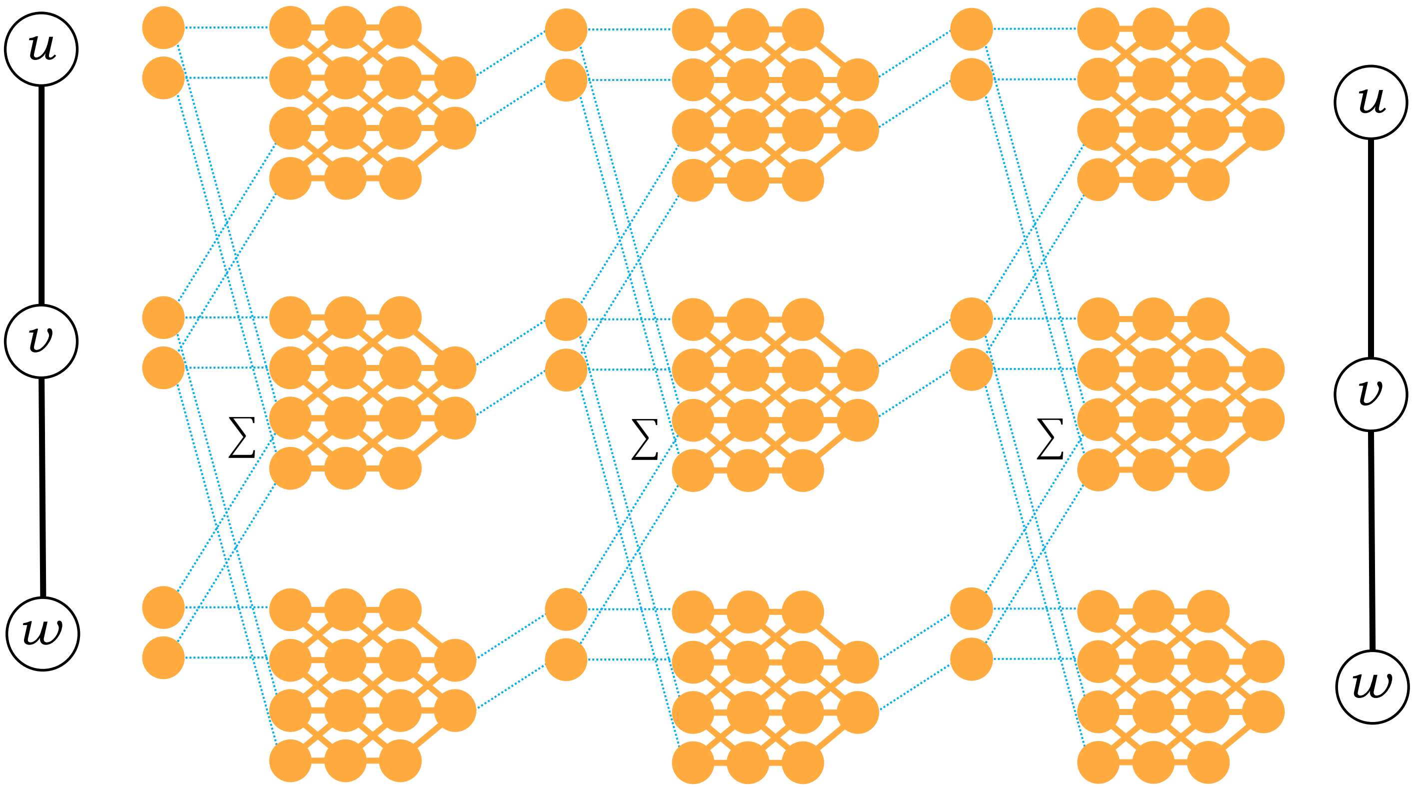
Graph Neural Networks



a_v = AGGREGATE ({{ h_u | $u \in N(v)$ }}) (Min, Max, Mean, Sum)

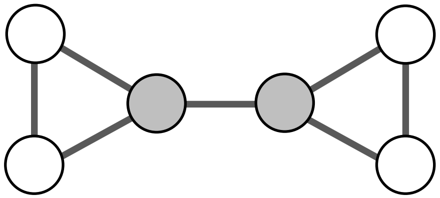
$h_v^{(t+1)}$ = UPDATE (h_v, a_v) (Little Neural Network)

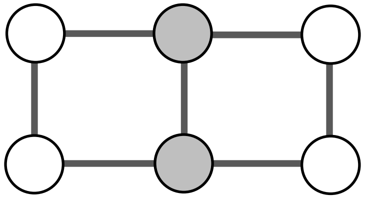
Graph Neural Networks



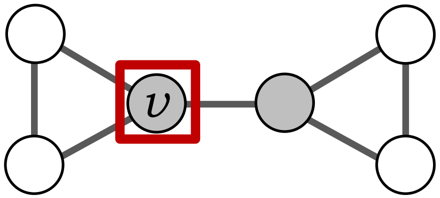
GNN Limitations?

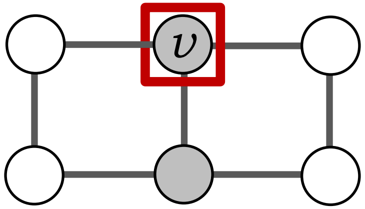
Limits of GNNs





Limits of GNNs





More Expressive GNNs?

DropGNN: Random Dropouts Increase the Expressiveness of Graph Neural Networks

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Roger Wattenhofer
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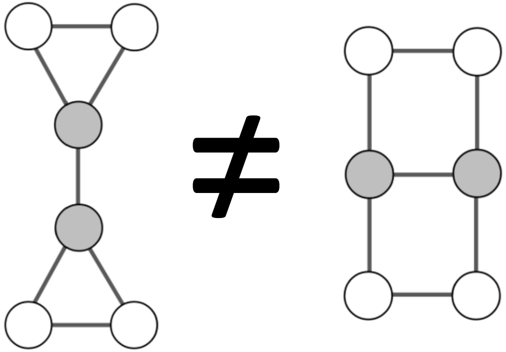
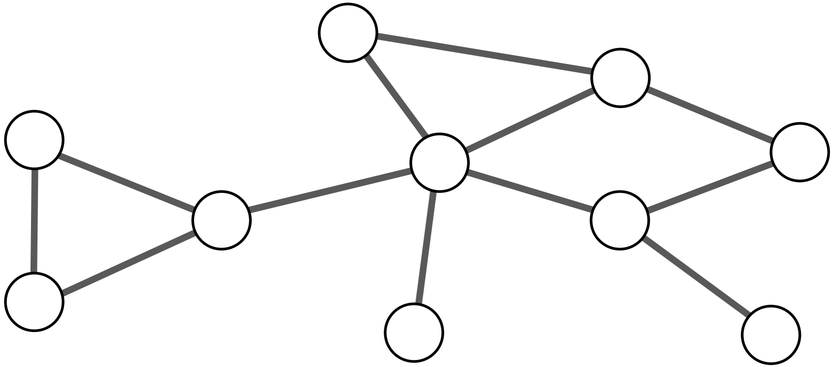


GNNs with Dropouts

Multiple runs of the GNN

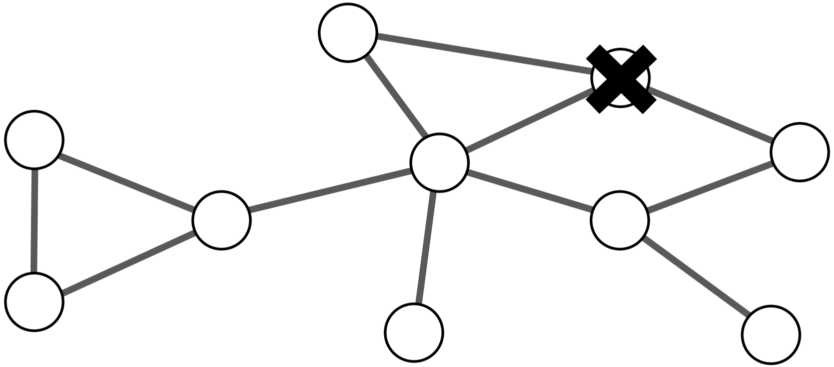
Each node removed with probability *p* independently



GNNs with Dropouts

Multiple runs of the GNN

Each node removed with probability p independently

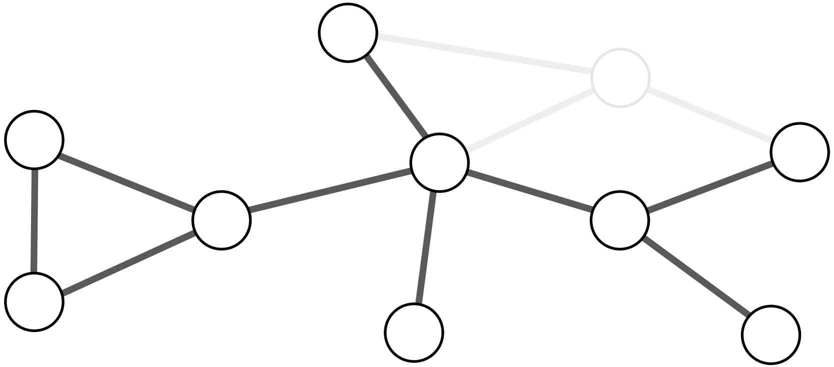


Run #1

GNNs with Dropouts

Multiple runs of the GNN

Each node removed with probability *p* independently

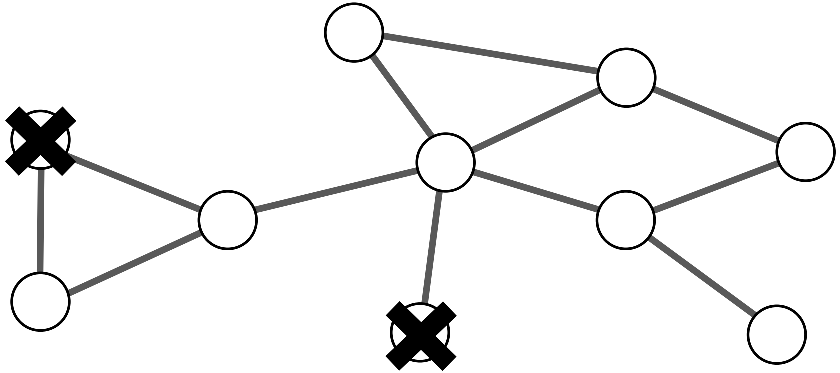


Run #1

GNNs with Dropouts

Multiple runs of the GNN

Each node removed with probability *p* independently

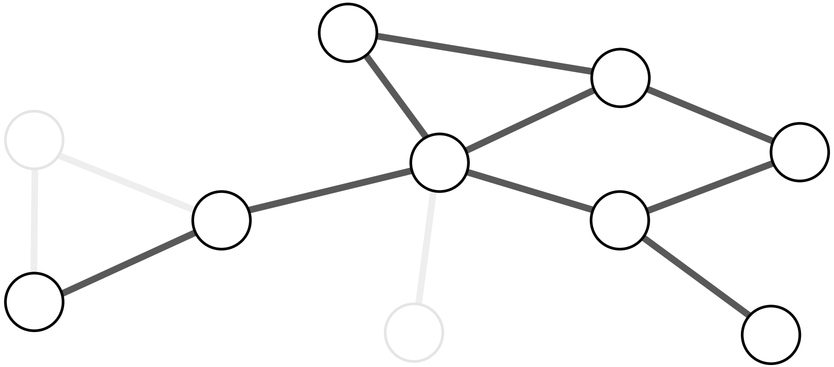


Run #2

GNNs with Dropouts

Multiple runs of the GNN

Each node removed with probability *p* independently

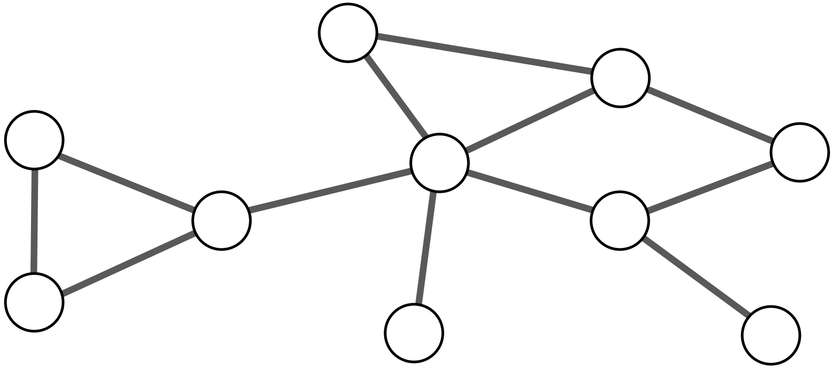


Run #2

GNNs with Dropouts

Multiple runs of the GNN

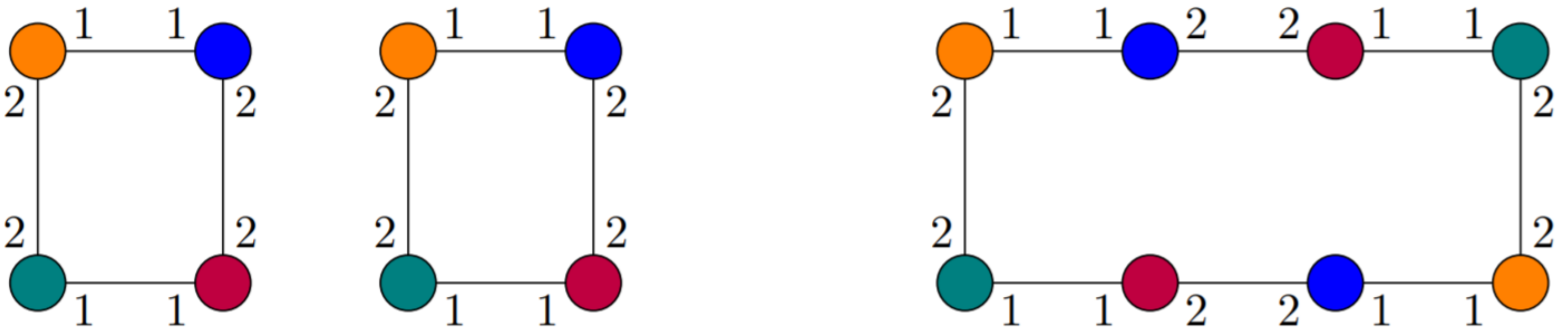
Each node removed with probability *p* independently



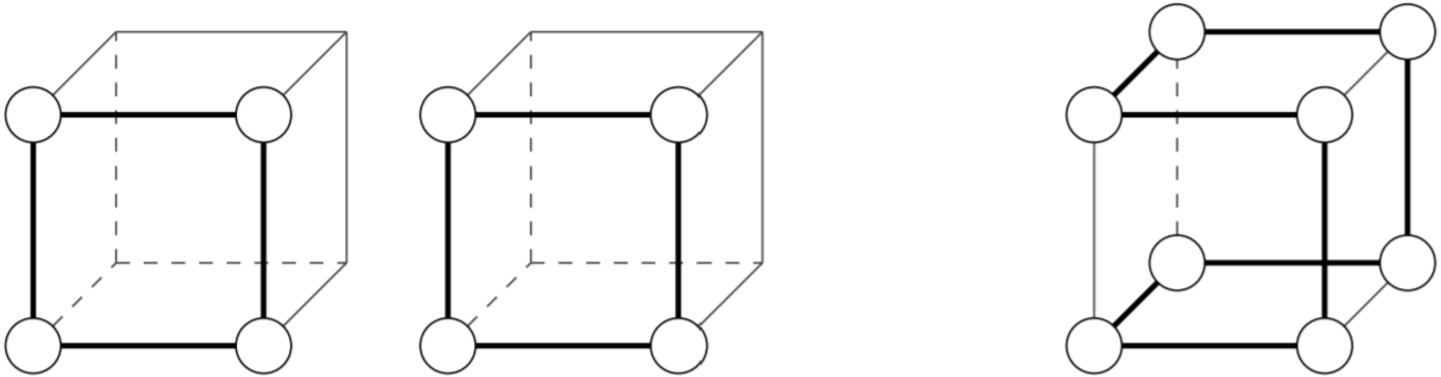
Run #3

GNNs with Dropouts

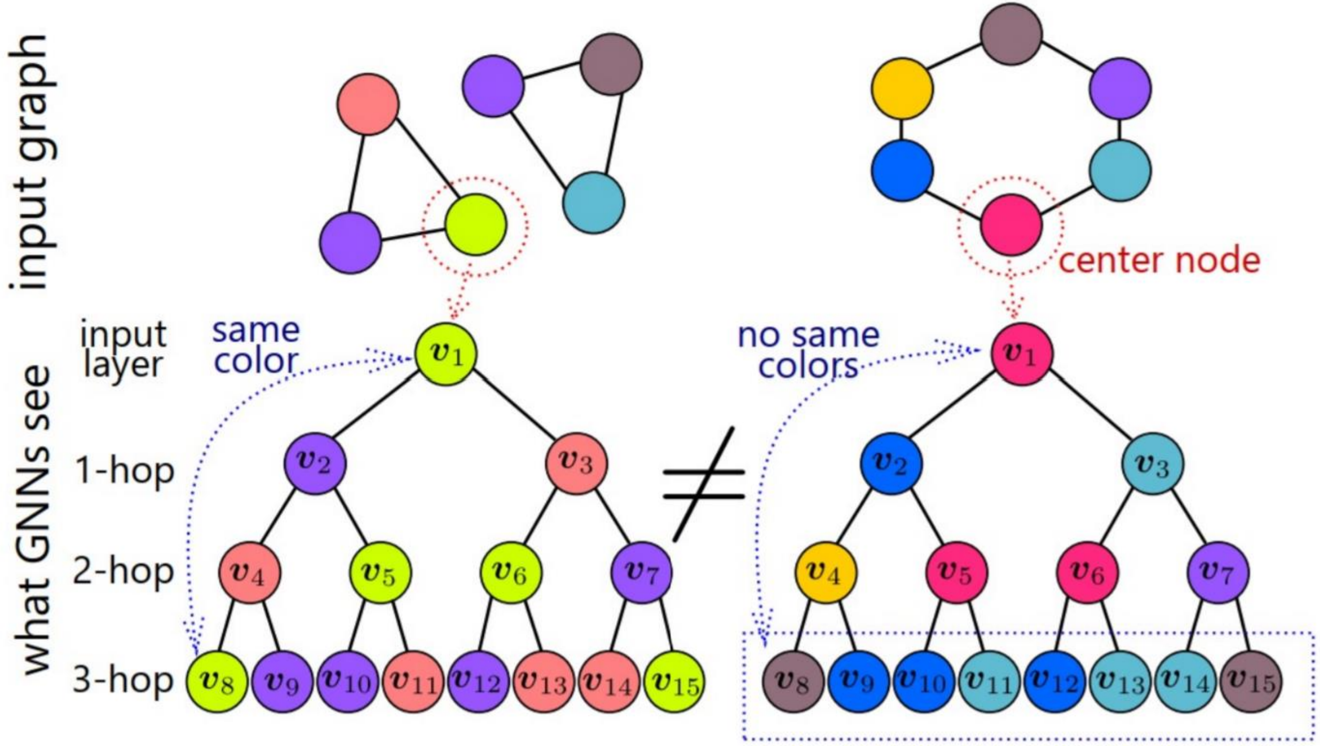
Port Numbers



Angle Features

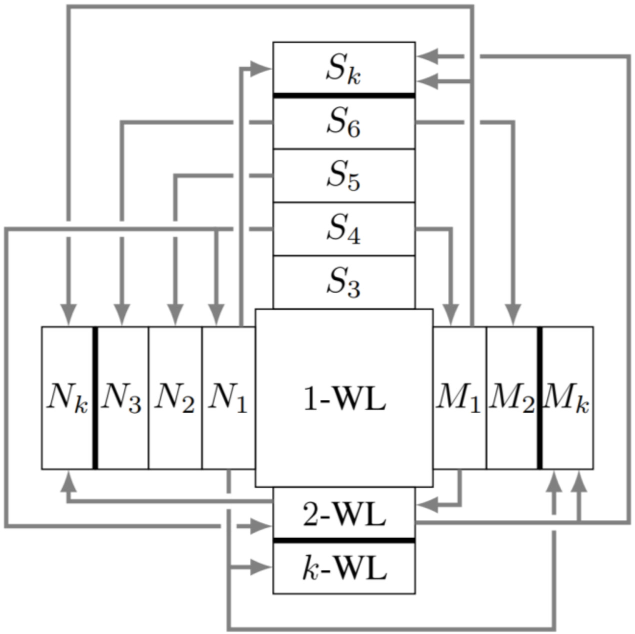


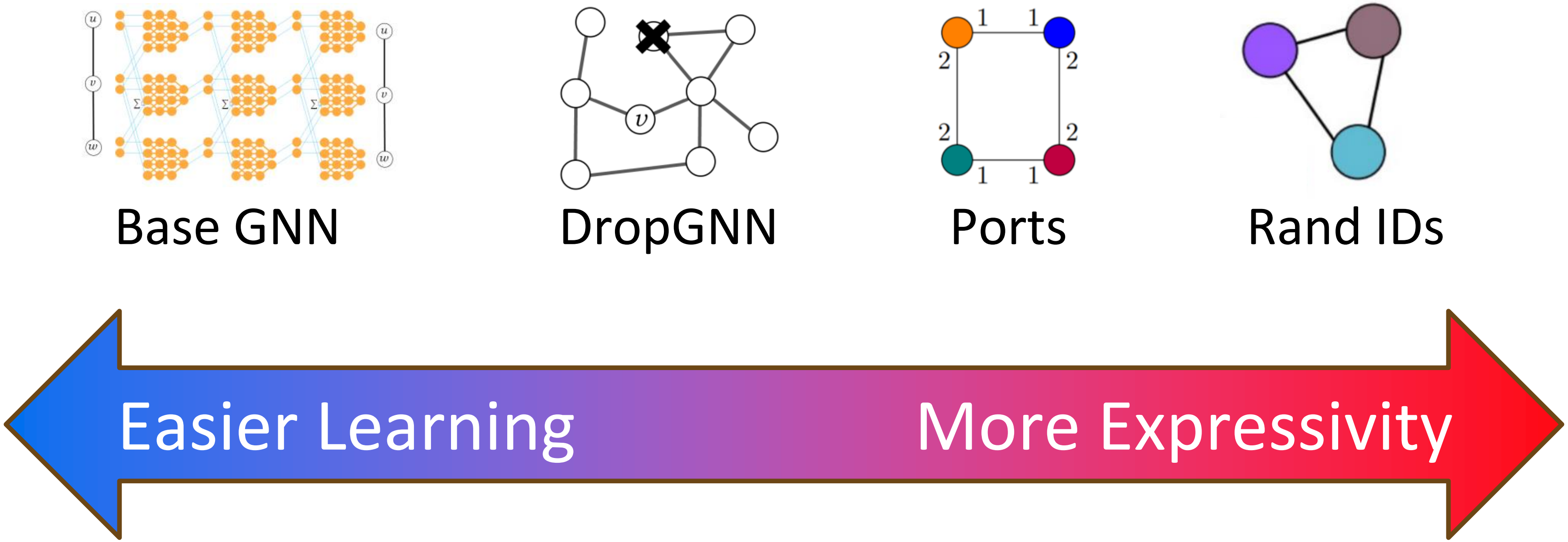
Random Features



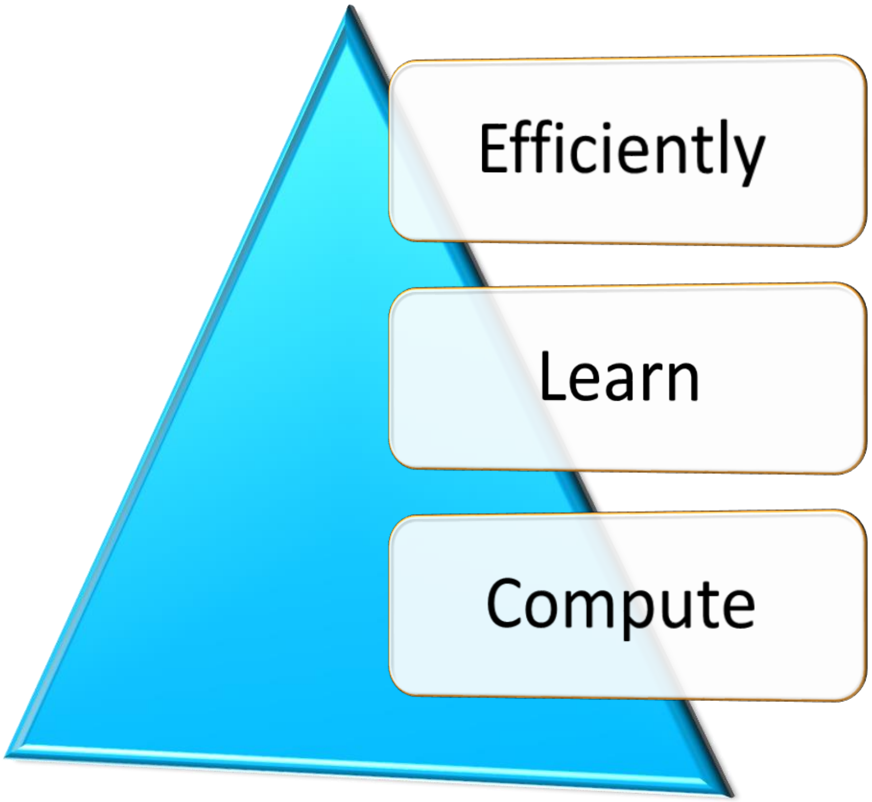
A Theoretical Comparison of Graph Neural Network Extensions

Pál András Papp [1] Roger Wattenhofer [1]





Base GNN
DropGNN
Ports
Rand IDs
Easier Learning
More Expressivity



Efficiently
Learn
Compute

Extrapolation

Without Aggregation?

GwAC: GNNs with Asynchronous Communication

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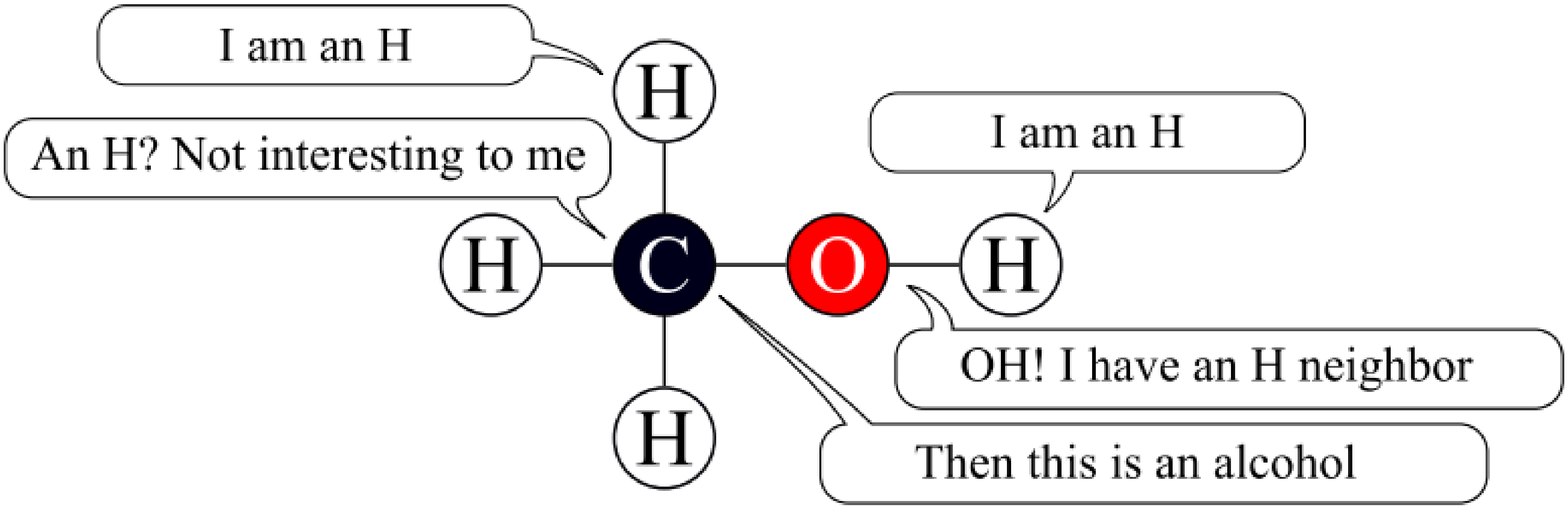
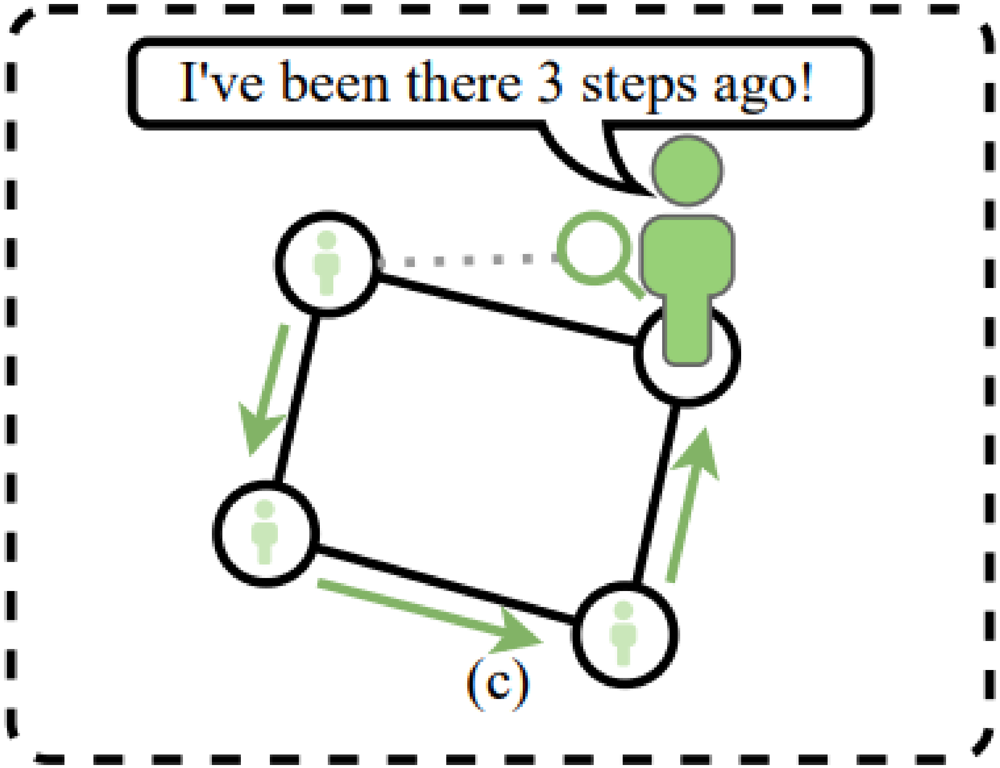
Roger Wattenhofer
ETH Zurich, Switzerland
wattenhofer@ethz.ch



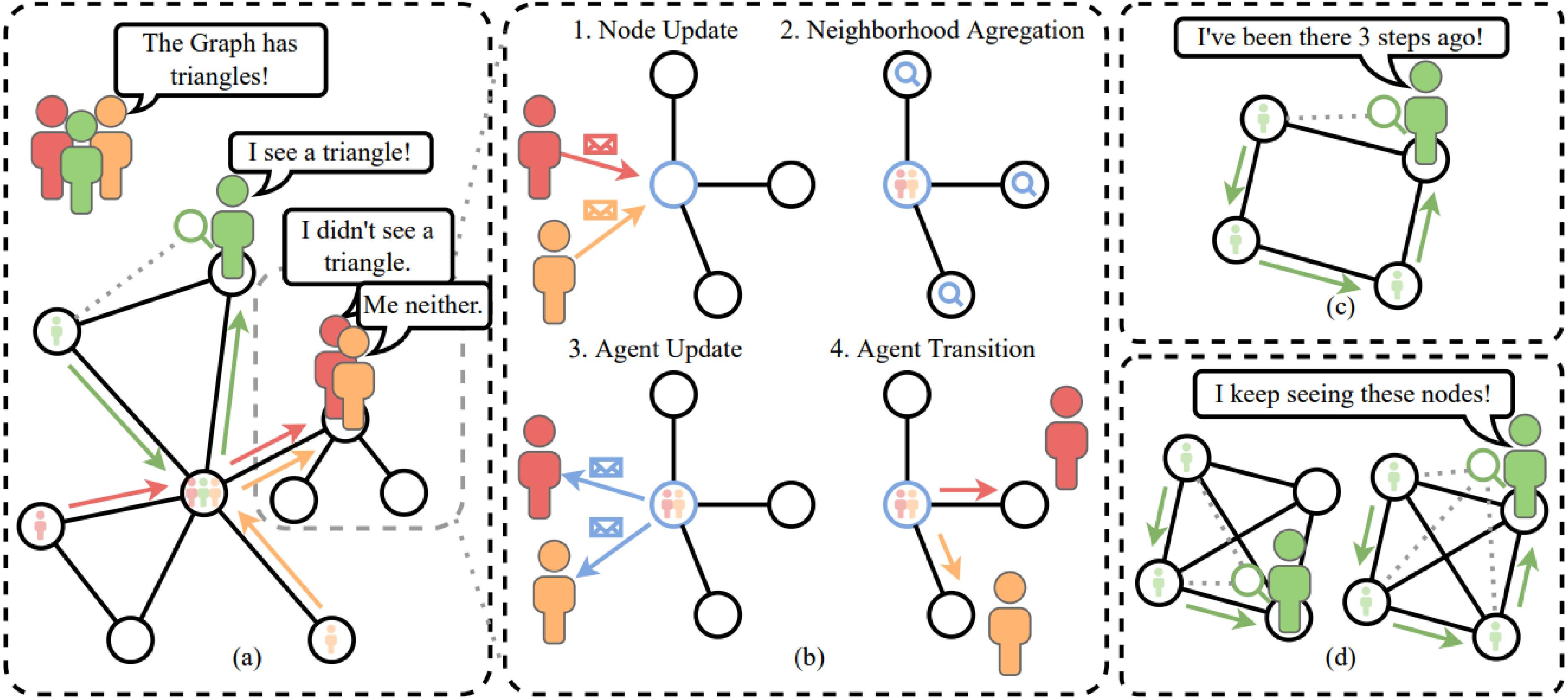
AGENT-BASED GRAPH NEURAL NETWORKS

Karolis Martinkus[1], **Pál András Papp**[2], **Benedikt Schesch**[1], **Roger Wattenhofer**[1]
[1]ETH Zurich [2]Computing Systems Lab, Huawei Zurich Research Center

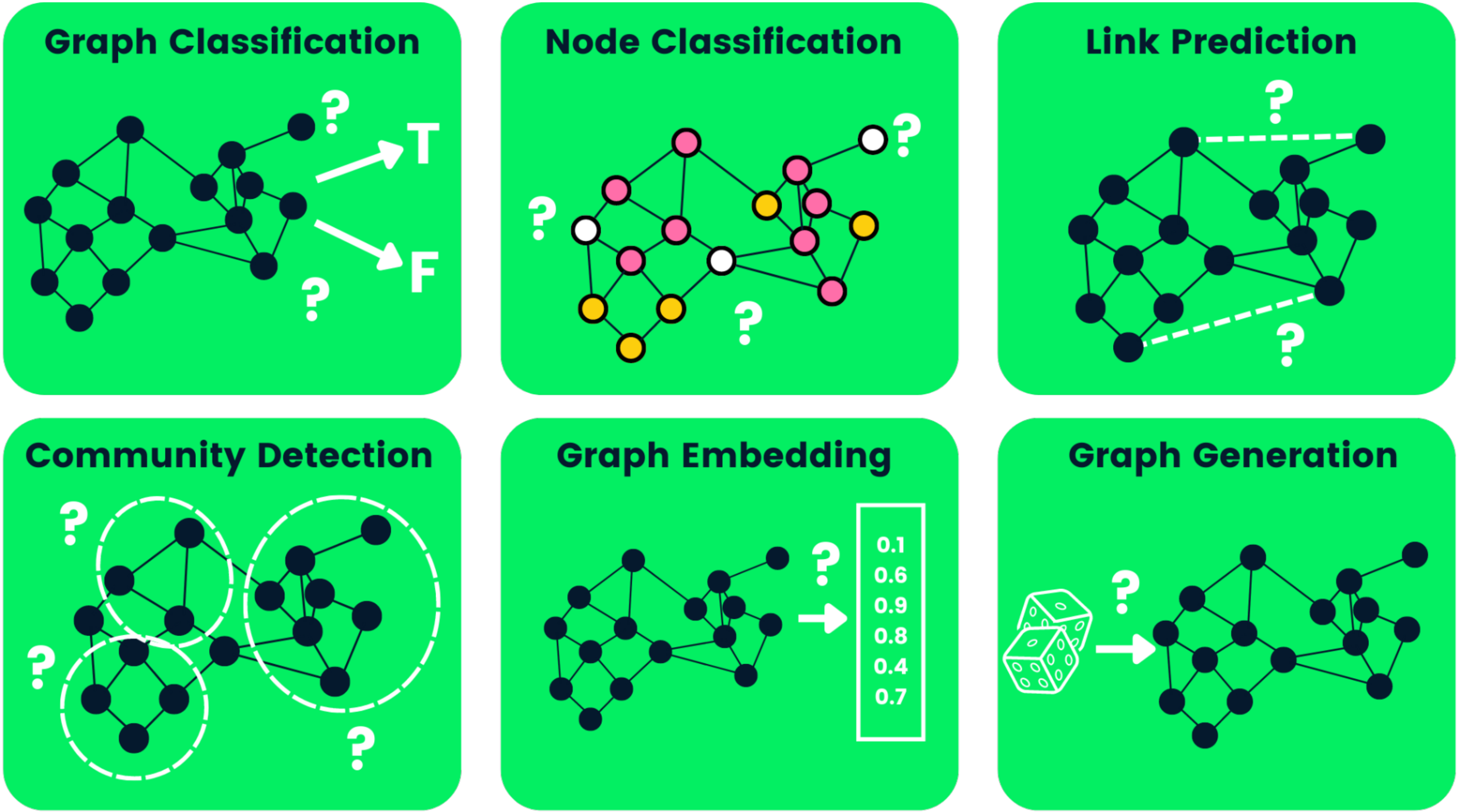


Agent-based Graph Neural Networks

Karolis Martinkus[1], Pál András Papp[2], Benedikt Schesch[1], Roger Wattenhofer[1]



Model	4-CYCLES [59]	CIRCULAR SKIP LINKS [15]	2-WL
GIN [75]	50.0 ±0.0	10.0 ±0.0	50.0 ±0.0
GIN with random features [64; 1]	99.7 ±0.4	95.8 ±2.1	92.4 ±1.6
SMP [71]	**100.0 ±0.0**	**100.0 ±0.0**	50.0 ±0.0
DROPGIN [59]	**100.0 ±0.0**	**100.0 ±0.0**	**100.0 ±0.0**
ESAN [8]	**100.0 ±0.0**	**100.0 ±0.0**	**100.0 ±0.0***
1-2-3 GNN [53]	**100.0 ±0.0**	**100.0 ±0.0**	**100.0 ±0.0†**
PPGN [51]	**100.0 ±0.0**	**100.0 ±0.0**	50.0 ±0.0
CRAWL [67]	**100.0 ±0.0**	**100.0 ±0.0**	**100.0 ±0.0**
RANDOM WALK AGENTNET	**100.0 ±0.0**	**100.0 ±0.0**	50.5 ±4.5
SIMPLIFIED AGENTNET	**100.0 ±0.0**	**100.0 ±0.0**	**100.0 ±0.0**
AGENTNET	**100.0 ±0.0**	**100.0 ±0.0**	**100.0 ±0.0**


Graph Classification
?
T
F
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Node Classification
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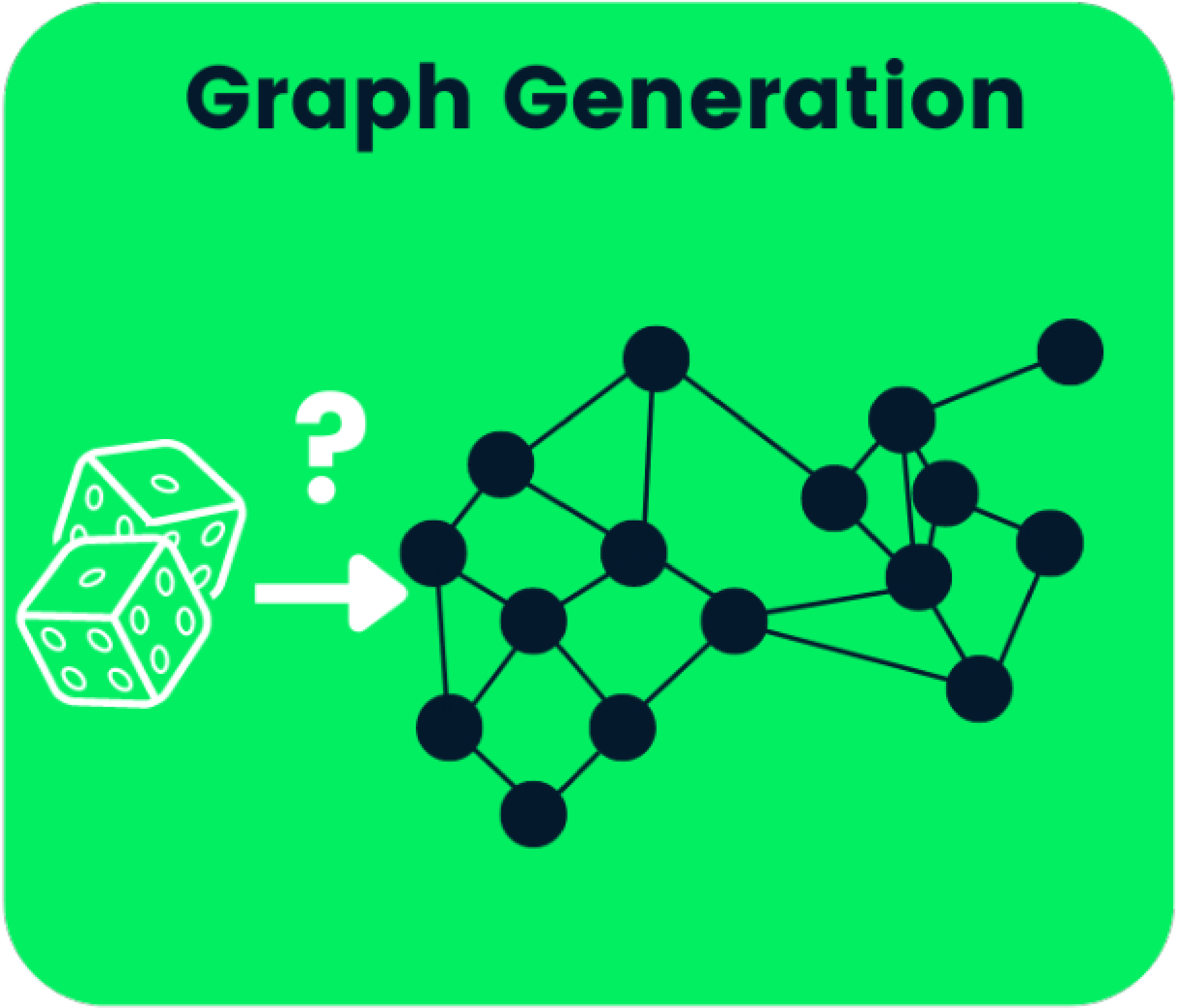
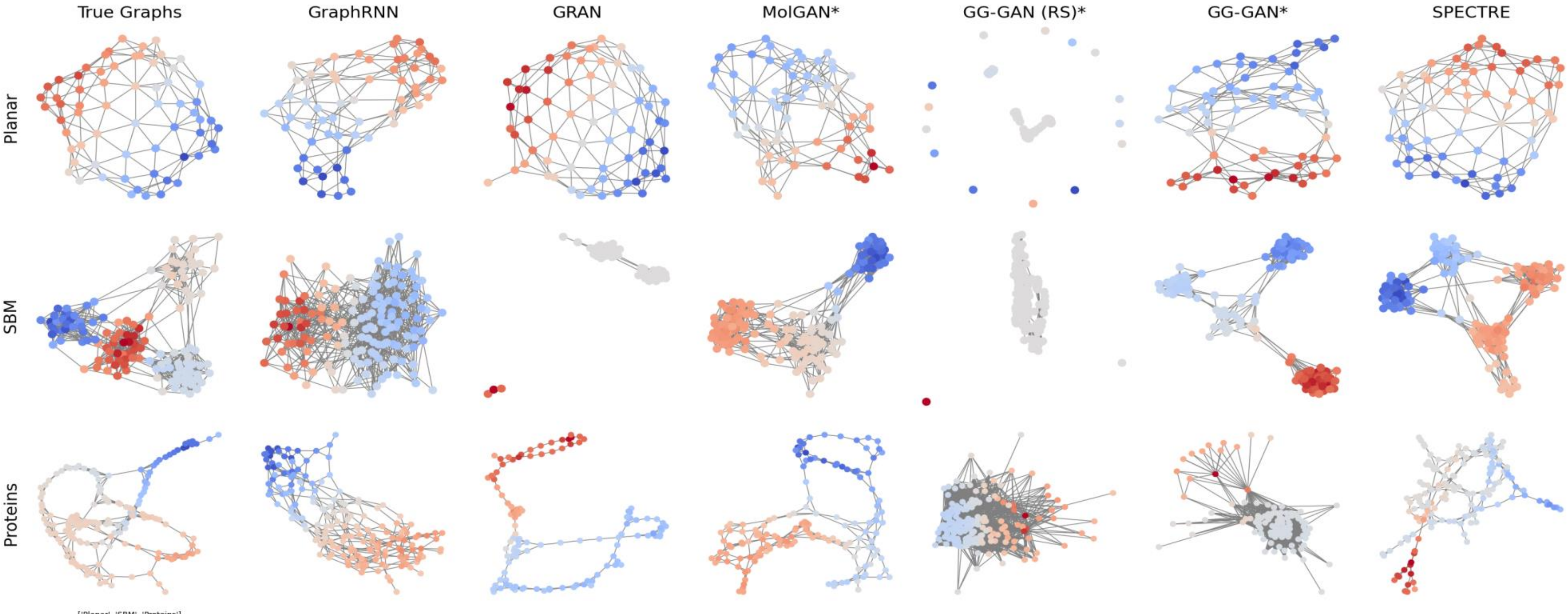
?
?
Link Prediction
?
?
Community Detection
?
?
?
Graph Embedding
?
0.1
0.6
0.9
0.8
0.4
0.7
Graph Generation
?


Graph Generation
?

SPECTRE : Spectral Conditioning Helps to Overcome the Expressivity Limits of One-shot Graph Generators

Karolis Martinkus [1] **Andreas Loukas** [* 2] **Nathanaël Perraudin** [* 3] **Roger Wattenhofer** [1]

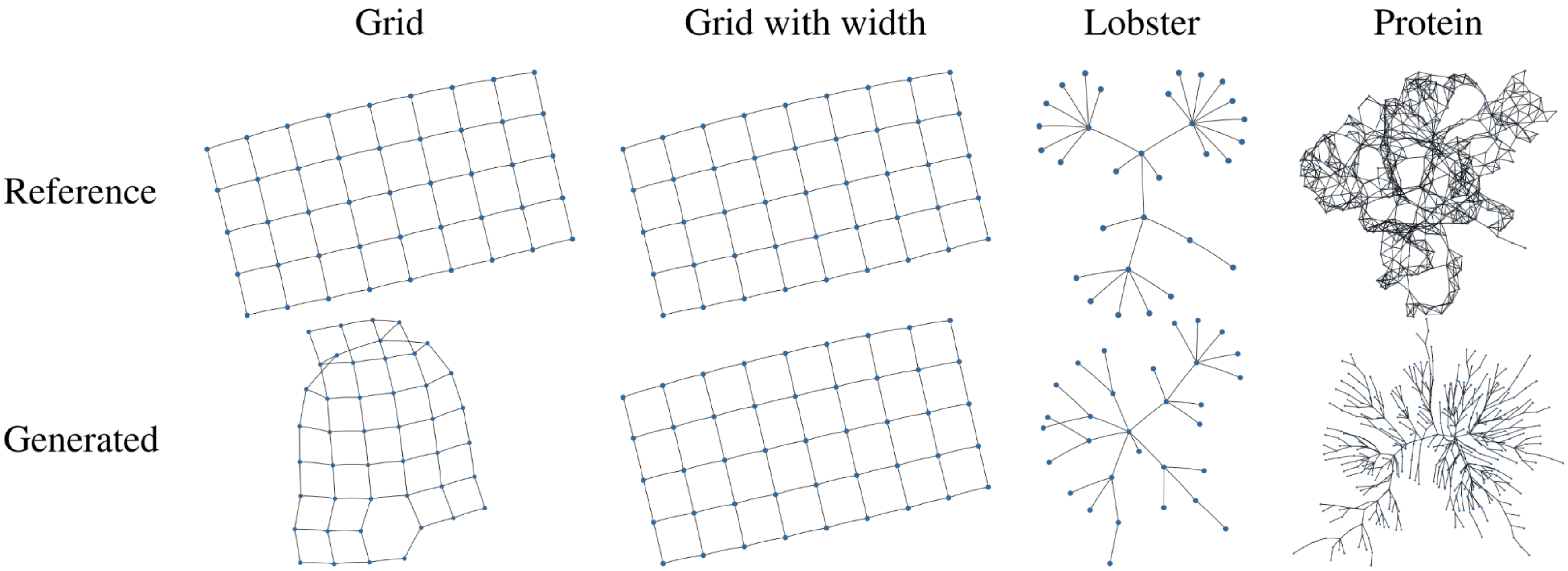


DISCOVERING GRAPH GENERATION ALGORITHMS

Mihai Babiac, Karolis Martinkus & Roger Wattenhofer
ETH Zurich
{mbabiac,martinkus,wattenhofer}@ethz.ch

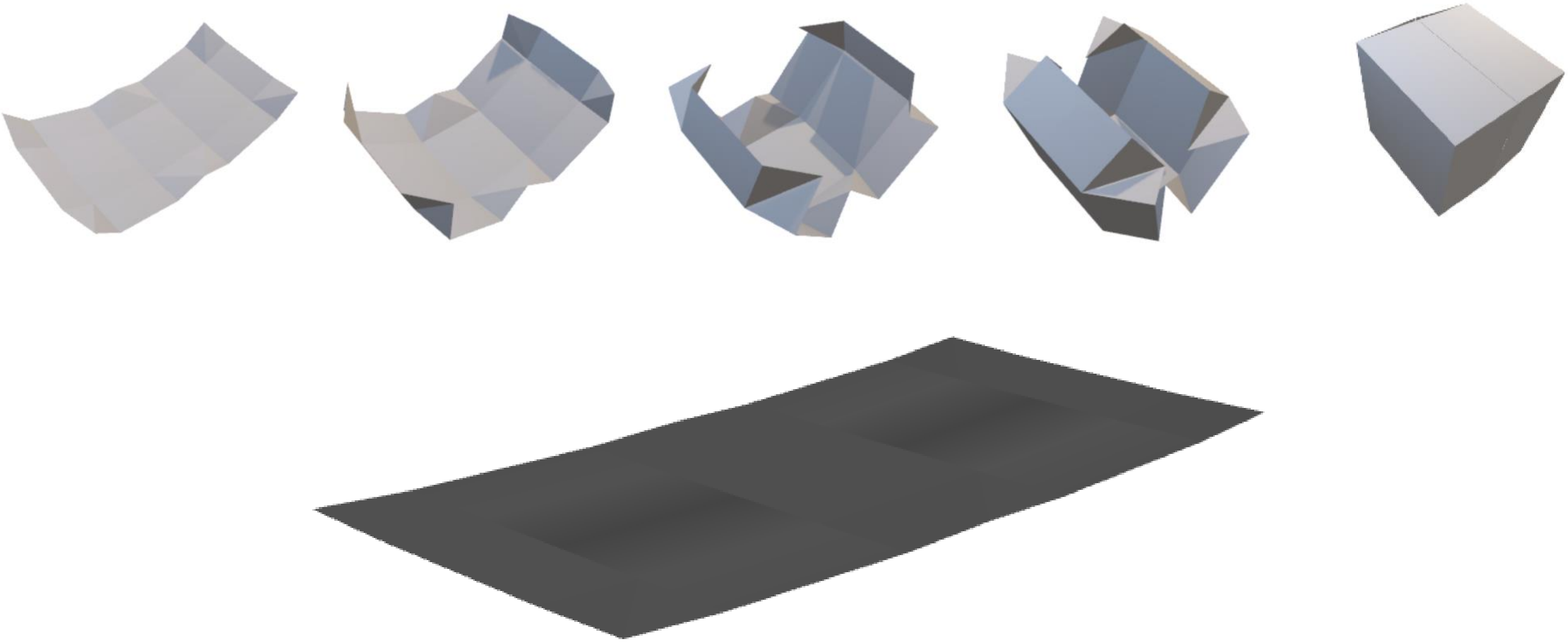
```
def outer_loop():
    for i in range(N):
        inner_loop()

def inner_loop():
    for j in range(i):
        float00 = random(0, 1)
        bool00 = float00 < 0.4
        if bool00:
            add_edge(i, j)

outer_loop()
```

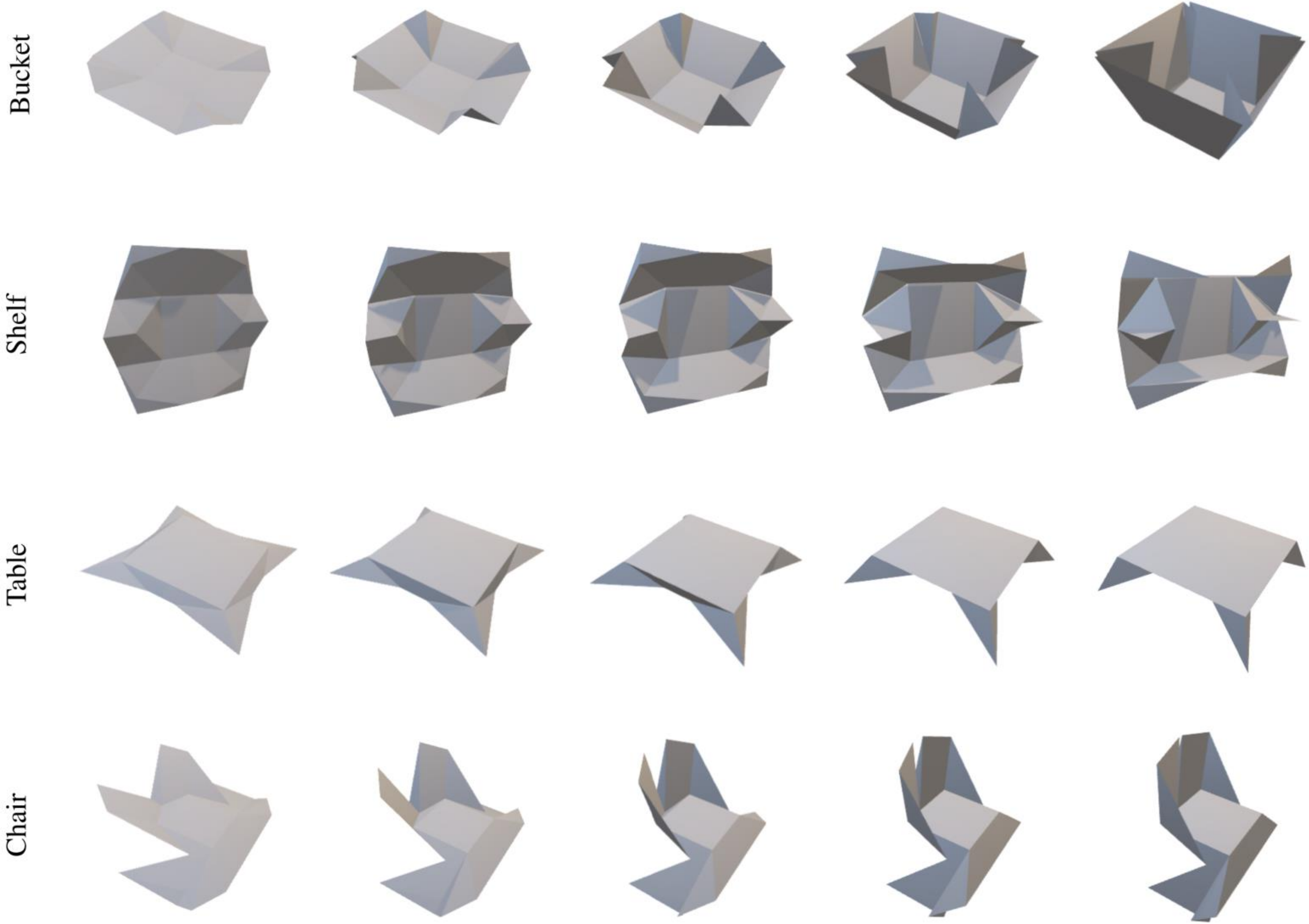
```
def outer_loop():
    for i in range(N):
        int00 = i + n
        add_edge(i, int00)

        int01 = i % n
        bool00 = int01 == 0
        if not bool00:
            int01 = i + 1
            add_edge(i, int01)

outer_loop()
```


Grid
Grid with width
Lobster
Protein
Reference
Generated

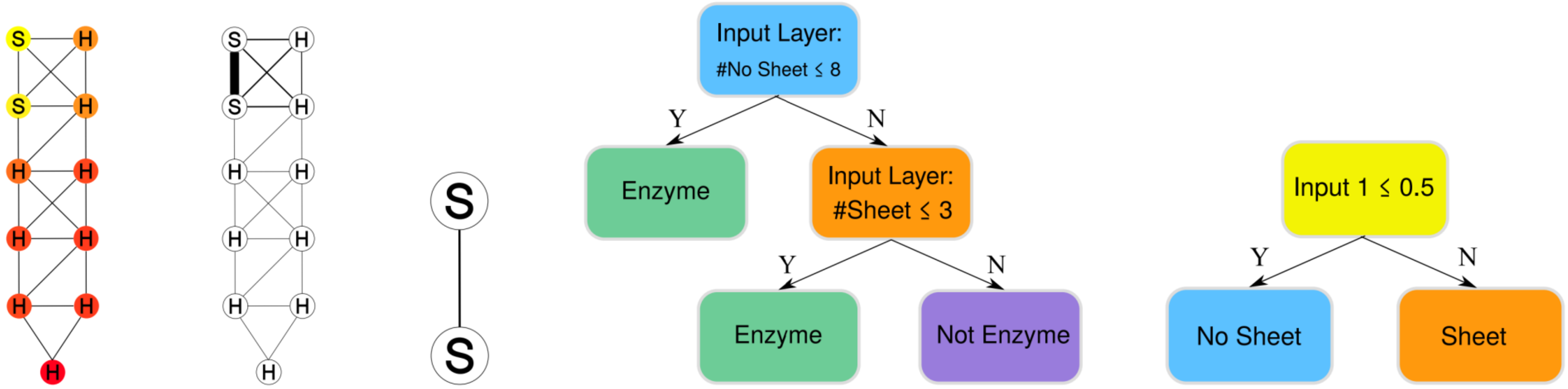
Automating Rigid Origami Design

Jeremia Geiger, Karolis Martinkus, Oliver Richter, Roger Wattenhofer



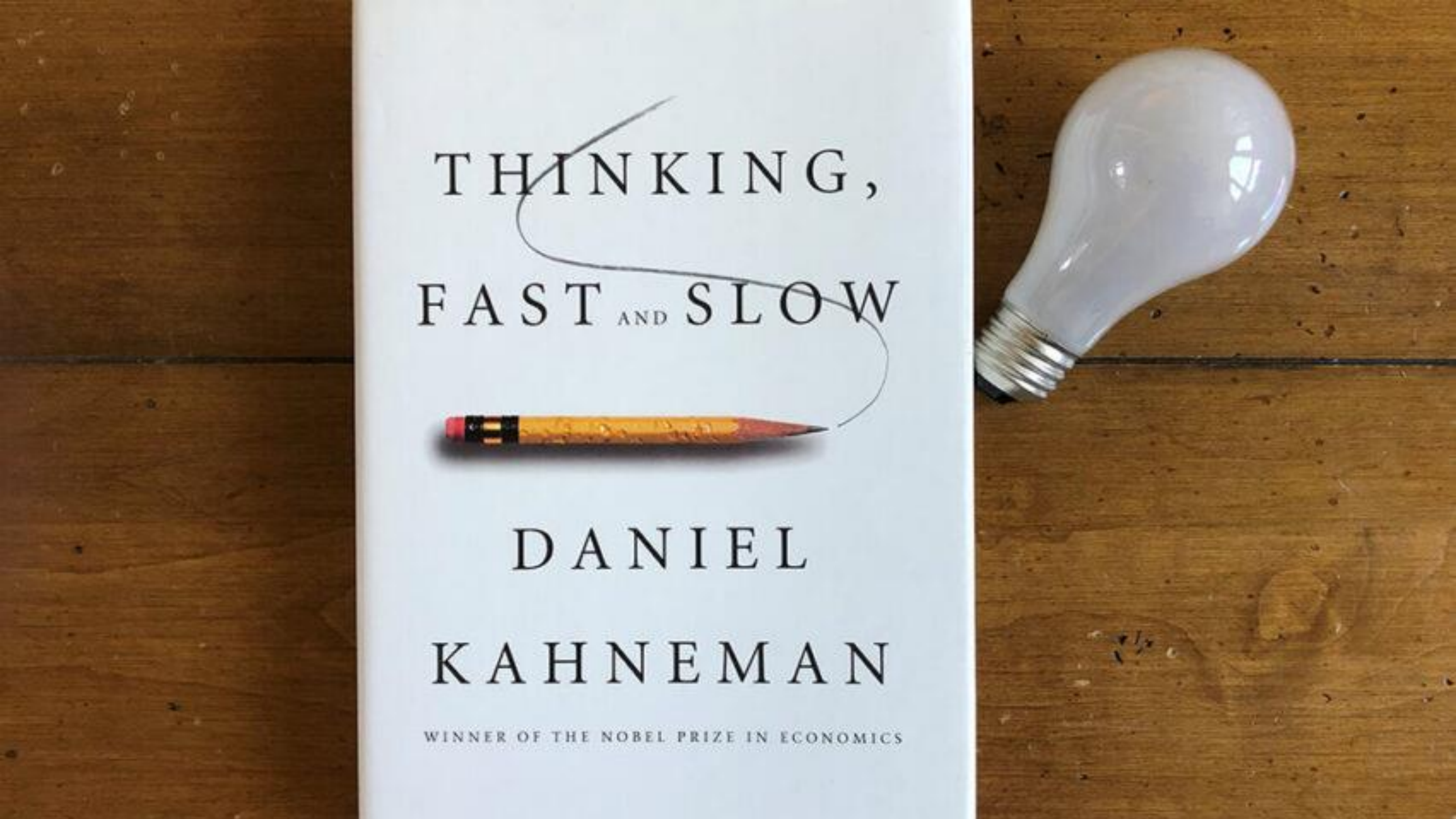

Bucket
Shelf
Table
Chair

Graph Explanation

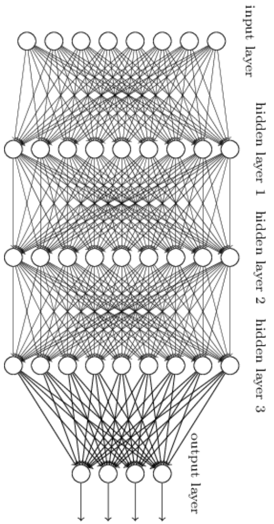

S
H
S
H
H
H
H
H
H
H
H
S
H
S
H
H
H
H
H
H
H
H
S
S
Input Layer:
#No Sheet ≤ 8
Y
N
Enzyme
Input Layer:
#Sheet ≤ 3
Y
N
Enzyme
Not Enzyme
Input 1 ≤ 0.5
Y
N
No Sheet
Sheet

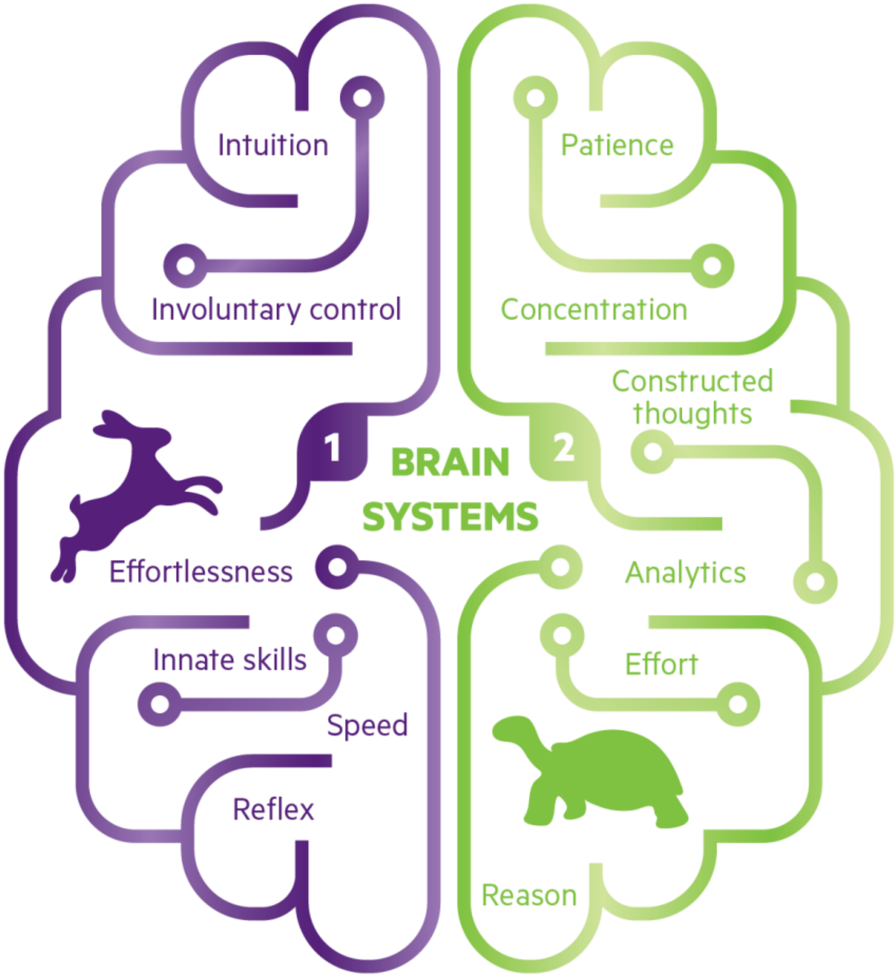
(a) (b) (c) (d) (e)

The Bigger Picture


THINKING,
FAST AND SLOW
DANIEL
KAHNEMAN
WINNER OF THE NOBEL PRIZE IN ECONOMICS

Deep Neural Networks





?

User

what is 5 times 7?

Assistant

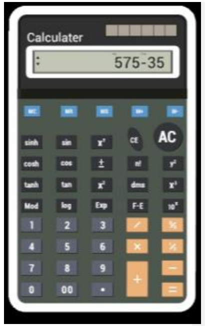
5 times 7 equals 35.

User

what is 384903720 times 538982734?

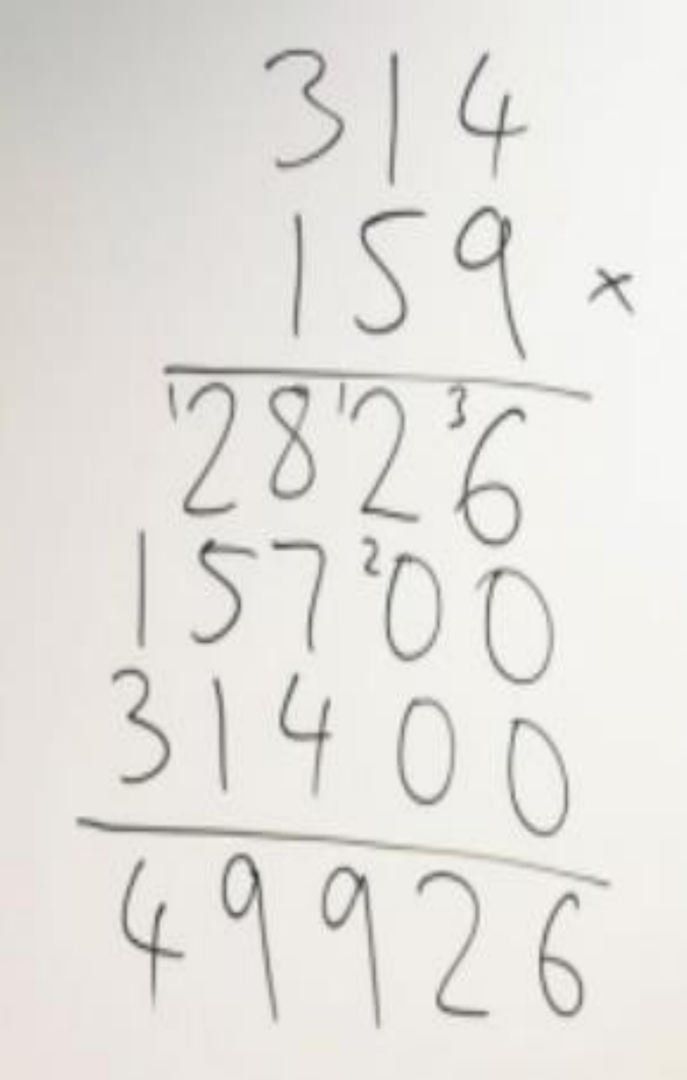
Assistant

384,903,720 times 538,982,734 equals 207,559,081,508,668,480.



$$384903720 \times 538982734 =$$

207,456,459,332,370,480



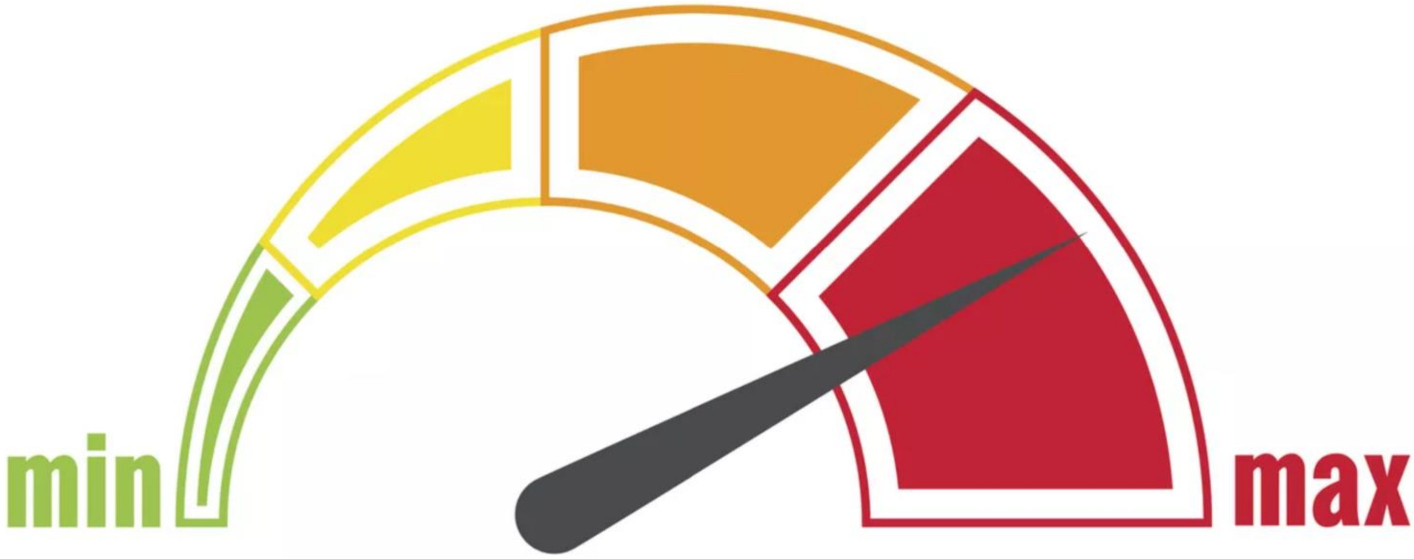
User

what is 384903720 times 538982734?

Assistant

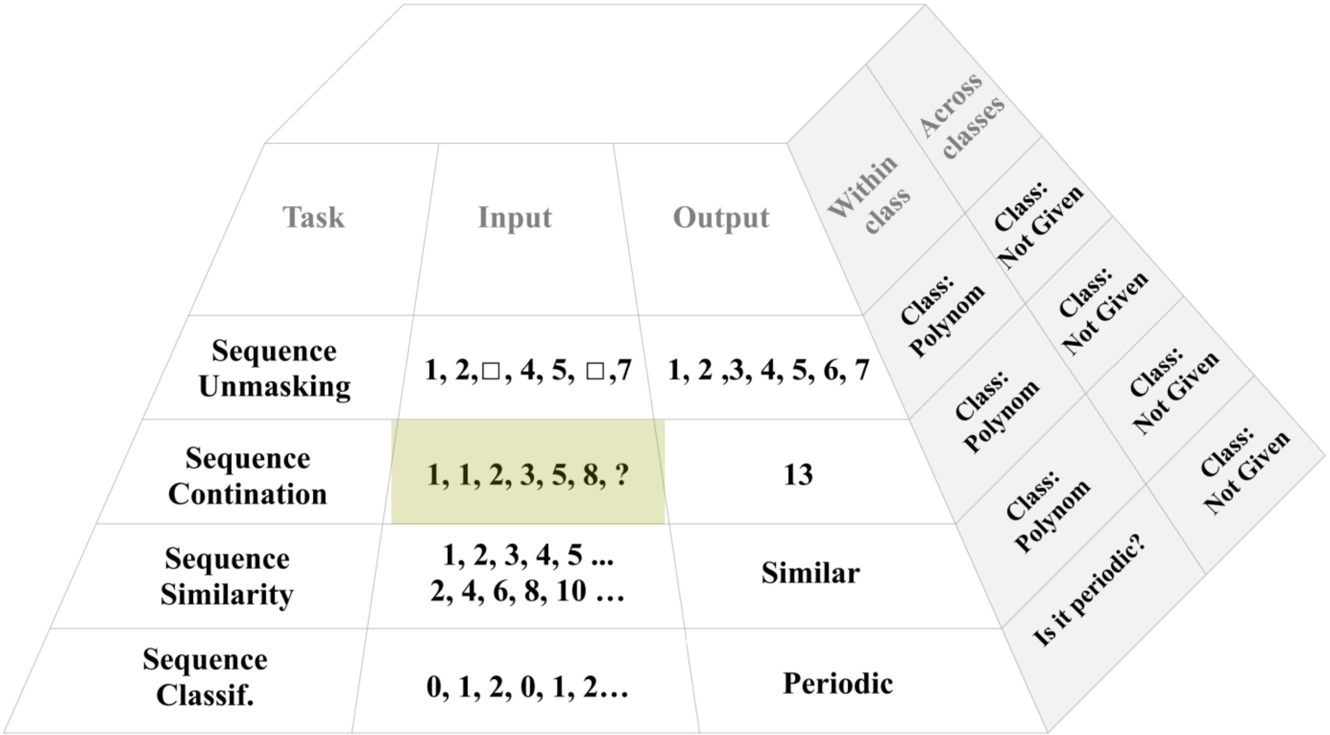
384,903,720 times 538,982,734 equals 207,559,081,508,668,480.

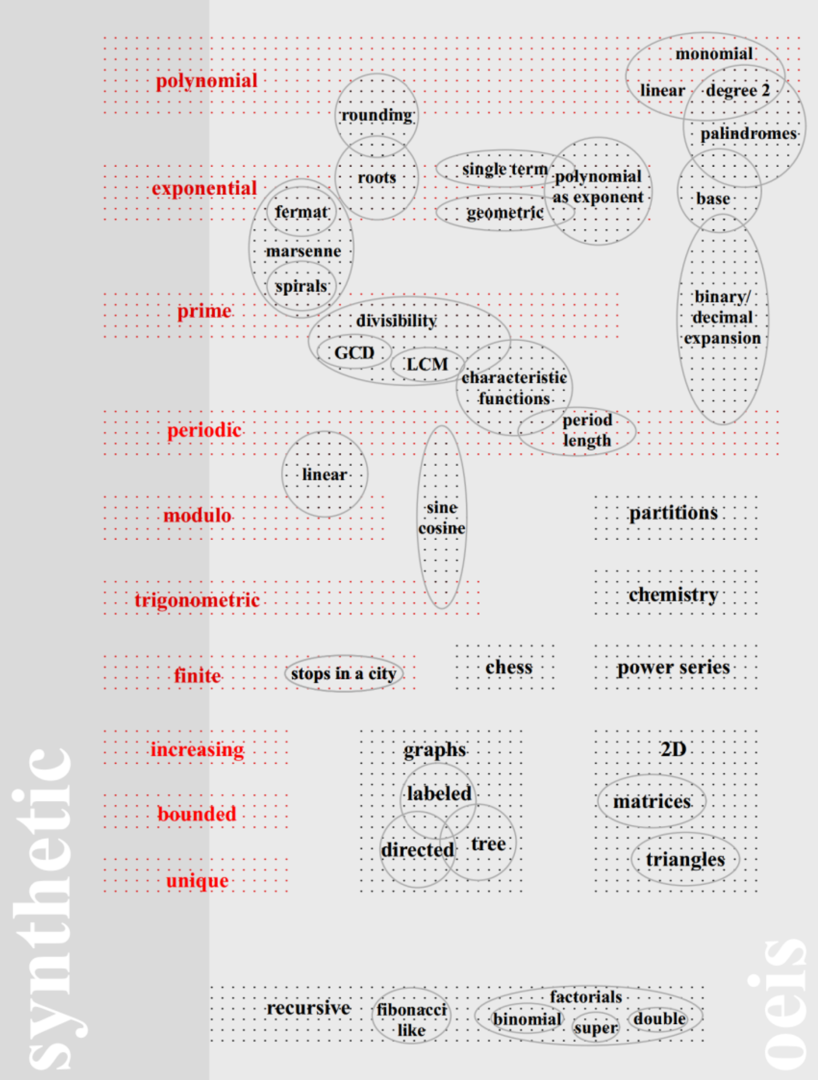
Thinking Slow Benchmark?



FACT: Learning Governing Abstractions Behind Integer Sequences

Peter Belcák, Ard Kastrati, Flavio Schenker, Roger Wattenhofer




synthetic
oeis
polynomial
exponential
prime
periodic
modulo
trigonometric
finite
increasing
bounded
unique
monomial
linear
degree 2
palindromes
rounding
roots
single term
geometric
polynomial as exponent
base
fermat
marsenne
spirals
divisibility
GCD
LCM
characteristic functions
binary/ decimal expansion
period length
linear
sine cosine
partitions
chemistry
stops in a city
chess
power series
graphs
labeled
directed
tree
2D
matrices
triangles
recursive
fibonacci like
factorials
binomial
super
double

Simon Tatham's Portable Puzzle Collection

Simon Tatham's Puzzles 4+

Greg Hewgill

Designed for iPad

★★★★★ 4.8 • 171 Ratings

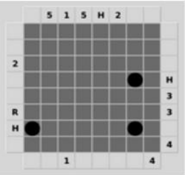
Free

Simon Tatham's Puzzles

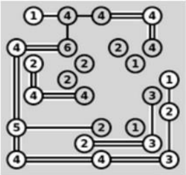
Chris Boyle

4.8★	500K+	E
14.5K reviews	Downloads	Everyone ⓘ

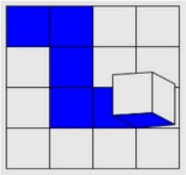
Black Box



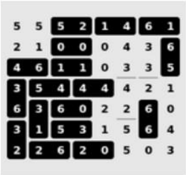
Bridges



Cube

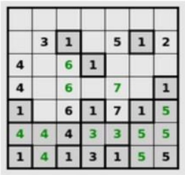


Dominosa

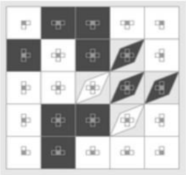


Fifteen

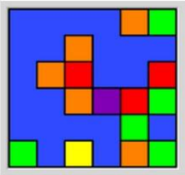
Filling



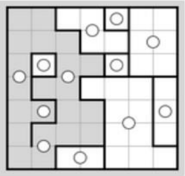
Flip



Flood

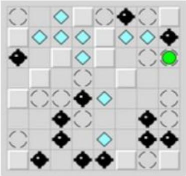


Galaxies



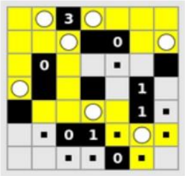
Guess

Inertia

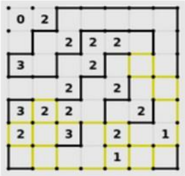


Keen

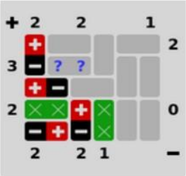
Light Up



Loopy



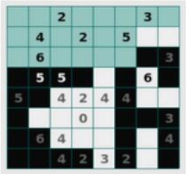
Magnets



Map

Mines

Mosaic



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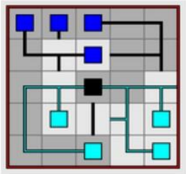
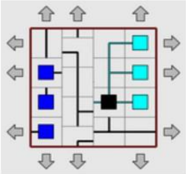
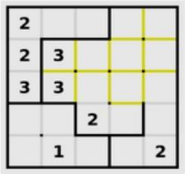


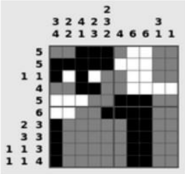
Netslide



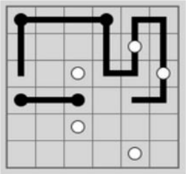
Palisade



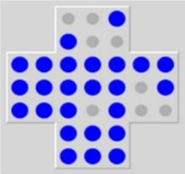
Pattern



Pearl



Pegs



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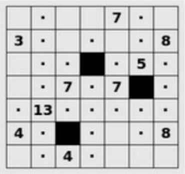
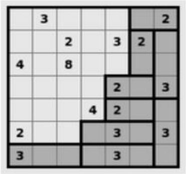
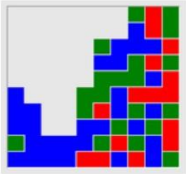


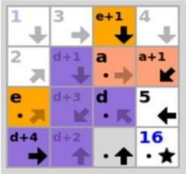
Rectangles



Same Game

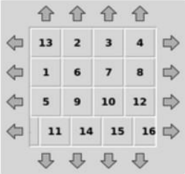


Signpost

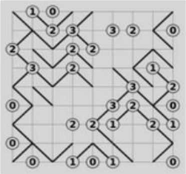


Singles

Sixteen

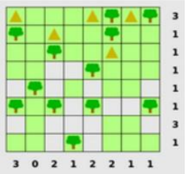


Slant

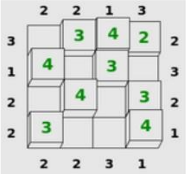


Solo

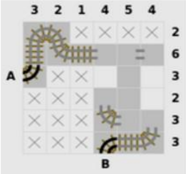
Tents



Towers

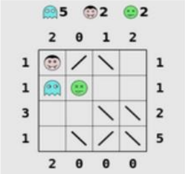


Tracks

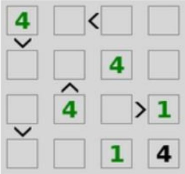


Twiddle

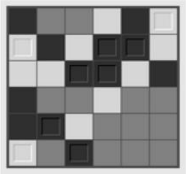
Undead



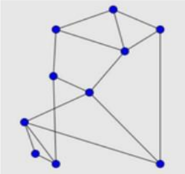
Unequal



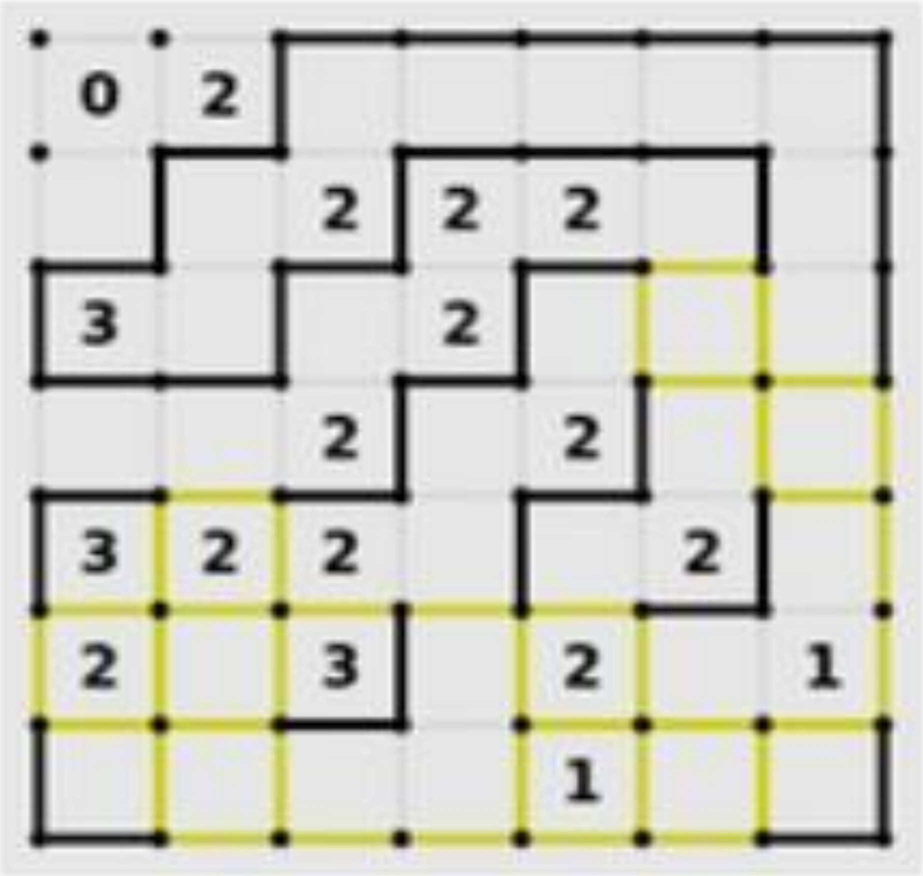
Unruly



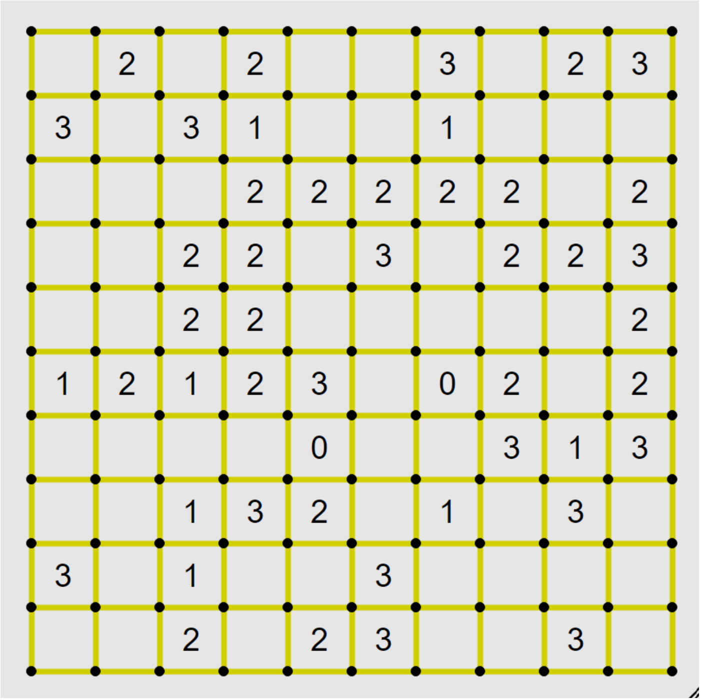
Untangle

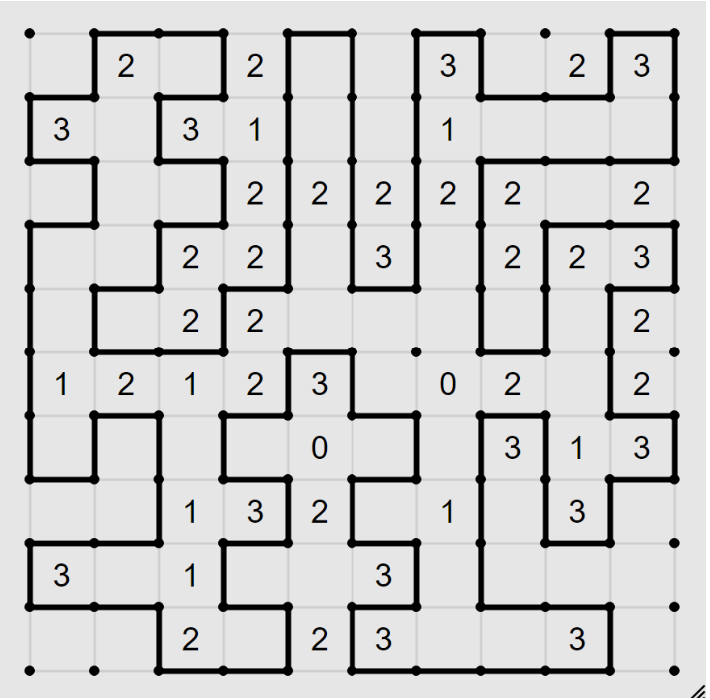


Loopy



Loopy (Takegaki, Slitherlink, Ouroboros, Suriza, …)





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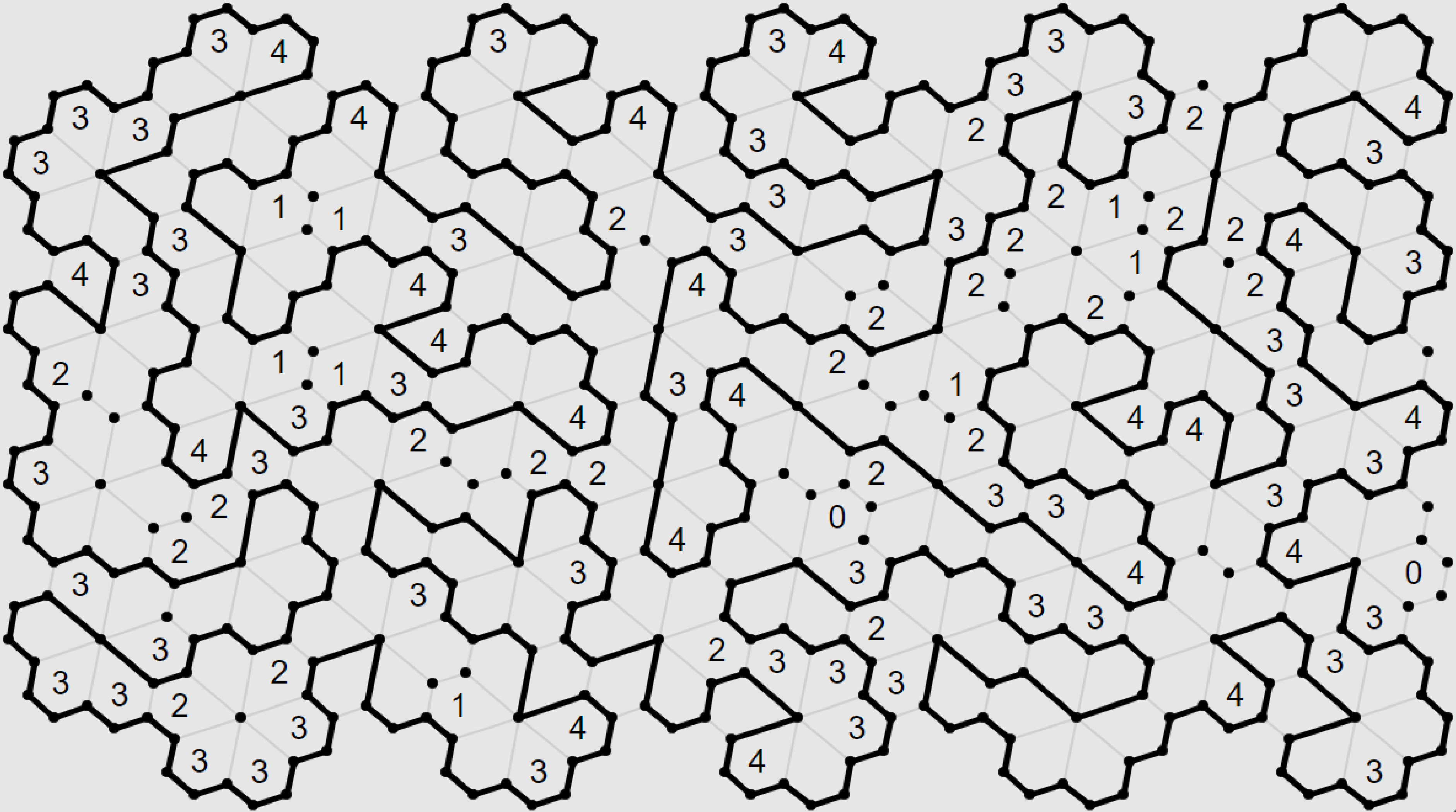
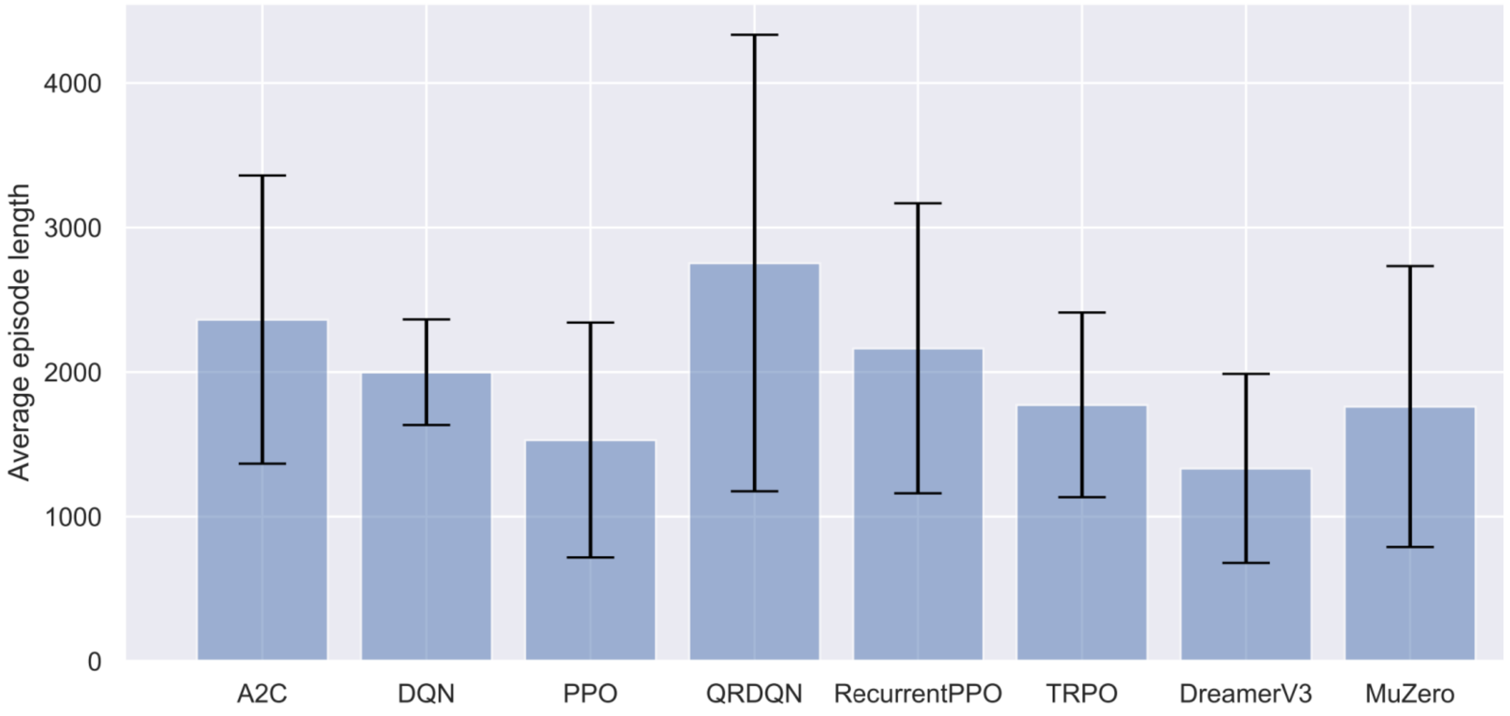
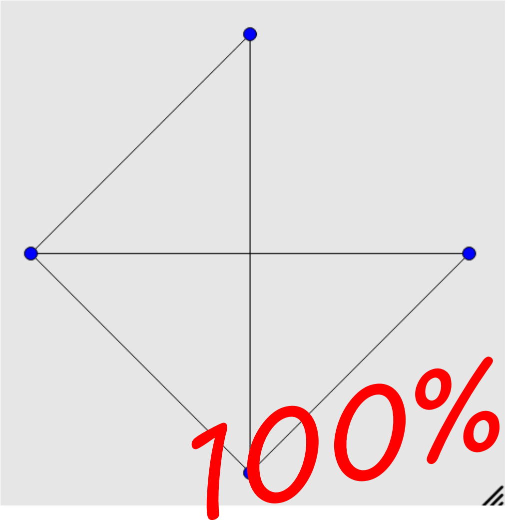
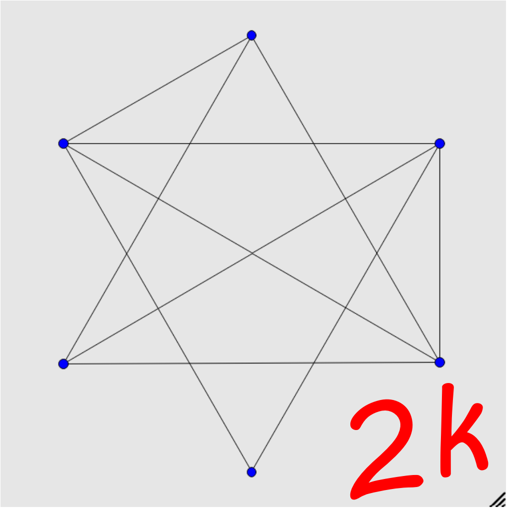
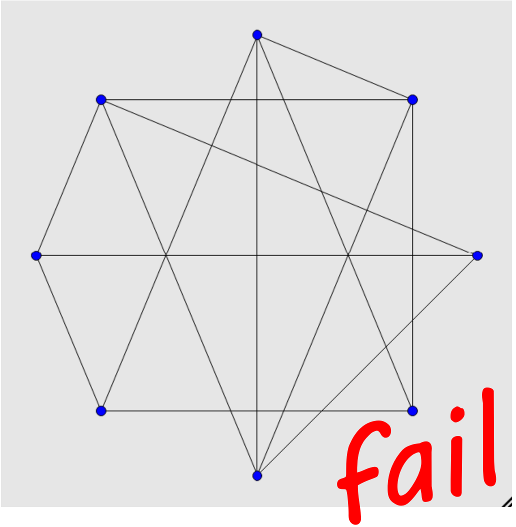



Average episode length
0
1000
2000
3000
4000
A2C
DQN
PPO
QRDQN
RecurrentPPO
TRPO
DreamerV3
MuZero

Puzzle	Parameters	PPO		DreamerV3	
Netslide	`2x3b1`	35.3 ± 0.7	(100.0%)	12.0 ± 0.4	(100.0%)
	`3x3b1`	4742.1 ± 2960.1	(9.2%)	3586.5 ± 676.9	(22.4%)
Same Game	`2x3c3s2`	11.5 ± 0.1	(100.0%)	7.3 ± 0.2	(100.0%)
	`5x5c3s2`	1009.3 ± 1089.4	(30.5%)	527.0 ± 162.0	(30.2%)
Untangle	`4`	34.9 ± 10.8	(100.0%)	6.3 ± 0.4	(100.0%)
	`6`	2294.7 ± 2121.2	(96.2%)	1683.3 ± 73.7	(82.0%)







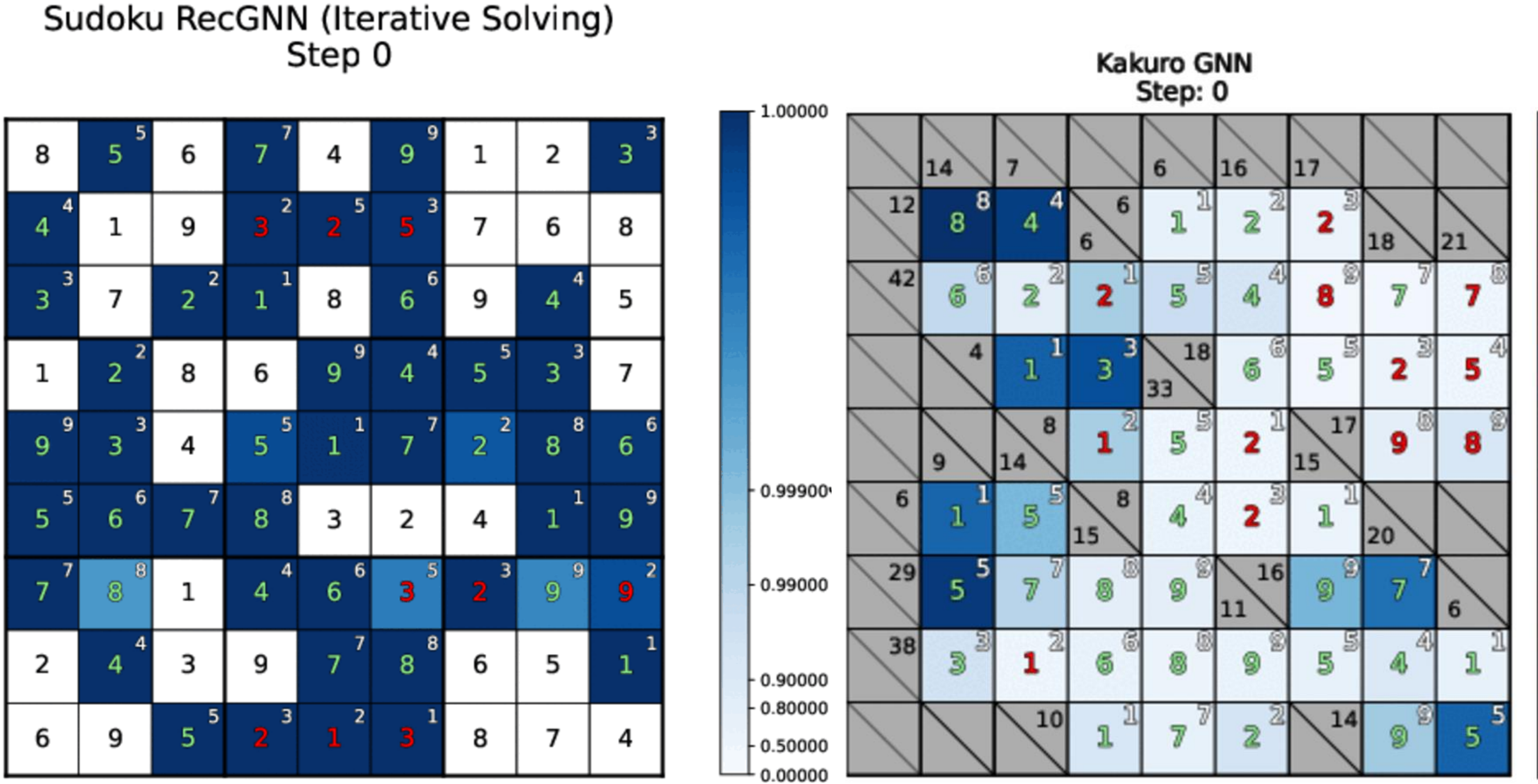
Sudoku

1		3	
	1		2

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

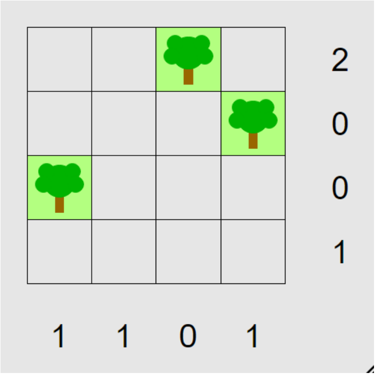
f		9		5			6						b	3	7
	6	b				1	f		7						8
				9		4						2	g		5
5	g	c	8			a	d	3		b		1			
		d	f			2				5		c			
9		4		c	5	g				d	1		e	7	
	b		5		9		3				a	6		f	4
								4	e				a	5	
	4	2				c	e								
a	d		e	1				9		4		f		8	
	5	g		f	2				d	6	8		7		9
			1		a				c			5	2		
			c		4		g	8	a			b	f	2	1
g		a	d						5		6				
7						9		e	b				6	d	
8	1	6						c			4		5		g

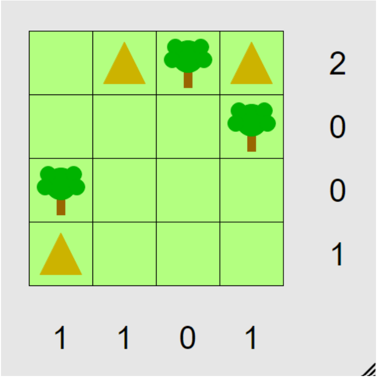
	4	6			2			
	3					7		
7		2		9	8			
		5					2	
	8		5		6		3	
	2					5		
			7	1		2	4	6
		9					5	
			4			8	9	

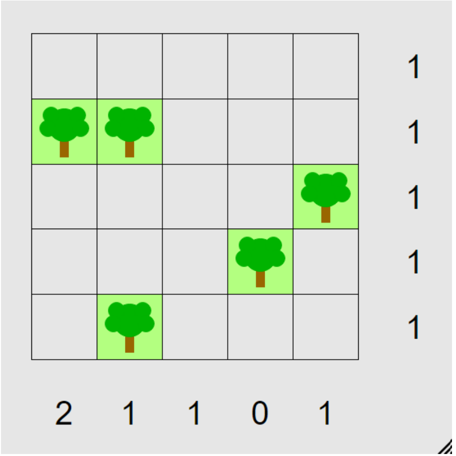


Sudoku RecGNN (Iterative Solving)
Step 0
Kakuro GNN
Step: 0
1.00000
0.99900
0.99000
0.90000
0.80000
0.50000
0.00000

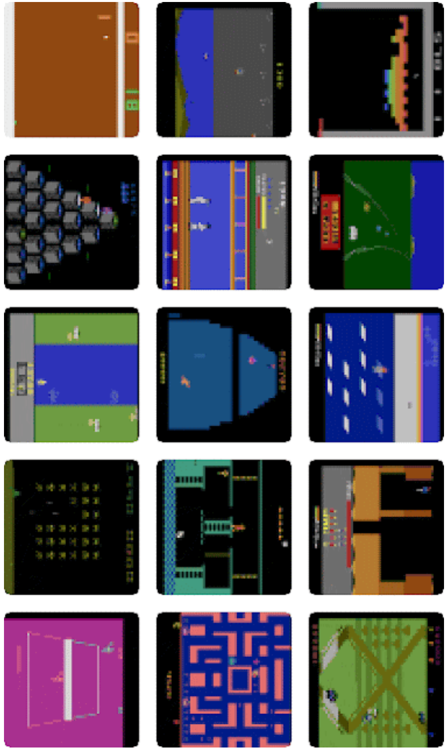
Tents

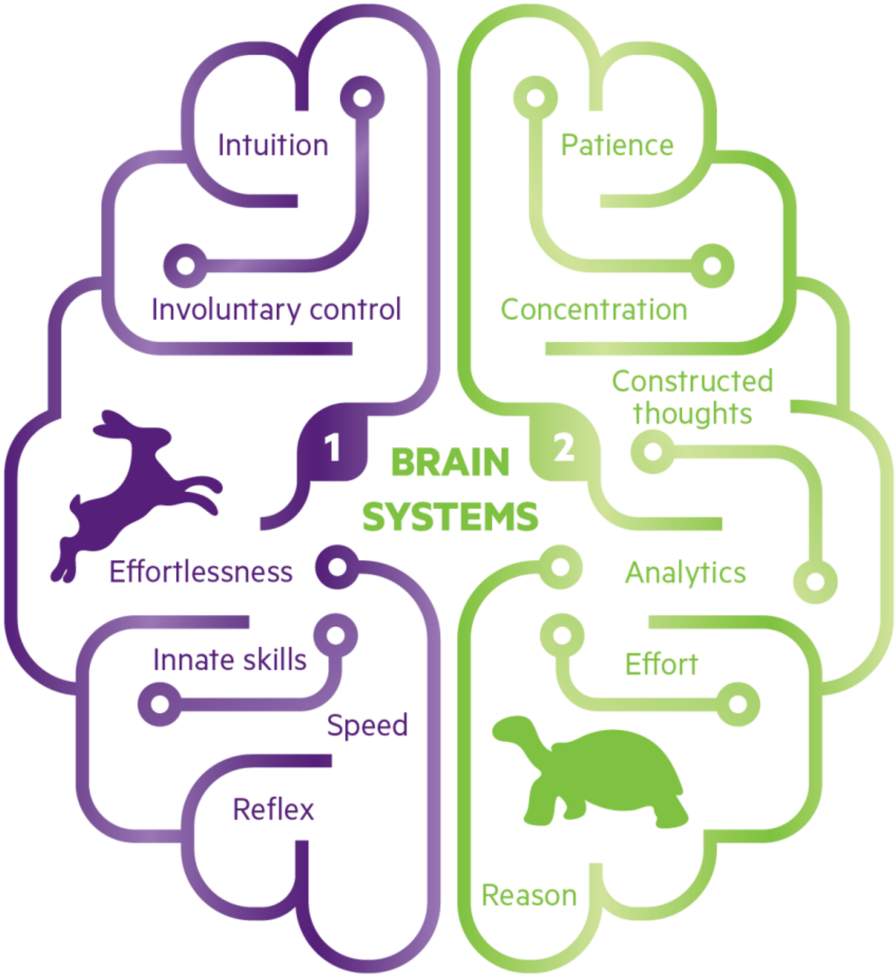




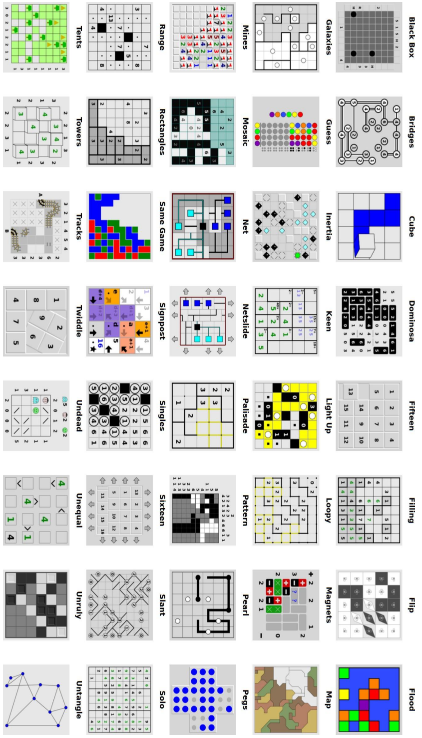


Atari Games

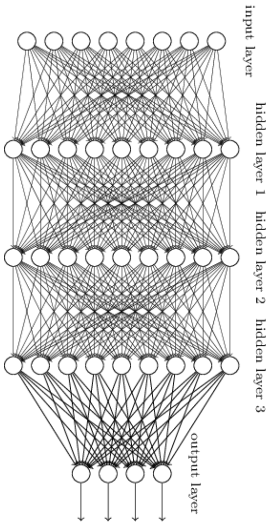


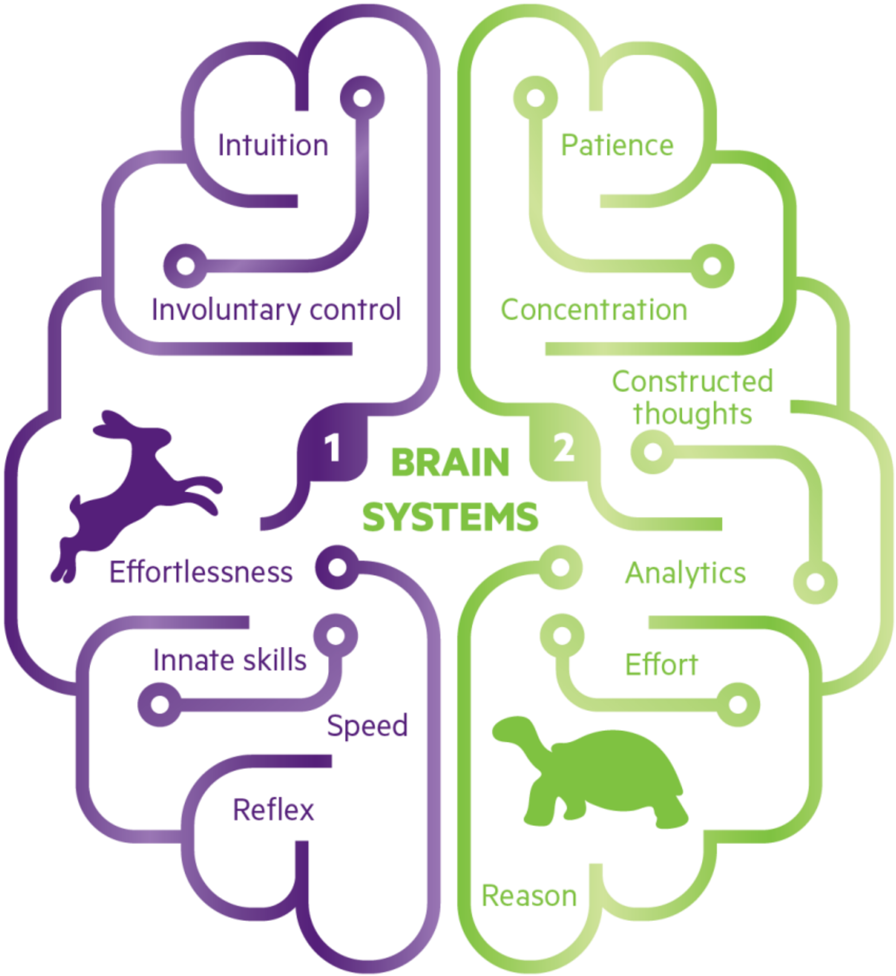


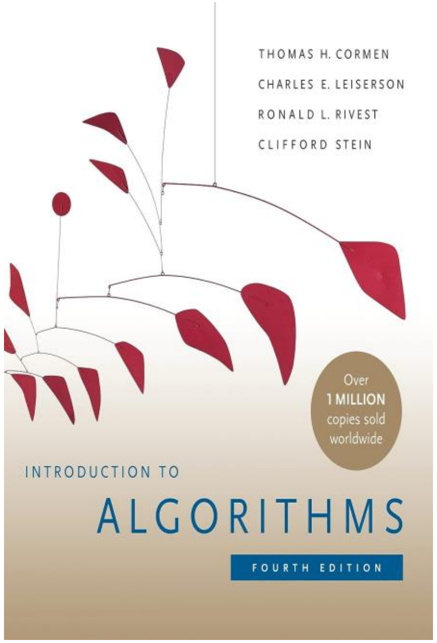
Puzzle Games



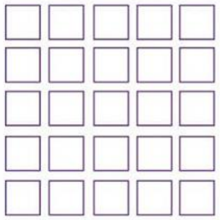
Deep Neural Networks

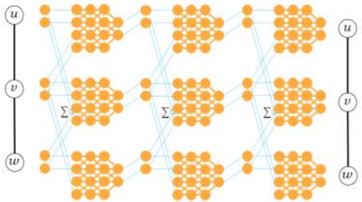






Summary




u
v
w
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Σ
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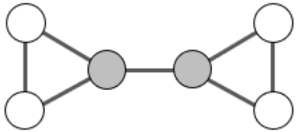
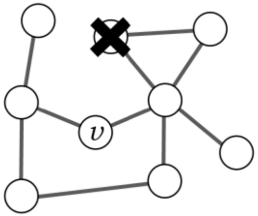
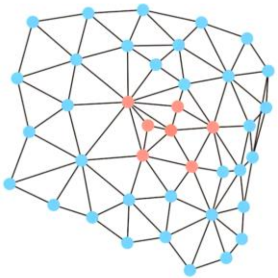
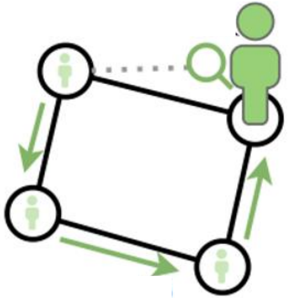
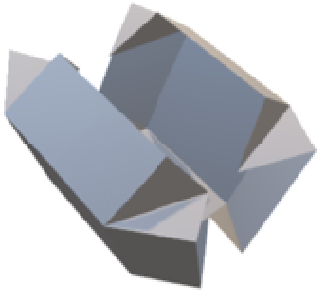
v
w

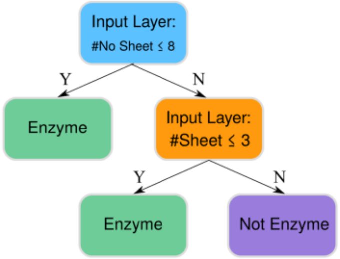



v





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Y
N
Enzyme
Input Layer:
#Sheet ≤ 3
Y
N
Enzyme
Not Enzyme

Thank You!

Any questions or comments?

Thanks to co-authors: Peter Belcak, Benjamin Estermann, Lukas Faber, Florian Grötschla, Luca Lanzendörfer, Karolis Martinkus, Joël Mathys, Pal Andras Papp, etc.

Roger Wattenhofer