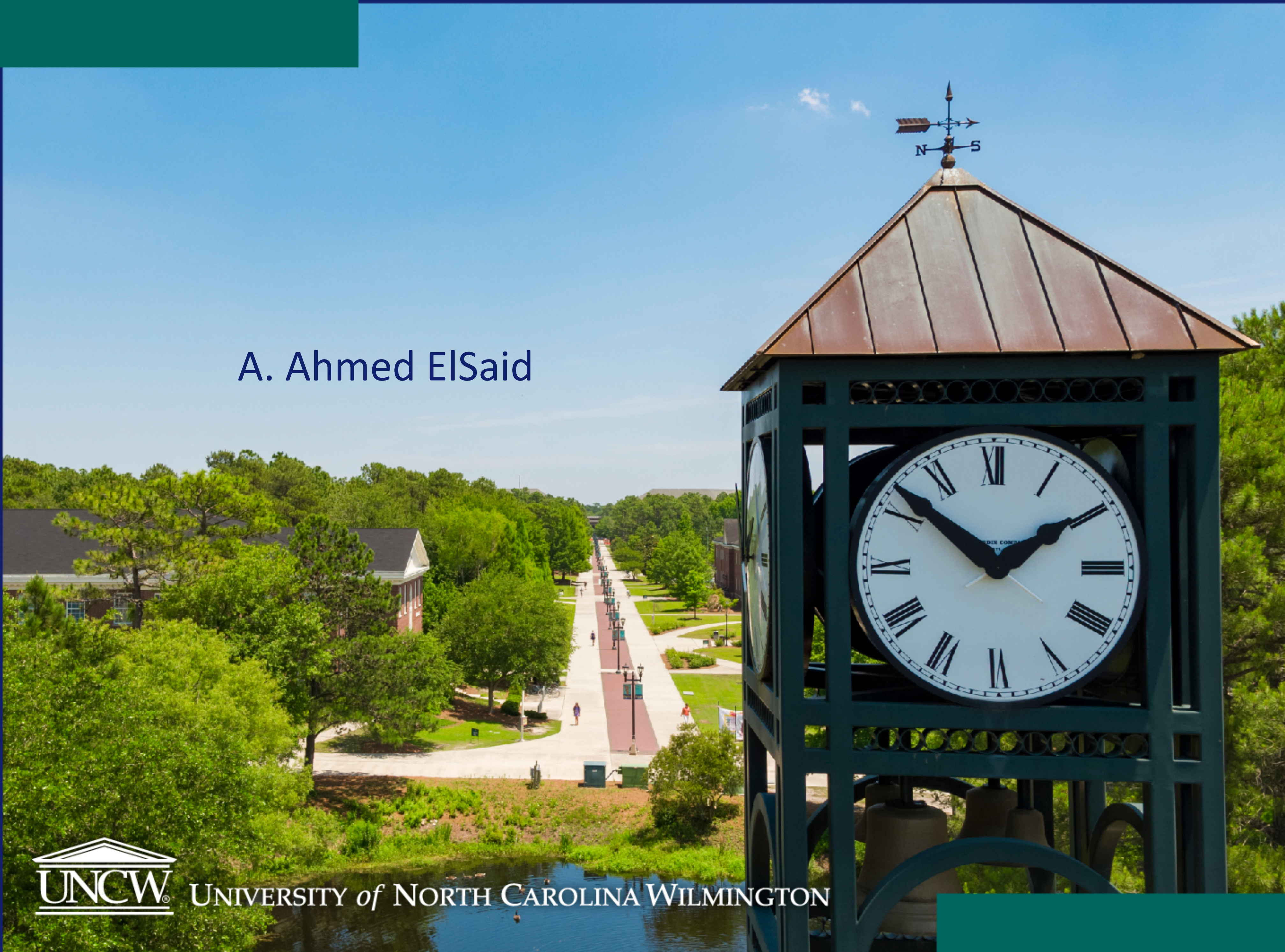


A. Ahmed ElSaid

UNCW UNIVERSITY of NORTH CAROLINA WILMINGTON

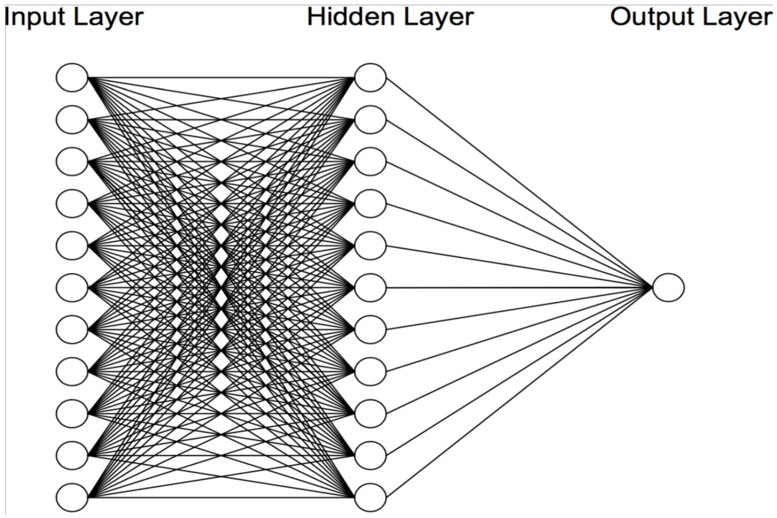
Overview

- NeuroEvolution (NE) & Neural Architecture Search (NAS)
- Ant-based Neural Topology Search (ANTS)
- Continuous ANTS (CANTS)
- BP-Free CANTS
- Future Research Directions

Neural Architecture Search (NAS)

NAS

- Deep RNN (powerful internal state): more data abstraction
- However, **More Structural Elements** = **More Computation + Noise**
- Neural networks are directed graphs - NAS: finding optimum graph-elements from inputs to outputs
- NAS traditionally: Hand Crafted through trail & Error (Time + Experience)
- **Metaheuristic method** = **automation** + **near-to-optimum structure**



- NAS methods include , random search, RL, Evolutionary algorithms, Bayesian optimization, Gradient based
- NAS strategies can be divided to: *a)* **ML**, *b)* **NE**, and *c)* **Nature Inspired**

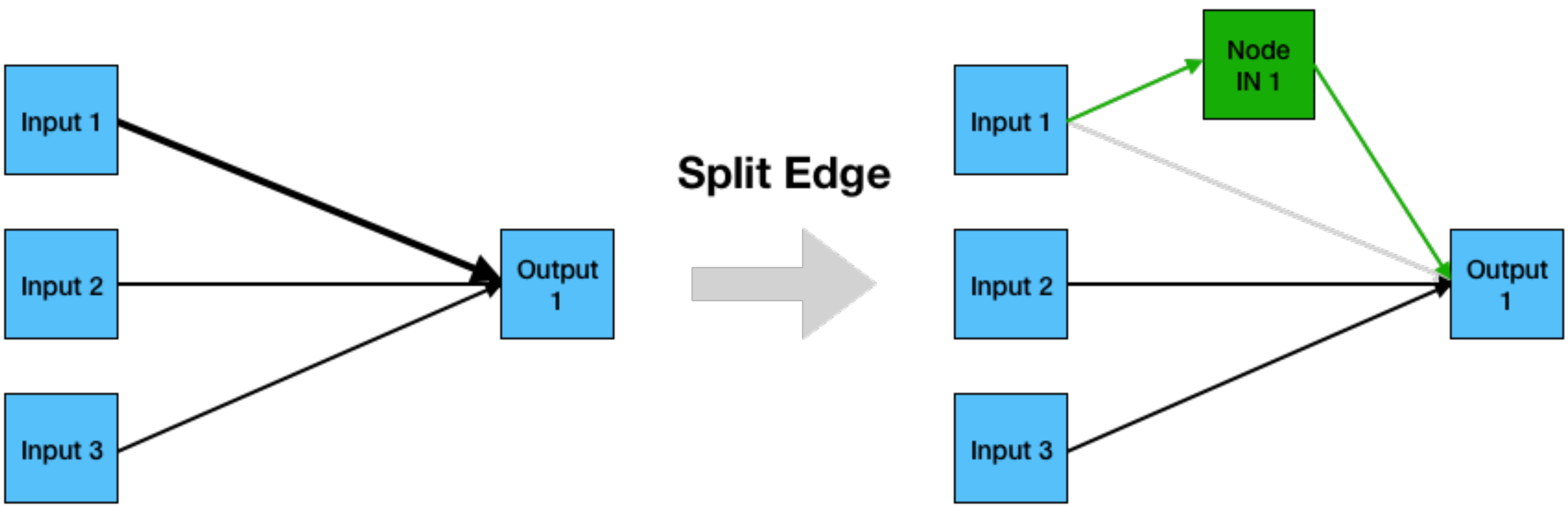
NAS

- Many of NAS are Nature-inspired
- Many NAS are GA-based (NEAT* and its inspirations)

*Stanley, K.O. and Miikkulainen, R., 2002. Evolving neural networks through augmenting topologies. *Evolutionary computation*, *10*(2), pp.99-127.

NAS

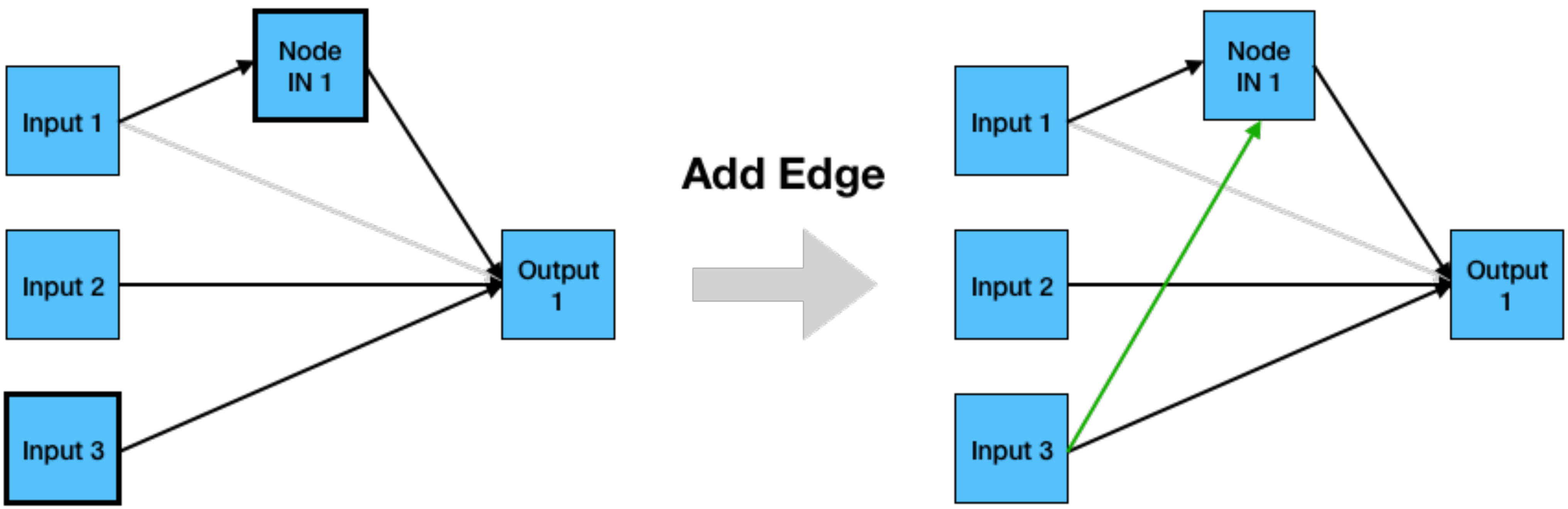
EXAMM Genetic Mutations: **Split Edge**



Alex Ororbia, AbdElRahman ElSaid, and Travis Desell. Investigating Recurrent Neural Network Memory Structures using Neuro-Evolution. The Genetic and Evolutionary Computation Conference (GECCO 2019). Prague, Czech Republic. July 8-12, 2019.

NAS

EXAMM Genetic Mutations: **Add Edge**



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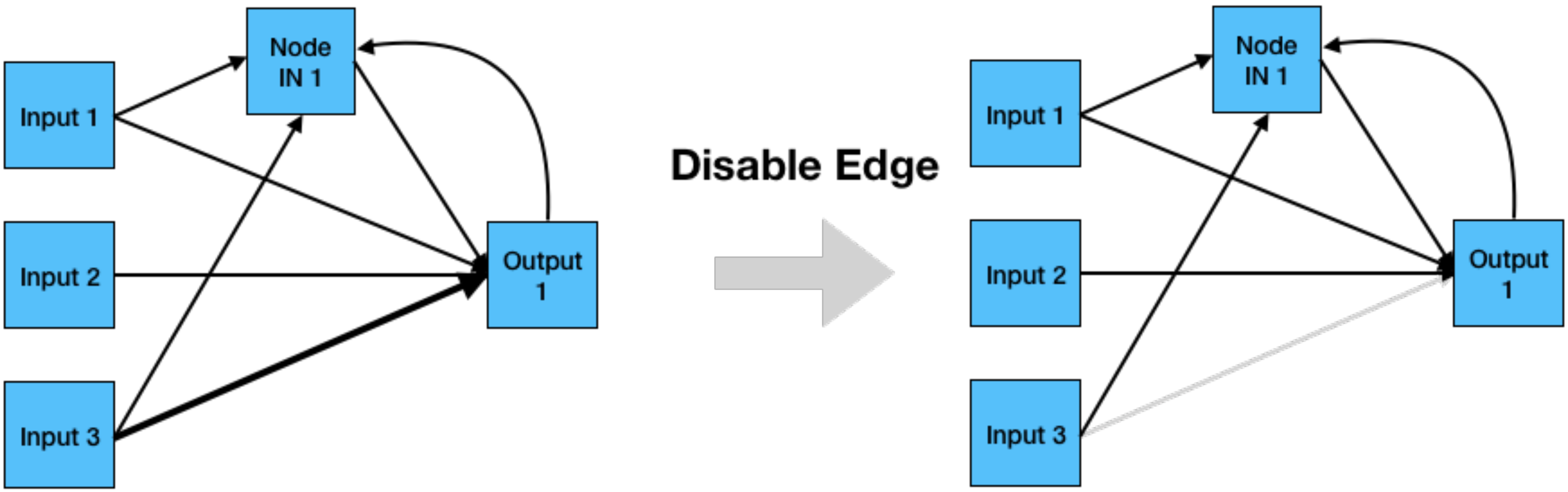
NAS

EXAMM Genetic Mutations: **Disable Edge**



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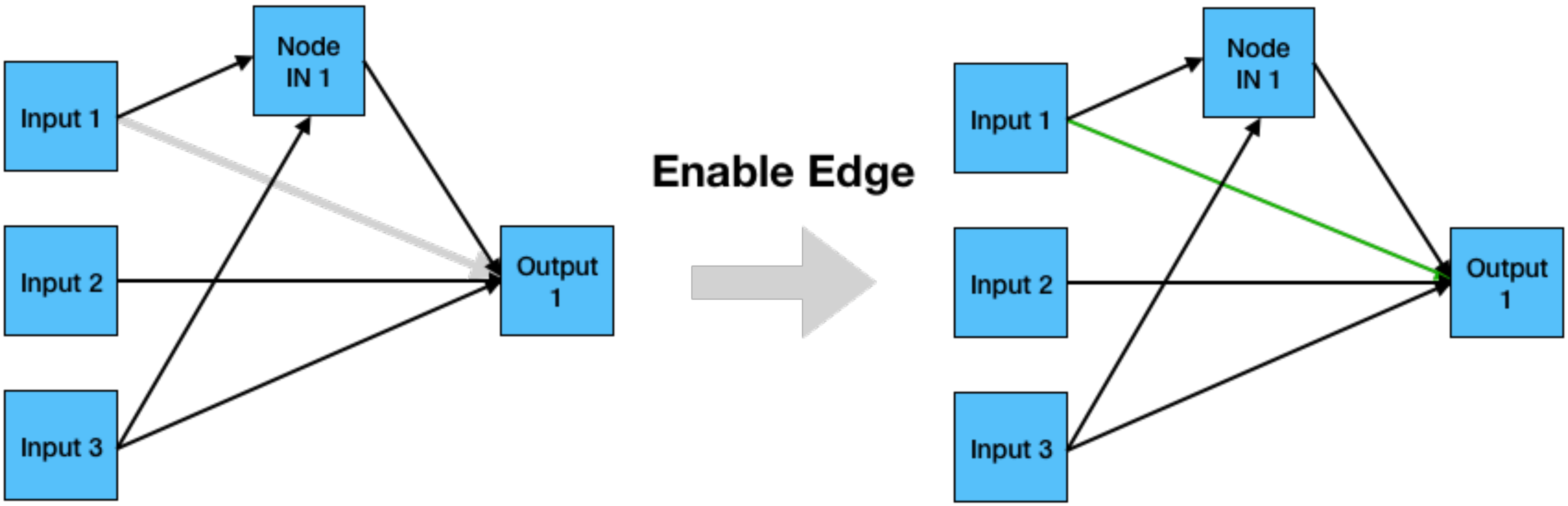

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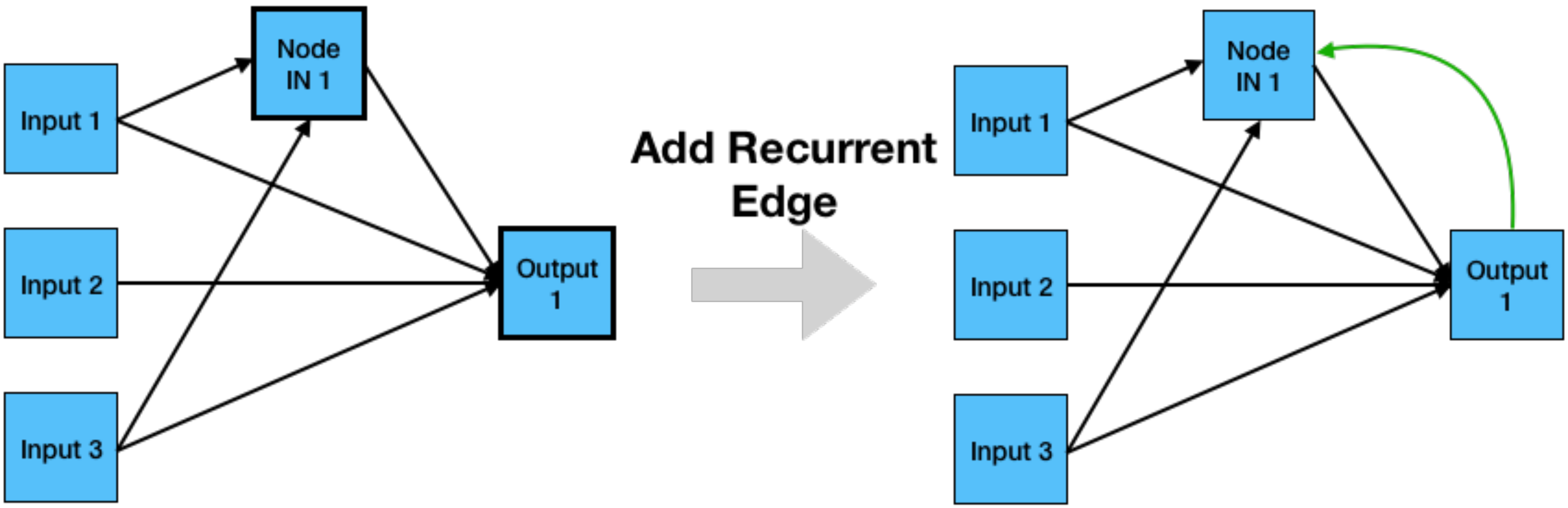
NAS

EXAMM Genetic Mutations: **Add Recurrent Edge**



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NAS

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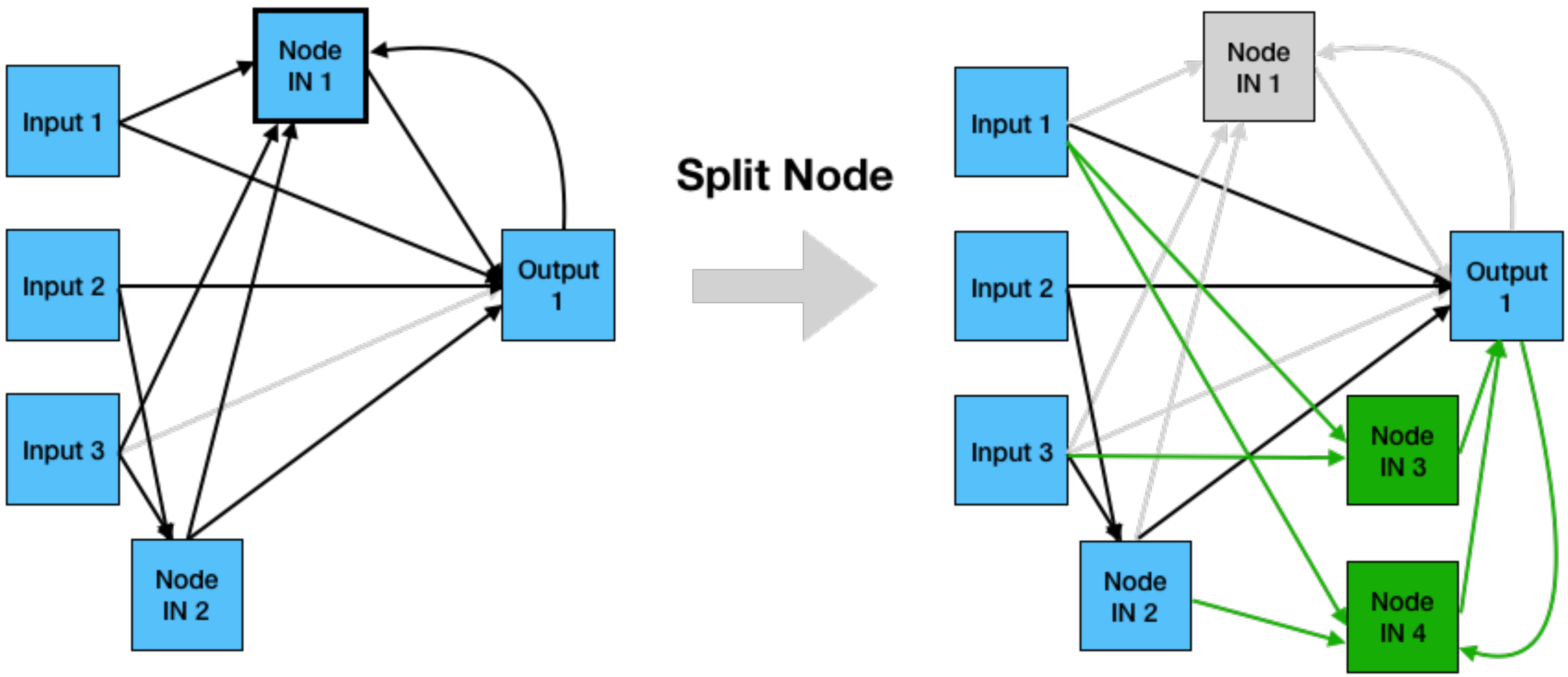

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NAS

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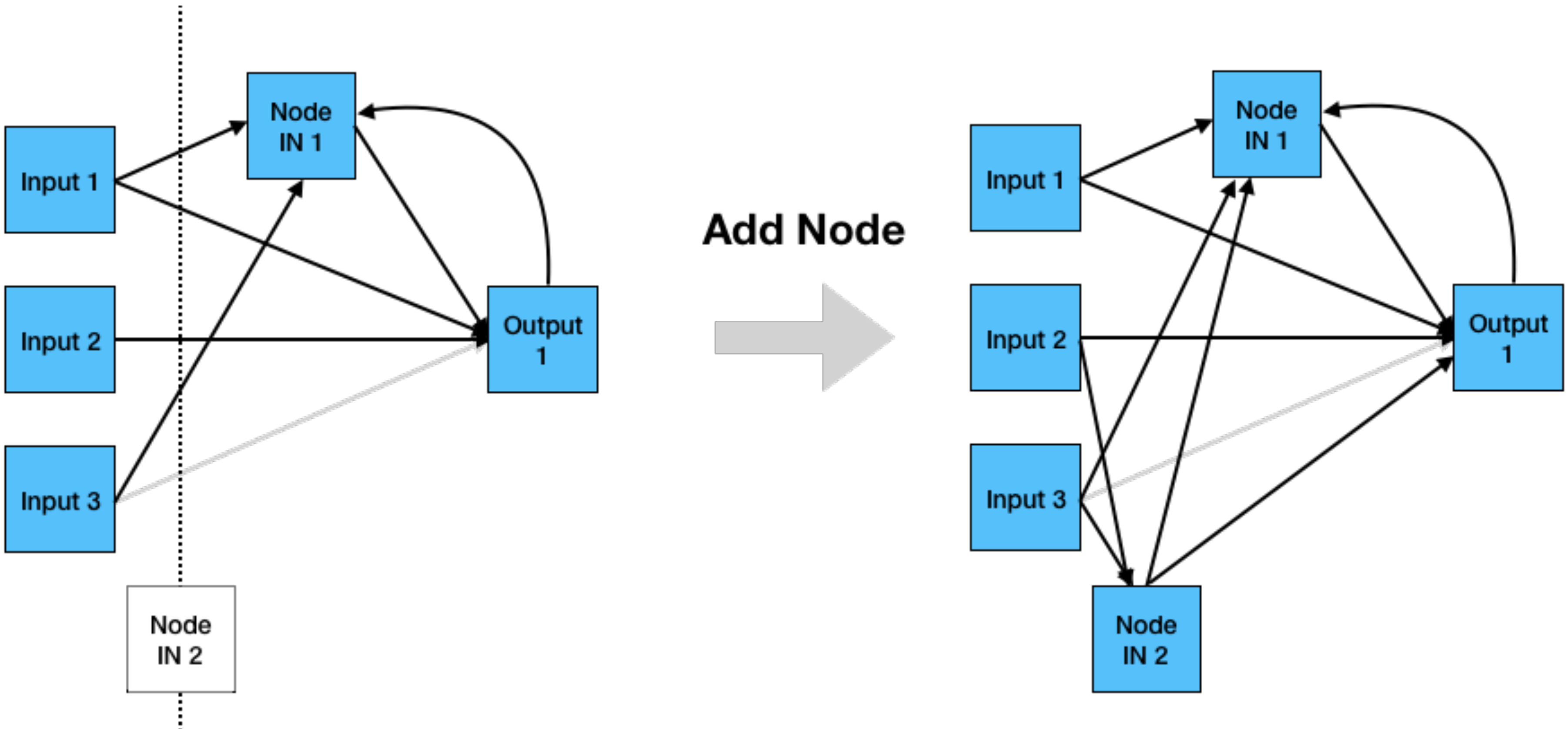

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NAS

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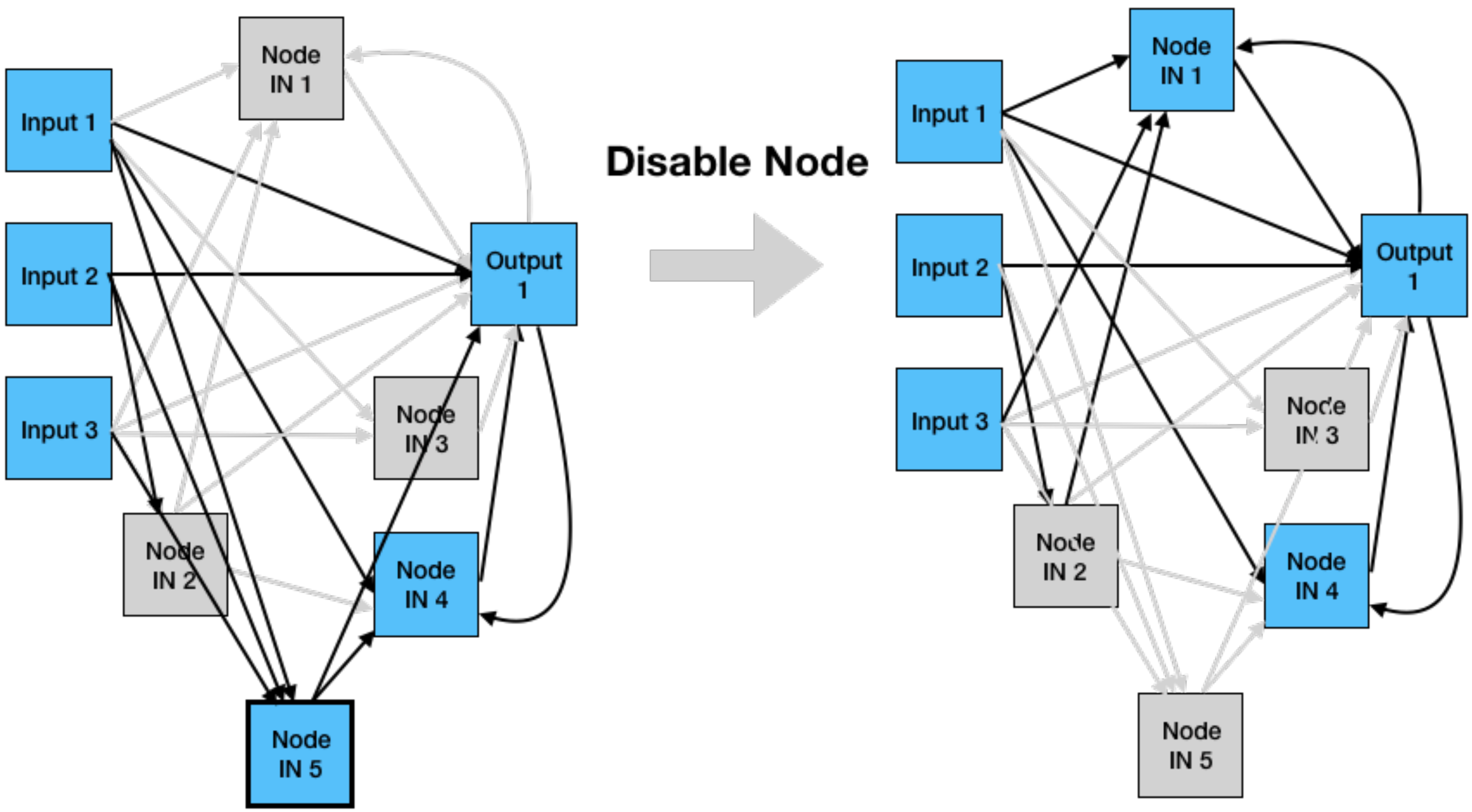

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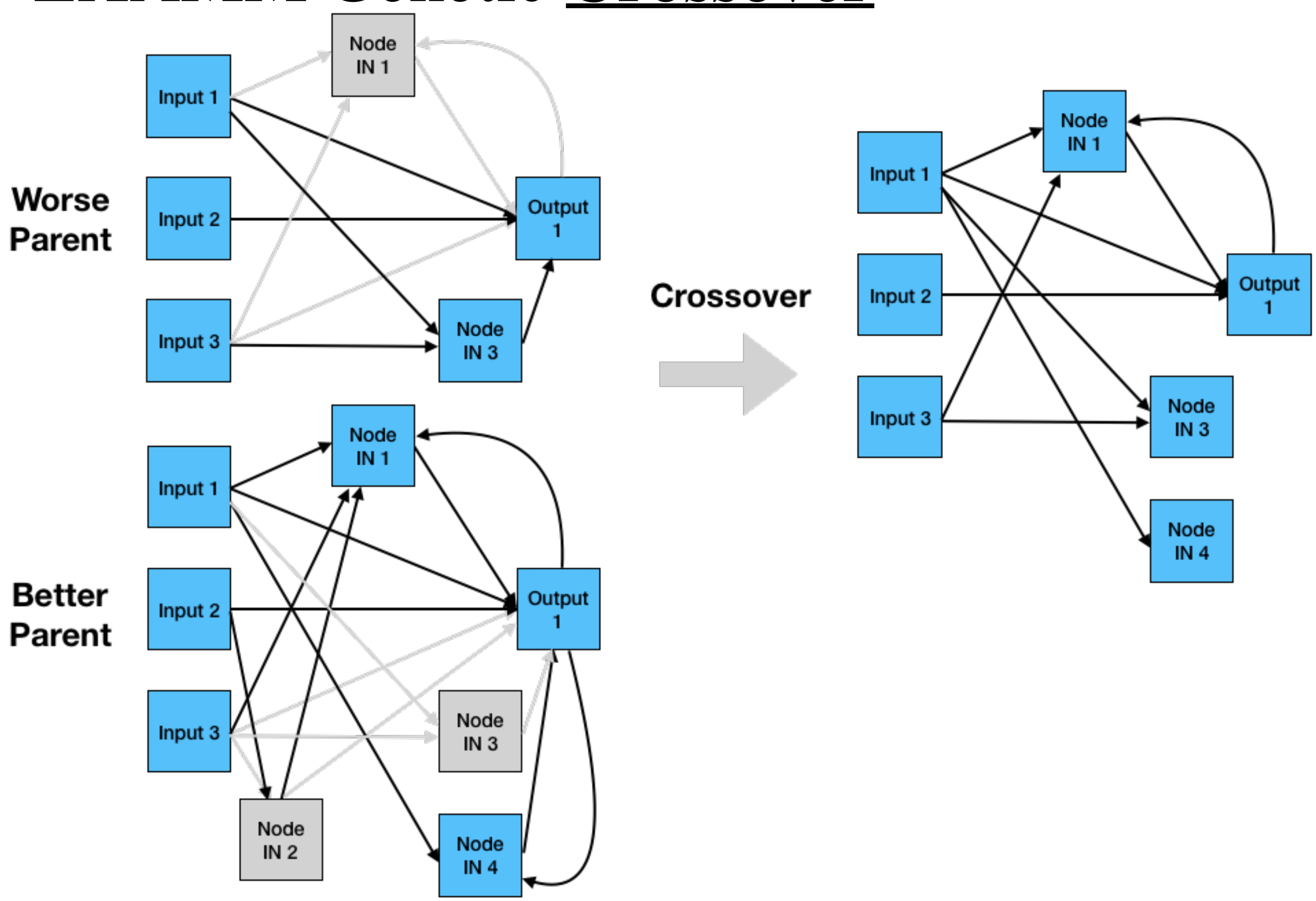
NAS

EXAMM Genetic **Crossover**



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NAS

- Many of NAS are Nature-inspired
- Many NAS are GA-based (NEAT and its inspirations)
- Our approach was different: Ant Colony Optimization: *Massive search space*

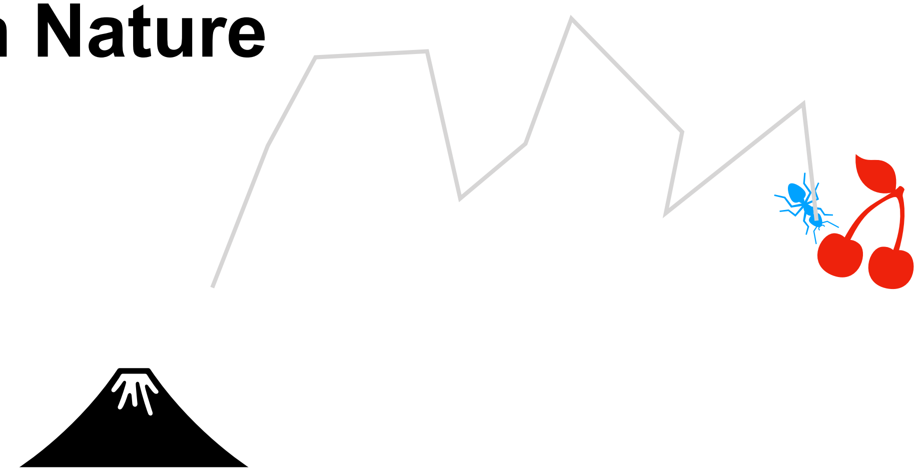
Ant Colony Optimization

- GA vs. Ant Colony Optimization: *Search Space*
- ACO showed good results since first introduced for the Traveling Salesman problem*
- ACO was used to pick the inputs[1] for NN and optimize NN weights[2]
- Method was never used for NAS (one exception**: simple Elman NN)

*Marco Dorigo, Vittorio Maniezzo, and Alberto Colorni. Ant system: optimization by a colony of cooperating agents. IEEE Transactions on Systems, Man, and Cybernetics, Part B (Cybernetics), 26(1):29–41, 1996
**Desell, T.; Clachar, S.; Higgins, J.; and Wild, B. 2015. Evolving deep recurrent neural networks using ant colony optimization. In European Conference on Evolutionary Computation in Combinatorial Optimization, 86–98. Springer
[1] Sivagaminathan, R.K. and Ramakrishnan, S., 2007. A hybrid approach for feature subset selection using neural networks and ant colony optimization. *Expert systems with applications*, *33*(1), pp.49-60.
[2] Liu, Y.P., Wu, M.G. and Qian, J.X., 2006, May. Evolving neural networks using the hybrid of ant colony optimization and BP algorithms. In International Symposium on Neural Networks (pp. 714-722). Springer, Berlin, Heidelberg

ACO: Ants in Nature

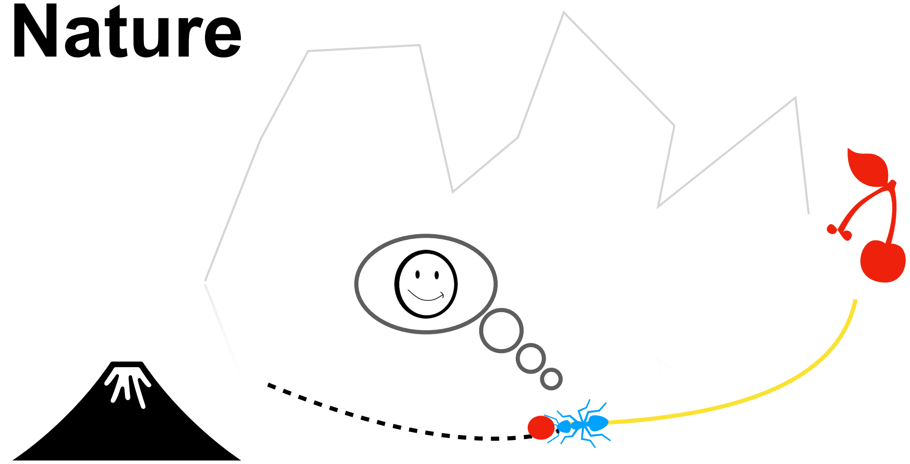
- Ants travers on paths to search for food



ACO: Ants in Nature

- Ants travers on paths to search for food

- When ant finds food, it deposits pheromone on the path it took in its return journey



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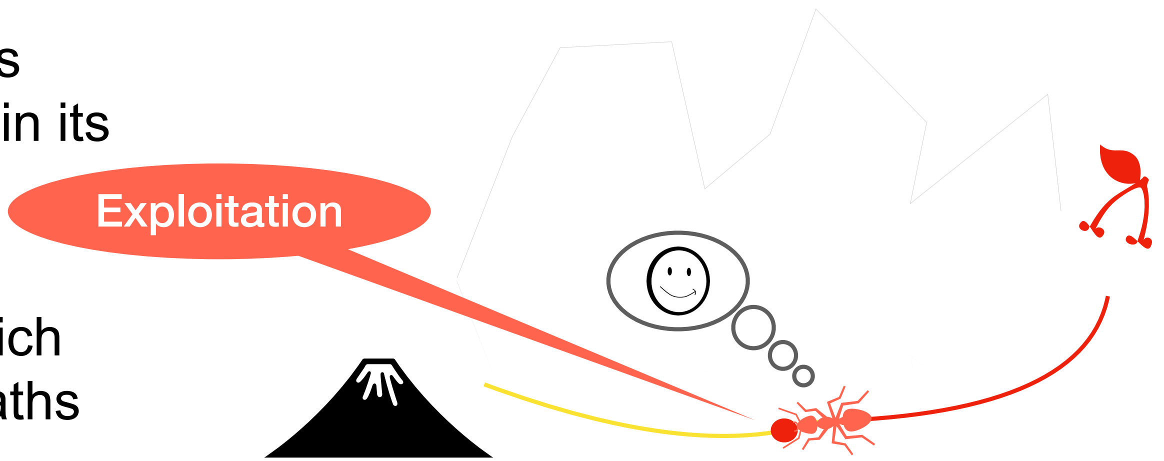

ACO: Ants in Nature

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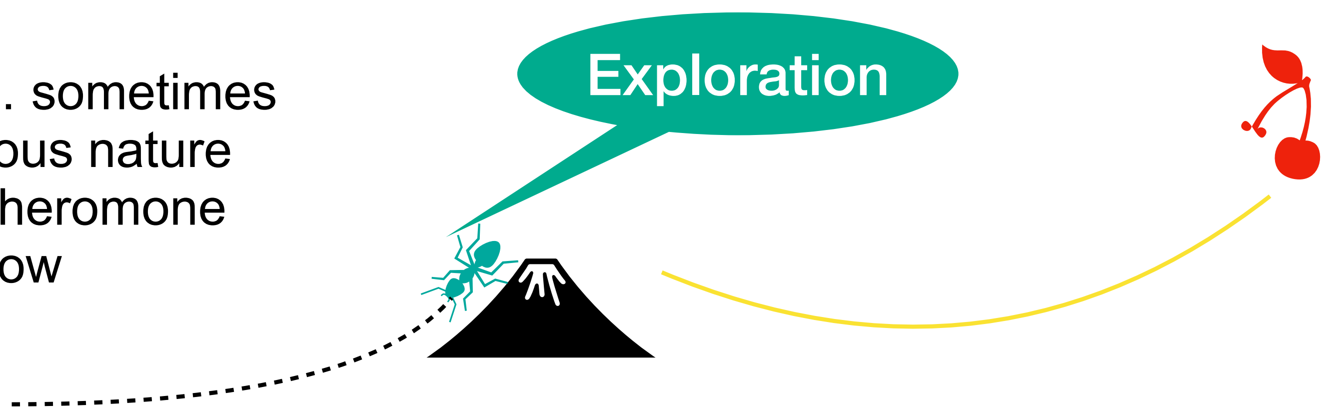
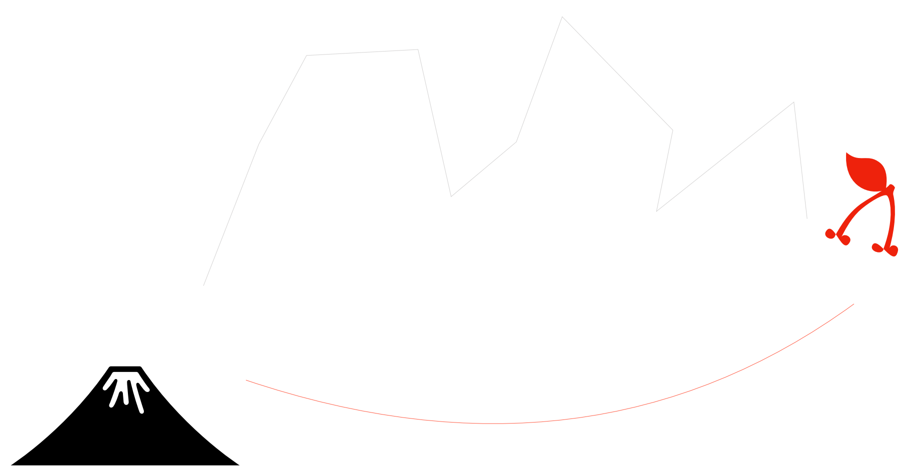
- Ants tend to take the paths which are food promising: i.e. take paths which has more pheromone deposits (***Exploitation nature***)
- Ants are also ***explorers***… sometimes ants follow their adventurous nature and take paths with low pheromone levels, or new path with now pheromone traces



ACO: Ants in Nature

- Pheromone also evaporates over time on paths not frequently traveled, which encourages ants to use their exploration nature

- This inspiring behavior makes ACO a very interesting algorithm for determining paths through graphs.



Ant Colony Based Optimization

Why ACO?

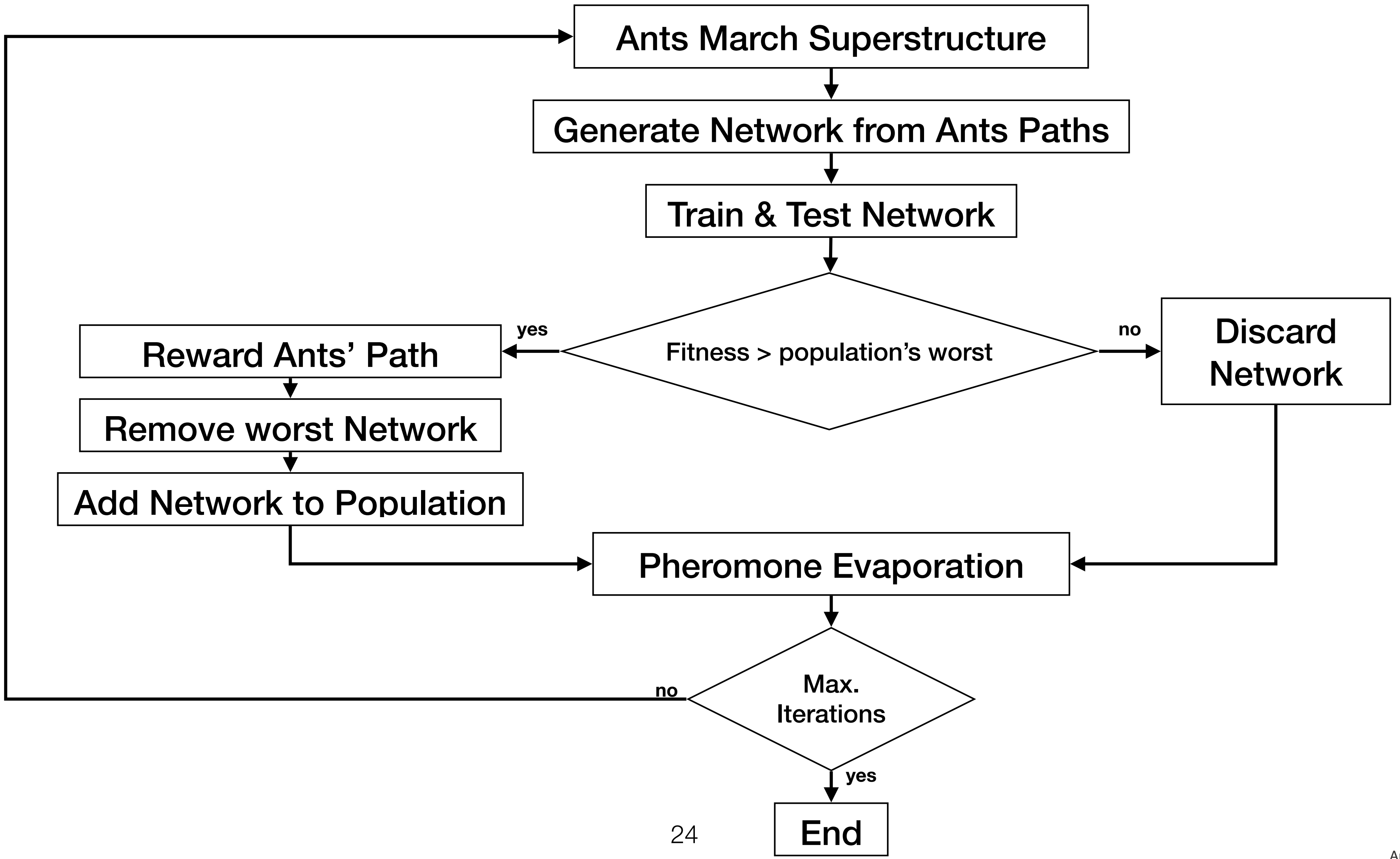
- NN are directed graphs

- ACO is* :
  - fault tolerant,
  - decentralized,
  - scalable, and
  - easily traceable

- ACO decentralization ==> perfect candidate for parallel and HPC ==> accelerates optimization

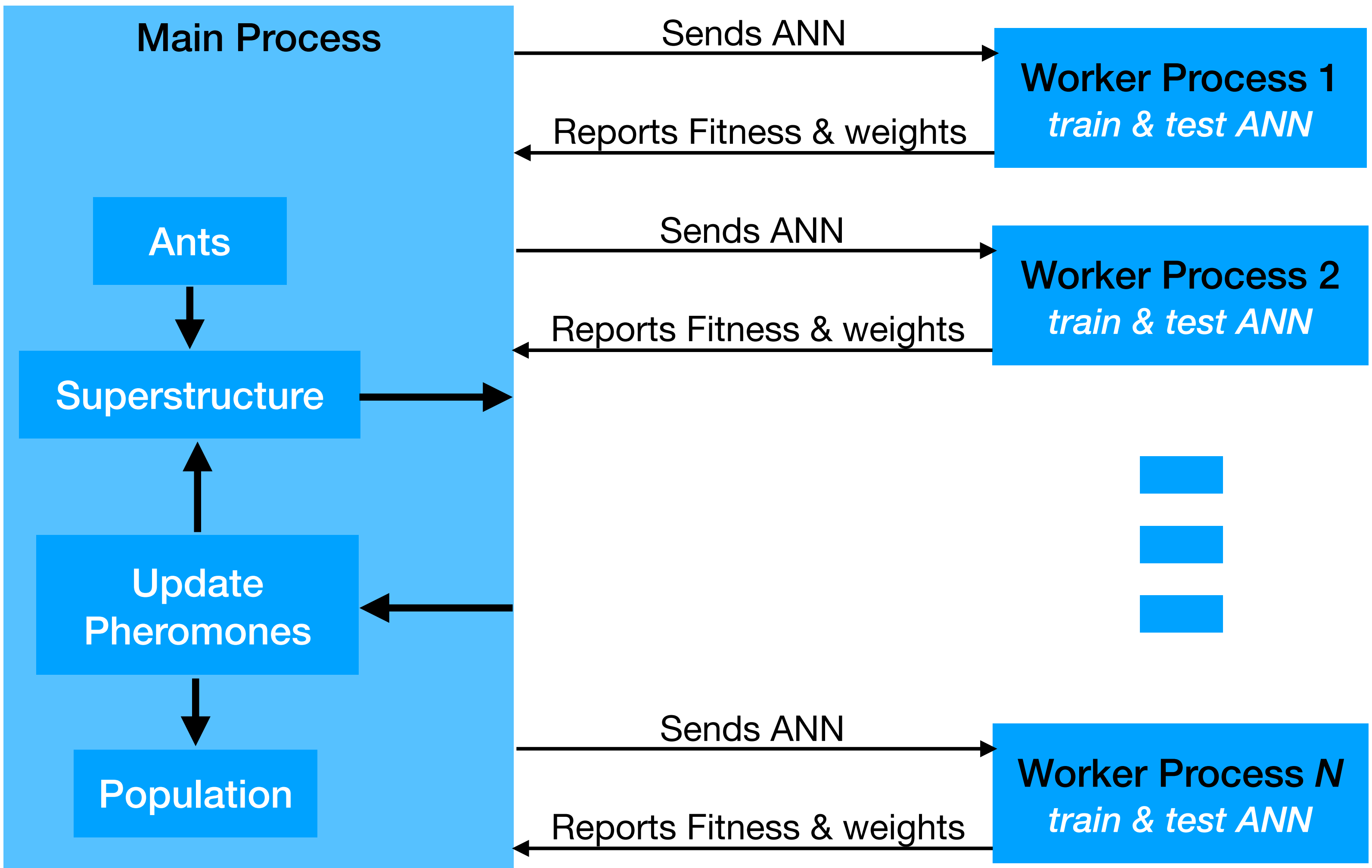
*Edvinas Byla and Wei Pang. Deepswarm: Optimising convolutional neural networks using swarm intelligence. arXiv preprint arXiv:1905.07350, 2019.

Ant Colony Based Optimization

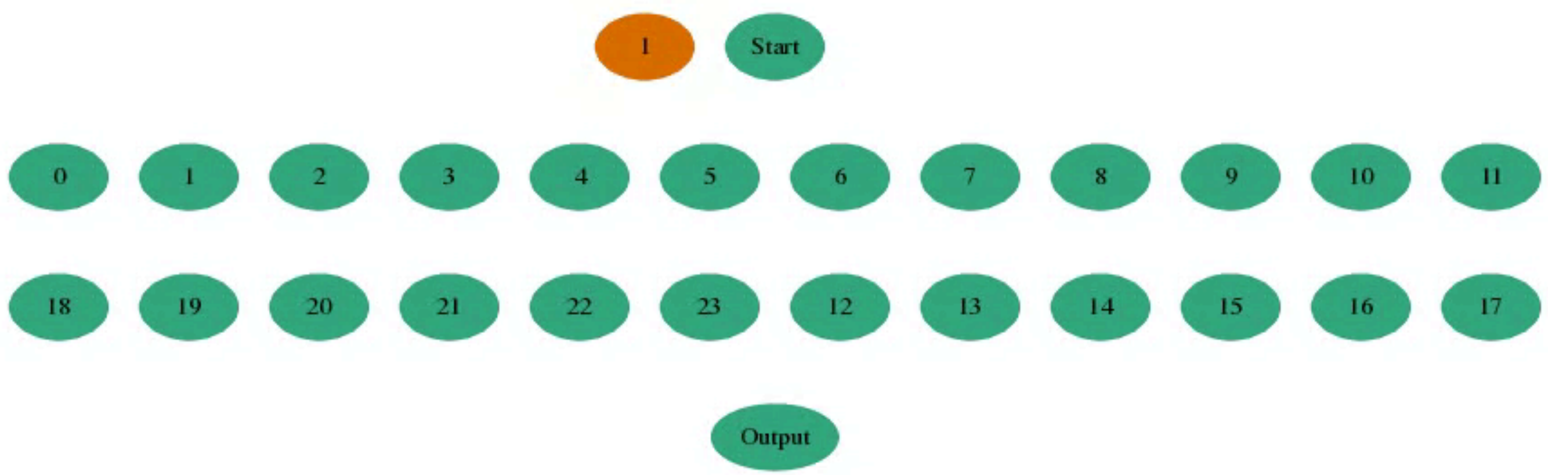


Ant Colony Based Optimization

Asynchronous Evolution



Ant Colony Based Optimization



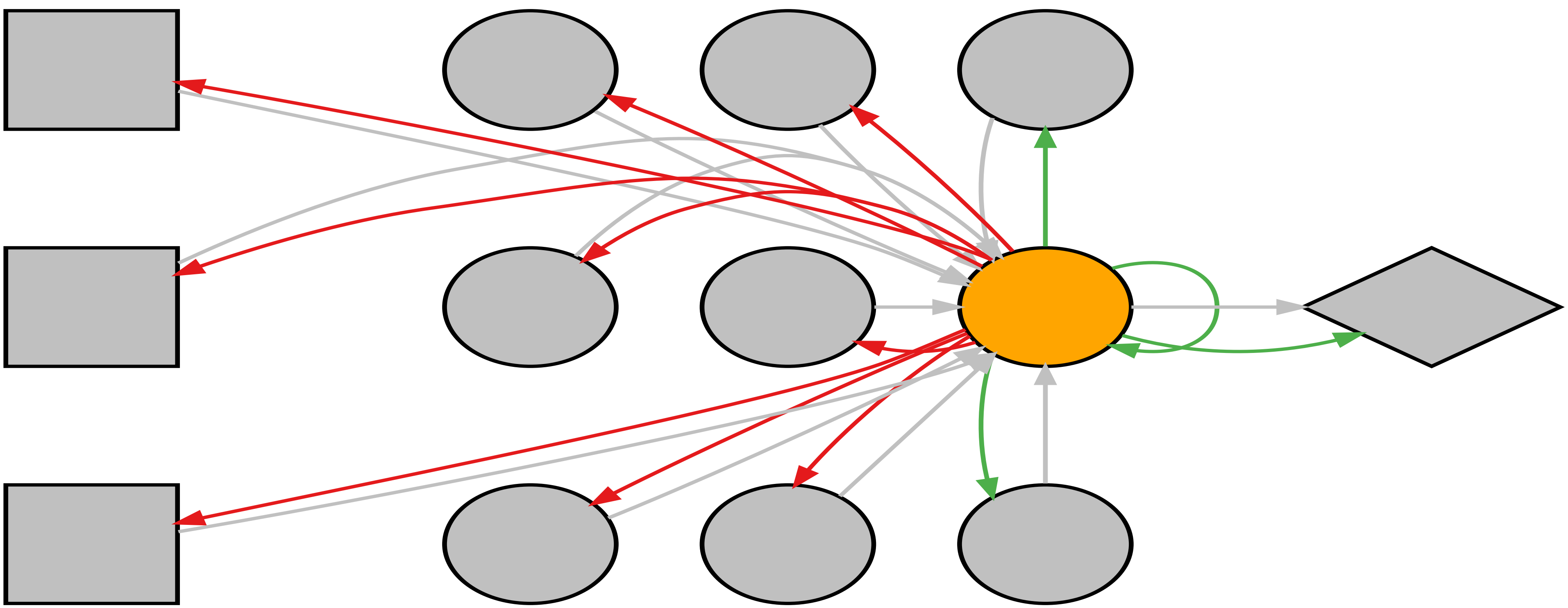
Ant-based Neural Topology Search (ANTS)

Ant Neural Topology Search (ANTS)

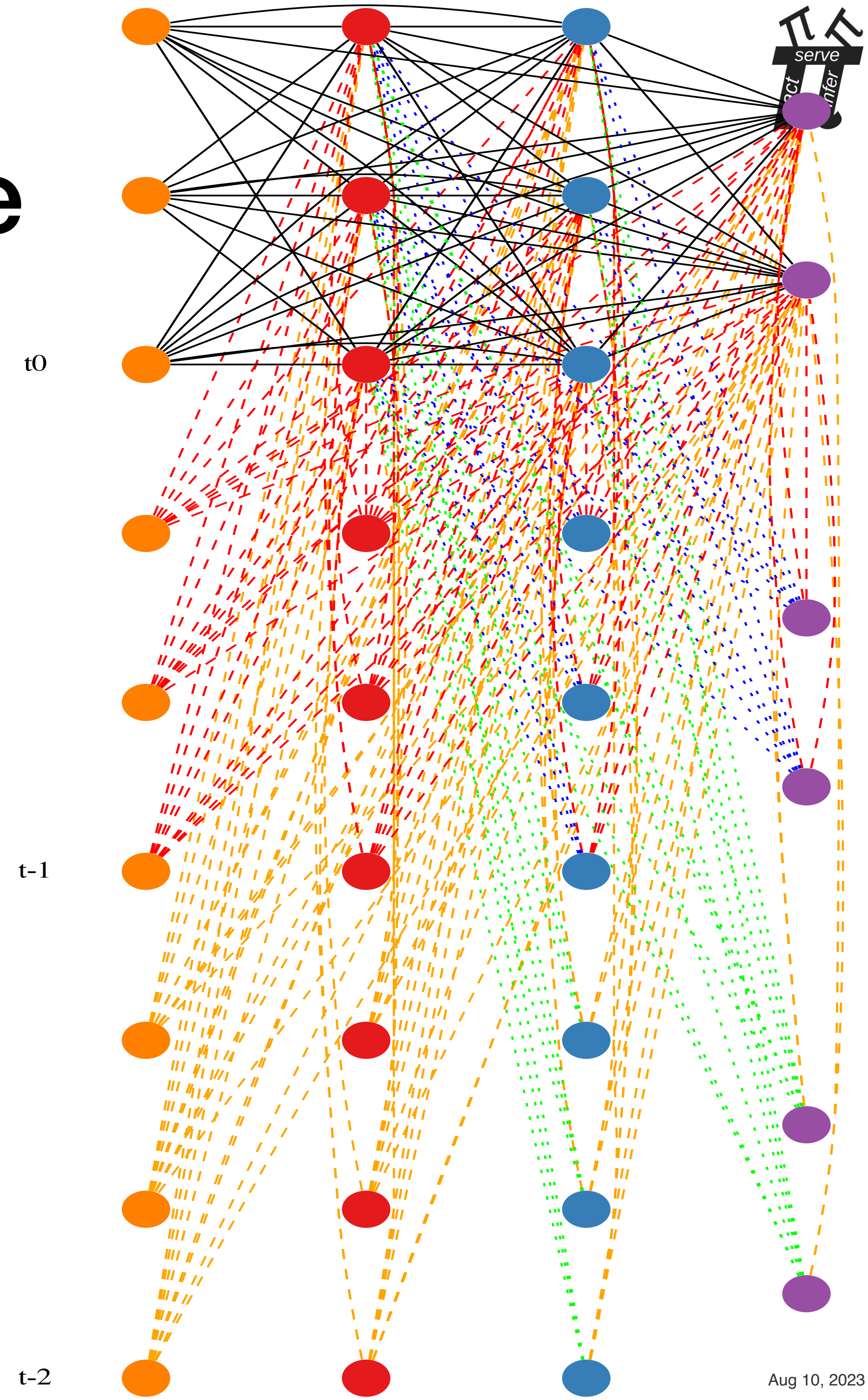
- ANTS is generic and powerful NE method which can optimize an entire RNN structure
- RNNs have a potentially larger architecture search space (than feed forward NNs or CNNs) due to recurrent connections over multiple time spans

1. Superstructure

- Superstructure representing a massively connected RNN is used to hold the pheromone value deposited by traversing ants



1. Superstructure



Input

Hidden 1

Hidden 2

Output

Edges

t-1 Fwd Recurrent Edges

t-2 Fwd Recurrent Edges

t-1 Bwd Recurrent Edges

t-2 Bck Recurrent Edges

2. Colony Weight Sharing

- ANTS utilizes a novel concept for initializing RNN weights: it keeps a pool of shared weights to save the weights of the best performing RNNs

- Those weights are passed to later generated RNNs instead of randomly initializing them and training the RNNs from scratch, which would slow the NE process

$$x = \frac{fit_{new} - fit_{pop\_best}}{fit_{pop\_worst} - fit_{pop\_best}}$$

$$\Phi(fit_{new}) = min\left(max\left((1-x),0\right),1\right)$$

$$W_{s\_structure_i} = \Phi W_{RNN_i} + (1-\Phi) W_{s\_structure_i}$$

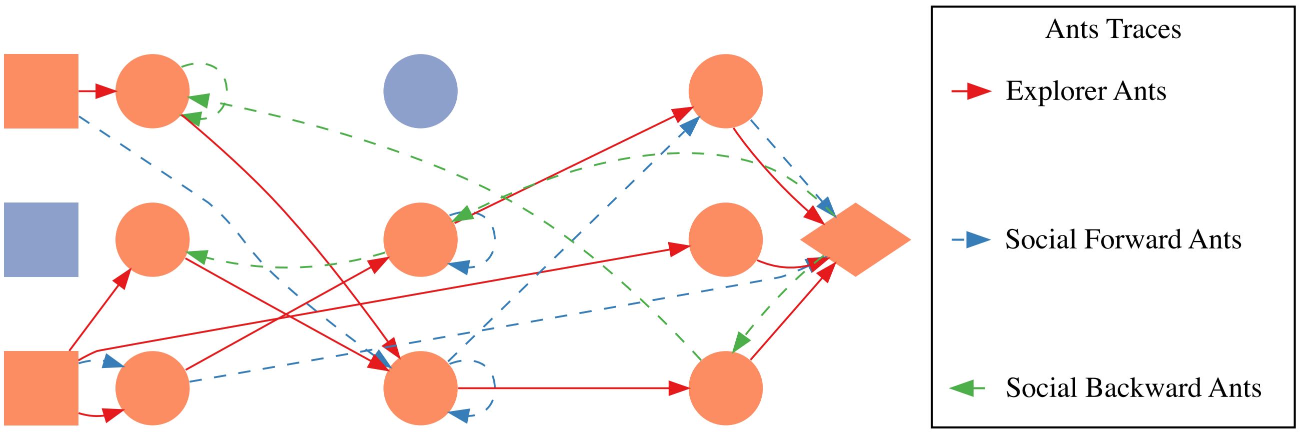
3. Multiple Memory Cells

- The superstructure also has a collection of memory based cells at each node for the ants to choose from when they move on the superstructure to construct their RNNs
- This further complicates ANTS optimization work… local search at each node of the superstructure
- The nodes types:
    - Gated Recurrent Unit (GRU) [1]
    - LSTM RNN [2]
    - Minimum Gated Unit (MGU) [3]
    - Update-Gated RNN (UGRNN) Unit [4]
    - Delta RNN Unit [5]

[1]Cho, Kyunghyun; van Merrienboer, Bart; Gulcehre, Caglar; Bahdanau, Dzmitry; Bougares, Fethi; Schwenk, Holger; Bengio, Yoshua (2014). Learning Phrase Representations using RNN Encoder-Decoder for Statistical Machine Translation. arXiv:1406.1078
[2]Felix A. Gers; Jürgen Schmidhuber; Fred Cummins (2000). Learning to Forget: Continual Prediction with LSTM. Neural Computation. 12 (10): 2451–2471.
[3]Gou-Bing Zhou,Jianxin Wu, Chen-Lin Zhang and Zhi-Hua Zhou. Minimal gated unit for recurrent neural networks. International Journal of Automation and Computing 13.3 (2016): 226-234.
APA
[4]Collins, Jasmine, Jascha Sohl-Dickstein, and David Sussillo. Capacity and trainability in recurrent neural networks. arXiv preprint arXiv:1611.09913 (2016).
[5]Ororbia II, Alexander G., Tomas Mikolov, and David Reitter. Learning simpler language models with the differential state framework. Neural computation 29.12 (2017): 3327-3352.

4. Multiple Ant Species

- ANTS is also unique in using different ant species
- Members of each specie has their own properties, which makes these agents dependent unique in their effect
- There are:
    - *Explorer Ants*: they only move on edges.
    - *Social forward Ants*: they only move on forward recurrent edges.
    - *Social Backward Ants*: they only move on backward recurrent edges.
- Ant species and their movement behavior limit the tendency of the ants to wander around in the superstructure exploiting the massive number of recurrent edges.



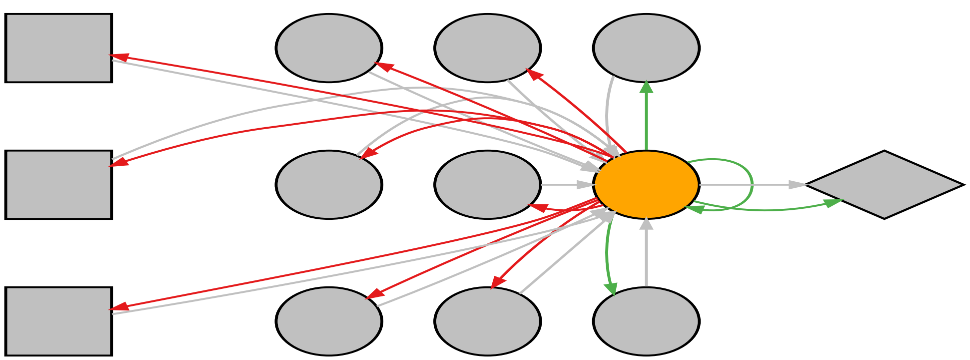
5. Regularization for Pheromone Placement

- ANTS regularize pheromone deposits using L1/L2 regularization using the weights of the evaluated RNNs
- This imposes a penalty on less sparse RNNs and give incentive for ants to work harder on RNN sparsity
- Applying regularization to pheromone deposits is another level of control, which was not introduced in previous simpler ways

$$\tau_{new} = (1-\alpha)\cdot\tau_{old} + \alpha\left\{\frac{1}{\eta + \frac{\gamma}{n}||W||}\right\}$$

6. Jumping Ants

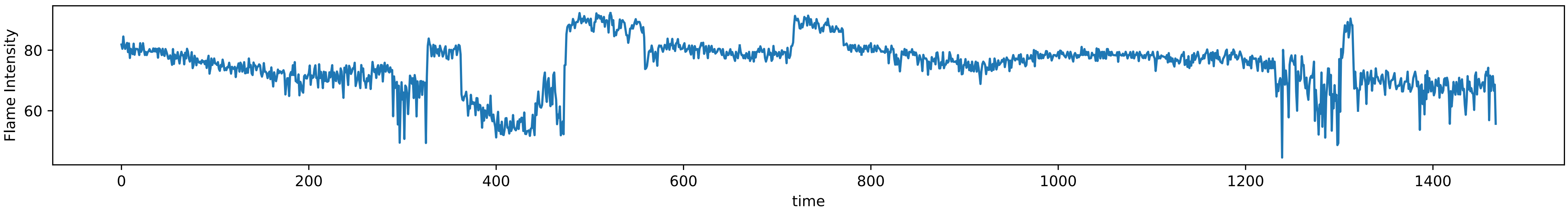
- Ants in ANTS can either:
  - move on edges/recurrent edges that jump over the superstructure layers.
  - be restricted to move only on edges/recurrent edges between consecutive layers with out jumping



ANTS

Experiments

- Time-series data used in these experiments came from a coal-fired power plant
- Part of data used:
  - Training data: 7200 per-minute time steps, 12 parameters (5 days)
  - Testing data: 7200 per-minute time steps, 12 parameters (5 days)
- The Flame Intensity of a plant's burner was the prediction target of the experiments for operation optimization
- Data & ANTS source code are open source and published in github **



ElSaid A., Ororbia A., and Desell, T. **Ant-based Neural Topology Search (ANTS) for Optimizing Recurrent Networks**, *EvoStar 2020.* Seville, Spain
https://github.com/travisdesell/exact

ANTS

Experiments

- 12 input parameters:
  - Conditioner Inlet Temp
  - Conditioner Outlet Temp
  - Coal Feeder Rate
  - Primary Air Flow
  - Primary Air Split
  - Secondary Air Flow Total
  - Secondary Air Flow
  - Secondary Air Split
  - Tertiary Air Split
  - Total Comb Air Flow
  - Auxiliary Fuel Flow
  - Flame Intensity

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ANTS

Experiments

- The experiments covered all ANTS heuristics:
    - Number of Ants: 20, 40, 80, 160
    - L1, L2 regularization parameter ($\alpha = \{.25,.65,.9\}$)
    - Combinations of ants species
    - Superstructure weight update parameter (constant version) ($\Phi = \{.3,.6,.9\}$)
    - Jumping or non-jumping ants

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ANTS

Experiments

- Superstructure:
  - 12 nodes input layer
  - 3 hidden layer, 12 nodes each
  - 1 node output layer
  - Recurrent connections spanned 1, 2, 3 time steps.
  - 49 nodes, 924 edges, 3626 recurrent edges.

- Superstructure unrolled over 7200 time steps by BPTT:
  - 352,800 nodes
  - 6,652,800 edges
  - 26,107,200 recurrent edge

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ANTS

Experiments

- Compared to:
  - EXAMM* (Evolutionary eXploration of Augmenting Memory Models) - generated 2k RNNs, each trained for 10 epochs for 10 repeats
  - NEAT** (NeuroEvolution of Augmenting Topologies) generated 420,000 RNNs (2k * 10 * 2)
  - Fixed architecture RNN - were allowed to train for 70 epochs:1, 2 and 3 layer LSTM, GRU, MGU, UGRNN, Delta-RNN networks

ElSaid A., Ororbia A., and Desell, T. **Ant-based Neural Topology Search (ANTS) for Optimizing Recurrent Networks**, *EvoStar 2020.* Seville, Spain
*AbdElRahman ElSaid, Steven Benson, Shuchita Patwardhan, David Stadem, and Travis Desell. Evolving Recurrent Neural Networks for Time Series Data Prediction of Coal Plant Parameters. The 22nd International Conference on the Applications of Evolutionary Computation (EvoStar: EvoApps 2019).
**Stanley, K.O. and Miikkulainen, R., 2002. Evolving neural networks through augmenting topologies. *Evolutionary computation*, *10*(2), pp.99-127.

ANTS

Experiments

- 1,600 experiments conducted to include all the combinations of ANTS heuristics combinations
- ANTS generated 2k RNNs for each experiment, each trained for 10 epochs
- Experiment repeated 10 times for statistical comparison
- ANTS generated, trained, and evaluated a total of **32 million** RNNs.
- Experiments were scheduled on HPC cluster with 64 Intel® Xeon® Gold 6150 CPU each with 36 cores and 375 GB RAM (total 2304 cores and 24 TB RAM)
- It took about a month to finish using 1000 cores.

ElSaid A., Ororbia A., and Desell, T. **Ant-based Neural Topology Search (ANTS) for Optimizing Recurrent Networks**, *EvoStar 2020.* Seville, Spain
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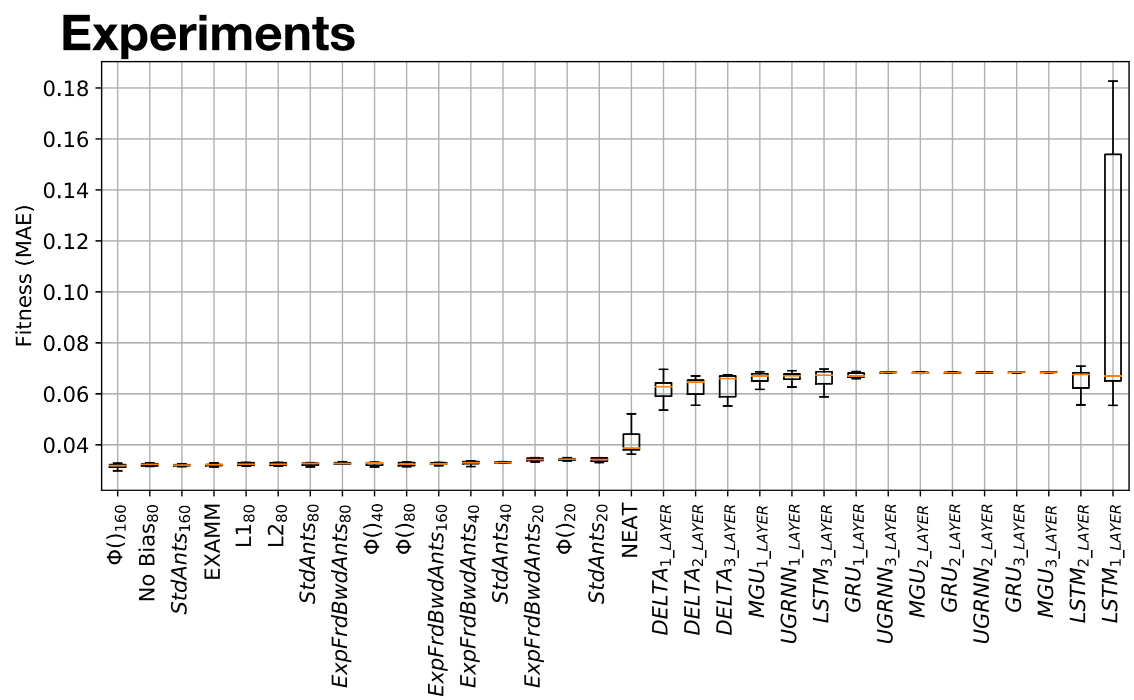
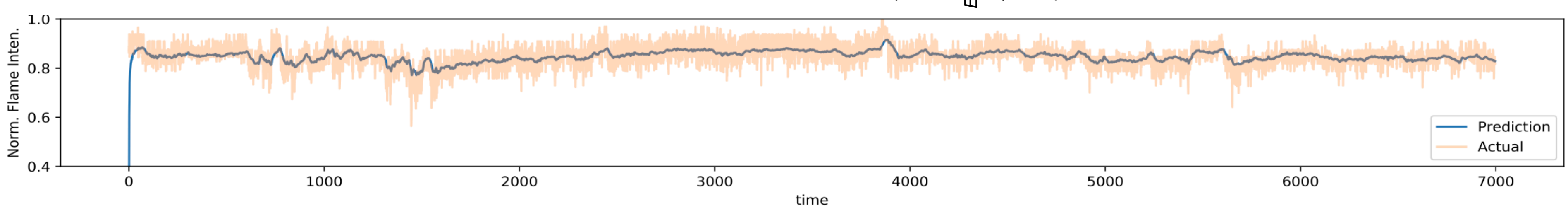
ANTS

- ANTS outperform NEAT
- ANTS outperformed the EXAMM





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[2]Alex Ororbia, AbdElRahman ElSaid, and Travis Desell. Investigating Recurrent Neural Network Memory Structures using Neuro-Evolution. The Genetic and Evolutionary Computation Conference (GECCO 2019). Prague, Czech Republic. July 8-12, 2019.

[3] Kenneth Stanley and Risto Miikkulainen. Evolving neural networks through augmenting topologies. Evolutionary computation: 10, 2. (2002), 99–127.

ANTS

Experiments

- ANTS heuristic ranking statistics

	Top 10			Top 25			Top 100			Top 250			Top 500		
	Mean	Median	Best	Mean	Median	Best	Mean	Median	Best	Mean	Median	Best	Mean	Median	Best
Φ()	3(0)	4(0)	3(0)	9(0)	7(0)	9(0)	26(0)	23(0)	31(8)	58(0)	54(0)	49(8)	108(1)	96(0)	100(14)
ConstΦ	7(0)	6(0)	7(0)	14(0)	14(0)	12(0)	60(0)	63(0)	54(8)	147(0)	149(0)	155(16)	294(0)	301(0)	299(43)
NoΦ	0(0)	0(0)	0(0)	2(0)	4(0)	4(0)	14(0)	14(0)	15(0)	45(0)	47(0)	46(0)	98(0)	103(0)	101(0)
L1	2(0)	4(0)	0(0)	9(0)	8(0)	3(3)	42(0)	34(0)	30(4)	96(0)	96(0)	91(4)	190(0)	186(1)	186(21)
L2	5(0)	5(0)	6(0)	13(0)	12(0)	16(1)	40(0)	45(0)	38(3)	100(0)	98(0)	95(12)	189(0)	192(0)	185(21)
StdAnts	0	0	0	1	0	0	3	0	0	20	19	0	80	77	7
StdBiasAnts	0	0	0	0	0	0	3	1	0	23	16	0	83	83	11
ExpAnts	0	0	10	0	0	25	1	0	100	10	6	250	92	85	440
ExpFrdAnts	6	7	0	14	15	0	45	49	0	98	103	0	123	128	40
ExpBkwAnts	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ExpFrdBkwAnts	4	3	0	10	10	0	48	50	0	99	106	0	122	127	2
No Jump	0	0	5	0	0	13	0	0	52	0	0	128	2	9	282
Layer Jump	10	10	5	25	25	12	100	100	48	250	250	122	498	491	218
20 Ants	0	0	2	0	0	6	0	0	24	0	0	65	3	6	220
40 Ants	2	0	3	5	1	7	14	15	23	50	57	63	97	87	120
80 Ants	4	3	2	8	11	6	44	45	26	82	80	60	175	173	80
160 Ants	4	7	3	12	13	6	42	40	27	118	113	62	225	234	80

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ANTS

Experiments

- ANTS is the first metaheuristic method to involve the core of ACO in RNN NE in massive search space
- ANTS heuristics to control ants tendency to wander around superstructure, exploiting recurrent connections, proved successful and efficient
- Allowing **ants to skip layer** proved effective in **RNNs sparsity and performance**
- Introduction of **L1/L2 regularization** into the ACO
- **Weights-pooling offered boost for training** RNNs which reflected in their performance
- **Formalized strategies are generic** and could be applied to any other ACO algorithm's pheromone update process
- **Pheromone deposition process is novel** if albeit a bit unconventional
- **ANTS beats NEAT** by over an order of magnitude, which is considered a **benchmark in NE**
- **ANTS** is not only unique, but **is now state of the art over EXAMM on this dataset**

ElSaid A., Ororbia A., and Desell, T. **Ant-based Neural Topology Search (ANTS) for Optimizing Recurrent Networks**, *EvoStar 2020.* Seville, Spain

Continuous Ant-based Neural Topology Search (CANTS)

CANTS

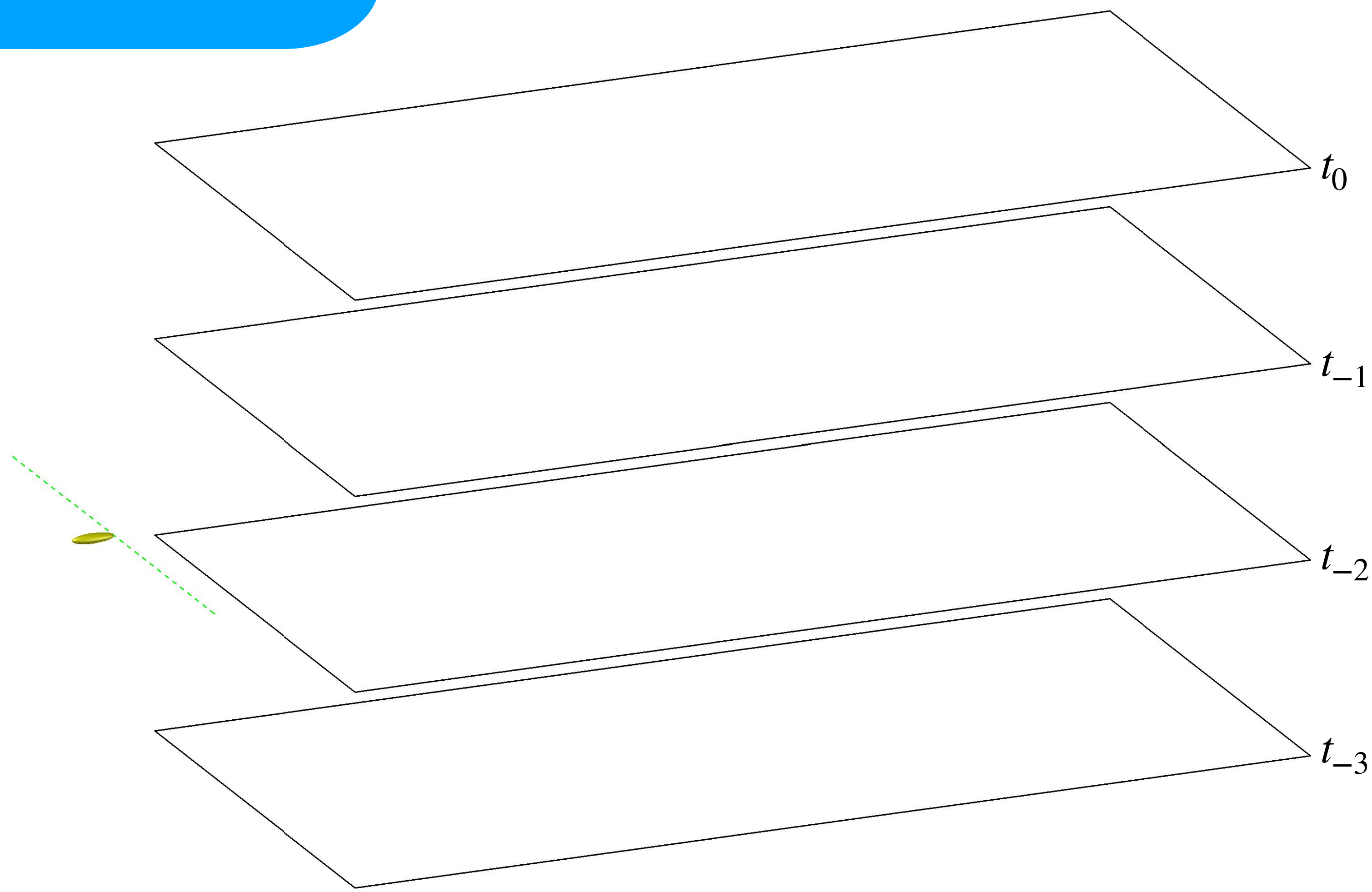
- Replaces main ANTS limitation: **Discrete => Continuous** *Search Space*

- New Search space is semi-continuous 3D:
  - Layers represent time lag: pure continuous movement
  - Jumping through time (between layers): discrete movement

ElSaid, A., Karns, J., Lyu, Z., Ororbia, A. and Desell, T., 2020. **Continuous Ant-Based Neural Topology Search.** arXiv preprint arXiv:2011.10831.

CANTS

Input Selection



ElSaid, A., Karns, J., Lyu, Z., Ororbia, A. and Desell, T., 2020. **Continuous Ant-Based Neural Topology Search.** arXiv preprint arXiv:2011.10831.

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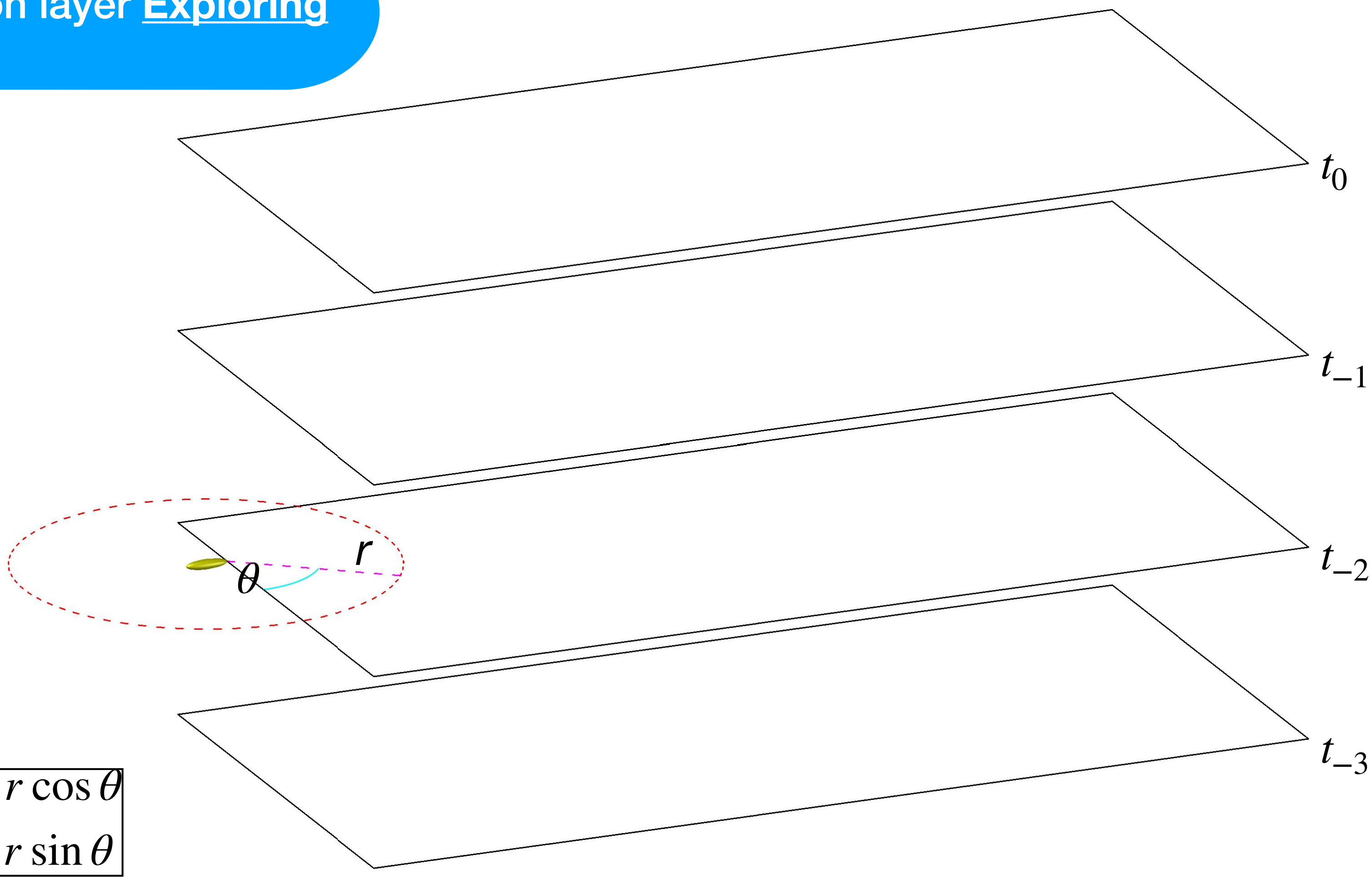
Picking Layer
&
Moving on layer **Exploring**



$$x = x_0 + r\cos\theta$$
$$y = y_0 + r\sin\theta$$

ElSaid, A., Karns, J., Lyu, Z., Ororbia, A. and Desell, T., 2020. **Continuous Ant-Based Neural Topology Search.** arXiv preprint arXiv:2011.10831.

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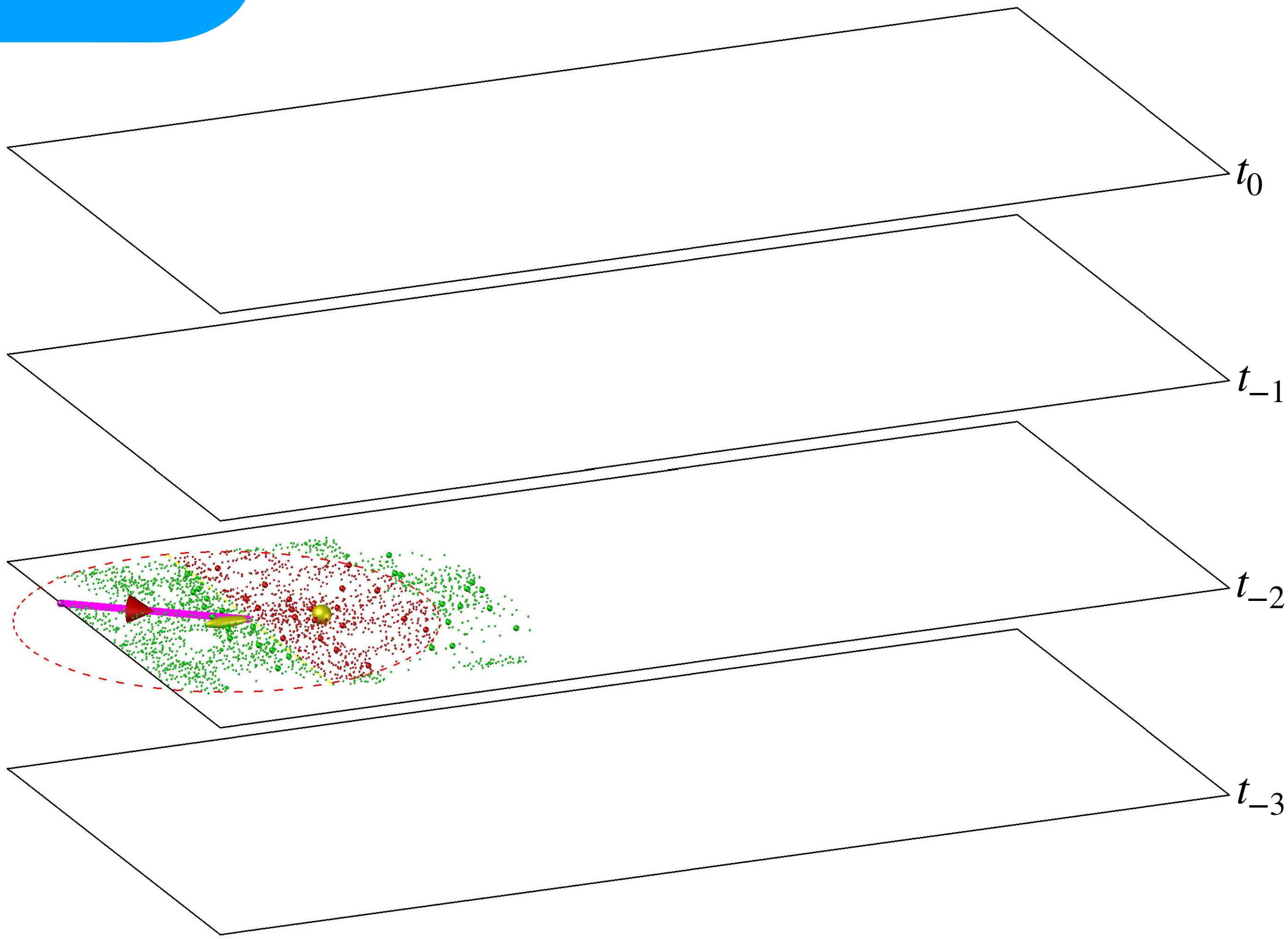
Moving on layer: **Exploiting**



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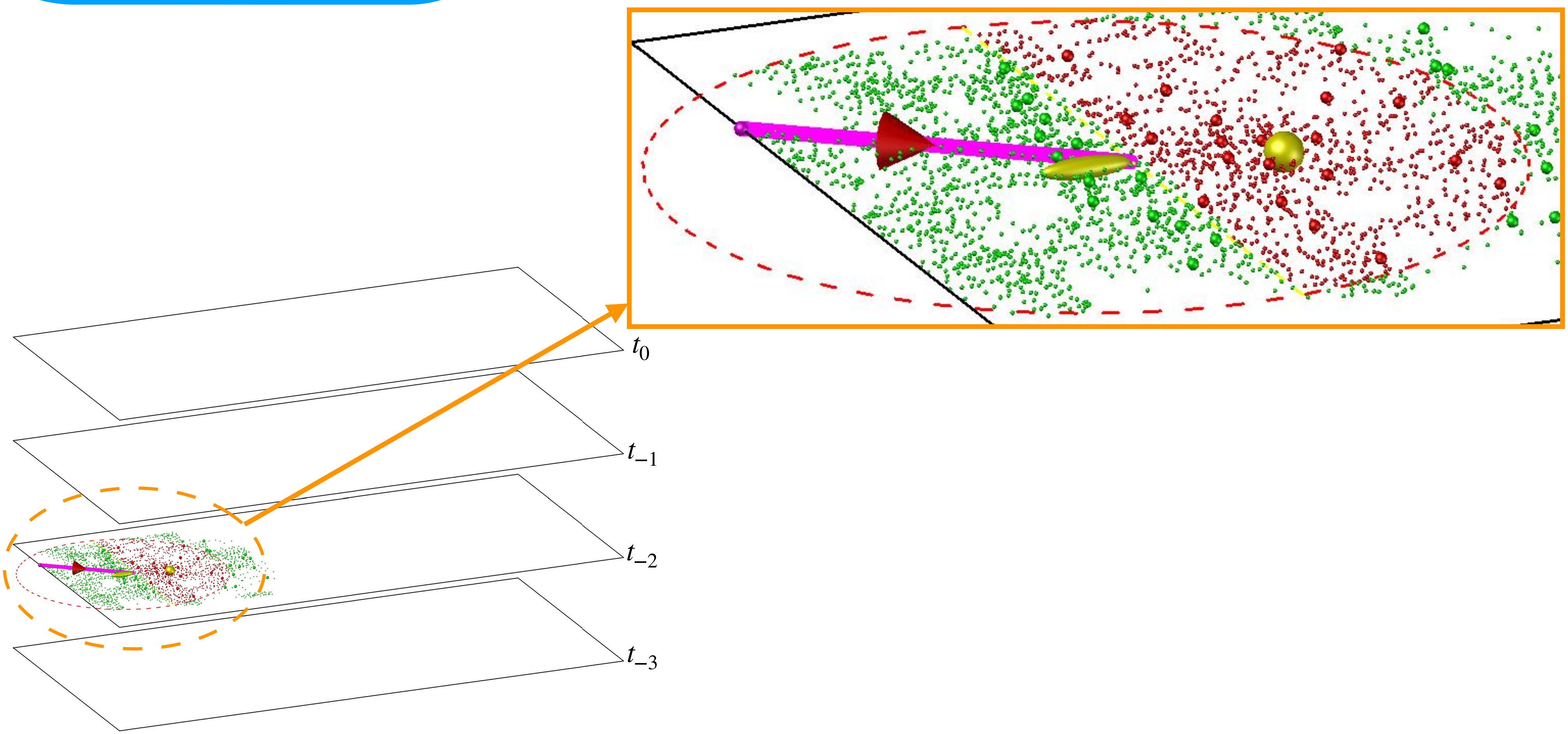
CANTS

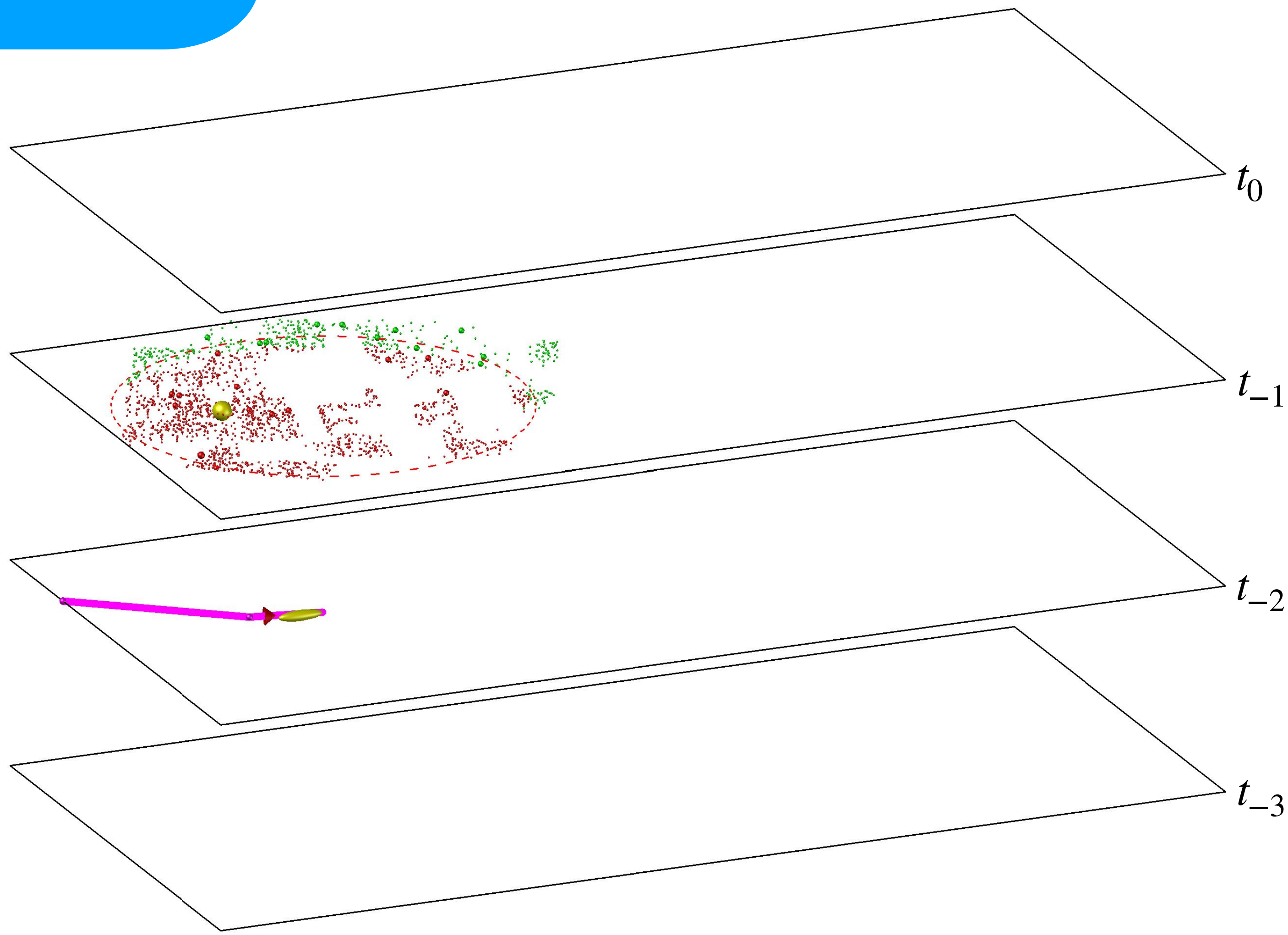
Moving on layer: **Exploiting**



ElSaid, A., Karns, J., Lyu, Z., Ororbia, A. and Desell, T., 2020. **Continuous Ant-Based Neural Topology Search.** arXiv preprint arXiv:2011.10831.

Backward Recurrent Edge

CANTS



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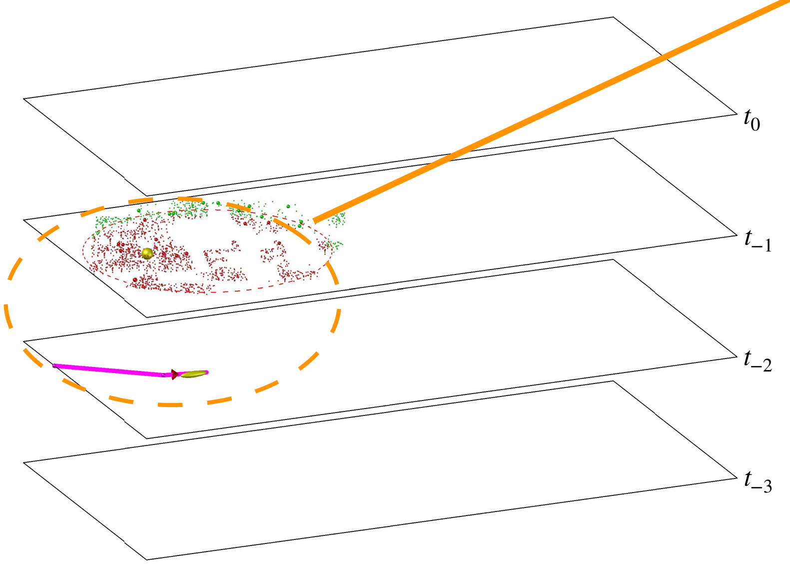
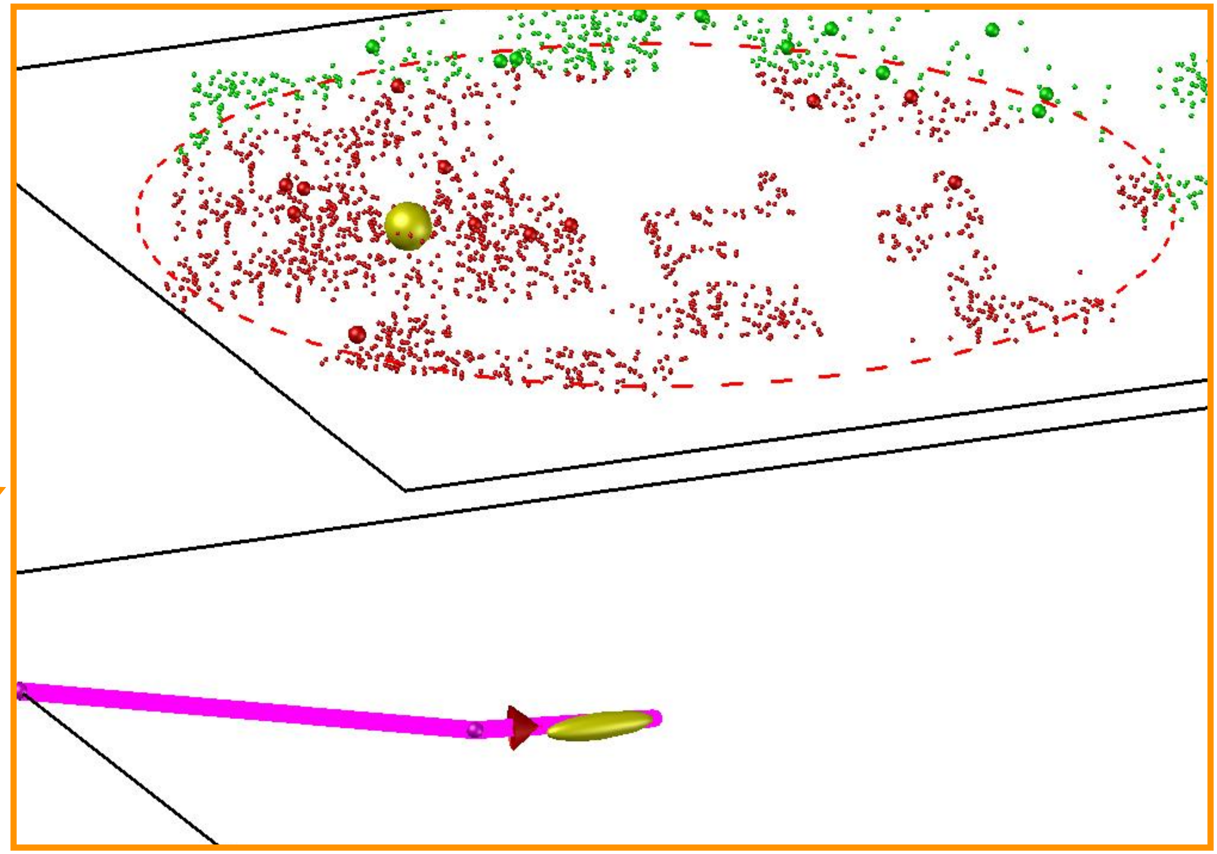
Backward Recurrent Edge

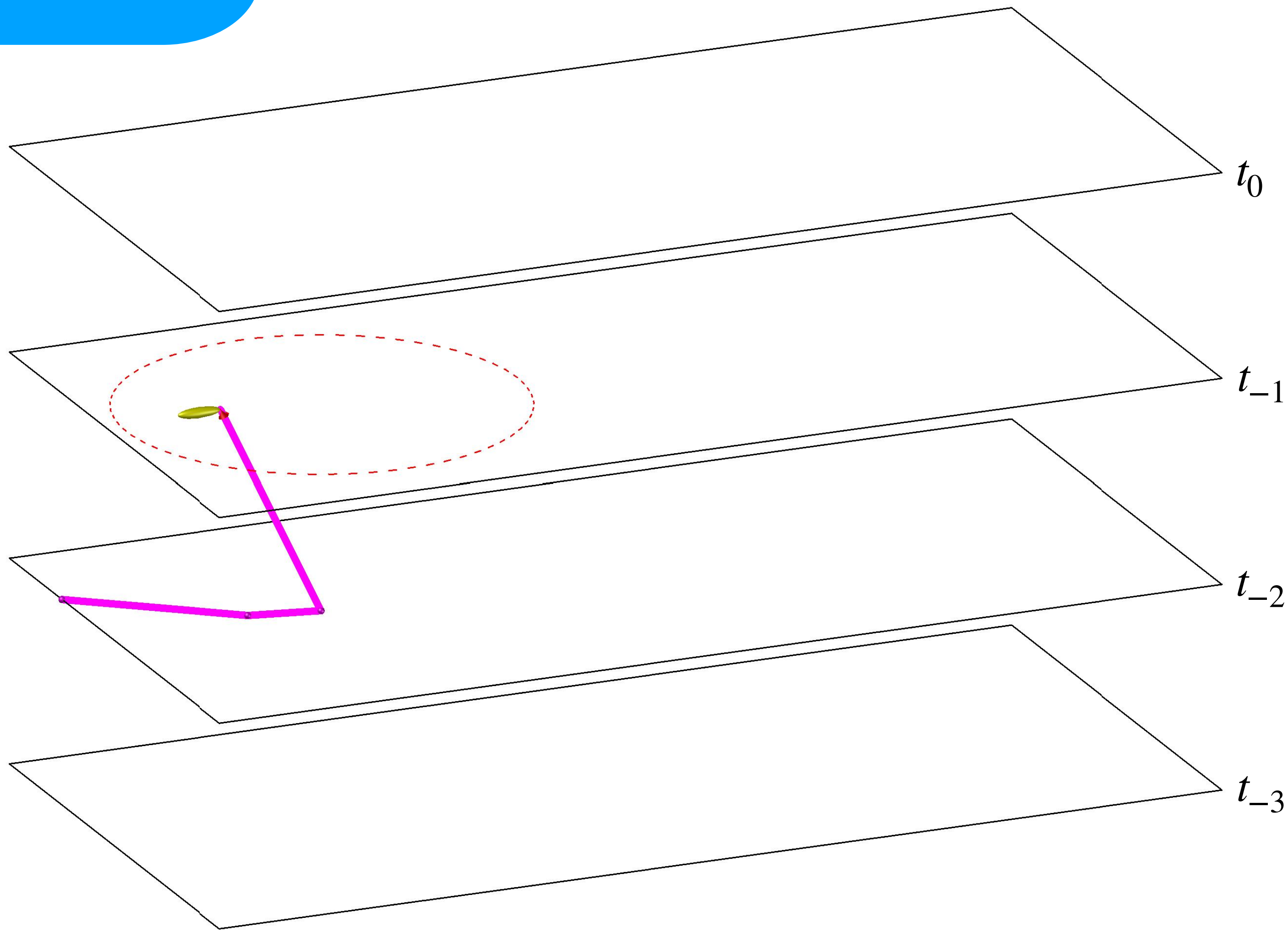




ElSaid, A., Karns, J., Lyu, Z., Ororbia, A. and Desell, T., 2020. **Continuous Ant-Based Neural Topology Search.** arXiv preprint arXiv:2011.10831.

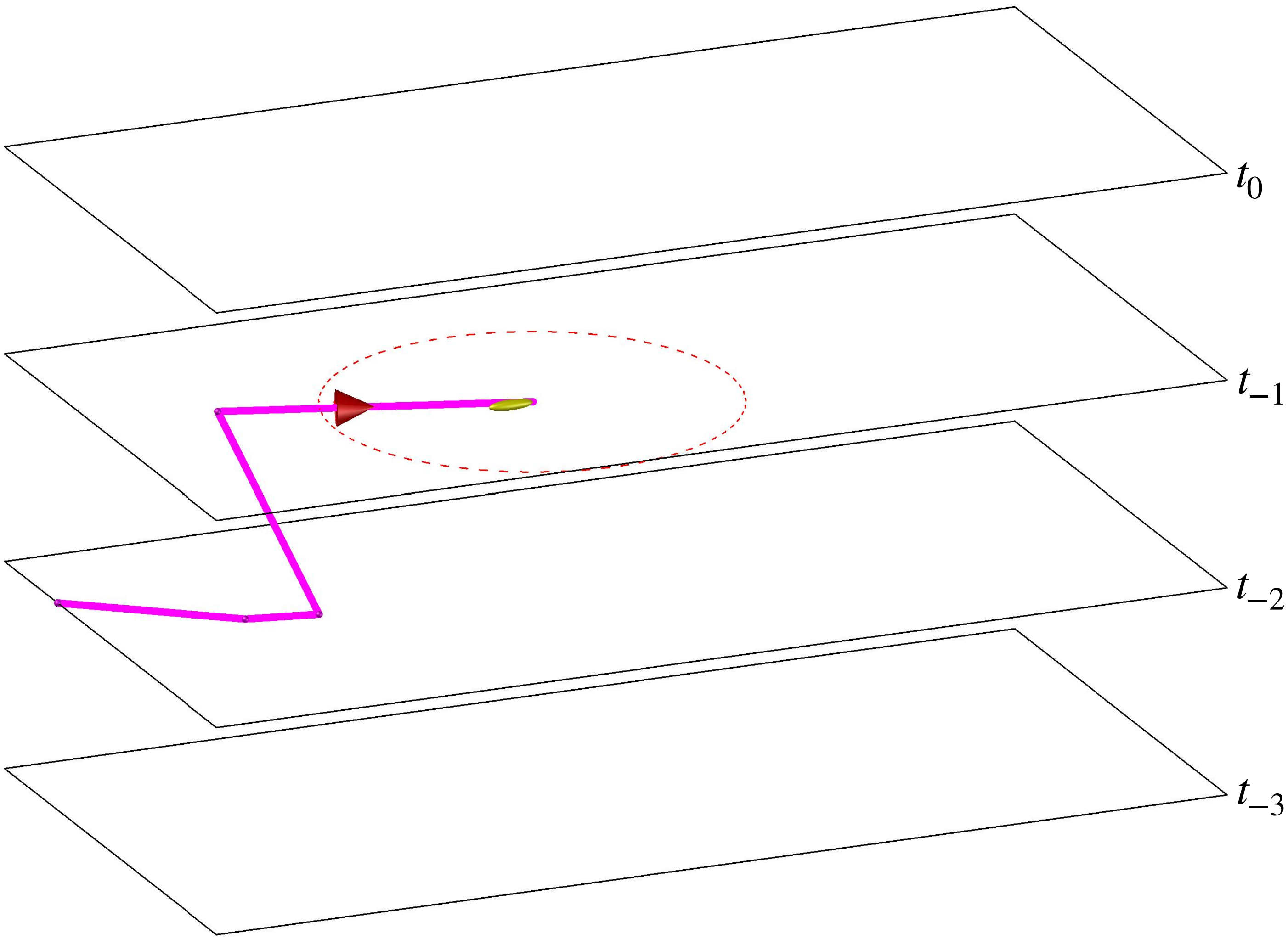
CANTS

Backward
Recurrent Edge



ElSaid, A., Karns, J., Lyu, Z., Ororbia, A. and Desell, T., 2020. **Continuous Ant-Based Neural Topology Search.** arXiv preprint arXiv:2011.10831.

CANTS



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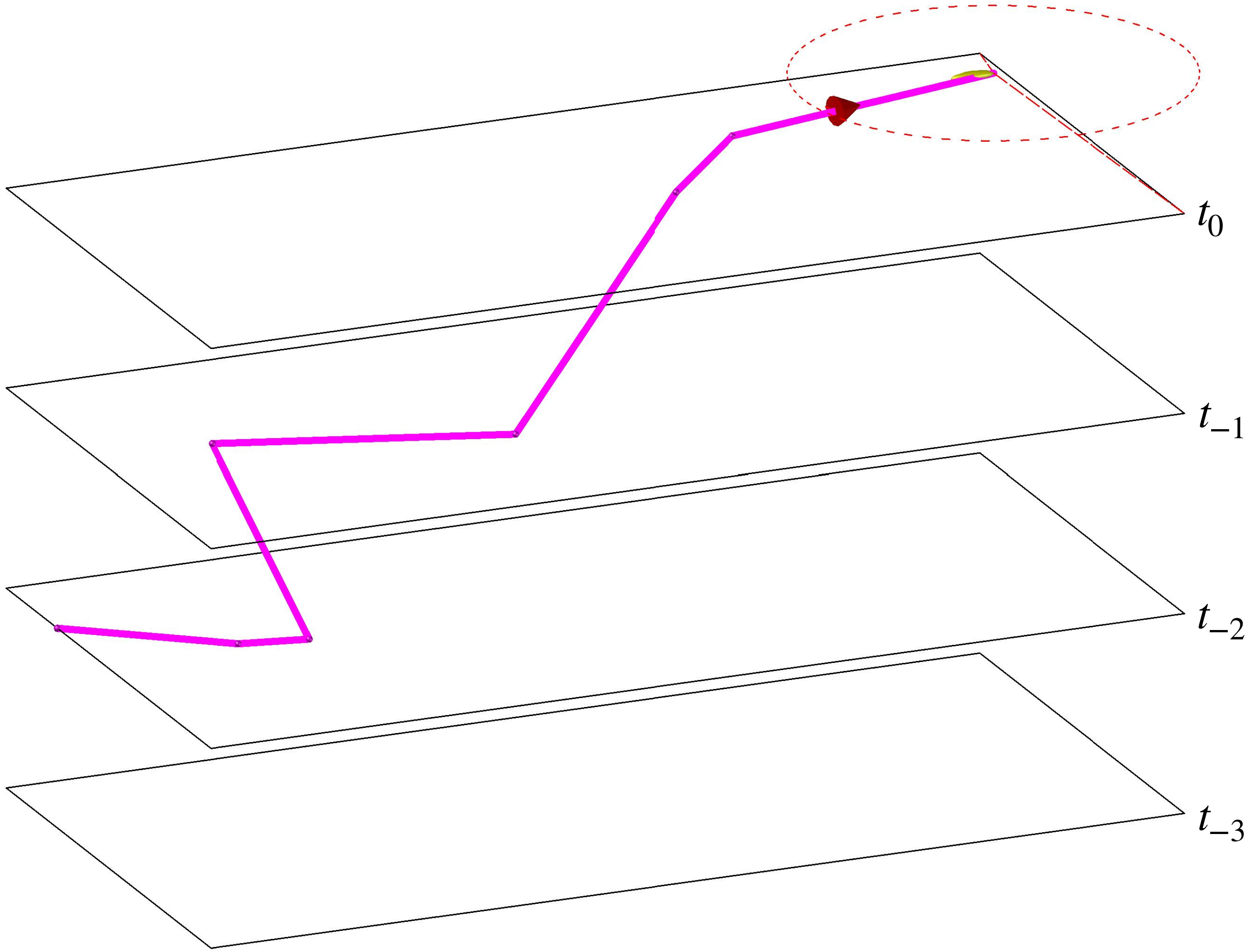
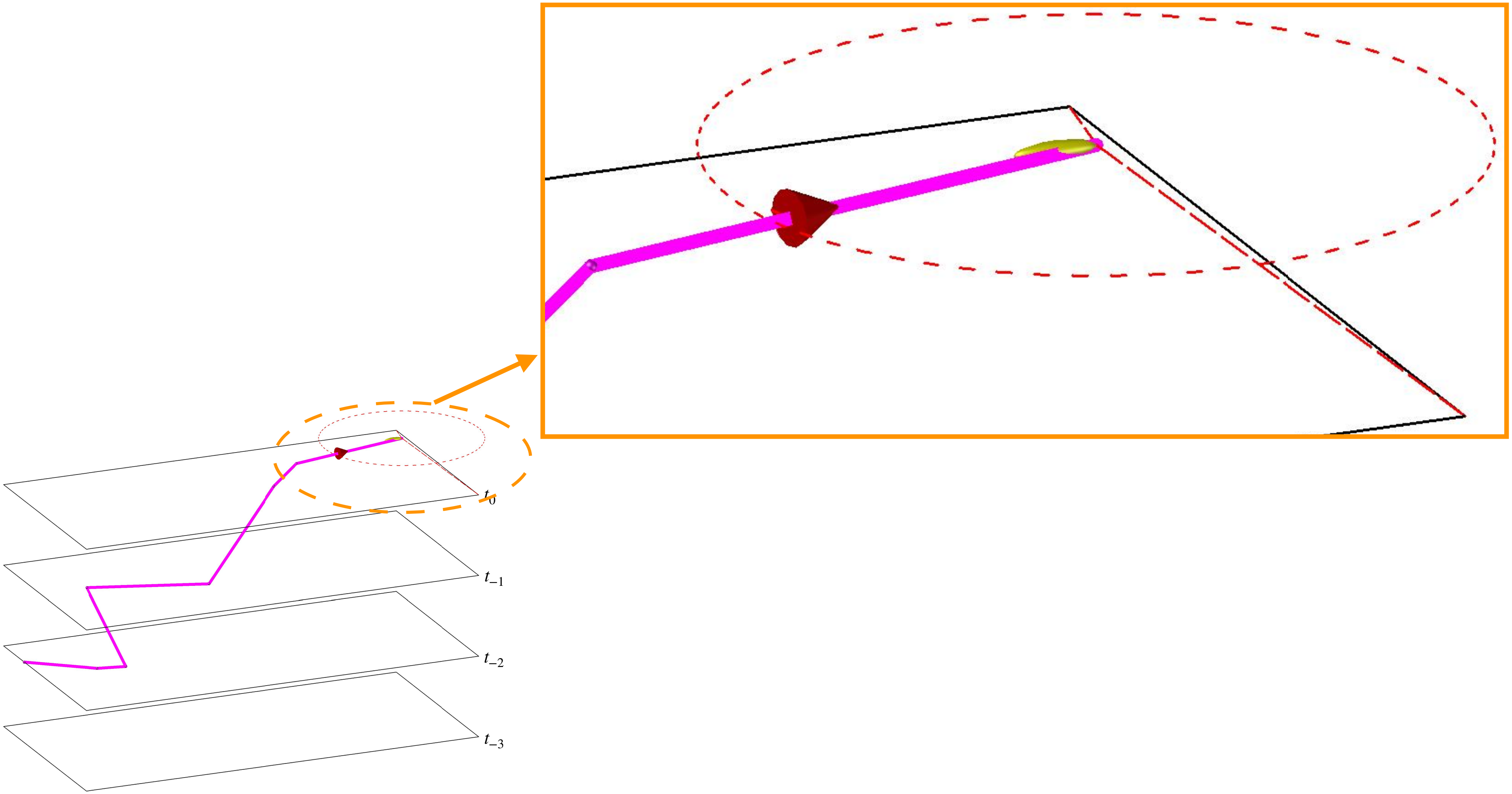
CANTS



ElSaid, A., Karns, J., Lyu, Z., Ororbia, A. and Desell, T., 2020. **Continuous Ant-Based Neural Topology Search.** arXiv preprint arXiv:2011.10831.

Output Selection

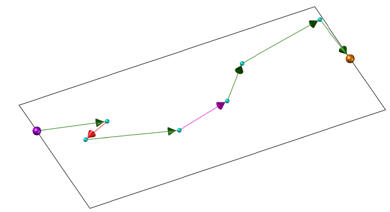
CANTS

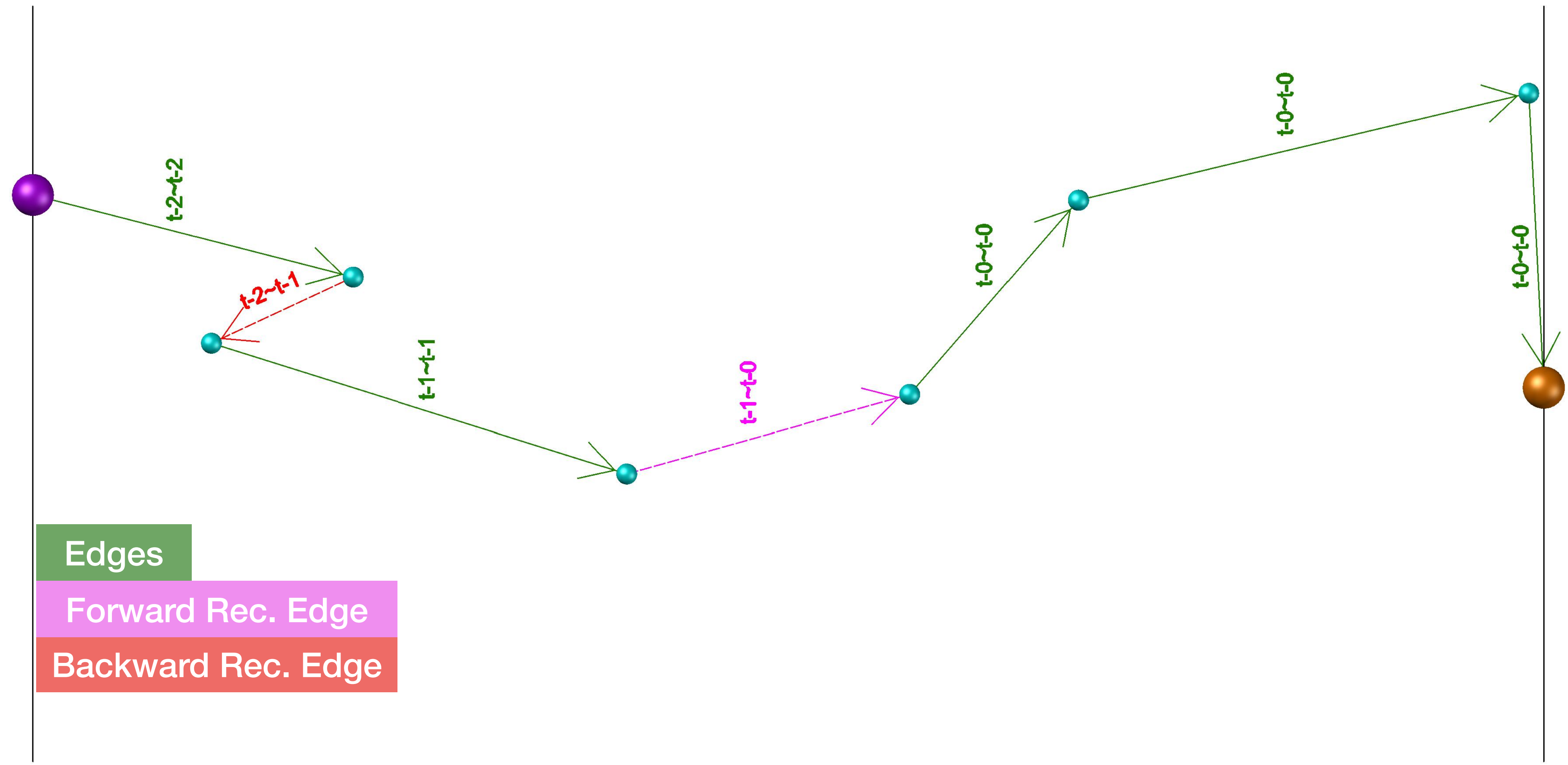


ElSaid, A., Karns, J., Lyu, Z., Ororbia, A. and Desell, T., 2020. **Continuous Ant-Based Neural Topology Search.** arXiv preprint arXiv:2011.10831.

CANTS

Projecting RNN on 2D



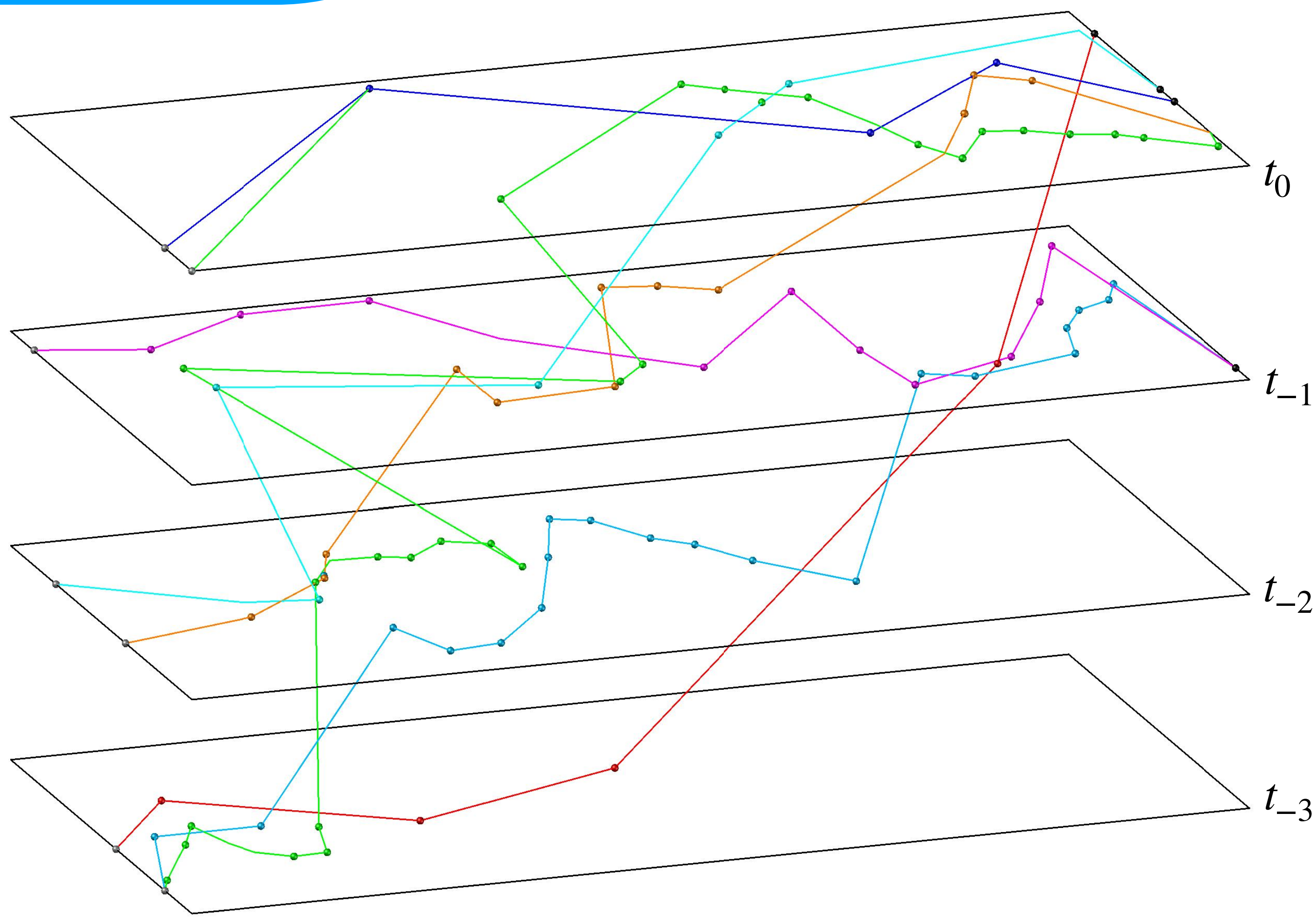


ElSaid, A., Karns, J., Lyu, Z., Ororbia, A. and Desell, T., 2020. **Continuous Ant-Based Neural Topology Search.** arXiv preprint arXiv:2011.10831.

CANTS

cants swarming

Input

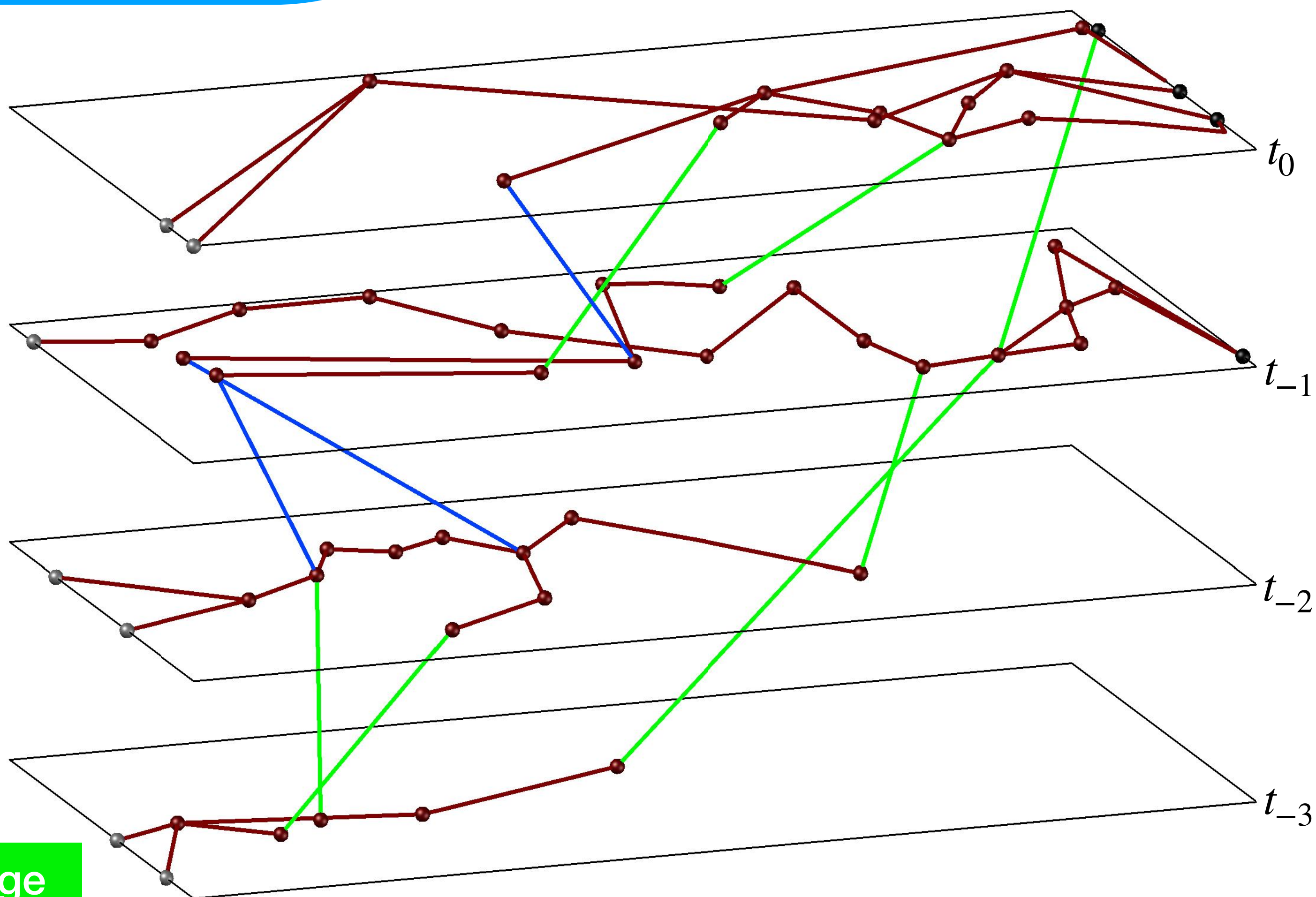


Output

ElSaid, A., Karns, J., Lyu, Z., Ororbia, A. and Desell, T., 2020. **Continuous Ant-Based Neural Topology Search.** arXiv preprint arXiv:2011.10831.

CANTS

Nodes condensation (DBSCAN)



Input

Output

Edges

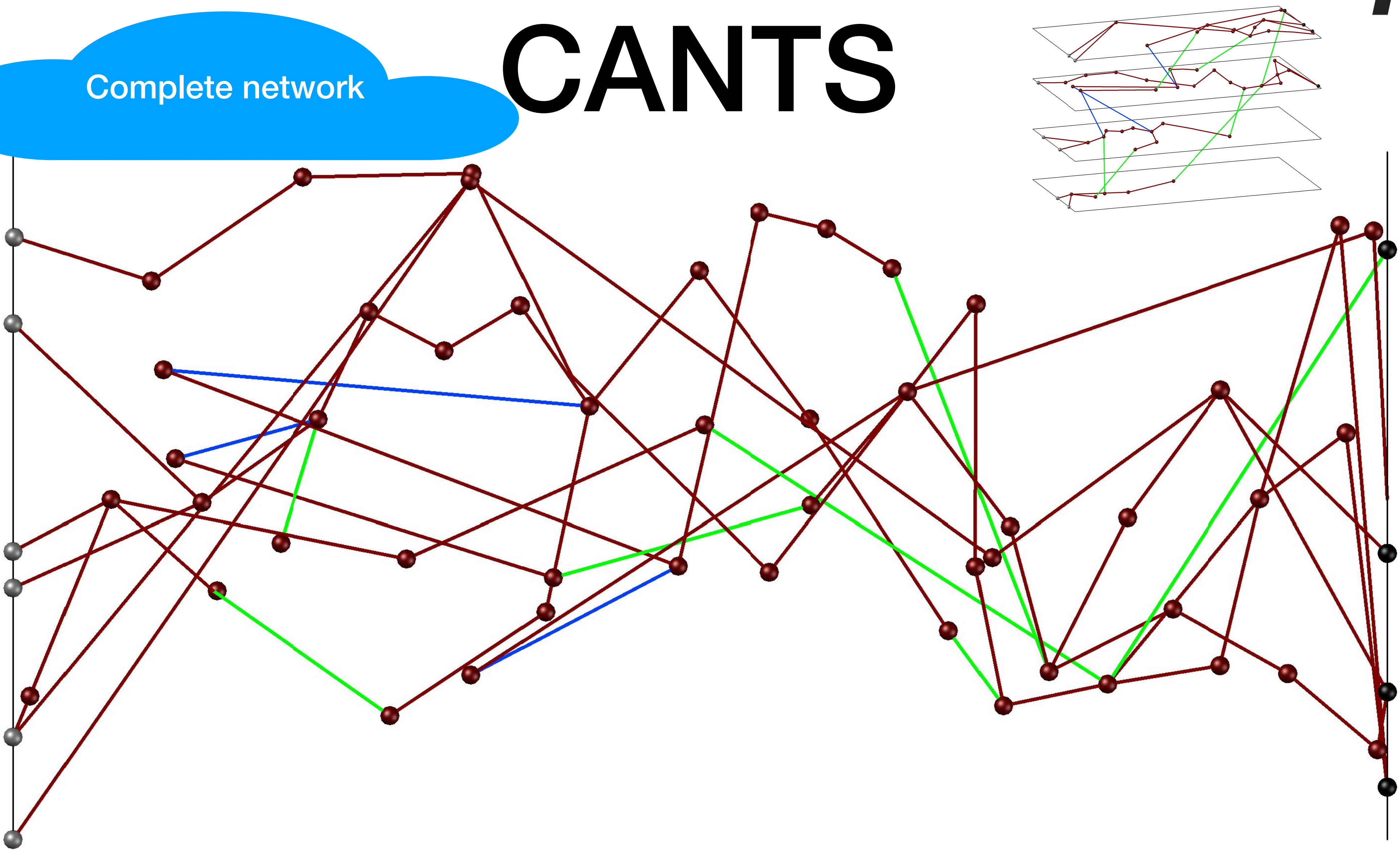
Forward Rec. Edge

Backward Rec. Edge

ElSaid, A., Karns, J., Lyu, Z., Ororbia, A. and Desell, T., 2020. **Continuous Ant-Based Neural Topology Search.** arXiv preprint arXiv:2011.10831.

CANTS

Complete network



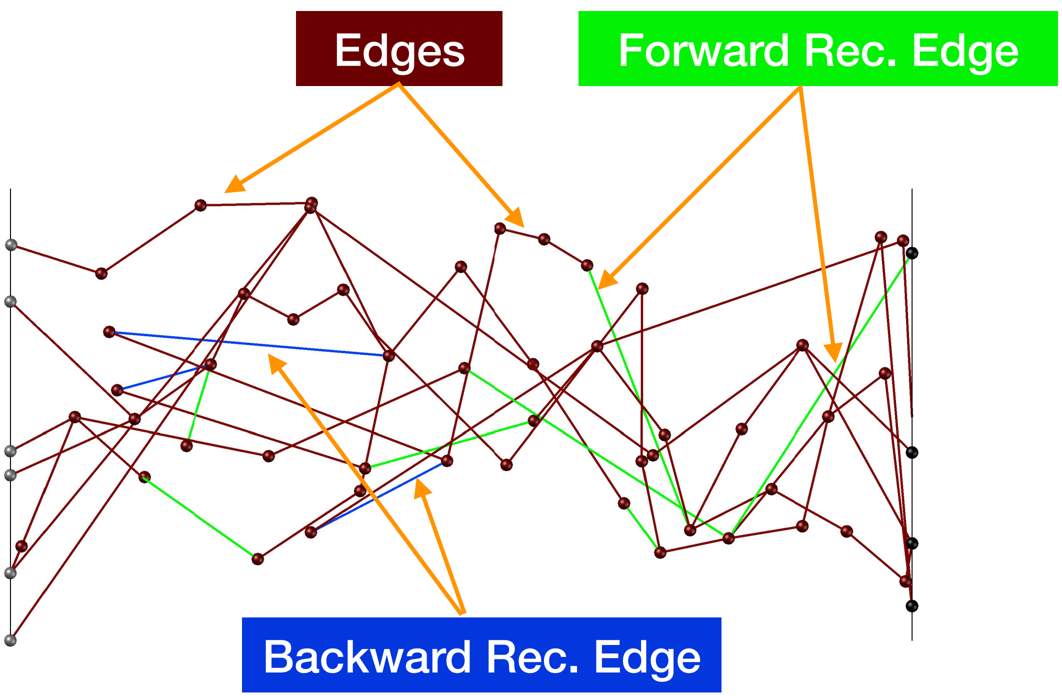
Input

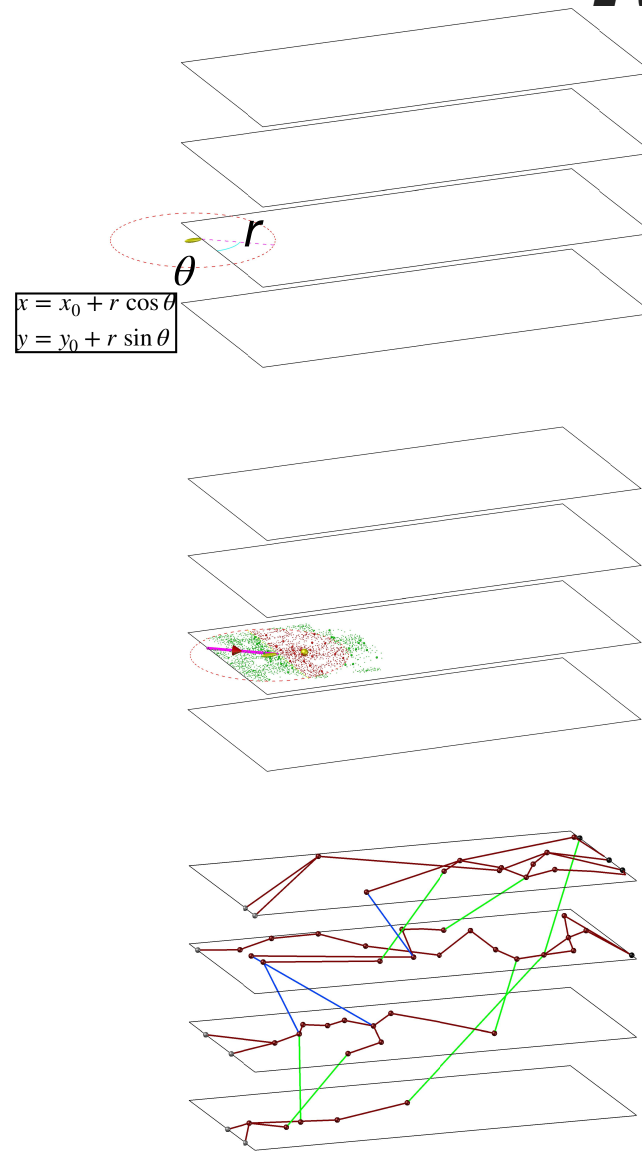
Output

ElSaid, A., Karns, J., Lyu, Z., Ororbia, A. and Desell, T., 2020. **Continuous Ant-Based Neural Topology Search.** arXiv preprint arXiv:2011.10831.

CANTS

Complete network





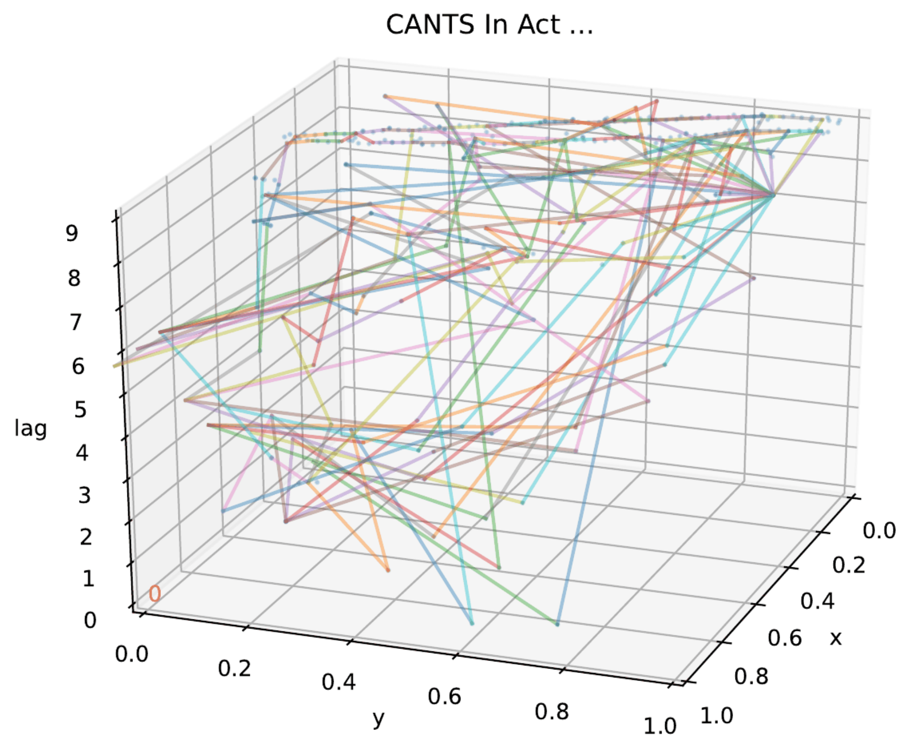
Input

Output

ElSaid, A., Karns, J., Lyu, Z., Ororbia, A. and Desell, T., 2020. **Continuous Ant-Based Neural Topology Search.** arXiv preprint arXiv:2011.10831.
*https://github.com/travisdesell/exact

CANTS

- CANTS gets rid of Superstructure ==> Continuous Search
- Unbounded search space
- Have 8 tunable hyperparameters (half of ANTS and EXAMM[1]):
  - No. Layers of Search Space
  - Number of agents
  - Agents sensing range
  - Agent's probability to create new node
  - Node condensation distance and min points (DBSCAN)
  - Pheromone updating parameter
  - Pheromone volatility parameter



"Continuous Ant-Based Neural Topology Search." Applications of Evolutionary Computation: 24th International Conference, EvoApplications 2021, Held as Part of EvoStar 2021, Virtual Event, April 7–9, 2021, Proceedings. Vol. 12694. Springer Nature, 2021.

CANTS

Experiments

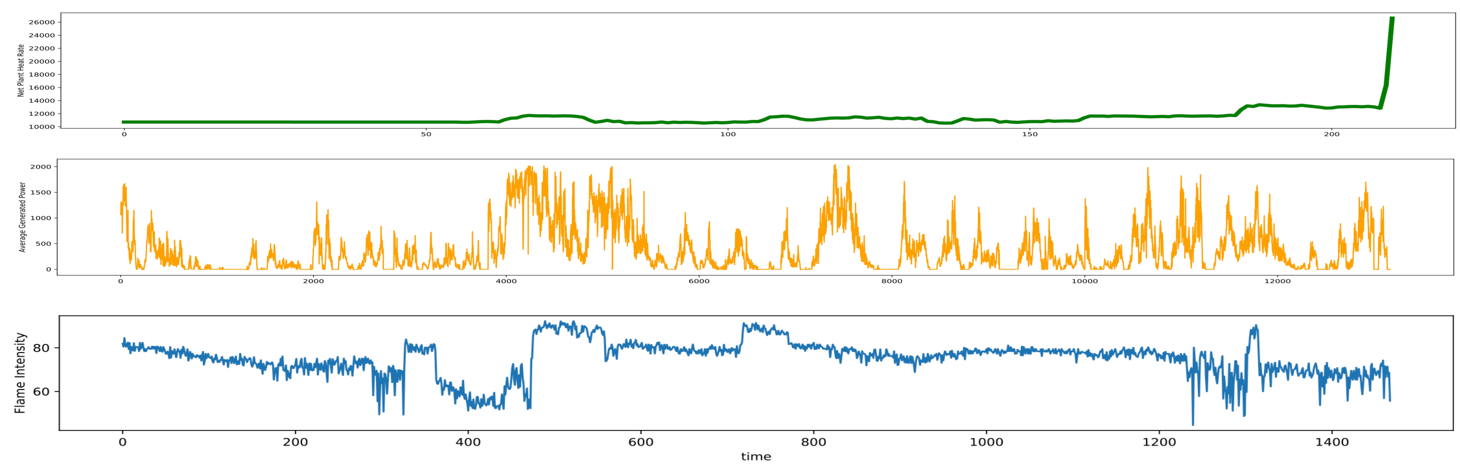
- 3 Time-series datasets:
  - Wind Power Generation (P_{avrg}),
  - coal-fired power plant Burner (Net Plant Heat Rate), and
  - coal-fired power plant Boiler (Main Flame Intensity)
- Data & CANTS source code are open source and published on GitHub*

	Flame Intensity	Net Plant Heat Rate	Average Generated Power
Number of Inputs	12	48	88
Training Records	7000	850	190,974
Testing Records	7000	211	37,514

Wind P_{avg_out}

Coal Plant $Heat\_Rate$

Coal Plant $Flame\_Intensity$



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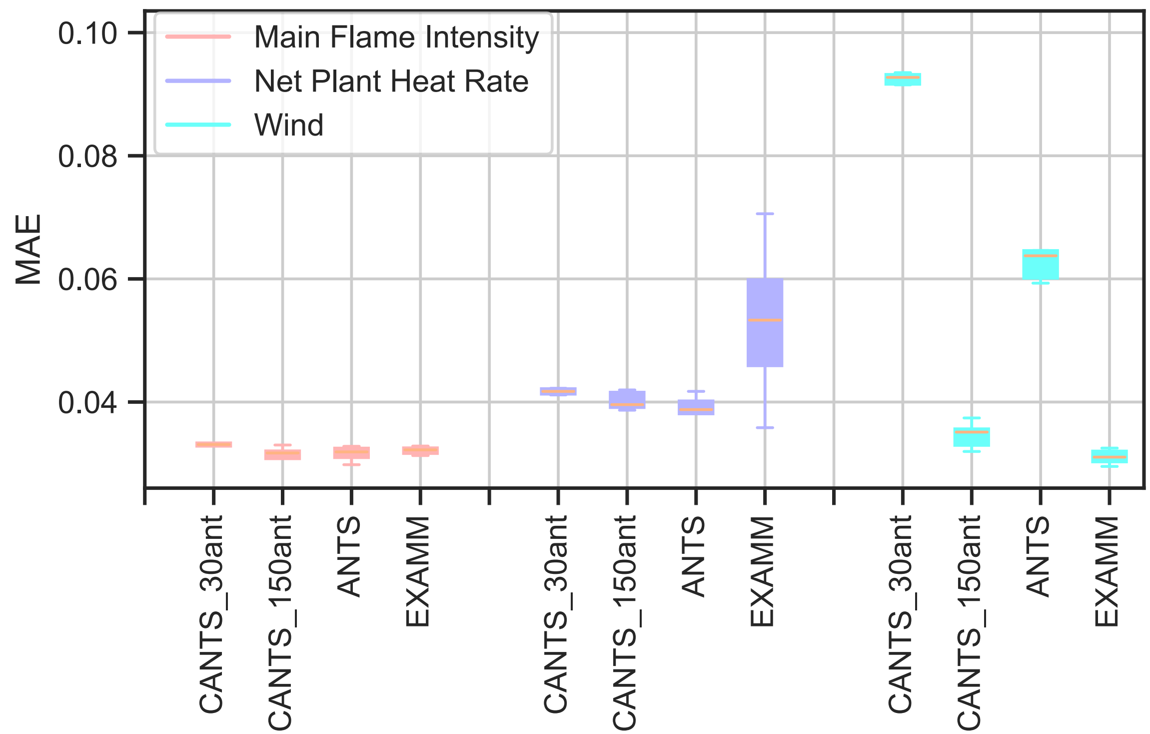
*https://github.com/travisdesell/exact

CANTS

Experiments

- Compared CANTS to:
    - ANTS best Flame Intensity heuristics
    - EXAMM
- Competed with ANTS & EXAMM on coal fired power plant parameters
- Competed with EXAMM on wind's avg. generated power
- CANTS performance more consistent



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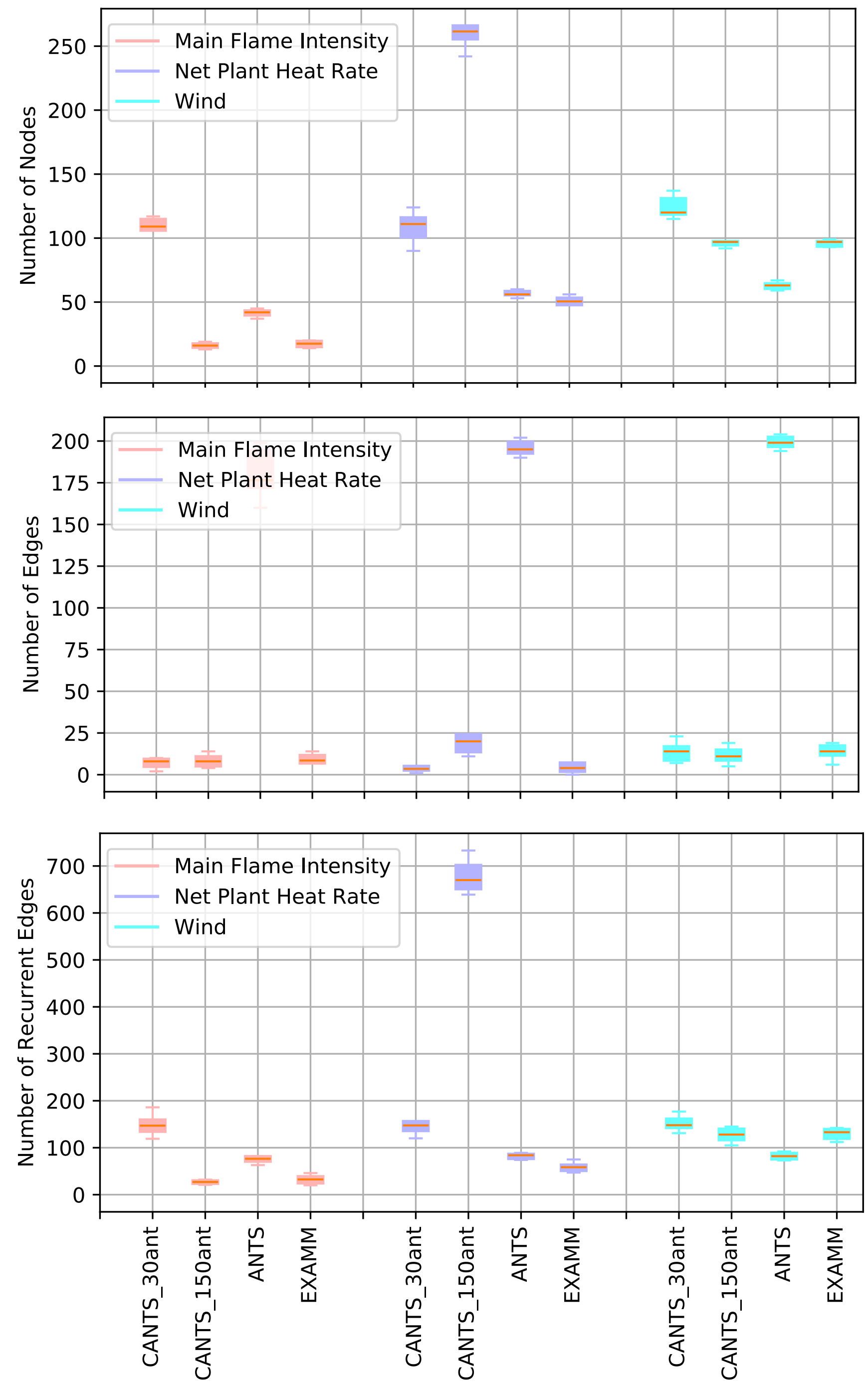
CANTS

Experiments

- CANTS’ structure were sparser than ANTS’
- CANTS’ structure sparsity competed with EXAMM’s



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*https://github.com/travisdesell/exact

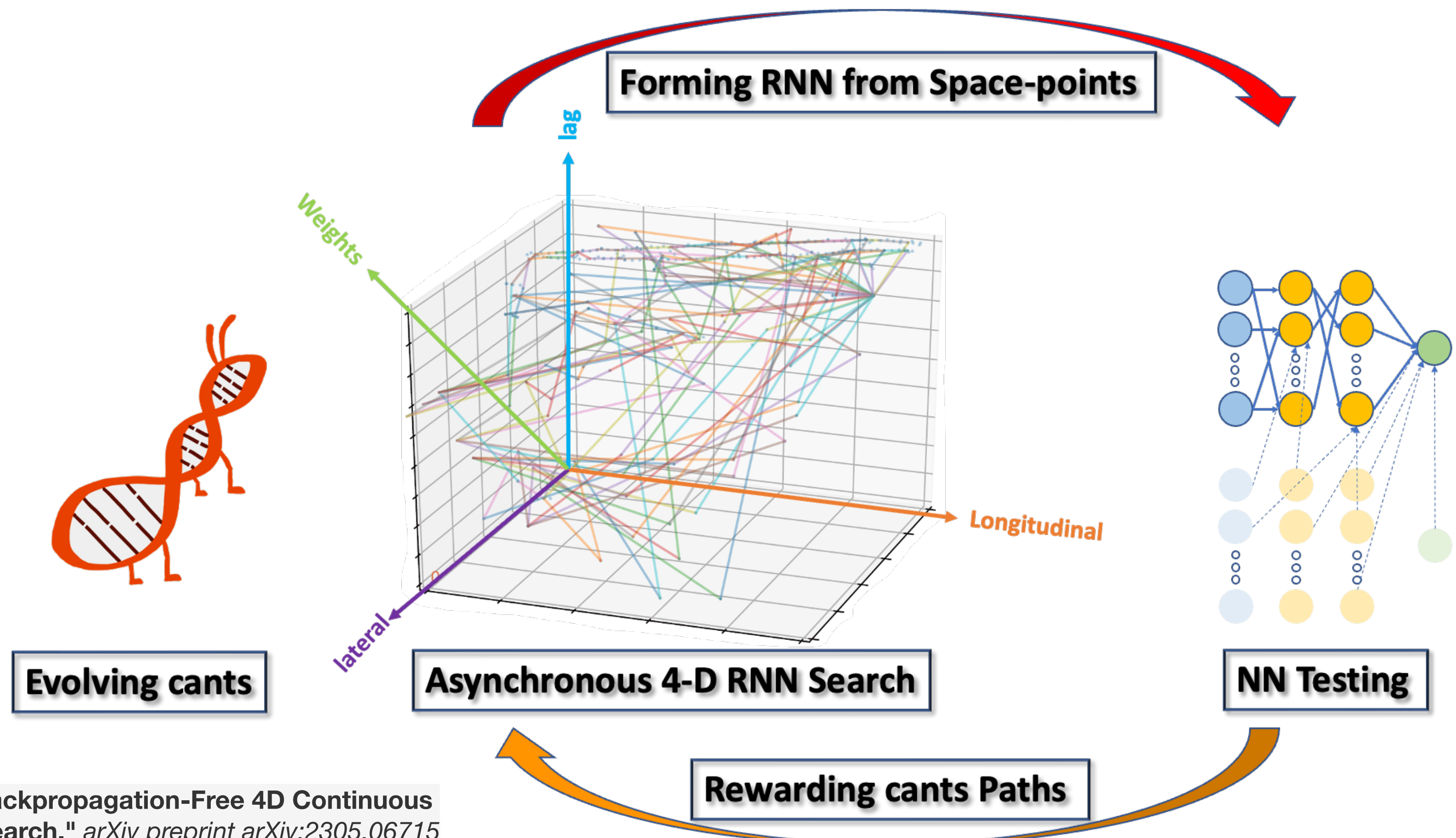
CANTS Summary

- Explores a **unbounded search space**
- Early results compete-with and outperforms ANTS
- **Hyperparameters are half** of ANTS' EXAMM's
- **Indirectly encode** the neural topology to 3D search space

AbdElRahman ElSaid, Alexander G. Ororbia and Travis Desell. **The Ant Swarm Neuro-Evolution Procedure for Optimizing Recurrent Networks**. *arXiv: Neural and Evolutionary Computing (cs.NE)*. September, 2019.
ElSaid, A., Karns, J., Lyu, Z., Ororbia, A. and Desell, T., 2020. Continuous Ant-Based Neural Topology Search. arXiv preprint arXiv:2011.10831.

CANTS for NeuroEvolution

- Adding a 4th dimension for the synaptic weights
- Turning the process from NAS to NE
- Dramatically reducing optimization time cost
- Intelligent evolving cants: learn their exploration/exploitation parameter & sensing radii => Reinforcement learning



ElSaid, AbdElRahman, et al. **"Backpropagation-Free 4D Continuous Ant-Based Neural Topology Search."** *arXiv preprint arXiv:2305.06715* (2023).

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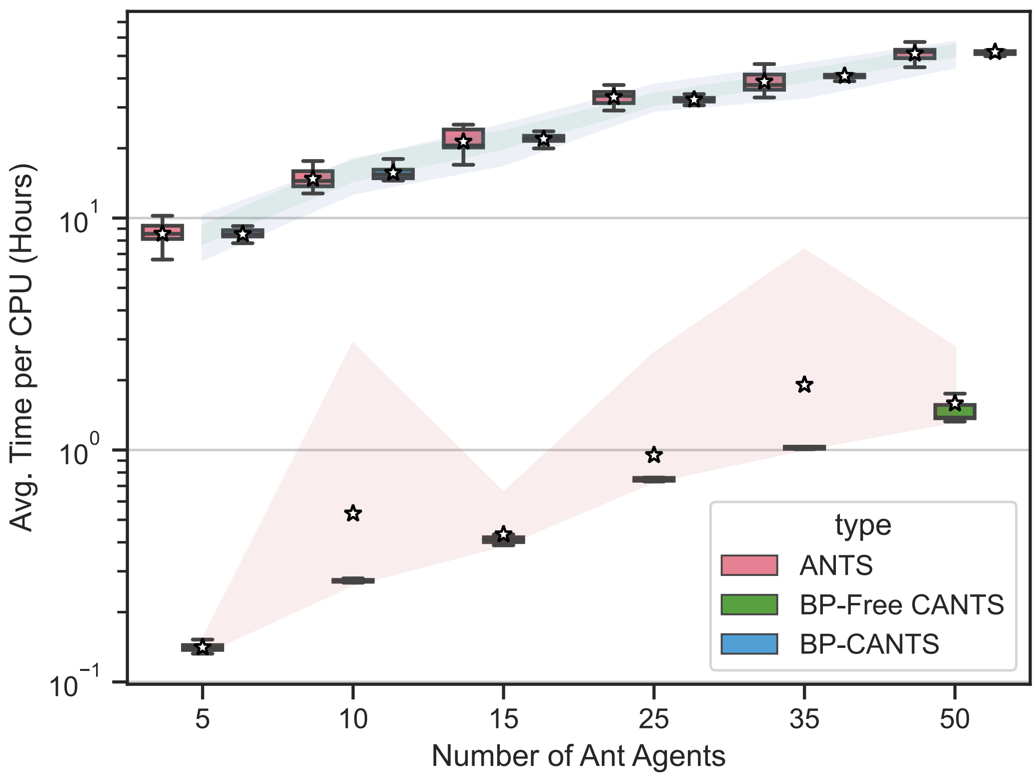

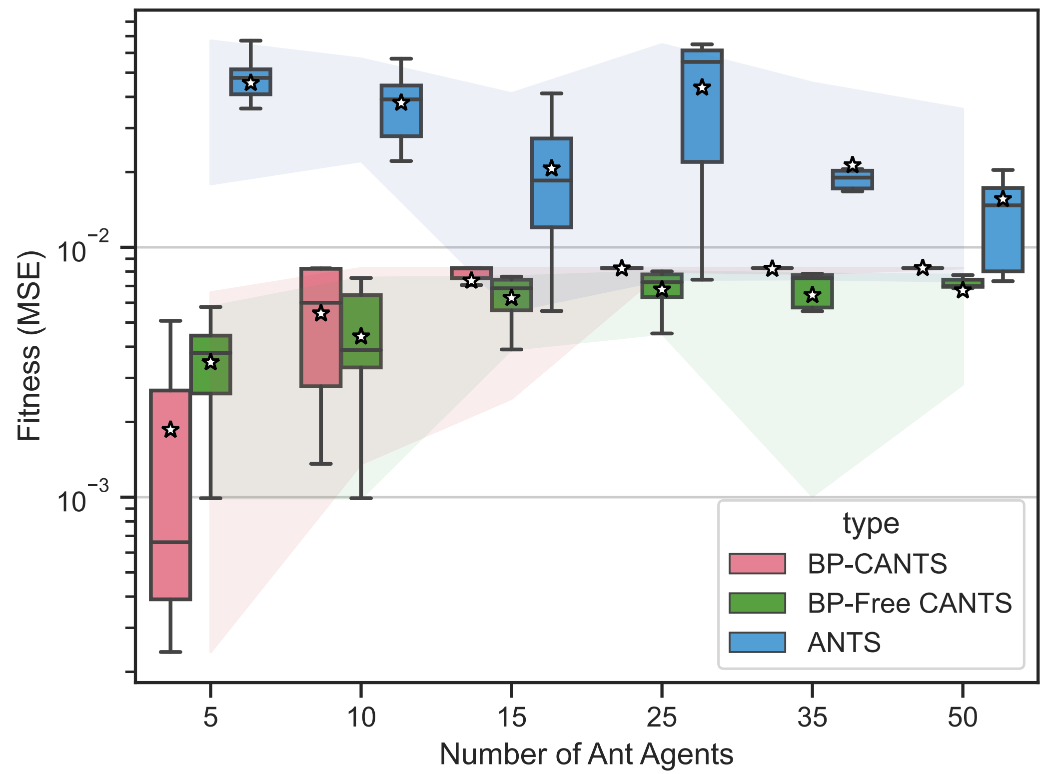

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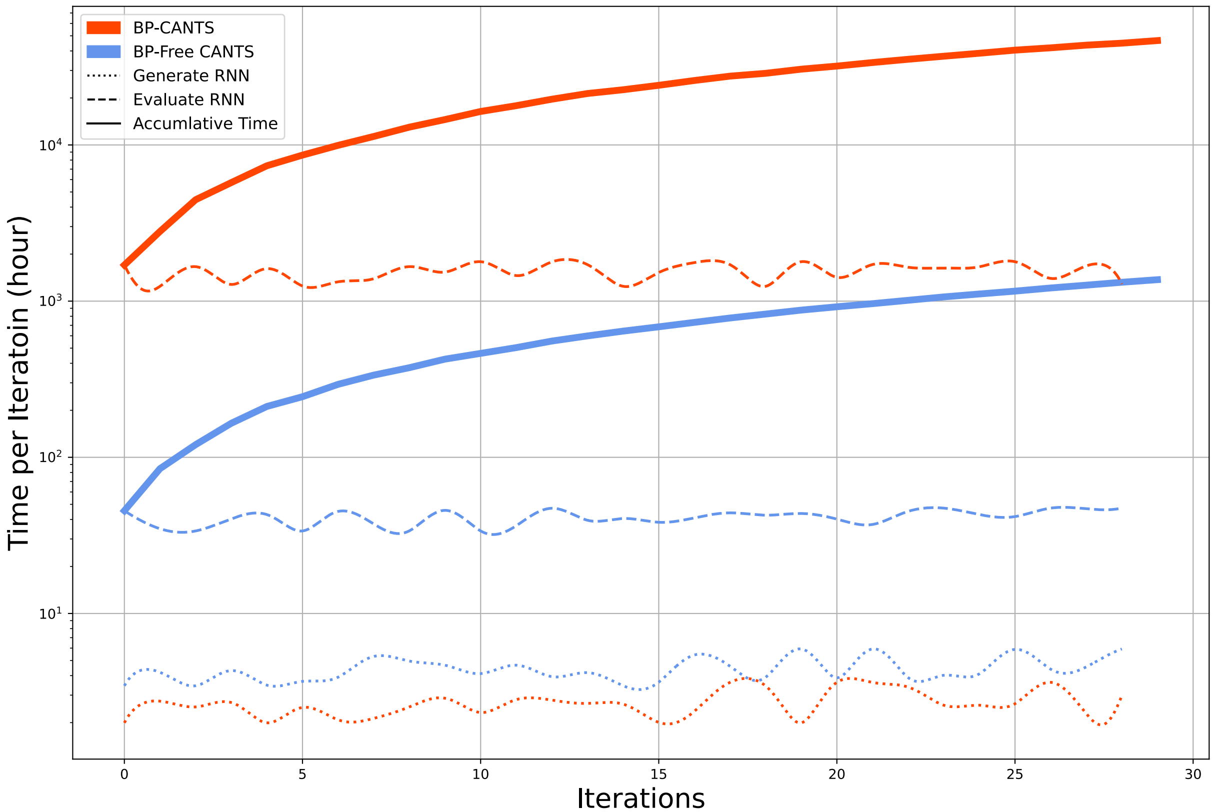

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Future Research Directions

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- Turn CANTS to complete continuous search space

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- Investigate the emergence of memory-based cells as an alternative to recurrent connections

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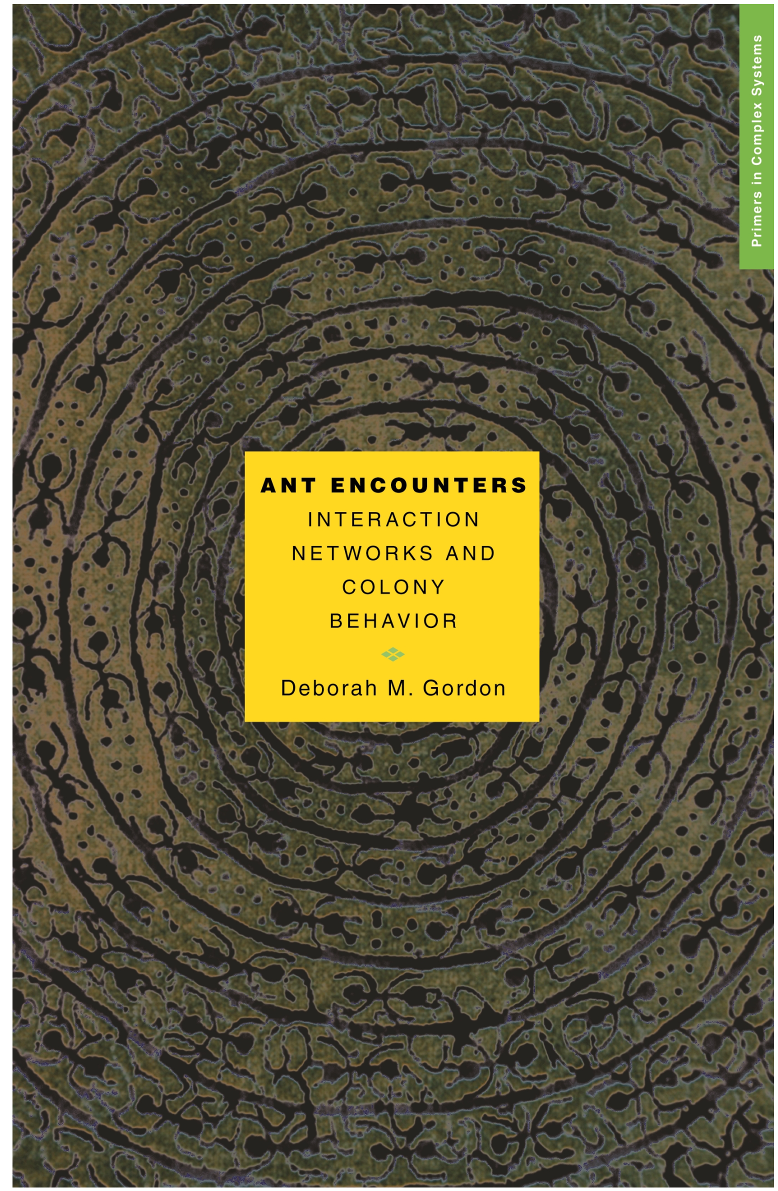
- Turn CANTS to complete continuous search space

- Investigate the emergence of memory-based cells as an alternative to recurrent connections

- Follow Myrmecology's view to colonies: colonies are the living organisms and ants are their cells => **Let Colonies Evolve Genetically**



Questions?