LABORATÓRIO DE INTELIGÊNCIA COMPUTACIONAL

DEPARTAMENTO DE CIÊNCIA DA COMPUTAÇÃO

Neural Architecture Search in Graph Neural Networks

Matheus Nunes and Gisele L. Pappa

9th Brazilian Conference on Intelligent Systems (BRACIS) - 2020

Motivation

- Graphs are ubiquitous (e.g. chemistry, social networks, movies, etc.)
- Graph Neural Networks (GNNs) are state-of-the-art techniques for ML in Graphs but their design is currently hand-made and error-prone

Motivation

- AutoML techniques such as Neural Architecture Search (NAS) have been successfully applied to CNNs for image data (e.g. CIFAR-10, ImageNet)

- However, there are very few works that explore NAS for GNNs
  - Auto-GNN (Zhou et. al., 2019)
  - GraphNAS (Gao et. al., 2020)

Motivation

- Both Auto-GNN and GraphNAS use Reinforcement Learning (RL) as an optimization technique
  - Evolutionary Algorithms (EAs) have been shown to be competitive for CNNs

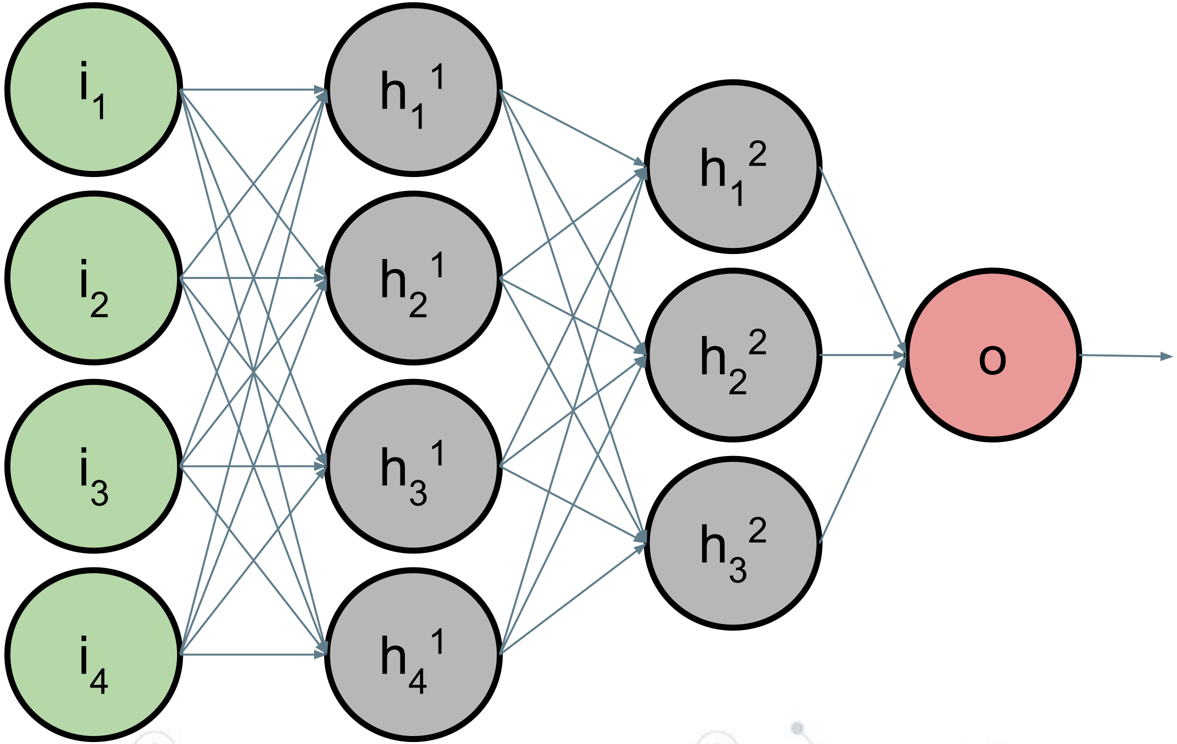
- Auto-GNN applies weight sharing to child arch. as speed up

In this work

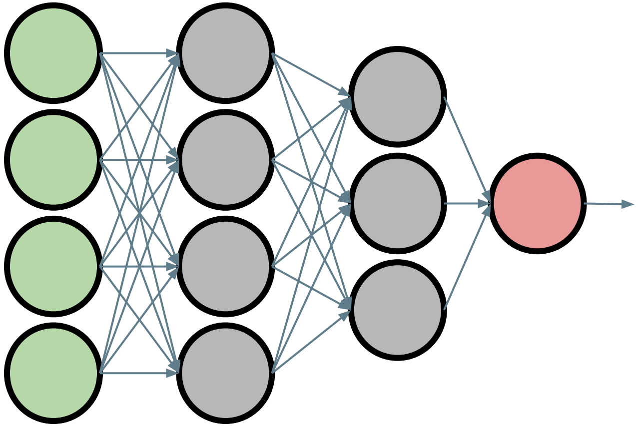
- Adapt and employ an EA previously proposed for image data on GraphNAS’ search space
  - Regularized evolution (Real et. al., 2019)

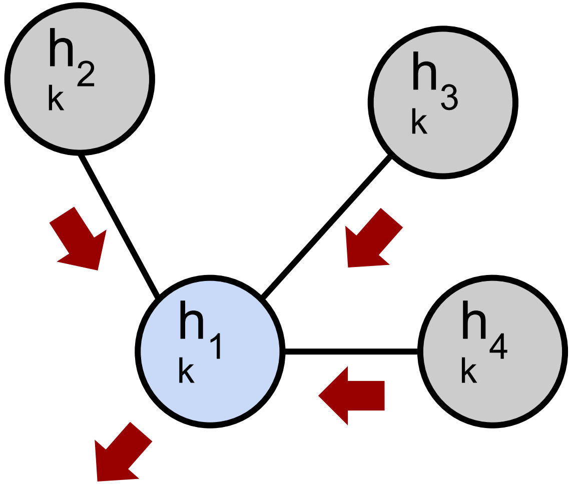
- Compare with RL and Random Search (RS) in terms of the validation accuracy of the best architecture found and overall execution runtime

Background: GNNs



Background: GNNs





$$h_i^0 = node\ features$$

$$h_1^{k+1} = act(\ cmb(\ agg(h_2^k, h_3^k, h_4^k),\ h_1^k))$$

$$out = softmax(h_i)$$

Background: NAS

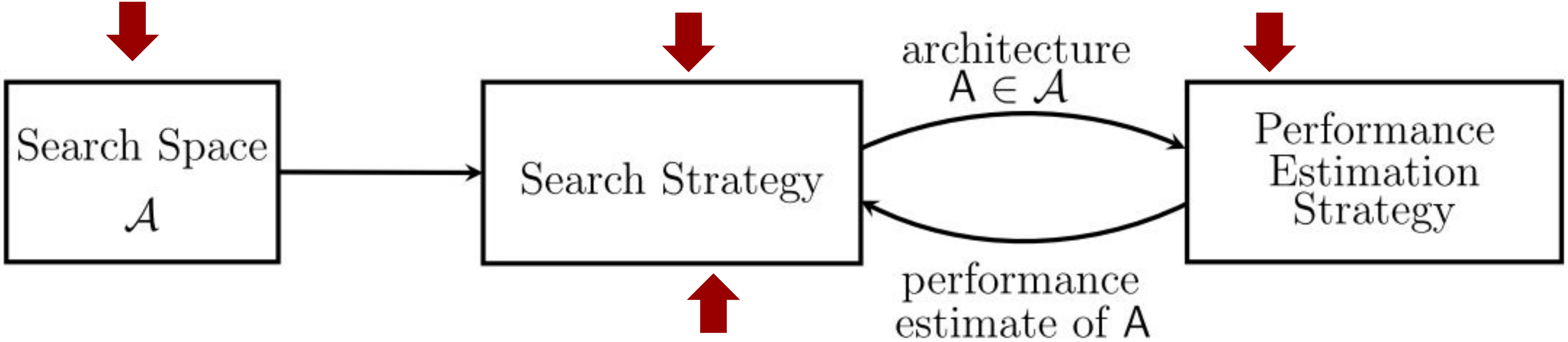


Image from: *Elsken et. al., Neural Architecture Search: A Survey. JMLR'19.*

In this work

- Evaluate the performance of 3 search methods (EA, RL, RS) over 2 search spaces from GraphNAS (Macro, Micro)
  - Spaces differ in structure and size

- Performance measure: **validation accuracy** after 300 training epochs in child arch.

Search Strategies

Reinforcement Learning (RL)

RNN controller generates child architectures

Policy gradient method with child arch. validation acc. as reward signal

Evolutionary Algorithm (EA)

Parent selected via tournament selection

Child arch. generated via mutation

Oldest individual removed from population

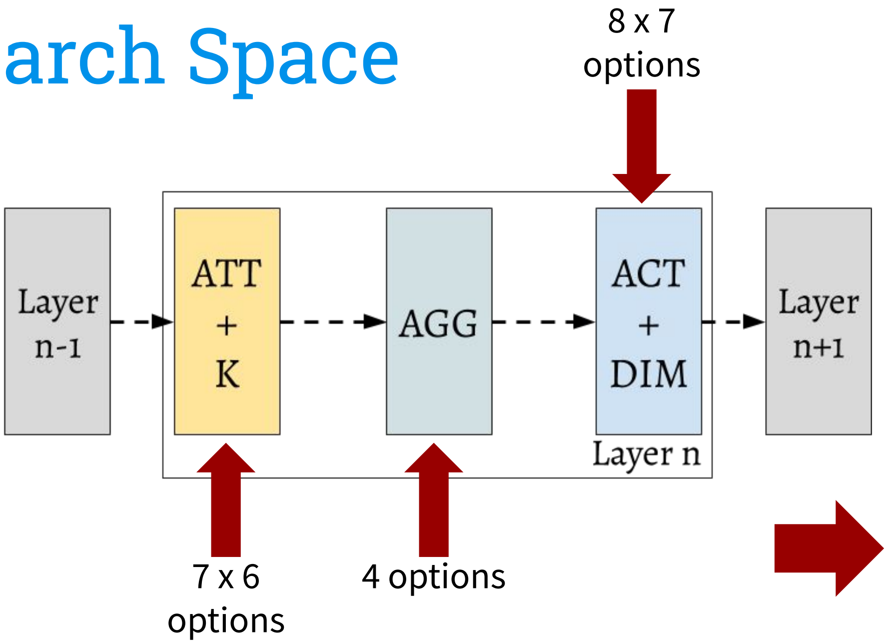
Random Search (RS)

Random architecture is generated

Trained and evaluated

Best architecture stored

Macro Search Space

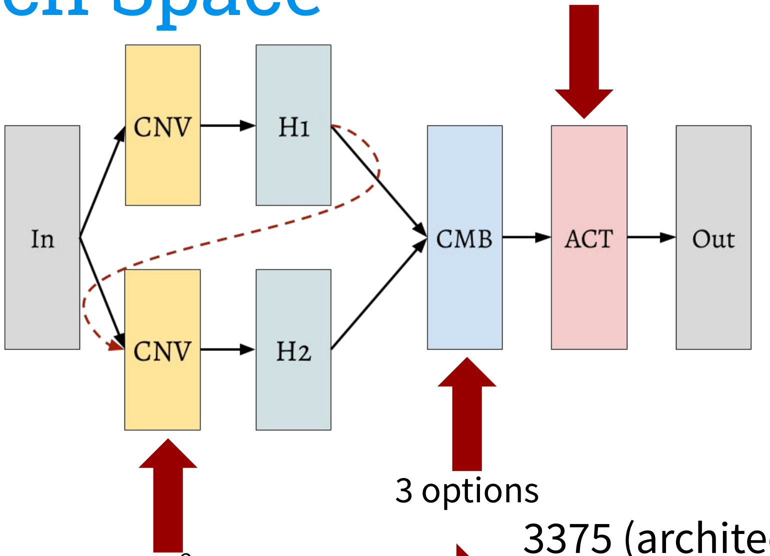


9408 possibilities in total!

Small space, **always** uses **graph attention**, **no hyperparameter tuning**

Micro Search Space

5 options



3 options

15^2 options

3375 (architectures)

x 3 x 10 x 5 x 7 options (hyperparameters)

= **3.5 x 10^6 possibilities in total**.

Larger space, **multiple** convolution operators, **hyperparameter tuning**

Experimental Analysis

- All search methods run over 7 datasets, for 1000 iterations, using 5 different random seeds
- Dataset split: 500 validation nodes, rest for training (same as GraphNAS' paper)
- Code (and additional results): https://github.com/mhnnunes/nas_gnn

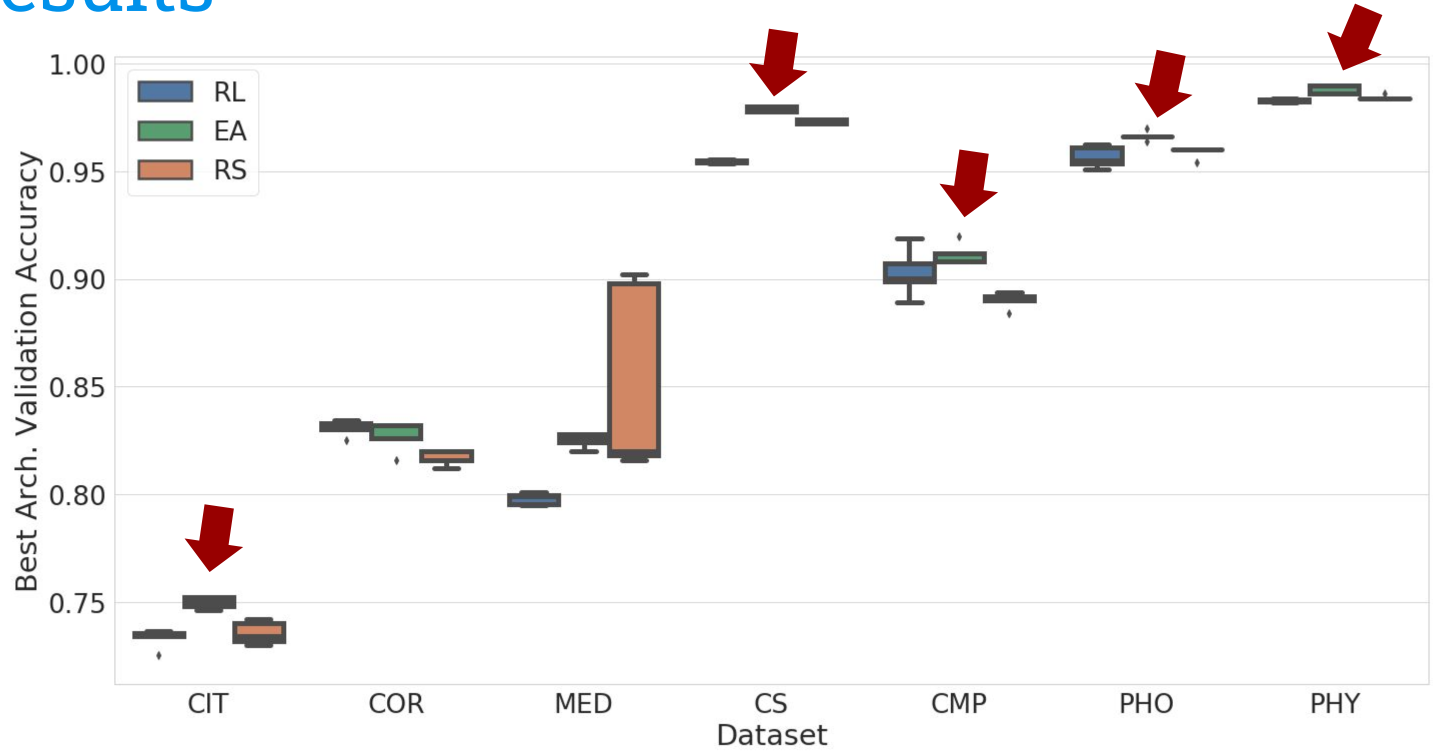
Experimental Analysis

- Search methods settings:
  - RL: one-layer LSTM, 100 HU, ADAM opt., LR 3.5×10^{-4}
  - EA: Pop. size = 100, tournament size = 3 (best)

- Evaluate search methods in terms of best found child architecture **validation accuracy** and overall **runtime**

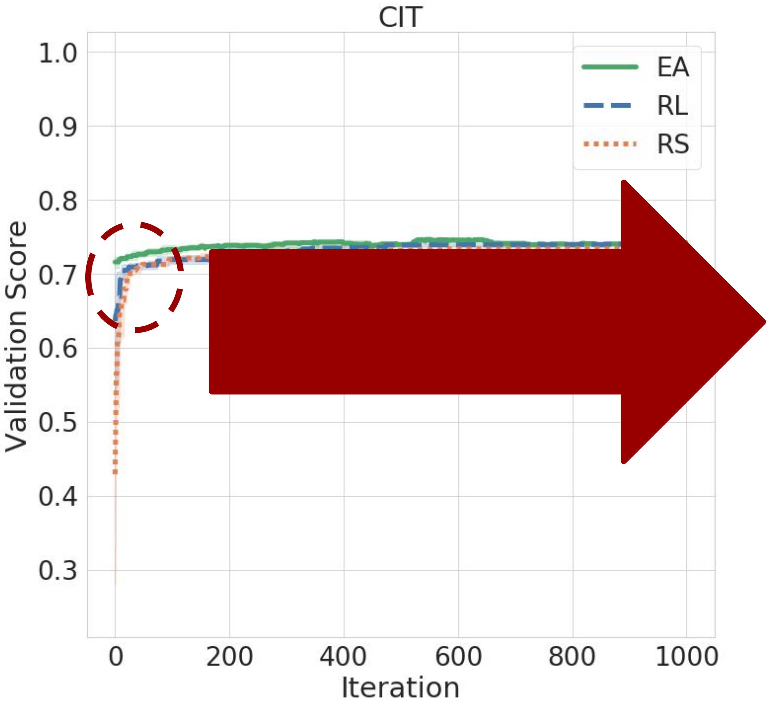
Results

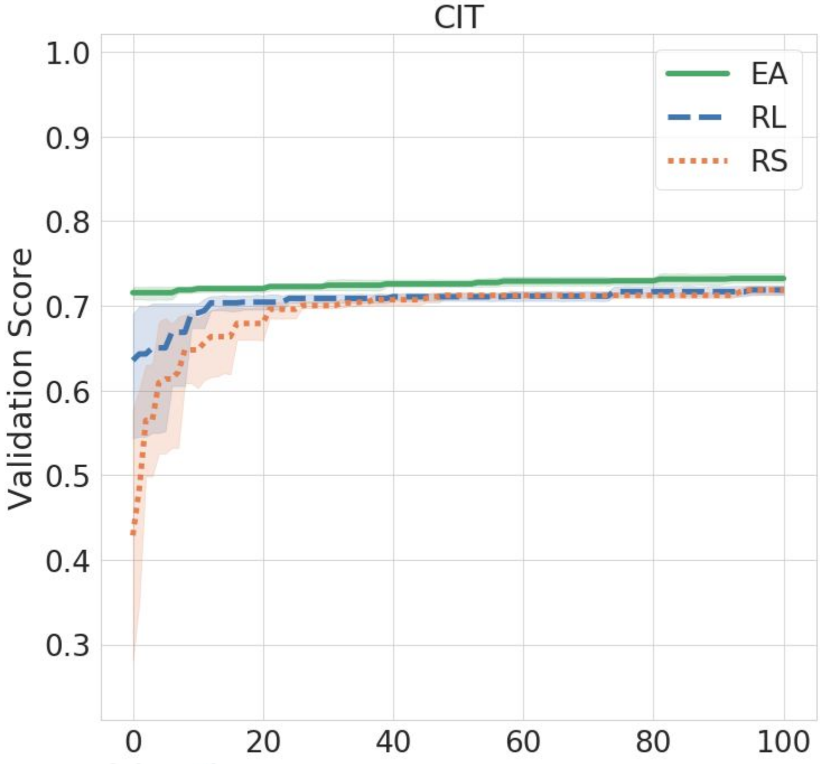
Despite not being statistically significant, EA wins in 5 of 7!



Results

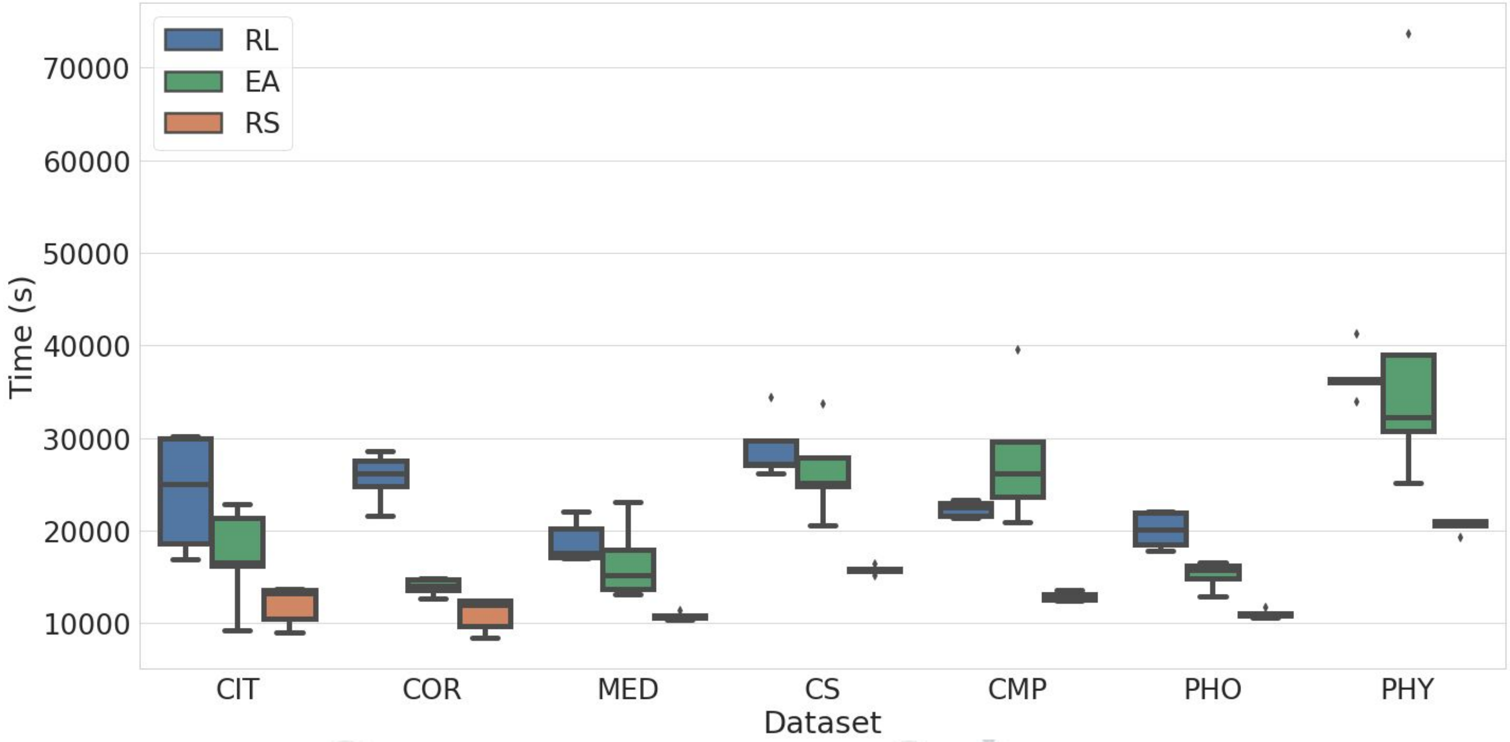
All methods converge
early in the search!
< 100 iterations



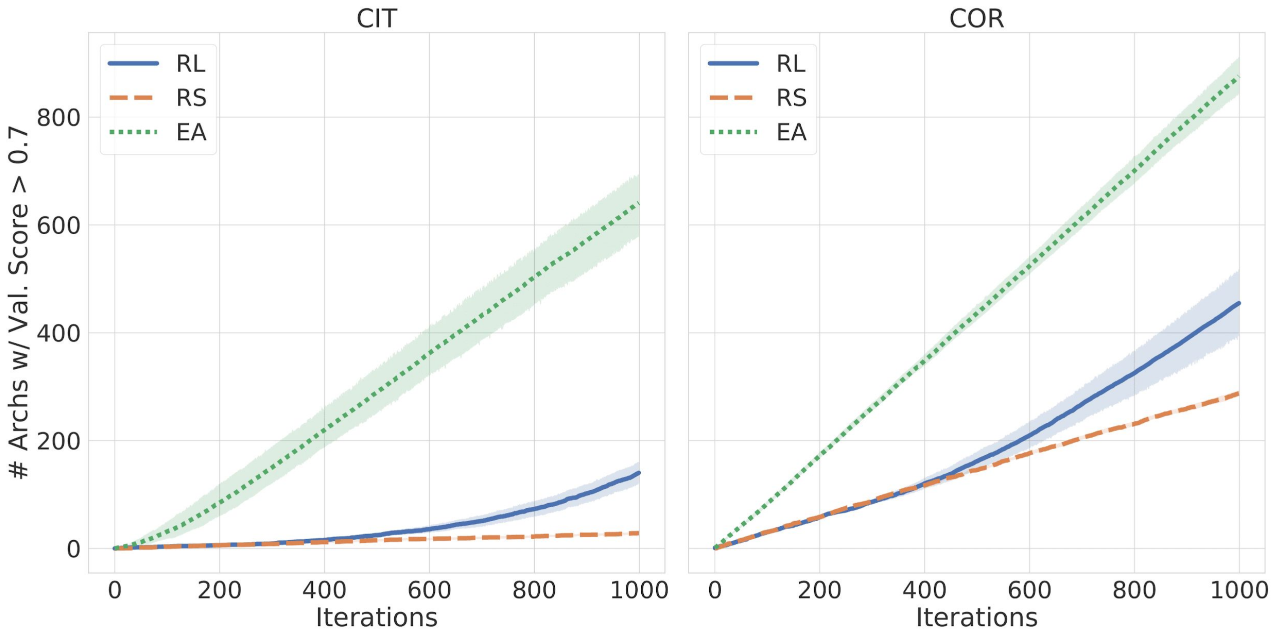


Results

RS is faster in most cases, with EA in second place!



Results



EA consistently generates and evaluates high accuracy architectures!

Conclusions

- All three optimization methods **converge fast** and find **similarly good performing architectures**:
  - Neutrality?

- **EA** tends to generate better performing arch. than the other methods, and **RS** tends to be **fastest**

LAIC
LABORATÓRIO DE INTELIGÊNCIA COMPUTACIONAL

DCC
DEPARTAMENTO DE CIÊNCIA DA COMPUTAÇÃO

UFMG

Neural Architecture Search in Graph Neural Networks

Matheus Nunes and Gisele L. Pappa

{mhnnunes, glpappa}@dcc.ufmg.br

9th Brazilian Conference on Intelligent Systems (BRACIS) - 2020

Presentation template by: [SlidesCarnival]