Bayesian Generational Population-Based Training

Xingchen Wan, Cong Lu, Jack Parker-Holder, Philip J. Ball, Vu Nguyen, Binxin Ru and Michael A. Osborne

Presented by
Ridwan Muheeb
rm2084

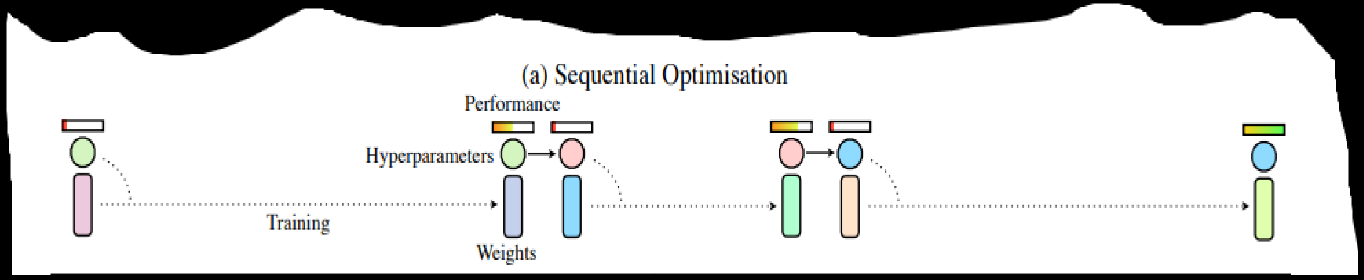
Historical Context

- It has been proven that success of a neural network depends upon the joint tuning of the model structure, its data and the details of how the model is optimized.
- Each of these components of a learning framework is controlled by a number of parameters i.e. hyperparameters (HP) which influence the learning process and must be properly tuned to fully unlock the network performance.
- There are two approaches for doing this:
- Parallel Search
- Sequential Search

Historical Context

1. **Sequential Search**:

- Run few optimizations in parallel but many times sequentially with outputs of previous epochs guiding later epochs in order to find the best case.
- E.g. hand tuning or Bayesian optimization.
- Works best but time consuming due long optimization processes.



Source: Jaderberg, et al, 2017

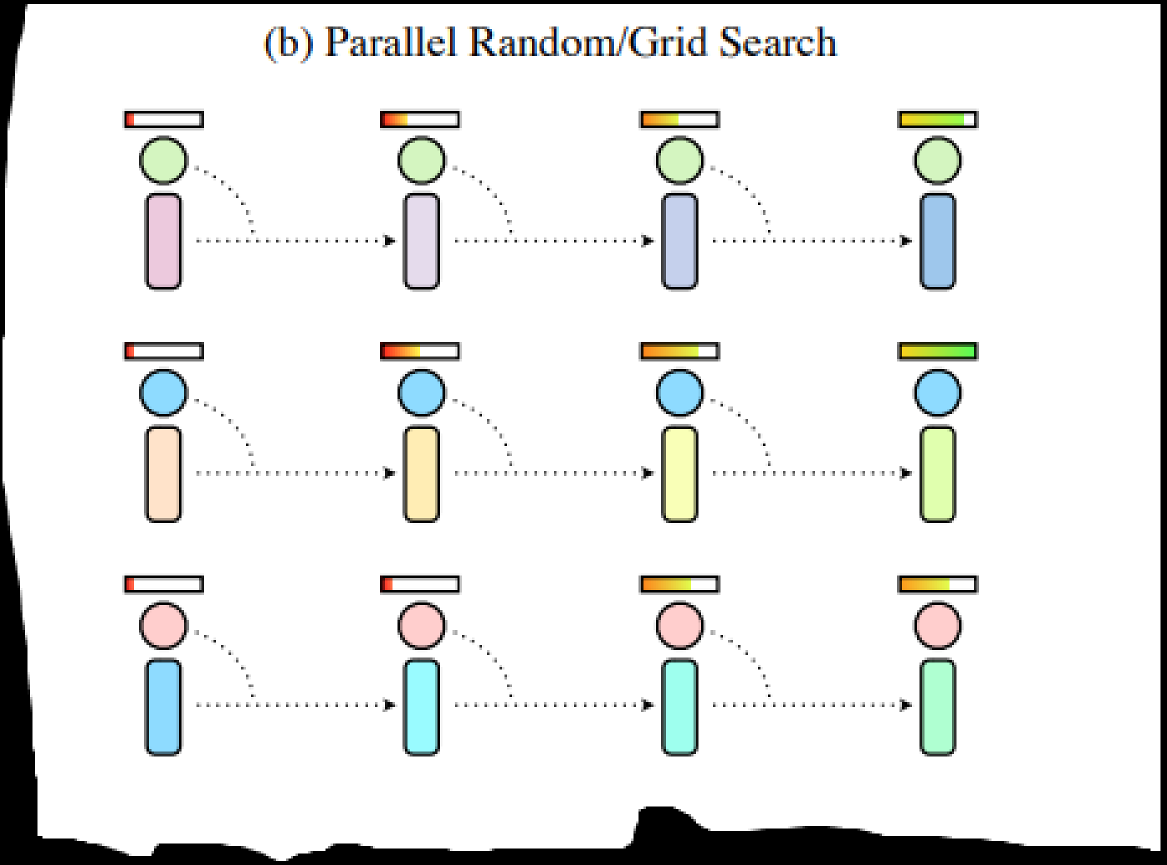
Start a simple rate and decrease by a fixed factor in each epoch e.g. start 0.005 decrease by factor of 10 for each 100 epochs

0.005 → 0.0005 → 0.00005 → 0.000005

Historical Context

2. Parallel Search:

- Run multiple optimizations in parallel in bid to find one best output.
- E.g. grid or random search.
- Time and computationally expensive.

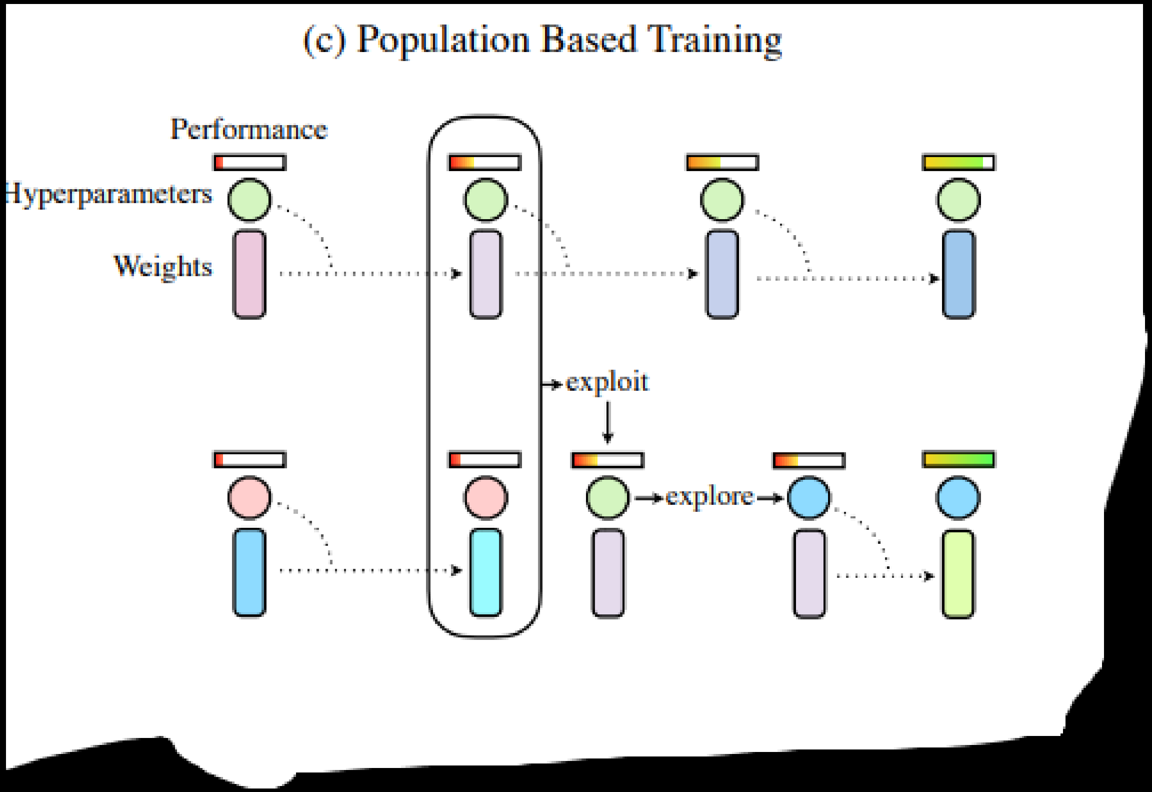


Source: Jaderberg, et al, 2017

Population Based Training Paradigm

3. Population Based Training:

- parallel + sequential optimization methods.
- Start like parallel search, randomly sampling HP and weight initializations.
- Underperforming population model replaces self with a better performing model and explore new HPs by modifying the better model's HPs before training is continued.
- Allow it to focus on weight space that has best potential to produce good results.
- Proven to be effective in Generative Adversarial Networks (GANs) and Machine Learning Translation



Source: Jaderberg, et al, 2017

Motivation

- Fragility of reinforcement learning to key hyperparameters and choice of network architecture.
- Expensive RL parameters tuning.
- Possibility of obtaining algorithmic optimality at different training points due to changing data distribution
- Evolving training and data and increased agent complexity.
- Existing Population Based Training styles are not scalable to higher dimensional data.
- **Solution -> Bayesian Generational Population Based Training**

Key Ideas

- Capable of tweaking a large proportion of agents configurations.
- On-the-fly and automatic finetuning of HPs and architectures during training epochs.
- Achieve these using two techniques:
  - Model based HPs architecture exploration steps built on local Bayesian optimization
  - Generational learning which combines PBT and network distillation.
- Experimented for Proximal Policy Optimization (PPO) on *Brax*, a less computing intensive differentiable physics engine simulation environments.

Key Ideas – Algorithmic representation

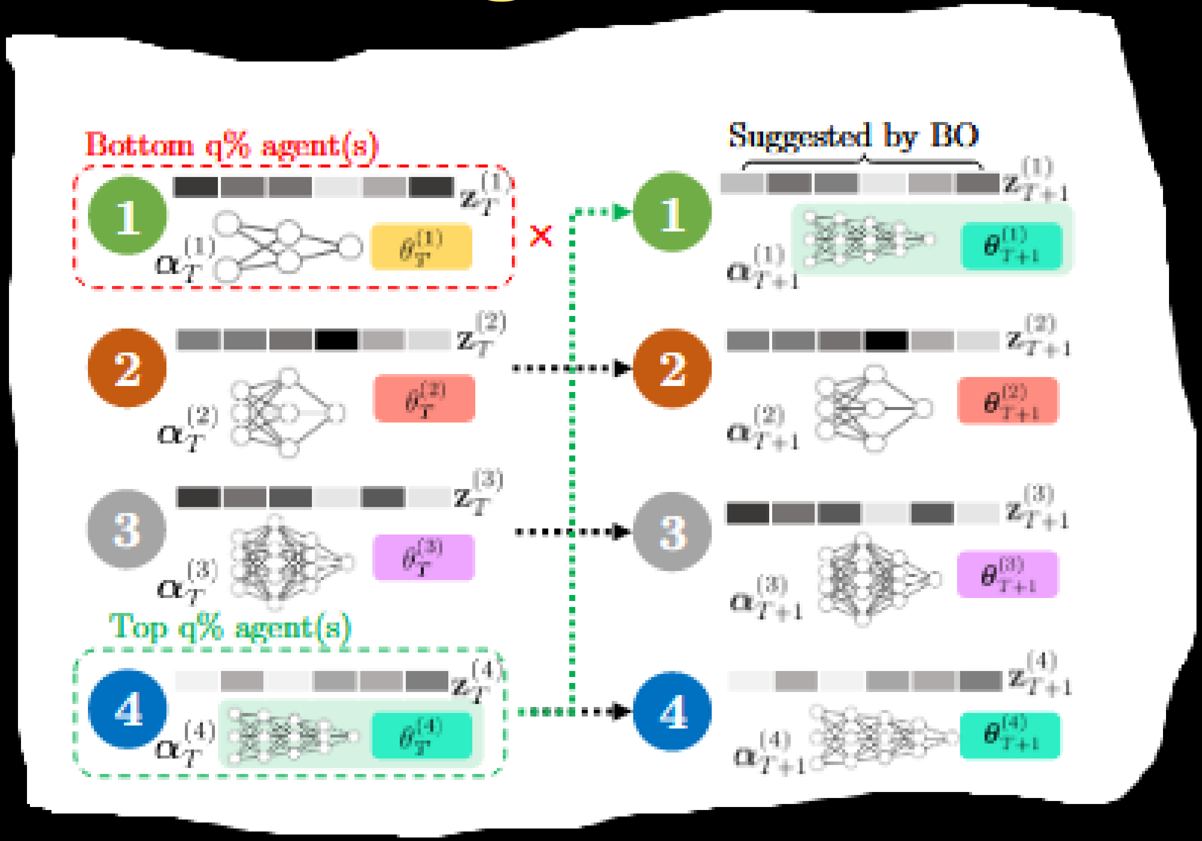
Algorithm 1 BG-PBT; distillation and NAS steps marked in magenta (§3.2)

```
Input: pop size B, t_ready, max steps T, q (% agents replaced per iteration)
Initialize B agents with weights {θ_0^(i)}_{i=1}^B, random hyperparameters {z_0^(i)}_{i=1}^B and architectures {y_0^(i)}_{i=1}^B,
for t = 1, . . . , T (in parallel for all B agents) do
    Train models & record data for all agents
    if t mod t_ready = 0 then
        Replace the weights & architectures of the bottom q% agents with those of the top q% agents.
        Update the surrogate with new observations & returns and adjust/restart the trust regions.
        Check whether to start a new generation (see §3.2).
        if start a new generation then
            Clear the GP training data.
            Create B agents with archs. from BO/random.
            Distill from a top-q% performing agent of the existing generation to new agents.
        else
            Select new hyperparameters z for the agents whose weights have been just replaced with randomly sampled configs (if D = ∅) OR using the suggestions from the BO agent described conditioned on y (otherwise).
```

- **Consists of three parts.**
- Use a Bayesian optimization approach to select new HP configurations z for agents.
- Extend the search space to accommodate architecture search to allowing agents to choose their own networks.
- Use on-policy distillation to transfer between different architectures.

Source: Wan, et al (2021)

Key Ideas
Within a generation

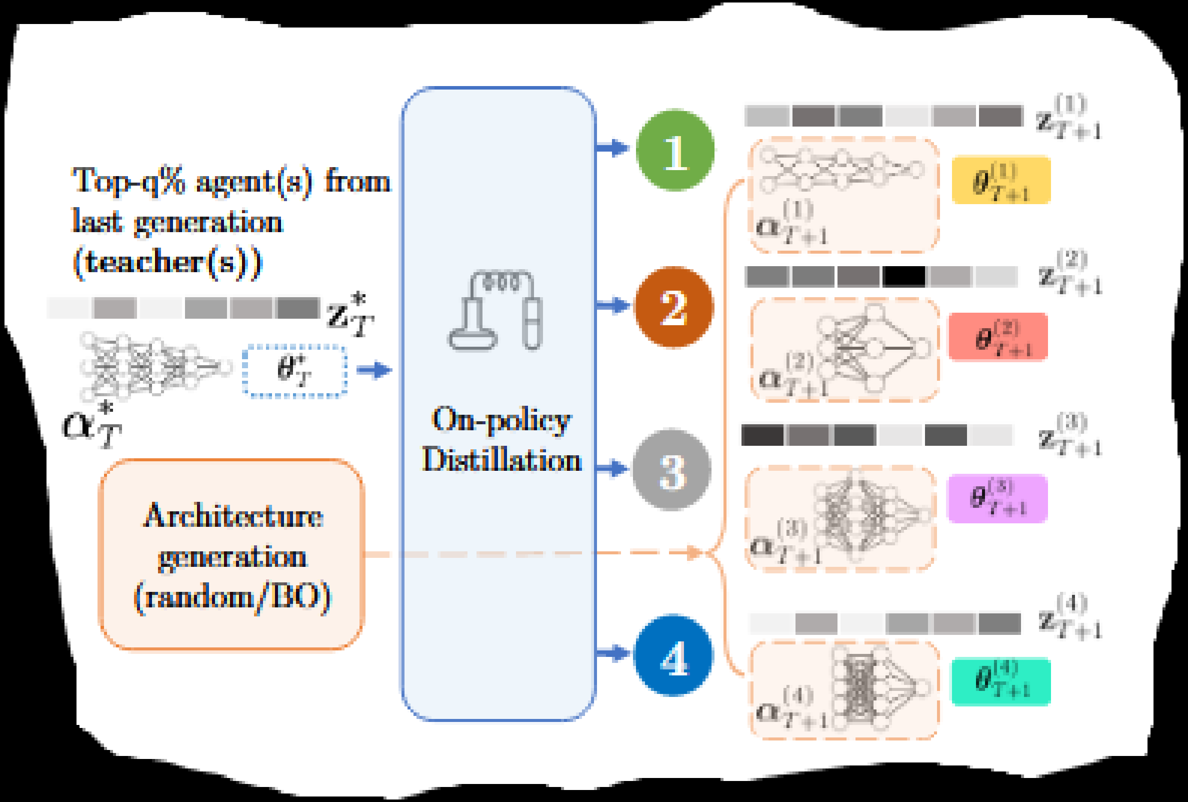


Source: Wan, et al (2021)

- Consist of three stages.
- **Initialization:** Random HP and weights of different architectures are used for training.
- **Exploitation:** Underperforming agents copies weight and architectures of the best-performing agent.
- **Exploration:** HPs suggestions by time-varying, high-dimensional BO agent.

Key Ideas

Across generations

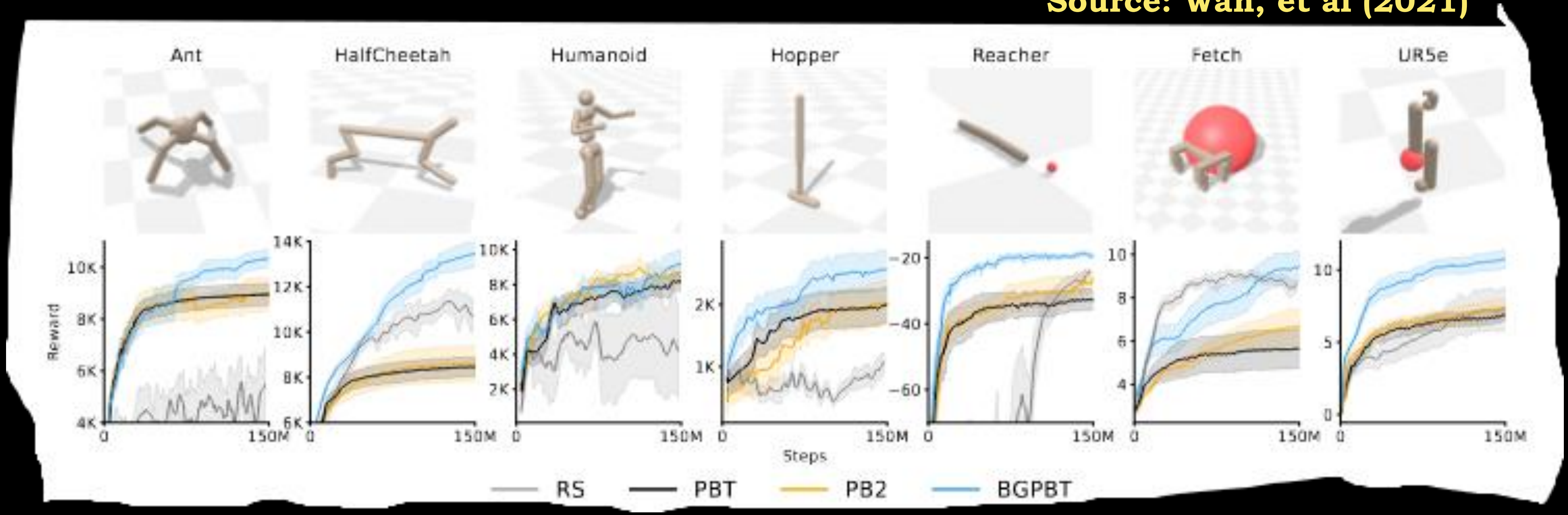


Source: Wan, et al (2021)

- Consist of two stages.
- **Initialization:** Generate 1 random architecture.
- Subsequent generations: BO agent performance of the previously generated is used to suggest new architectures.
- **Transfer Knowledge: (On-policy distillation):** Best agents from previous generation guides subsequent ones.

Performance – Comparative Evaluation

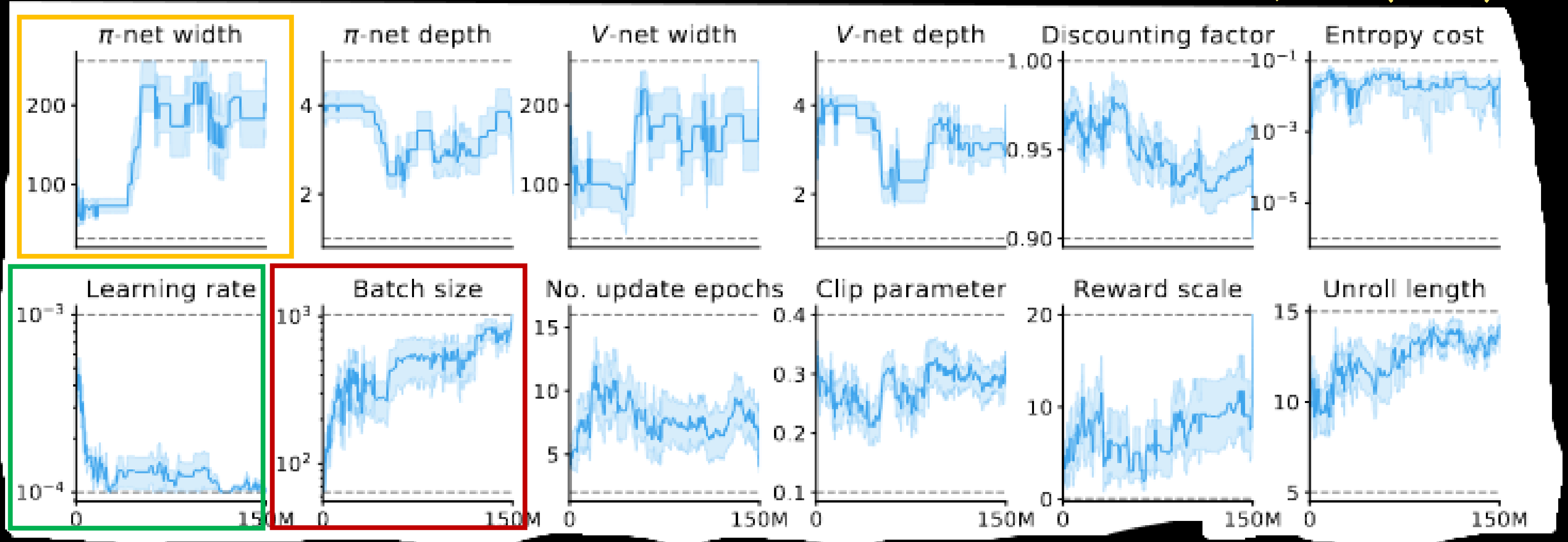
Source: Wan, et al (2021)



- Experiments conducted on 7 Brax environments.
- Outperforms Random Search, Population Based Training (Jaderberg et al, 2017), PB2 (Parker-Holder et al, 2020) in all the 7 environments

Performance on Discovered Hyperparameter and Architecture Schedules

Source: Wan, et al (2021)



- Increasing HP size over time during training to model complex behaviors.
- Start with few hyperparameter sizes and increase accordingly to model complex behaviors
- BG-PBT achieved declining learning rate and batch size increment over time without any pre-defined schedule.
- Result consistent with common practices in deep and reinforcement learning.

Pros

- On-the-fly hyperparameters finetuning to achieve optimal results with less computing resources.
- Results consistent with trends in deep and reinforcement learning domain (declining learning rate and increasing batch size).
- Outperforms existing architectures of PBT based solutions in the simulation environments.

Limitations

- Although the researchers was able to automate Reinforcement Learning hyperparameters using BG-PBT, they recognized need to automate PBT parameters themselves e.g. no. of iterations/epochs needed to achieve optimal result.
- Environmental complexity, network architecture sensitivity and poor selection of architectures can affect the system performance.

Suggestion for Future Research

- Applicability of BG-PBT to other domains outside of reinforcement learning such as GANs, Machine Learning Translation/NLP.

Bibliography

- Jaderberg, Max, et al. "Population based training of neural networks." *arXiv preprint arXiv:1711.09846* (2017).
- Wan, Xingchen, et al. "Bayesian Generational Population-Based Training." *First Conference on Automated Machine Learning (Main Track)*. 2022.