Bayesian Generational Population-Based Training

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Abstract Reinforcement learning (RL) offers the potential for training generally capable agents that can interact autonomously in the real world. However, one key limitation is the brittleness of RL algorithms to core hyperparameters and network architecture choice. Furthermore, non-stationarities such as evolving training data and increased agent complexity mean that different hyperparameters and architectures may be optimal at different points of training. This motivates AutoRL, a class of methods seeking to automate these design choices. One prominent class of AutoRL methods is Population-Based Training (PBT), which have led to impressive performance in several large scale settings. In this paper, we introduce two new innovations in PBT-style methods. First, we employ trust-region based Bayesian Optimization, enabling full coverage of the high-dimensional mixed hyperparameter search space. Second, we show that using a *generational* approach, we can also learn both architectures and hyperparameters jointly on-the-fly in a single training run. Leveraging the new highly parallelizable Brax physics engine, we show that these innovations lead to large performance gains, significantly outperforming the tuned baseline while learning entire configurations on the fly.

1 Introduction

Reinforcement Learning (RL) (Sutton and Barto, 2018) has proven to be a successful paradigm for training agents across a variety of domains and tasks (Kalashnikov et al., 2018; Mnih et al., 2013; Nguyen et al., 2021b; Silver et al., 2017), with some believing it could be enough for training generally capable agents (Silver et al., 2021). However, a crucial factor limiting the wider applicability of RL to new problems is the notorious sensitivity of algorithms with respect to their hyperparameters (Andrychowicz et al., 2021; Engstrom et al., 2020; Henderson et al., 2018), which often require expensive tuning. Indeed, it has been shown that when tuned effectively, good configurations often lead to dramatically improved performance in large scale settings (Chen et al., 2018).

To address these challenges, recent work in *Automated Reinforcement Learning* (AutoRL) (Parker-Holder et al., 2022) has shown that rigorously searching these parameter spaces can lead to previously unseen levels of performance, even capable of breaking widely used simulators (Zhang et al., 2021). However, AutoRL contains unique challenges, as different tasks even in the same suite are often best solved with different network architectures and hyperparameters (Furuta et al., 2021; Xu et al., 2022). Furthermore, due to the non-stationarities present in RL (Igl et al., 2021), such as changing data distributions and the requirement for agents to model increasingly complex behaviors over time, optimal hyperparameters and architectures may not remain constant. To address this, works have shown adapting hyperparameters through time (Jaderberg et al., 2017; Parker-Holder et al., 2021; Paul et al., 2019; Zhang et al., 2021) and defining fixed network architecture schedules (Czarnecki et al., 2018) can be beneficial for performance. However, architectures and hyperparameters are inherently linked (Park et al., 2019), and to date, no method combines the ability to jointly and continuously adapt both on the fly.

In this paper we focus on Population-based Training (PBT) (Jaderberg et al., 2017) methods, where a population of agents is trained in parallel, copying across stronger weights and enabling adaption of hyperparameters in a single training run. This allows PBT methods to achieve impressive performance on many large-scale settings (Jaderberg et al., 2019; Liu et al., 2021). However, PBT-style

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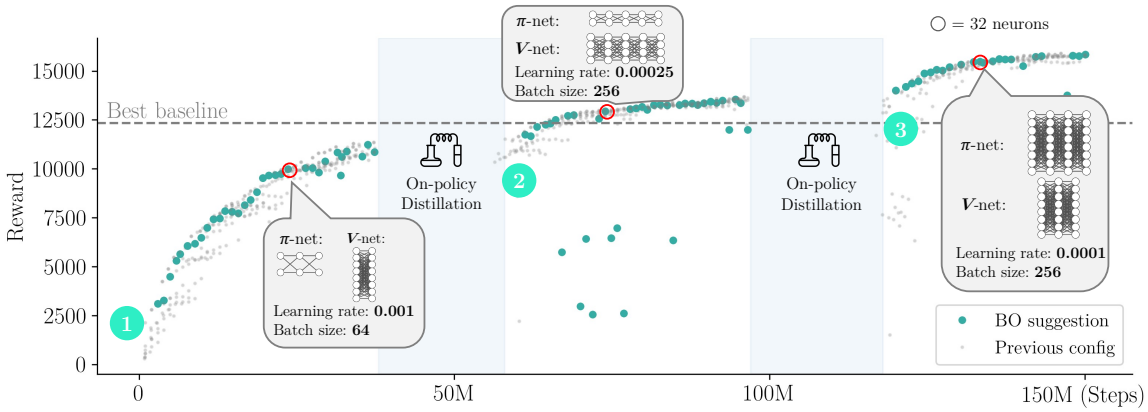

Figure 1: An example run of BG-PBT on HalfCheetah task in BRAX: BG-PBT combines population-based training with high-dimensional Bayesian optimization, generational training (different generations marked with numbers in the figure) and on-policy distillation between generations to transfer across RL agents with different neural architectures: at different points during training, both hyperparameters and the architectures of policy & value networks are tuned on-the-fly, leading to significant improvement over the baseline.

methods are typically limited in scope due to two key factors: 1) they only optimize a handful of hyperparameters, either due to using random search (Jaderberg et al., 2017), or model-based methods that do not scale to higher dimensions (Parker-Holder et al., 2021, 2020); 2) PBT methods are usually restricted to the same fixed architecture since weights are copied between agents.

We seek to overcome both of these issues in this paper, and propose *Bayesian Generational Population-based Training (BG-PBT)*, with an example run demonstrated in Fig. 1. BG-PBT is capable of tuning a significantly greater proportion of the agent's configuration, thanks to two new ideas. First, we introduce a new model-based *hyperparameter and architecture* exploration step motivated by recent advances in local Bayesian optimization (Wan et al., 2021). Second, we take inspiration from Stooke et al. (2021) who showed that PBT can be particularly effective when combined with network distillation (Igl et al., 2021), in an approach known as generational learning. As prior works in generational training (Stooke et al., 2021; Vinyals et al., 2019) show, the use of successive generations of architectures with distillation results in significantly reduced training time for new agents. This provides us with an algorithm-agnostic framework to create agents which continuously discover their *entire configuration*. Thus, for the first time, we can tune hyperparameters and architectures during one training run as part of a single unified algorithm.

We run a series of exhaustive experiments tuning both the architectures and hyperparameters for a Proximal Policy Optimization (PPO) (Schulman et al., 2017) agent in the newly introduced BRAX environment suite (Freeman et al., 2021). BRAX enables massively parallel simulation of agents, making it perfect for testing population-based methods without vast computational resources. Our agents significantly outperform both the tuned baseline and a series of prior PBT methods. Notably, we observe that BG-PBT often discovers a *schedule of networks* during training—which would be infeasible to train from scratch. Furthermore, BG-PBT discovers entirely new modes of behavior for these representative environments, which we show at `https://sites.google.com/view/bgpbt`.

To summarize, the main contributions of this paper are as follows:

1. We show for the first time it is possible to select architectures as part of a PBT framework, using *generational training with policy distillation* with Neural Architecture Search (NAS).
2. We propose a novel and efficient algorithm, **BG-PBT**, especially designed for high-dimensional mixed search spaces, which can select both architectures and hyperparameters on-the-fly with provable efficiency guarantees.
3. We show in a series of experiments our *automatic architecture curricula* make it possible to achieve significantly higher performance than previous methods.

2 Preliminaries

We begin by introducing the reinforcement learning framework, population-based training, which our method is based on, and the general problem setup we investigate in this paper.

Reinforcement Learning. We model the environment as a Markov Decision Process (MDP) (Sutton and Barto, 2018), defined as a tuple $M = (\mathcal{S}, \mathcal{A}, P, R, \rho_0, \gamma)$, where $\mathcal{S}$ and $\mathcal{A}$ denote the state and action spaces respectively, $P(s_{t+1}|s_t, a_t)$ the transition dynamics, $R(s_t, a_t)$ the reward function, ρ_0 the initial state distribution, and $\gamma \in (0, 1)$ the discount factor. The goal is to optimize a policy $\pi(a_t|s_t)$ that maximizes the expected discounted return $\mathbb{E}_{\pi,P,\rho_0}\left[\sum_{t=0}^{\infty} \gamma^t R(s_t, a_t)\right]$. Given a policy π, we may define the state value function $V^\pi(s) = \mathbb{E}_{\pi,P}\left[\sum_{t=0}^{\infty} \gamma^t R(s_t, a_t)|s_0 = s\right]$ and the state-action value-function $Q^\pi(s, a) = \mathbb{E}_{\pi,P}\left[\sum_{t=0}^{\infty} \gamma^t R(s_t, a_t)|s_0 = s, a_0 = a\right]$. The advantage function is then defined as the difference $A^\pi(s, a) = Q^\pi(s, a) - V^\pi(s)$.

A popular algorithm for online continuous control that we use is PPO (Schulman et al., 2017). PPO achieves state-of-the-art results for popular benchmarks (Cobbe et al., 2020) and is hugely parallelizable, making it an ideal candidate for population-based methods (Parker-Holder et al., 2020). PPO approximates TRPO (Schulman et al., 2015) and uses a clipped objective to stabilize training:

$$\mathcal{L}_{\text{PPO}}(\theta) = \min\left(\frac{\pi_\theta(a \mid s)}{\pi_\mu(a \mid s)} A^{\pi_\mu}, g(\theta, \mu) A^{\pi_\mu}\right), \text{ where } g(\theta, \mu) = \text{clip}\left(\frac{\pi_\theta(a \mid s)}{\pi_\mu(a \mid s)}, 1 - \epsilon, 1 + \epsilon\right) \quad (1)$$

where π_μ is a previous policy and ϵ is the clipping parameter.

Population-Based Training. RL algorithms, including PPO, are typically quite sensitive to their hyperparameters. PBT (Jaderberg et al., 2017) is an evolutionary method that tunes RL hyperparameters on-the-fly. It optimizes a population of B agents in parallel, so that their weights and hyperparameters may be dynamically adapted within a single training run. In the standard paradigm without architecture search, we consider two sub-routines, explore and exploit. We train for a total of T steps and evaluate performance every $t_{\text{ready}} < T$ steps. In the exploit step, the weights of the worst-performing agents are replaced by those from an agent randomly sampled from the set of best-performing ones, via *truncation selection*. To select new hyperparameters, we perform the explore step. We denote the hyperparameters for the bth agent in a population at timestep t as $\mathbf{z}_t^b \in \mathcal{Z}$; this defines a *schedule* of hyperparameters over time $\left(z_t^b\right)_{t=1,\ldots T}$. Let $f_t(z_t)$ be an objective function (e.g. the return of a RL agent) under a given set of hyperparameters at timestep t, our goal is to maximize the final performance $f_T(z_T)$.

The original PBT uses a combination of random sampling and evolutionary search for the explore step by suggesting new hyperparameters mutated from the best-performing agents. Population Based Bandit (PB2) and PB2-Mix (Parker-Holder et al., 2021, 2020) improve on PBT by using *Bayesian optimization (BO)* to suggest new hyperparameters, relying on a time-varying *Gaussian Process (GP)* (Rasmussen and Williams, 2006) to model the data observed. We will also use GP-based BO in our method, and we include a primer of GPs and BO in App. A.

Problem Setup. We follow the notation used in Parker-Holder et al. (2020) and frame the hyperparameter optimization problem in the lens of optimizing an expensive, time-varying, black-box reward function $f_t : \mathcal{Z} \to \mathbb{R}$. Every t_{ready} steps, we observe and record noisy observations, $y_t = f_t(\mathbf{z}_t) + \epsilon_t$, where $\epsilon_t \sim \mathcal{N}(0, \sigma^2\mathbf{I})$ for some fixed variance σ^2. We follow the typical PBT setup by defining a hyperparameter space, $\mathcal{Z}$, which for the Brax (Freeman et al., 2021) implementation of PPO we follow in the paper, consists of 9 parameters: learning rate, discount factor (γ), entropy coefficient (c), unroll length, reward scaling, batch size, updates per epoch, GAE parameter (λ) and clipping parameter (ϵ). To incorporate the architecture hyperparameters, $\mathbf{y} \in \mathcal{Y}$, we add 6 additional parameters leading to a 15-dimensional joint space $\mathcal{J} = \mathcal{Y} \times \mathcal{Z}$. For both the policy and value networks, we add the width and depth of the Multi-layer Perceptron (MLP) and a binary flag on whether to use spectral normalization.

3 Bayesian Generational Population-Based Training (BG-PBT)

We present BG-PBT in Algorithm 1 which consists of two major components. First, a BO approach to select new hyperparameter configurations $\mathbf{z}$ for our agents (§3.1). We then extend the search space to accommodate architecture search, allowing agents to choose their own networks (parameterized by $\mathbf{y} \in \mathcal{Y}$) and use on-policy distillation to transfer between different architectures (§3.2).

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 $\{\theta_0^{(i)}\}_{i=1}^B$, random hyperparameters $\{\mathbf{z}_0^{(i)}\}_{i=1}^B$ and architectures $\{\mathbf{y}_0^{(i)}\}_{i=1}^B$,
for $t = 1, \ldots, T$ (in parallel for all B agents) **do**
  Train models & record data for all agents
  if $t \bmod t_{\text{ready}} = 0$ **then**
    Replace the weights & architectures of the bottom q% agents with those of the top q% agents.
    Update the surrogate with new observations & rewards 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 $\mathbf{z}$ for the agents whose weights have been just replaced with randomly sampled configs (if $\mathbf{D} = \emptyset$) **OR** using the suggestions from the BO agent described conditioned on $\mathbf{y}$ (otherwise).

3.1 High-dimensional BO agents in mixed-input configuration space for PBT

Existing population-based methods ignore (PB2) or only partially address (PB2-Mix, which does not consider ordinal variables such as integers) the heterogeneous nature of the mixed hyperparameter space $\mathcal{Z}$. Furthermore, both previous methods are equipped with standard GP surrogates which typically scale poorly beyond low-dimensional search spaces, and are thus only used to tune a few selected hyperparameters deemed to be the most important based on human expertise. To address these issues, BG-PBT explicitly accounts for the characteristics of typical RL hyperparameter search space by making several novel extensions to CASMOPOLITAN (Wan et al., 2021), a state-of-the-art BO method for high-dimensional, mixed-input problems for our setting. In this section, we outline the main elements of our design, and we refer the reader to App. B.1 for full technical details of the approach.

Tailored treatment of mixed hyperparameter types. Hyperparameters in RL can be continuous (e.g. discounting factor), ordinal (discrete variables with ordering, e.g. batch size) and categorical (discrete variables without ordering, e.g. activation function). BG-PBT treats each variable type differently: we use tailored kernels for the GP surrogate, and utilize interleaved optimization for the acquisition function, alternating between local search for the categorical/ordinal variables and gradient descent for the continuous variables. BG-PBT extends both CASMOPOLITAN and PB2-Mix by further accommodating ordinal variables, as both previous works only considered continuous and categorical variables.

Trust Regions (TR). TRs have proven success in extending GP-based BO to higher-dimensional search spaces, which were previously intractable due to the curse of dimensionality, by limiting exploration to promising regions in the search space based on past observations (Eriksson et al., 2019; Wan et al., 2021). In the PBT context, TRs also implicitly avoid large jumps in hyperparameters, which improves training stability. We adapt the TRs used in the original CASMOPOLITAN to the time-varying setup by defining TRs around the current best configuration, and then adjusting them dynamically: similar to Eriksson et al. (2019) and Wan et al. (2021), TRs are expanded or shrunk upon consecutive "successes" or "failures". We define a proposed configuration to be a "success" if it appears in the top q%-performing agents and a "failure" otherwise. When the TRs shrink below some specified minimum, a *restart* is triggered, which resets the GP surrogate to avoid becoming stuck at a local optimum. We adapt the Upper Confidence Bound (UCB)-based criterion proposed in Wan et al. (2021) which is based on a global, auxiliary GP model to the time-varying setting to re-initialize the population when a restart is triggered. Full details are provided in App. B.2.

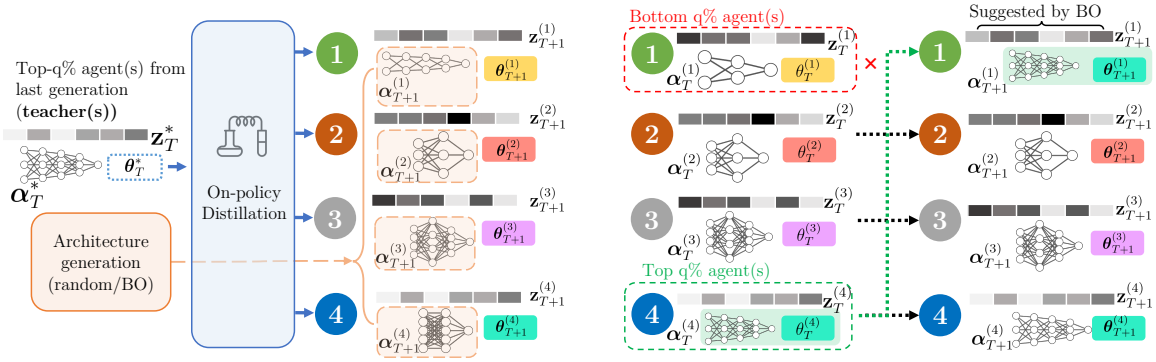

Figure 2: BG-PBT (a) at the *beginning* of a generation (**left**) and (b) *during* a generation (**right**). At the start of a generation, agents with diverse architectures are suggested and on-policy distillation is used to transfer information across generations & different architectures (§3.2). Within a generation, a high-dimensional, mixed-input BO agent suggests hyperparameters (§3.1, we copy weights across fixed architectures).

Theoretical Properties. Following Wan et al. (2021), we show that under typical assumptions (presented in App. C) used for TR-based algorithms (Yuan, 1999), our proposed BG-PBT converges to the global optimum asymptotically. Furthermore, we derive an upper bound on the cumulative regret and show that under certain conditions it achieves sublinear regret. We split the search space into $\mathcal{Z} = [\mathcal{H}, \mathcal{X}]$ (categorical/continuous parts respectively). We note that Assumption C.3 considers the minimum TR lengths $L^x_{\min}, L^h_{\min}$ are set to be small enough so that the GP approximates f accurately in the TRs. In practice, this assumption only holds asymptotically, i.e. when the observed datapoints in the TRs goes to infinity. We present the main result, the time-varying extension to Theorem 3.4 from Wan et al. (2021), and then refer to App. C for the derivation.

Theorem 3.1. *Assume Assumptions C.2 & C.3 hold. Let $f_i : [\mathcal{H}, \mathcal{X}] \to \mathbb{R}$ be a time-varying objective defined over a mixed space and $\zeta \in (0, 1)$. Suppose that: (i) there exists a class of functions g_i in the RKHS $\mathcal{G}_k([\mathcal{H}, \mathcal{X}])$ corresponding to the kernel k of the global GP model, such that g_i passes through all the local maximas of f_i and shares the same global maximum as f_i; (ii) the noise at each timestep ϵ_i has mean zero conditioned on the history and is bounded by σ; (iii) $\|g_i\|_k^2 \leq B$. Then BG-PBT obtains a regret bound*

$$Pr\left\{R_{IB} \leq \sqrt{\frac{C_1 I \beta_I}{B} \gamma(IB; k; [\mathcal{H}, \mathcal{X}])} + 2 \quad \forall I \geq 1\right\} \geq 1 - \zeta,$$

with $C_1 = 8/\log(1 + \sigma^{-2})$, $\gamma(T; k; [\mathcal{H}, \mathcal{X}])$ defined in Theorem C.1 and β_I is parameter balancing exploration-exploitation as in Theorem 2 of Parker-Holder et al. (2020).

Under the same ideal conditions assumed in Bogunovic et al. (2016); Parker-Holder et al. (2020) where the objective does not vary significantly through time, the cumulative regret bound is sublinear with $\lim_{I\to\infty} \frac{R_{IB}}{I} = 0$, when $\omega \to 0$ and $\tilde{N} \to I$.

3.2 Adapting architectures on the fly

Now that we are equipped with an approach to optimize in high-dimensional $\mathcal{Z}$, we focus on choosing *network architectures*. Despite their importance in RL (Cobbe et al., 2019; Furuta et al., 2021), architectures remain underexplored as a research direction. Adapting architectures for PBT methods is non-trivial as we further enlarge the search space, and weights cannot readily be copied across different networks. Inspired by Stooke et al. (2021), our key idea is that when beginning a new *generation* we can distill behaviors into new architectures (see Fig. 2). Specifically:

- *Starting each generation:* We fill the population of B agents by generating a diverse set of architectures for both the policy and value networks. For the first generation, this is done via random

sampling. For subsequent generations, we use suggestions from BO and/or random search with successive halving over the architecture space $\mathcal{Y}$ only; the BO is trained on observations of the best performance each architecture has achieved in previous generations. We initialize a new generation when the evaluated return stagnates beyond a pre-set patience during training.

- *Transfer between generations:* Apart from the very first generation, we transfer information from the best agent(s) of the previous generation to each new agent, in a similar fashion to Stooke et al. (2021), using on-policy distillation with a joint supervised and RL loss between *different architectures* as shown in Fig. 2a. Given a learned policy π_i and value function V_i from a previous generation, the new joint loss optimized is:

$$\mathbb{E}_{(s_t,a_t)\sim\pi_{i+1}}\left[\alpha_{\text{RL}}\mathcal{L}_{\text{RL}} + \alpha_V \left\|V_i(s_t) - V_{i+1}(s_t)\right\|_2 + \alpha_\pi \mathbb{D}_{\text{KL}}\big(\pi_i(\cdot \mid s_t) \,||\, \pi_{i+1}(\cdot \mid s_t)\big)\right] \tag{2}$$

  for weights $\alpha_{\text{RL}} \geq 0$, $\alpha_V \geq 0$, $\alpha_\pi \geq 0$, and RL loss $\mathcal{L}_{\text{RL}}$ taken from Equation (1). We linearly anneal the supervised losses over the course of each generation, so that by the end, only the RL loss remains.
- *During a generation:* We follow standard PBT methods to evolve the hyperparameters of each agent by copying weights $\boldsymbol{\theta}$ *and the architecture* $\mathbf{y}$ from a top-q% performing agent to a bottom-q% agent, as shown in Fig. 2b. This creates an effect similar to successive halving (Jamieson and Talwalkar, 2016; Karnin et al., 2013) where poorly-performing architectures are quickly removed from the population in favor of more strongly-performing ones; typically at the end of a generation, 1 or 2 architectures dominate the population. While we do not introduce new architectures within a generation, the hyperparameter suggestions are conditioned on the current policy and value architectures by incorporating the architecture parameters $\mathbf{y}$ as contextual fixed dimensions in the GP surrogate described in §3.1.

4 Experiments

While BG-PBT provides a framework applicable to any RL algorithm, we test our method on 7 environments from the new BRAX environment suite, using PPO. We begin by presenting a comparative evaluation of BG-PBT against standard baselines in population-based training to both show the benefit of searching over the full hyperparameter space with local BO and of automatically adapting architectures over time. We further show that our method beats end-to-end BO, showing the advantage of dynamic schedules. Next, we analyze these learned hyperparameter and architecture schedules using BG-PBT and we show analogies to similar trends in learning rate and batch size in supervised learning. Finally, we perform ablations on individual components of BG-PBT. Additional experiments showing the ability of BG-PBT to scale to problems which require higher computational budget and larger population sizes B are shown in App. F. For all population-based methods, we use a population size $B = 8$ and a total budget of 150M steps. We note that BG-PBT with architectures uses additional on-policy samples from the environment in order to distill between architectures. We instantiate the BRAX environments with an action repeat of 1. We use t_{ready} of 1M for all PBT-based methods on all environments except for Humanoid and Hopper, where we linearly anneal t_{ready} from 5M to 1M. The remaining hyperparameters and implementation details used in this section are listed in App. E.

Comparative evaluation of BG-PBT. We first perform a comparative evaluation of BG-PBT against standard baselines in PBT-methods and the PPO baseline provided by the BRAX authors. We show the benefit of using local BO and treating the whole RL hyperparameter space $\mathcal{Z}$, by comparing BG-PBT against PBT (Jaderberg et al., 2017), PB2 (Parker-Holder et al., 2020) and Random Search (RS) using the default architecture in BRAX. In RS, we simply sample from the hyperparameter space and take the best performance found using the same compute budget as the PBT methods. Next, we include architecture search into BG-PBT using the full space $\mathcal{J}$ and show significant gains in performance compared to BG-PBT without architectures; we use random search over $\mathcal{J}$ as a

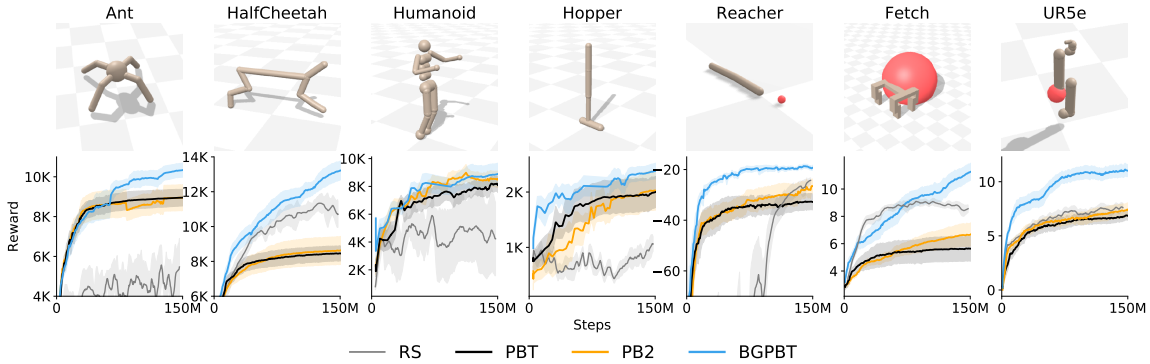

Figure 3: Visualization of each environment (**top row**) and mean evaluated return over the population with ±1 SEM (shaded) across 7 random seeds (**bottom row**) in all environments. RS refers to the higher performing of RS-$\mathcal{Z}$ or RS-$\mathcal{J}$ in Table 1.

Table 1: Mean evaluated return ±1SEM across 7 seeds shown. For PBT-style methods (PBT, PB2 and BG-PBT), the mean best-performing agent in the population is shown. Methods performing within 1 SEM of the best-performing method are bolded (the same applies to all tables).

Method Search space	PPO* $\mathcal{Z}$	RS $\mathcal{Z}$	RS $\mathcal{J}$	PBT $\mathcal{Z}$	PB2 $\mathcal{Z}$	BG-PBT $\mathcal{J}$
Ant	$3853_{\pm 676}$	$6780_{\pm 317}$	$4781_{\pm 515}$	$8955_{\pm 385}$	$8954_{\pm 594}$	$\mathbf{10349}_{\pm 326}$
HalfCheetah	$6037_{\pm 236}$	$9502_{\pm 76}$	$10340_{\pm 329}$	$8455_{\pm 400}$	$8629_{\pm 746}$	$\mathbf{13216}_{\pm 503}$
Humanoid	$9109_{\pm 987}$	$4004_{\pm 519}$	$4652_{\pm 1002}$	$7954_{\pm 437}$	$\mathbf{8452}_{\pm 512}$	$\mathbf{8894}_{\pm 716}$
Hopper	$120_{\pm 43}$	$339_{\pm 25}$	$943_{\pm 185}$	$2002_{\pm 254}$	$2027_{\pm 323}$	$\mathbf{2381}_{\pm 127}$
Fetch	$14.0_{\pm 0.2}$	$5.2_{\pm 0.4}$	$8.6_{\pm 0.2}$	$5.5_{\pm 0.8}$	$6.6_{\pm 0.7}$	$\mathbf{11.3}_{\pm 0.6}$
Reacher	$-189.3_{\pm 43.7}$	$-24.2_{\pm 1.4}$	$-95.2_{\pm 25.3}$	$-32.9_{\pm 2.8}$	$-26.6_{\pm 2.6}$	$\mathbf{-19.2}_{\pm 0.9}$
UR5e	$5.2_{\pm 0.2}$	$5.3_{\pm 0.4}$	$7.7_{\pm 0.3}$	$6.9_{\pm 0.4}$	$7.4_{\pm 0.6}$	$\mathbf{11.0}_{\pm 0.5}$

*From the BRAX authors and implemented in a different framework (JAX) to ours (PyTorch)

baseline. The optimized PPO implementation from the BRAX authors is provided as a sequential baseline. We present the results in Table 1 and the training trajectories in Fig. 3.

We show that BG-PBT significantly outperforms the RS baselines and the existing PBT-style methods in almost all environments considered. We also observe that RS is a surprisingly strong baseline, performing on par or better than PBT and PB2 in HalfCheetah, Reacher, Fetch and UR5e — this is due to a well-known failure mode in PBT-style algorithms where they may be overly greedy in copying sub-optimal behaviors early on and then fail to sufficiently explore in weight space when the population size is modest. BG-PBT avoids this problem by *re-initializing networks each generation* and distilling, which prevents collapse to suboptimal points in weight space.

Comparison against sequential BO. We further compare against BO in the traditional sequential setup (Table 2): for each BO iteration, the agent is trained for the full 150M timesteps before a new hyperparameter suggestion is made. To enable BO to improve on RS, we allocate a budget of 50 evaluations, *which is approx. 6× more expensive* than our method and up to 50× more costly in terms of wall-clock time if vanilla, non-parallel BO is used. We implement this baseline using SMAC3 (Lindauer et al., 2022) in both the $\mathcal{Z}$ and $\mathcal{J}$ search spaces (denoted BO-$\mathcal{Z}$ and BO-$\mathcal{J}$ respectively in Table 2). While, unsurprisingly, BO improves over the RS baseline, BG-PBT still outperforms it in a majority of environments. One reason for this is that BG-PBT naturally discovers a dynamic schedule of hyperparameters and architectures, which is strictly more flexible than a carefully tuned but still static configuration – we analyze this below.

Analysis of discovered hyperparameter and architecture schedules. We present the hyperparameter and architecture schedules learned by BG-PBT in our main comparative evaluation on Ant in Fig. 4 (results on other environments are presented in App. F). We find consistent trends across environments such as the decrease of learning rate and increase in batch sizes over time, consistent to common practices in both RL (Engstrom et al., 2020) and supervised learning, but crucially BG-PBT discovers the same *without any pre-defined schedule*. We also find that different networks

Table 2: Comparison against sequential BO*

Method	BO-$\mathcal{Z}^*$	BO-$\mathcal{J}^*$	BG-PBT
Ant	$6975_{\pm 1013}$	$7149_{\pm 507}$	$\mathbf{10349}_{\pm 326}$
HalfCheetah	$11202_{\pm 204}$	$10859_{\pm 174}$	$\mathbf{13216}_{\pm 503}$
Humanoid	$\mathbf{9040}_{\pm 1303}$	$4845_{\pm 962}$	$\mathbf{8894}_{\pm 716}$
Hopper	$358_{\pm 60}$	$1254_{\pm 154}$	$\mathbf{2381}_{\pm 127}$
Fetch	$\mathbf{13.2}_{\pm 0.2}$	$11.6_{\pm 0.1}$	$11.3_{\pm 0.6}$
Reacher	$\mathbf{-17.3}_{\pm 0.3}$	$-51.7_{\pm 18.3}$	$-19.2_{\pm 0.9}$
UR5e	$9.0_{\pm 0.5}$	$6.3_{\pm 1.4}$	$\mathbf{11.0}_{\pm 0.5}$

*More resources required compared to BG-PBT.

Table 3: Ablation studies

Method	No TR/NAS	No NAS	BG-PBT
Ant	$8954_{\pm 594}$	$9352_{\pm 402}$	$\mathbf{10349}_{\pm 326}$
HalfCheetah	$8629_{\pm 746}$	$9483_{\pm 626}$	$\mathbf{13216}_{\pm 503}$
Humanoid	$8452_{\pm 512}$	$\mathbf{10359}_{\pm 647}$	$8894_{\pm 716}$
Hopper	$2027_{\pm 323}$	$\mathbf{2511}_{\pm 154}$	$\mathbf{2381}_{\pm 127}$
Fetch	$6.6_{\pm 0.7}$	$7.3_{\pm 0.8}$	$\mathbf{11.3}_{\pm 0.6}$
Reacher	$-26.6_{\pm 2.6}$	$\mathbf{-17.6}_{\pm 0.8}$	$-19.2_{\pm 0.9}$
UR5e	$7.4_{\pm 0.6}$	$9.0_{\pm 0.8}$	$\mathbf{11.0}_{\pm 0.5}$

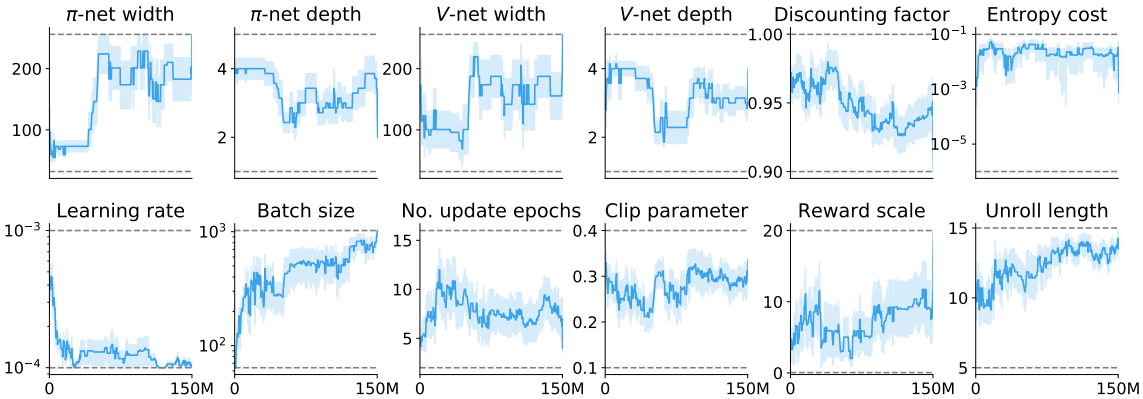

Figure 4: The hyperparameter and architecture schedule discovered by BG-PBT on Ant: we plot the hyperparameters of the best-performing agent in the population averaged across 7 seeds with ± 1 SEM shaded. Gray dashed lines denote the hyperparameter bounds.

are favored at different stages of training, but the exact patterns differ across environments: for Ant (Fig. 4), we find that larger networks are preferred towards the end of training, with the policy and value network widths increasing over time: Prior work has shown that larger networks like those we automatically find towards the end of training *can be notoriously unstable and difficult to train from scratch* (Czarnecki et al., 2018; Ota et al., 2021), which further supports our use of generational training to facilitate this.

Ablation Studies. BG-PBT improves on existing methods by using local TR-based BO (§3.1) and NAS & distillation (§3.2). We conduct an ablation study by removing either or both components in Table 3, where "No NAS" does not search architectures or distill but uses the default BRAX architectures, and "No TR/NAS" further only uses a vanilla GP surrogate and is identical to PB2. We find the tailored BO agent in §3.1 improves performance across the board. On the importance of NAS & distillation, in all environments except for Humanoid and Reacher, BG-PBT matches or outperforms "No NAS", despite $\mathcal{J}$ being a more complicated search space and the "No NAS" baseline is conditioned on strongly-performing default architectures. We also see a particularly large gain for HalfCheetah and Fetch when we include architectures, demonstrating the effectiveness of the generational training and NAS in our approach. We include additional ablation studies in App. F.

5 Related Work

On-the-fly hyperparameter tuning. Our work improves on previous PBT (Jaderberg et al., 2017; Parker-Holder et al., 2020; Zhang et al., 2021) style methods. In particular, we build upon Parker-Holder et al. (2021), using a more scalable BO step, and adding architecture search with generational learning. Dalibard and Jaderberg (2021) introduce an approach for increasing diversity in the weight space for PBT, orthogonal to our work. There have also been non-population-based methods for dynamic hyperparameter optimization, using bandits (Badia et al., 2020; Ball et al., 2020; Moskovitz et al., 2021; Parker-Holder et al., 2020), gradients (Flennerhag et al., 2021; Paul et al., 2019; Xu et al., 2018; Zahavy et al., 2020) or Evolution (Tang and Choromanski, 2020). Crucially, none of the methods described searches over architectures.

Architecture search. In RL, Czarnecki et al. (2018) showed increasing agent complexity over time could be effective, albeit with a pre-defined schedule. Miao et al. (2021) showed that DARTS (Liu et al., 2019) could be effective in RL, finding high performing architectures on the Procgen benchmark. Auto-Agent-Distiller (Fu et al., 2020) deals with the problem of finding optimal architectures for compressing the model size of RL agents, and also find that using distillation between the teacher and student networks improves stability of NAS in RL. BO has been used as a powerful tool for searching over large architecture spaces (Kandasamy et al., 2018; Nguyen et al., 2021a; Ru et al., 2021; Wan et al., 2021, 2022; White et al., 2021). Conversely, we only consider simple MLPs and the use of spectral normalization. There has been initial effort (Izquierdo et al., 2021) combining NAS and hyperparameter optimization in sequential settings, which is distinct to our on-the-fly approach.

Generational Training and Distillation. Stooke et al. (2021) recently introduced generational training, using policy distillation to transfer knowledge between generations, accelerating training. Our method is based on this idea, with changing generations. The use of distillation is further supported by Igl et al. (2021) who recently used this successfully to adapt to non-stationarities in reinforcement learning, however keeping hyperparameters and architectures fixed.

6 Conclusion & Discussion

In this paper, we propose BG-PBT: a new algorithm that significantly increases the capabilities of PBT methods for RL. Using recent advances in Bayesian Optimization, BG-PBT is capable of searching over drastically larger search spaces than previous methods. Furthermore, inspired by recent advances in generational learning, we show it is also possible to efficiently learn architectures on the fly as part of a unified algorithm. The resulting method leads to significant performance gains across the entire Brax environment suite, achieving high performance even in previously untested environments. We believe BG-PBT is a significant step towards truly environment agnostic RL algorithms, while also offering a path towards open-ended learning where agents never stop tuning themselves and continuously expand their capabilities over time.

Limitations & Future Work. We note that while our method shows a significant boost in performance by including architectures for most environments, in some environments, such as Humanoid, we achieve better results without architecture search. We hypothesize this is due to the complexity of the environment and an increased sensitivity to the network architecture. Furthermore, while we provide a theoretical guarantee for our method in Theorem 3.1 for searching purely over architectures, no such guarantees exist when we transfer between architectures across generations. Indeed, we occasionally see poor architectures being selected, which are then discarded during truncation selection. Therefore, an immediate future direction is to address these issues and to improve the architecture selection process. Another limitation is that while all RL-related hyperparameters are included in the search space, certain hyperparameters of BG-PBT could also be automatically searched for, including but not limited to distillation hyperparameters, which are currently fixed, and PBT parameters such as t_{ready}, which could allow us to avoid myopic and greedy behavior. Beyond these limitations, our algorithm readily transfers to other RL problems with high-dimensional mixed spaces, and thus we would readily accommodate more complicated architecture search spaces (e.g. vision-based environments) and incorporate environment parameters (Paul et al., 2016) into the search space to generalize to new tasks.

Broader Impact. We open-source our code so that practitioners in the field can accelerate their own deployment of RL systems. However, in doing so, we should be wary of the risk of also improving malicious use of RL; in particular, down-stream applications which could have an impact on people's security and privacy. To mitigate these risks, we encourage research on RL governance and safe RL. As a general purpose framework for improving any RL algorithm, our method should be part of that conversation.

7 Reproducibility Checklist

1. For all authors...

   (a) Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope? [Yes] [The abstract and introduction's content is substantiated in §4]

   (b) Did you describe the limitations of your work? [Yes] We discuss them in §6.

   (c) Did you discuss any potential negative societal impacts of your work? [Yes] We discuss them in §6.

   (d) Have you read the ethics review guidelines and ensured that your paper conforms to them? [Yes] We have ensured our paper conforms to the guidelines.

2. If you are including theoretical results...

   (a) Did you state the full set of assumptions of all theoretical results? [Yes] The full set of assumptions are provided in Appendix C.

   (b) Did you include complete proofs of all theoretical results? [Yes] Complete proofs provided in Appendix C.

3. If you ran experiments...

   (a) Did you include the code, data, and instructions needed to reproduce the main experimental results, including all requirements (e.g., `requirements.txt` with explicit version), an instructive `README` with installation, and execution commands (either in the supplemental material or as a URL)? [Yes] We have included this in the supplementary material.

   (b) Did you include the raw results of running the given instructions on the given code and data? [Yes] We include raw numbers produced by the code.

   (c) Did you include scripts and commands that can be used to generate the figures and tables in your paper based on the raw results of the code, data, and instructions given? [Yes] We include notebooks that produce the plots.

   (d) Did you ensure sufficient code quality such that your code can be safely executed and the code is properly documented? [Yes] Yes, the code is documented and appropriate commands provided.

   (e) Did you specify all the training details (e.g., data splits, pre-processing, search spaces, fixed hyperparameter settings, and how they were chosen)? [Yes] Implementation details are discussed in Appendix D and Appendix E.

   (f) Did you ensure that you compared different methods (including your own) exactly on the same benchmarks, including the same datasets, search space, code for training and hyperparameters for that code? [Yes] All methods benchmarked on the same Brax environment suite, we used the same computational budget and population size for all other PBT methods.

   (g) Did you run ablation studies to assess the impact of different components of your approach? [Yes] We include ablations in Section 4 and in Appendix F.

   (h) Did you use the same evaluation protocol for the methods being compared? [Yes] All PBT methods are evaluated by best performance in the population.

   (i) Did you compare performance over time? [Yes] We regularly evaluate the evaluated performance through the course of training.

(j) Did you perform multiple runs of your experiments and report random seeds? [Yes] All our experiments are averaged over 7 random seeds.

(k) Did you report error bars (e.g., with respect to the random seed after running experiments multiple times)? [Yes] We report the mean performance and indicate ± 1 standard error.

(l) Did you use tabular or surrogate benchmarks for in-depth evaluations? [N/A]

(m) Did you include the total amount of compute and the type of resources used (e.g., type of GPUs, internal cluster, or cloud provider)? [Yes] We describe our compute and resource usage in Appendix E.

(n) Did you report how you tuned hyperparameters, and what time and resources this required (if they were not automatically tuned by your AutoML method, e.g. in a NAS approach; and also hyperparameters of your own method)? [Yes] The RL hyperparameters were tuned by our AutoRL method. The hyperparameters for BG-PBT were tuned by hand with ablations performed in Appendix F.

4. If you are using existing assets (e.g., code, data, models) or curating/releasing new assets…

(a) If your work uses existing assets, did you cite the creators? [Yes] We cite the creators of the codebase we use in Appendix E.

(b) Did you mention the license of the assets? [Yes] We mention the license of the codebase we use in Appendix E.

(c) Did you include any new assets either in the supplemental material or as a URL? [Yes] We include figures in a url link in the introduction.

(d) Did you discuss whether and how consent was obtained from people whose data you're using/curating? [N/A] No personal data used. All data for our algorithm is generated from RL environments.

(e) Did you discuss whether the data you are using/curating contains personally identifiable information or offensive content? [N/A] No personal data used. All data for our algorithm is generated from RL environments.

5. If you used crowdsourcing or conducted research with human subjects…

(a) Did you include the full text of instructions given to participants and screenshots, if applicable? [N/A] [We are not crowdsourcing or conducting research with human subjects.]

(b) Did you describe any potential participant risks, with links to Institutional Review Board (IRB) approvals, if applicable? [N/A] [We are not crowdsourcing or conducting research with human subjects.]

(c) Did you include the estimated hourly wage paid to participants and the total amount spent on participant compensation? [N/A] [We are not crowdsourcing or conducting research with human subjects.]

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A Primer on GPs and BO

Cong: *Copied from previous introduction, maybe we just want to delete this.* In order to effectively trade-off exploration and exploitation in the presence of uncertainty, Parker-Holder et al. (2020) model the data using a Gaussian Process (GP, Rasmussen and Williams (2006)), which assumes the data follows a Gaussian distribution with mean $\mu_t(z')$ and variance $\sigma_t^2(z')$ as:

$$\mu_t(z') \coloneqq \mathbf{k}_t(z')^T(\mathbf{K}_t + \sigma^2\mathbf{I})^{-1}\mathbf{f}_t \tag{3}$$

$$\sigma_t^2(z') \coloneqq k(z', z') - \mathbf{k}_t(z')^T(\mathbf{K}_t + \sigma^2\mathbf{I})^{-1}\mathbf{k}_t(z'), \tag{4}$$

where $\mathbf{K}_t \coloneqq \{k(z_i, z_j)\}_{i,j=1}^t$ and $\mathbf{k}_t \coloneqq \{k(z_i, z_t')\}_{i=1}^t$.

B Bayesian Optimization for PBT

In this section, we provide specific details for the modifications to Casmopolitan to make it amenable for PBT.

B.1 Proposing new configurations

A BO agent selects new configurations by selecting configuration(s) which maximize the acquisition function $\mathbf{z}_{\text{next}} = \arg\max_{\mathbf{z}} \text{acq}(\mathbf{z})$, in our case Upper Confidence Bound (UCB). This is typically achieved via off-the-shelf first-order optimizers, which is challenging in a mixed-input space as the discrete (ordinal and categorical) variables lack gradients and naïvely casting them into continuous variables yield invalid solutions which require rounding. To address this issue, Parker-Holder et al. (2021) select $\mathbf{h}$ first via time-varying bandits (using the proposed TV.EXP3.M algorithm) and then select $\mathbf{x}$ by optimizing the BO acquisition function, *conditioned on* the chosen $\mathbf{h}$. This method scales poorly to spaces with a large number of categorical choices, as bandit problems generally require pulling each arm at least once. Instead, we develop upon *interleaved acquisition optimization* introduced in Wan et al. (2021) which unifies all variables under a single GP, and alternates between optimization of the continuous and discrete variables:

Algorithm 2 Interleaved optimization of $\text{acq}(\mathbf{z})$

1: **while** not converged **do**
2: **Continuous**: Do a single step of gradient descent on the continuous dimensions.
3: **Ordinal and Categorical**: Conditioned on the new continuous values, do a single step of local search: randomly select an ordinal/categorical variable and choose a different (categorical), or an adjacent (ordinal) value, if the new value leads to an improvement in $\text{acq}(\cdot)$.

Compared to the approach in Wan et al. (2021), we include ordinal variables, which are optimized alongside the categorical variables via local search during acquisition optimization but are treated like continuous variables by the kernel. During acquisition, we define adjacent ordinals to be the neighboring values. For example, for an integer variable with a valid range $[1, 5]$ and current value 3, its neighboring values are 2 and 4. This allows us to exploit the natural ordering for ordinal variables whilst still ensuring that suggested configurations remain local and only explore *valid* neighboring solutions.

B.2 Restarting trust regions

We adapt the UCB-based criterion proposed in Wan et al. (2021) to the time-varying setting to re-initialize the population when a restart is triggered. For the i-th restart, we consider a global, auxiliary GP model trained on a subset of observed configurations and returns $D_{i-1}^* = \{\mathbf{z}_j^*, f_j^*\}_{j=1}^i$ and denote $\mu_g(\mathbf{z}; D_{i-1}^*)$ and $\sigma_g^2(\mathbf{z}; D_{i-1}^*)$ as the posterior mean and variance of the auxiliary GP.

The new trust region center is given by the configuration $\mathbf{z}_i^{(0)}$ that maximizes the UCB score: $\mathbf{z}_i^{(0)} = \arg\max_{\mathbf{z}\in\mathcal{Z}} \mu_g(\mathbf{z}; D_{i-1}^*) + \sqrt{\beta_i}\sigma_g(\mathbf{z}; D_{i-1}^*)$ where β_i is the UCB trade-off parameter. In the original CASMOPOLITAN, D^* consists of the best configurations in all previous restarts $1, ..., i-1$, which is invalid for the time-varying setting. Instead, we construct D_{i-1}^* using the following:

$$D_{i-1}^* = \{\mathbf{z}_j^*, \mu_T(\mathbf{z}_j^*)\}_{j=1}^{i=1} \text{ where } \mathbf{z}_j^* = \arg\max_{\mathbf{z}_j\in\mathcal{D}_j} \mu_T(\mathbf{z}_j), \tag{5}$$

where $\mathcal{D}_j$ denotes the set of previous configurations evaluated during the j-th restart and $\mu_T(\cdot)$ denotes the posterior mean of the time-varying GP surrogate *at the present timestep* $t = T$. Thus, instead of simply selecting the configurations of each restart that *led* to the highest observed reward, we select the configurations that *would have led to the highest reward if they were evaluated now*, according to the GP surrogate. Such a configuration preserves the convergence property of BG-PBT shown in Theorem 3.1.

C Theoretical Guarantees

C.1 Bound on the maximum information gain

We start by deriving the maximum information gain which extends the result presented in Wan et al. (2021) for the time-varying setting. Note that this result is defined over the number of local restarts I.

Theorem C.1. *Let* $\gamma(I; k; V) := \max_{A\subseteq V, |A|\leq I} \frac{1}{2}\log|\mathbf{I} + \sigma^{-2}[k(\mathbf{v}, \mathbf{v}')]_{\mathbf{v},\mathbf{v}'\in A}|$ *be the maximum information gain achieved by sampling* I *points in a* GP *defined over a set* V *with a kernel* k*. Denote the constant* $\eta := \prod_{j=1}^{d_h} n_j$*. Then we have, for the time-varying mixed kernel* k*,*

$$\gamma(I; k; [\mathcal{H}, \mathcal{X}]) \lessapprox \frac{I}{\tilde{N}}\left(\lambda\eta\gamma(I; k_x; \mathcal{X}) + (\eta - 2\lambda)\log I + \sigma_f^{-2}\tilde{N}^3\omega\right) \tag{6}$$

where the time steps $\{1, ..., I\}$ *are split into into* $I/\tilde{N}$ *blocks of length* $\tilde{N}$*, such that the function* f_t *does not vary significantly within each block.*

Proof. Following the proof used in Bogunovic et al. (2016)), we split the time steps $\{1, ..., I\}$ into $I/\tilde{N}$ blocks of length $\tilde{N}$, such that within each block the function f_i does not vary significantly. Then, we have that the maximum information gain of the time-varying kernel Bogunovic et al. (2016)) is bounded by

$$\gamma_I \leq \left(\frac{I}{\tilde{N}} + 1\right)\left(\tilde{\gamma}_{\tilde{N}} + \sigma_f^{-2}\tilde{N}^3\omega\right)$$

where $\omega \in [0, 1]$ is the forgetting-remembering trade-off parameter, and we consider the kernel for time $1 - k_{time}(t, t') \leq \omega|t - t'|$. We denote $\tilde{\gamma}_{\tilde{N}}$ as the maximum information gain for the time-invariant kernel counterpart in each block length of $\tilde{N}$.

Next, by using the bounds for the (time-invariant) mixed kernel in Wan et al. (2021) that $\tilde{\gamma}_{\tilde{N}} \leq \mathcal{O}\big((\lambda\eta + 1 - \lambda)\gamma(I; k_x; \mathcal{X}) + (\eta + 2 - 2\lambda)\log I\big)$, we get the new time-varying bound $\gamma(I; k; [\mathcal{H}, \mathcal{X}]) \lessapprox \frac{I}{\tilde{N}}\left(\lambda\eta\gamma(I; k_x; \mathcal{X}) + (\eta - 2\lambda)\log I + \sigma_f^{-2}\tilde{N}^3\omega\right)$ where we have suppressed the constant term for simplicity. □

C.2 Proof of the Local Convergence in Each Trust Region

Assumption C.2. *The time-varying objective function* $f_t(\mathbf{z})$ *is bounded in* $[\mathcal{H}, \mathcal{X}]$*, i.e.* $\exists F_l, F_u \in \mathbb{R}$: $\forall \mathbf{z} \in [\mathcal{H}, \mathcal{X}], F_l \leq f_t(\mathbf{z}) \leq F_u, \forall t \in [1, ..., T]$.

Assumption C.3. *Let us denote $L^h_{\min}$, $L^x_{\min}$ and L^h_0, L^x_0 be the minimum and initial TR lengths for the categorical and continuous variables, respectively. Let us also denote α_s as the shrinking rate of the TRs. The local GP approximates $f_t, \forall t \leq T$ accurately within any TR with length $L^x \leq \max\left(L^x_{\min}/\alpha_s, L^x_0(\lceil (L^h_{\min}+1)/\alpha_s\rceil - 1)/L^h_0\right)$ and $L^h \leq \max\left(\lceil (L^h_{\min}+1)/\alpha_s\rceil - 1, \lceil L^h_0 L^x_{\min}/(\alpha_s L^x_0)\rceil\right)$.*

Theorem C.4. *Given Assumptions C.2 & C.3, after a restart, BG-PBT converges to a local maxima after a finite number of iterations or converges to the global maximum.*

Proof. We may apply the same proof by contradiction used in Wan et al. (2021) for our time-varying setting, given the assumptions C.2 and C.3. For completeness, we summarize it below.

We show that our algorithm converges to (1) to a global maximum of f (if does not terminate after a finite number of iterations) or (2) a local maxima of f (if terminated after a finite number of iterations).

Case 1: when $t \to \infty$ and the TR lengths L^h and L^x have not shrunk below $L^h_{\min}$ and $L^x_{\min}$. From the algorithm description, the TR is shrunk after `fail_tol` consecutive failures. Thus, if after $N_{\min} = \texttt{fail_tol} \times m$ iterations where $m = \max(\lceil \log_{\alpha_e}(L^h_0/L^h_{\min})\rceil, \lceil \log_{\alpha_e}(L^x_0/L^x_{\min})\rceil)$, there is no success, BG-PBT terminates. This means, for case (1) to occur, BG-PBT needs to have at least one improvement per $N_{\min}$ iterations. Let consider the increasing series $\{f(\mathbf{z}^k)\}_{k=1}^{\infty}$ where $f(\mathbf{z}^k) = \max_{t=(k-1)N_{\min}+1,\ldots,kN_{\min}}\{f(\mathbf{z}_t)\}$ and $f(\mathbf{z}_i)$ is the function value at iteration t. Thus, using the monotone convergence theorem (Bibby, 1974), this series converges to the global maximum of the objective function f given that $f(\mathbf{z})$ is bounded (Assumption C.2).

Case 2: when BG-PBT terminates after a finite number of iterations, BG-PBT converges to a local maxima of $f(\mathbf{z})$ given Assumption C.3. Let us remind that BG-PBT terminates when either the continuous TR length $\leq L^x_{\min}$ or the categorical TR length $\leq L^h_{\min}$.

Let L_s be the largest TR length that after being shrunk, the algorithm terminates, i.e., $\lfloor \alpha_s L_s \rfloor \leq L^h_{\min}$.[1] Due to $\lfloor \alpha_s L_s \rfloor \leq \alpha_s L_s < \lfloor \alpha_s L_s \rfloor + 1$, we have $L_s < (L^h_{\min} + 1)/\alpha_s$. Because L_s is an integer, we finally have $L_s \leq \lceil (L^h_{\min} + 1)/\alpha_s \rceil - 1$. This means that $L_s = \lceil (L^h_{\min} + 1)/\alpha_s \rceil - 1$ is the largest TR length that after being shrunk, the algorithm terminates. We may apply a similar argument for the largest TR length (before terminating) for the continuous $L^x_{\min}/\alpha_s$.

In our mixed space setting, we have two separate trust regions for categorical and continuous variables. When one of the TR reaches its terminating threshold ($L^x_{\min}/\alpha_s$ or $\lceil (L^h_{\min}+1)/\alpha_s\rceil - 1$), the length of the other one is $(\lceil L^h_0 L^x_{\min}/(\alpha_s L^x_0)\rceil)$ or $L^x_0(\lceil (L^h_{\min}+1)/\alpha_s\rceil - 1)/L^h_0)$. Based on Assumption C.3, the GP can accurately fit a TR with continuous length $L^x \leq \max\left(L^x_{\min}/\alpha_s, L^x_0(\lceil (L^h_{\min}+1)/\alpha_s\rceil - 1)/L^h_0\right)$ and $L^h \leq \max\left(\lceil (L^h_{\min} + 1)/\alpha_s\rceil - 1, \lceil L^h_0 L^x_{\min}/(\alpha_s L^x_0)\rceil\right)$. Thus, if the current TR center is not a local maxima, BG-PBT can find a new data point whose function value is larger than the function value of current TR center. This process occurs iteratively until a local maxima is reached, and BG-PBT terminates. □

C.3 Proof of Theorem 3.1

Proof. Under the time-varying setting, at the i-th restart, we first fit the global time-varying GP model on a subset of data $D^*_{i-1} = \{\mathbf{z}^*_j, f(\mathbf{z}^*_j)\}_{j=1}^{i-1}$, where $\mathbf{z}^*_j$ is the local maxima found after the j-th restart, or, a random data point, if the found local maxima after the j-th restart is same as in the previous restart.

Let $\mathbf{z}^{**}_i = \arg\max_{\forall \mathbf{z} \in [\mathcal{H}, \mathcal{X}]} f_t(\mathbf{z})$ [2] be the global optimum location at time step i. Let $\mu_{gl}(\mathbf{z}; D^*_{i-1})$ and $\sigma^2_{gl}(\mathbf{z}; D^*_{i-1})$ be the posterior mean and variance of the global GP learned from D^*_{i-1}. Then, at the i-th restart, we select the following location $\mathbf{z}^{(0)}_i$ as the initial centre of the new TR:

$$\mathbf{z}^{(0)}_i = \arg\max_{\mathbf{z} \in [\mathcal{H}, \mathcal{X}]} \mu_{gl}(\mathbf{z}; D^*_{i-1}) + \sqrt{\beta_i}\sigma_{gl}(\mathbf{z}; D^*_{i-1}),$$

[1] The operator $\lfloor . \rfloor$ denotes the floor function

[2] Notationally, at the i-th restart, $\mathbf{z}^{**}_i$ is the global optimum location while $\mathbf{z}^*_i$ is the local maxima found by BG-PBT.

where β_i is the trade-off parameter in PB2 (Parker-Holder et al., 2020).

We follow Wan et al. (2021) to assume that at the i-th restart, there exists a function $g_i(\mathbf{z})$: (a) lies in the RKHS $\mathcal{G}_k([\mathcal{H}, \mathcal{X}])$ and $\|g_i\|_k^2 \leq B$, (b) shares the same global maximum $\mathbf{z}^*$ with f, and, (c) passes through all the local maxima of f and any data point $\mathbf{z}'$ in $\mathcal{D}_{i-1}^* \cup \{\mathbf{z}_i^{(0)}\}$ which are not local maxima (i.e. $g_i(\mathbf{z}') = f(\mathbf{z}'), \forall \mathbf{z}' \in D_{i-1}^* \cup \{\mathbf{z}_i^{(0)}\}$). In other words, the function $g_i(\mathbf{z})$ is a function that passes through the maxima of f whilst lying in the RKHS $\mathcal{G}_k([\mathcal{H}, \mathcal{X}])$ and satisfying $\|g_i\|_k^2 \leq B$.

Using β_i defined in Theorem 2 in Srinivas et al. (2010) for function g_i, $\forall i$, $\forall z \in [\mathcal{H}, \mathcal{X}]$, we have,

$$\Pr\{|\mu_{gl}(\mathbf{z}; D_{i-1}^*) - g_i(\mathbf{z})| \leq \sqrt{\beta_i}\sigma_{gl}(\mathbf{z}; D_{i-1}^*)|\} \geq 1 - \zeta. \tag{7}$$

In particular, with probability $1 - \zeta$, we have that,

$$\mu_{gl}(\mathbf{z}_i^{(0)}; D_{i-1}^*) + \sqrt{\beta_i}\sigma_{gl}(\mathbf{z}_i^{(0)}; D_{i-1}^*) \geq \mu_{gl}(\mathbf{z}_i^{**}; D_{i-1}^*) + \sqrt{\beta_i}\sigma_{gl}(\mathbf{z}_i^{**}; D_{i-1}^*) \geq g_i(\mathbf{z}_i^{**}). \tag{8}$$

Thus, $\forall i$, with probability $1 - \zeta$ we have

$$g_i(\mathbf{z}_i^{**}) - g_i(\mathbf{z}_i^{(0)}) \leq \mu_{gl}(\mathbf{z}_i^{(0)}; D_{i-1}^*) + \sqrt{\beta_i}\sigma_{gl}(\mathbf{z}_i^{(0)}; D_{i-1}^*) - g_i(\mathbf{z}_i^{(0)}) \leq 2\sqrt{\beta_i}\sigma_{gl}(\mathbf{z}_i^{(0)}; D_{i-1}^*).$$

Since $g_i(\mathbf{z}_i^{(0)}) = f(\mathbf{z}_i^{(0)})$, and $g_i(\mathbf{z}_i^{**}) = f(\mathbf{z}_i^{**})$, hence, $f_i(\mathbf{z}_i^{**}) - f(\mathbf{z}_i^{(0)}) \leq 2\sqrt{\beta_i}\sigma_{gl}(\mathbf{z}_i^{(0)}; D_{i-1}^*)$ with probability $1-\zeta$. With $\mathbf{z}_i^*$ as the local maxima found by BG-PBT at the i-th restart. As $f(\mathbf{z}_i^{(0)}) \leq f(\mathbf{z}_i^*)$, we have,

$$f_i(\mathbf{z}_i^{**}) - f_i(\mathbf{z}_i^*) \leq 2\sqrt{\beta_i}\sigma_{gl}(\mathbf{z}_i^{(0)}; D_{i-1}^*). \tag{9}$$

Let $\mathbf{z}_{i,b}$ be the point chosen by our algorithm at iteration i and batch element b, we follow Parker-Holder et al. (2020) to define the time-varying instantaneous regret as $r_{i,b} = f_i(\mathbf{z}_i^{**}) - f_i(\mathbf{z}_{i,b})$. Then, the time-varying batch instantaneous regret over B points is as follows

$$r_i^B = \min_{b \leq B} r_{i,b} = \min_{b \leq B} f_i(\mathbf{z}_i^{**}) - f_i(\mathbf{z}_{i,b}), \forall b \leq B \tag{10}$$

Using Equation (9) and Theorem 2 in Parker-Holder et al. (2020), we bound the cumulative batch regret over I restarts and B parallel agents

$$R_{IB} = \sum_{i=1}^{I} r_i^B \leq \sqrt{\frac{C_1 I \beta_I}{B}\gamma(IB; k; [\mathcal{H}, \mathcal{X}])} + 2 \tag{11}$$

where $C_1 = 32/\log(1 + \sigma_f^2)$, β_I is the explore-exploit hyperparameter defined in Theorem 2 in Parker-Holder et al. (2020) and $\gamma(IB; k; [\mathcal{H}, \mathcal{X}]) \lessapprox \frac{IB}{\tilde{N}}\left(\lambda\eta\gamma(I; k_x; \mathcal{X}) + (\eta - 2\lambda)\log IB + \sigma_f^{-2}\tilde{N}^3\omega\right)$ is the maximum information gain defined over the mixed space of categorical and continuous $[\mathcal{H}, \mathcal{X}]$ in the time-varying setting defined in Theorem C.1.

□

We note that given Theorem 3.1, if we use the squared exponential kernel over the continuous variables, $\gamma(\tilde{N}B; k; \mathcal{X}) = \mathcal{O}(\left[\log \tilde{N}B\right]^{d+1})$ (Srinivas et al., 2010), the bound becomes $R_{IB} \leq \sqrt{\frac{C_1 I^2 \beta_I}{\tilde{N}}\left(\lambda\eta\left[\log \tilde{N}B\right]^{d+1} + (\eta - 2\lambda)\log IB + \sigma_f^{-2}\tilde{N}^3\omega\right)} + 2$ where $\tilde{N} \leq I$, $B \ll T$ and $\omega \in [0, 1]$.

D Full PPO Hyperparameter Search Space

We list the full search space for PPO in Table 4. The architecture and hyperparameters form a complex 15-dimensional mixed search space.

Table 4: The hyperparameters for PPO form a 15-dimensional mixed search space.

Hyperparameter	Type	Range
learning rate	log-uniform	[1e-4, 1e-3]
discount factor (γ)	uniform	[0.9, 0.9999]
entropy coefficient (c)	log-uniform	[1e-6, 1e-1]
unroll length	integer	[5, 15]
reward scaling	uniform	[0.05, 20]
batch size	integer (power of 2)	[32, 1024]
no. updates per epoch	integer	[2, 16]
GAE parameter (λ)	uniform	[0.9, 1]
clipping parameter (ϵ)	uniform	[0.1, 0.4]
π network width	integer (power of 2)	[32, 256]
π network depth	integer	[1, 5]
π use spectral norm	binary	[True, False]
V network width	integer (power of 2)	[32, 256]
V network depth	integer	[1, 5]
V use spectral norm	binary	[True, False]

Table 5: Hyperparameters for BG-PBT.

Hyperparameter	Value
no. agents (B)	8
t_{ready}	5m
$t_{\max}$	150m
α_{RL}	1
α_V	0
α_π	5
no. distill timesteps	25m

E Implementation Details

We list the hyperparameters for our method BG-PBT in Table 5. **Cong**: *Describe annealling*

Our method is built using the PyTorch version of the BRAX (Freeman et al., 2021) codebase at `https://github.com/google/brax/tree/main/brax`. The codebase is open-sourced under the Apache 2.0 License. The BRAX environments are often subject to change, for full transparency, our evaluation is performed using the 0.10.0 version of the codebase.

We note that the PPO baseline used in Table 1 is implemented in a different framework (JAX) to ours, which has some differences in network weight initialization. The hyperparameters for the PPO baseline are tuned via grid-search on a reduced hyperparameter search space (Freeman et al., 2021). Since no hyperparameters were provided for the Hopper environment, we use the default in Freeman et al. (2021).

For the Humanoid and Hopper environments, we note that PBT-style methods performed poorly across the board. This was ameliorated by linearly annealing the interval t_{ready} to not encourage myopic behavior at the start.

We run our experiments on Tesla V100 GPUs. **Cong**: *Fill in running times.*

F Additional Experiments