

Automated Reinforcement Learning (AutoRL): A Survey and Open Problems

Jack Parker-Holder^{*1}, Raghu Rajan^{*2}, Xingyou Song^{*3},
André Biedenkapp², Yingjie Miao³, Theresa Eimer⁴, Baohe Zhang², Vu Nguyen⁵,
Roberto Calandra⁶, Aleksandra Faust^{†3}, Frank Hutter^{†2,7} & Marius Lindauer^{†4}

* co-first authors (alphabetical order)

† co-last authors (alphabetical order)

¹ University of Oxford

² University of Freiburg

³ Google Research, Brain Team

⁴ Leibniz University Hannover

⁵ Amazon Australia

⁶ Facebook AI Research

⁷ Bosch Center for Artificial Intelligence

jackph@robots.ox.ac.uk, rajanr@cs.uni-freiburg.de, xingyousong@google.com

Abstract

The combination of Reinforcement Learning (RL) with deep learning has led to a series of impressive feats, with many believing (deep) RL provides a path towards generally capable agents. However, the success of RL agents is often highly sensitive to design choices in the training process, which may require tedious and error-prone manual tuning. This makes it challenging to use RL for new problems, while also limits its full potential. In many other areas of machine learning, AutoML has shown it is possible to automate such design choices and has also yielded promising initial results when applied to RL. However, *Automated Reinforcement Learning* (AutoRL) involves not only standard applications of AutoML but also includes additional challenges unique to RL, that naturally produce a different set of methods. As such, AutoRL has been emerging as an important area of research in RL, providing promise in a variety of applications from RNA design to playing games such as Go. Given the diversity of methods and environments considered in RL, much of the research has been conducted in distinct subfields, ranging from meta-learning to evolution. In this survey we seek to unify the field of AutoRL, we provide a common taxonomy, discuss each area in detail and pose open problems which would be of interest to researchers going forward.

1. Introduction

In the past decade, we have seen a series of breakthroughs using Reinforcement Learning (RL, (Sutton & Barto, 2018)) to train agents in a variety of domains, such as games (Mnih et al., 2013; Berner et al., 2019; Silver et al., 2016; Vinyals et al., 2019) and robotics (OpenAI et al., 2018), with successes emerging in real world applications (Bellemare et al., 2020; Nguyen et al., 2021). As such, there has been a surge of interest in the research community.

However, while RL has achieved some impressive feats, many of the headline results rely on heavily tuned implementations, which fail to generalize beyond the intended domain. Indeed, RL algorithms have been shown to be incredibly sensitive to hyperparameters and architectures of deep neural networks (Henderson et al., 2018; Andrychowicz et al., 2021; Engstrom et al., 2020), while there are a growing number of additional design choices, such as the agent’s objective (Hessel et al., 2019) and update rule (Oh et al., 2020). It is tedious, expensive and potentially even error-prone for humans to manually optimize so many design choices at once. There has been significant success in other areas of machine learning (ML) with *Automated Machine Learning* (AutoML, Hutter et al. (2019)). However, these methods have not yet had a significant impact in RL, with applications typically challenging given the diversity of environments and algorithms, and the nonstationarity of the RL problem.

The goal of this survey is to present the field of *Automated Reinforcement Learning* (AutoRL), as a suite of methods automating a varying degree of the RL pipeline. AutoRL serves to tackle a variety of challenges: on the one hand, the fragility of RL algorithms hinders applications in novel fields, especially those where practitioners lack vast resources to search for optimal configurations. In many settings it may be prohibitively expensive to manually find even a moderately strong set of hyperparameters for a completely unseen problem. AutoRL has already been shown to aid in such a situation for important problems, such as designing RNA (Runge et al., 2019). On the other hand, for those with the benefit of more compute, it is clear that increasing the flexibility of the algorithm can boost performance (Xu et al., 2020; Zahavy et al., 2020; Jaderberg et al., 2017). This has already been exhibited with the famed AlphaGo agent, which was significantly improved through the use of Bayesian Optimization (Chen et al., 2018).

Methods that can be considered AutoRL algorithms were shown to be effective as early as the 1980s (Barto & Sutton, 1981). However, in recent times the prevalence of AutoML has led to the nascent application of more advanced techniques (Runge et al., 2019; Chiang et al., 2019). Meanwhile the evolutionary community has been evolving neural networks alongside their weights for decades (Stanley & Miikkulainen, 2002), with methods inspired by those proving effective for modern RL (Jaderberg et al., 2017). In addition, the recent popularity of meta-learning has led to a series of works that seek to automate the RL process (Houthoofd et al., 2018; Xu et al., 2018; Kirsch et al., 2020).

In this paper we seek to provide a taxonomy of these methods. In doing so, we hope to open up a swathe of future work through the cross-pollination of ideas, while also introducing RL researchers to a suite of techniques to improve the performance of their algorithms. We believe AutoRL has a significant part to play in aiding the potential impact of reinforcement learning, both in open-ended research and practical real-world applications, and this survey could form a starting point for those looking to harness its potential.

Furthermore, we hope to attract researchers interested in AutoML more broadly to the AutoRL community, since AutoRL poses unique challenges. In particular, RL suffers from non-stationarity, as the data the agent is training on is a function of the current policy. In addition, AutoRL also encompasses environment and algorithm design specific to RL problems. We believe these challenges will require significant future work and thus outline open problems throughout this paper.

Notation	Meaning
\mathcal{S}	State space
\mathcal{A}	Action space
P	Transition function
R	Reward function
\mathcal{O}	Observation space
ρ_o	Initial state distribution
T	Set of terminal states
γ	Discount factor
V	State-value function
Q	Action-value function
J	Expected total reward function
L	Loss function
f	Objective function
θ	Neural network parameters
ϕ	Secondary neural network parameters
B	Batch size
λ	Bootstrapping hyperparameter
ζ	All hyperparameters
η	Subset of hyperparameters that are differentiable

Table 1: Table of notation used.

2. Preliminaries and Notation

We begin by defining a Markov Decision Process (MDP) as a 7-tuple $(\mathcal{S}, \mathcal{A}, P, R, \rho_o, T, \gamma)$, where \mathcal{S} is the set of states, \mathcal{A} is the set of actions, $P : \mathcal{S} \times \mathcal{A} \rightarrow \mathcal{S}$ describes the transition dynamics, $R : \mathcal{S} \times \mathcal{A} \times \mathcal{S} \rightarrow \mathbb{R}$ describes the reward dynamics, $\rho_o : \mathcal{S} \rightarrow \mathbb{R}^+$ is the initial state distribution, T is the set of terminal states and $\gamma \leq 1$ is the discount factor¹.

We further define a POMDP with two additional components: \mathcal{O} represents the set of observations and $\Omega : \mathcal{S} \times \mathcal{A} \times \mathcal{O} \rightarrow \mathbb{R}^+$ describes the probability density function of an observation given a state and action. This makes it an 9-tuple $(\mathcal{S}, \mathcal{A}, P, R, \mathcal{O}, \Omega, \rho_o, T, \gamma)$.

Note that in many cases this is not sufficient to fully define the task considered (for example, if the dynamics are sampled from a parameterized distribution, such as having a cartpole environment where the length of the pole is drawn from a distribution). Where necessary we will discuss this alongside the methods which require it. Many of the algorithms we discuss are designed to optimize agents to maximize reward in a MDP/POMDP with a fixed parameterization. However, we also discuss those which seek to learn or automate components of the environment itself.

To provide sufficient background information, we briefly define the predominant classes of RL algorithms. In almost all cases, RL considers the problem of finding a *policy* $\pi_\theta : \mathcal{S} \rightarrow \mathcal{A}$

1. γ in many instances is treated as a hyperparameter, e.g., to make optimization tractable during training, while evaluation usually reports undiscounted rewards (i.e. $\gamma = 1$).

parameterized by θ (e.g., the weights of a neural network) to maximize cumulative reward:

$$\max_{\theta} J(\theta; \zeta) \quad \text{where} \quad J(\theta; \zeta) = \mathbb{E}_{\tau \sim \pi_{\theta}} \left[\sum_{t \geq 0} \gamma^t r_t \right], \quad (1)$$

where ζ is a set of hyperparameters of the pipeline, $\tau = (s_0, a_0, r_0, s_1, \dots)$ is a trajectory (consisting of observed states, actions and rewards denoted by s_t , a_t and r_t at timestep t) via π_{θ} 's interaction with the MDP, and $\sum_{t \geq 0} \gamma^t r_t$ is the total discounted reward.

However, other objectives $f(\zeta, \theta)$ may be considered along with extra parameters ζ , and may usually be framed in terms of a general bi-level optimization, i.e.

$$\max_{\zeta} f(\zeta, \theta^*) \quad \text{s.t.} \quad \theta^* \in \arg \max_{\theta} J(\theta; \zeta), \quad (2)$$

where $\max_{\zeta} f(\zeta, \theta^*)$ can be considered the *outer loop*, while $\max_{\theta} J(\theta; \zeta)$ can be considered the *inner loop*, which may be equivalent to minimizing some *loss*, i.e. $\min_{\theta} \mathcal{L}(\theta; \zeta)$, for some methods requiring automatic differentiation. The notation used in the paper is summarized in Table 1.

Example objectives for f include *generalization* (Zhang et al., 2018), where ζ may consist of hyperparameters or architectures, and $f(\zeta, \theta^*)$ can be defined as the *validation* reward, i.e. the reward in the outer loop, whereas $J(\theta^*; \zeta)$ can be considered the *training* reward, i.e. the reward in the inner loop. In other cases, $f(\zeta, \theta^*)$ may be a weighted sum of policy inference speed and rewards. **Optimizing ζ will be the main purpose of this survey**, with common definitions of ζ outlined in Section 3, while optimization methods will be outlined in Section 4.

We now provide a brief background on popular methods of optimizing the inner loop, i.e., θ .

2.1 Inner Loop Optimization

There are several classes of methods used to optimize θ (Sutton & Barto, 2018). At a high level, such methods may be classified into *model-free* and *model-based* methods depending on whether they use a model of the environment or not.

Model-free methods: A common class of model-free methods is *policy gradients* (Sutton et al., 1999a), which seeks to optimize $J(\theta)$ via gradient descent using the fact that

$$\nabla_{\theta} J(\theta) = \mathbb{E}_{\tau \sim \pi_{\theta}} \left[\sum_{t \geq 0} r_t \nabla_{\theta} \log \pi_{\theta}(a_t | s_t) \right], \quad (3)$$

assuming the notion of an action distribution from the policy: $a \sim \pi_{\theta}(\cdot | s)$. Policy gradient algorithms have been used extensively in robotics (Haarnoja et al., 2018; Tan et al., 2018), with several large scale applications (Berner et al., 2019).

In contrast, *value-based* methods seek to learn an action-value function predicting the expected discounted cumulative reward from a given state if an action is taken (Watkins &

Dayan, 1992) and policy π_θ is followed thereafter:

$$Q_\theta(s, a) = \mathbb{E}_{\tau \sim \pi_\theta} \left[\sum_{t \geq 0} r_t \middle| s_0 = s, a_0 = a \right], \quad (4)$$

for each initial state-action pair $(s, a) \in \mathcal{S} \times \mathcal{A}$. The policy therefore seeks to take the action maximizing the so-called *Q-values*, i.e. $\pi_\theta(s) \in \arg \max_a Q_\theta(s, a)$. A prototypical method based on temporal difference learning (Sutton & Barto, 2018) is Q-learning (Watkins & Dayan, 1992); in its most basic form, it maintains an estimate $Q_\theta : \mathcal{S} \times \mathcal{A} \rightarrow \mathbb{R}$ of the optimal value function, and given a sequence of transition tuples $(s_t, a_t, r_t, s_{t+1})_{t \geq 0}$, updates $Q_\theta(s_t, a_t)$ towards the target $r_t + \gamma \max_{a \in \mathcal{A}} Q_\theta(s_{t+1}, a)$, for each $t \geq 0$. The canonical value-based method in deep RL is DQN (Mnih et al., 2013). Since then, there has been an explosion of interest in the field, and a swathe of improvements to this algorithm (van Hasselt et al., 2016; Schaul et al., 2016; Wang et al., 2016; Bellemare et al., 2017; Fortunato et al., 2018). These innovations were combined in the Rainbow algorithm (Hessel et al., 2018).

Actor-critic methods (Sutton and Barto (2018)) usually combine policy gradient and value-based methods. In this case, the actor represents the policy which is learned using policy gradients based on the value function learnt by the critic (see e.g., Lillicrap, Hunt, Pritzel, Heess, Erez, Tassa, Silver, & Wierstra, 2016; Mnih, Badia, Mirza, Graves, Lillicrap, Harley, Silver, & Kavukcuoglu, 2016).

The model-free methods mentioned above can be practically organized into three components: a learner, a replay buffer, and potentially multiple actors. The *learner* performs gradient descent optimization over the *replay buffer*, which contains trajectory data collected by *actors* interacting with the MDP.

Model-based methods: Alternatively, *Model-Based* Reinforcement Learning (MBRL) methods make use of models of the environment, such as the transition function P and the reward function R . This may be in the form of the *true* model provided to the agent, famously used by the AlphaGo (Silver et al., 2016) algorithm, or the model may also be *learned* during training to predict the environment dynamics, either for training a policy (Sutton, 1991; Hafner et al., 2020; Ha & Schmidhuber, 2018; Kaiser et al., 2020) or for planning (Hafner et al., 2019; Chua et al., 2018; Tassa et al., 2012; Schrittwieser et al., 2020). In addition to minimizing the losses involved for model-free methods above, this may entail further minimizing, e.g., a mean-squared error (MSE) loss or negative log likelihood (NLL) loss on learning P and R .

Planning based approaches led to one of the most prominent successes in RL, with the AlphaGo agent making use of Monte Carlo Tree Search (MCTS, Browne et al. (2012)) guided by neural network approximators for the policy and value functions. MCTS performs a heuristic search by randomly sampling rollouts for a given state. This requires the true model of the environment. MuZero (Schrittwieser et al., 2020) takes these ideas one step further. It matches the performance of AlphaZero on Go, chess and shogi, while also performing well on Atari games with a learned model. An alternative planning approach is Model Predictive Control (MPC, Garcia et al. (1989)), which solves an optimization problem online. This has been used in Deep RL, for example, in the PETS algorithm (Chua et al., 2018) or PlaNet (Hafner et al., 2019).

In contrast, Dyna (Sutton, 1991) is a canonical MBRL algorithm that essentially treats a learned dynamics model as an environment for model-free RL. Dyna-style approaches are popular since they facilitate faster inference at deployment time (forward-pass of the policy rather than an optimization loop) and have been shown to be highly sample-efficient both from proprioceptive states (Janner et al., 2019) and pixels (Hafner et al., 2020).

2.2 Non-Stationarity of the Optimization Problem

In various domains of AI, such as evolutionary algorithms or deep learning, it is well known that some hyperparameters need to be adapted over time to achieve the best performance (see e.g., Moulines & Bach, 2011; Doerr & Doerr, 2020). A prime example for this are learning rates in deep learning. Keeping static learning rates might result in very slow learning or even in diverging learning behavior. As deep neural networks are the commonly used method of function approximation in the current landscape of RL, it is to be expected that similar dynamic treatments of hyperparameters are needed in RL. In fact, existing optimization experiments have observed that dynamically adapting learning rates is also beneficial for model-free and model-based RL (Jaderberg et al., 2017; Zhang et al., 2021).

Additionally, the nature of RL further amplifies the potential non-stationarity of hyperparameters, even in stationary environments (Igl et al., 2021). With the trial-and-error approach to learning, an RL agent constantly (re-)generates its own training data, which is highly dependent on the current instantiation of the agent. Thus, hyperparameter settings might require very different values over the whole training run. Indeed, besides classical static optimization approaches, methods for AutoRL typically include approaches for dynamically selecting configurations. We will discuss these more in Section 4 when we introduce the current state of methods for AutoRL.

3. What Needs to be Automated?

In this section, we introduce the set of problems AutoRL seeks to solve. Figure 1 demonstrates some of the tunable components in a standard RL pipeline, which range from entire algorithms to a single hyperparameter. The following subsections begin at a high level, approximately equating to the sequence of decisions that need to be made when first considering using RL to solve a problem.

3.1 How Do We Design Tasks?

When using RL for a new problem setting, designing the learning environment is usually the first problem to be considered. First of all, the user must specify a reward function $R(s, a, s')$. This is typically assumed to be provided in many RL papers and common benchmarks (Bellemare et al., 2012; Brockman et al., 2016), yet it is certainly non-trivial to be set for many real world problems. For example, for robotic manipulation, the reward could be provided once the task is completed, or given based on some intermediate goal, such as reaching the object of interest. These differences can often have a dramatic impact on the success of policy optimization (Gleave et al., 2021).

Often, it is also necessary to determine what should be provided as an observation for the agent. For example, when training from pixels, it is common to deploy a series of

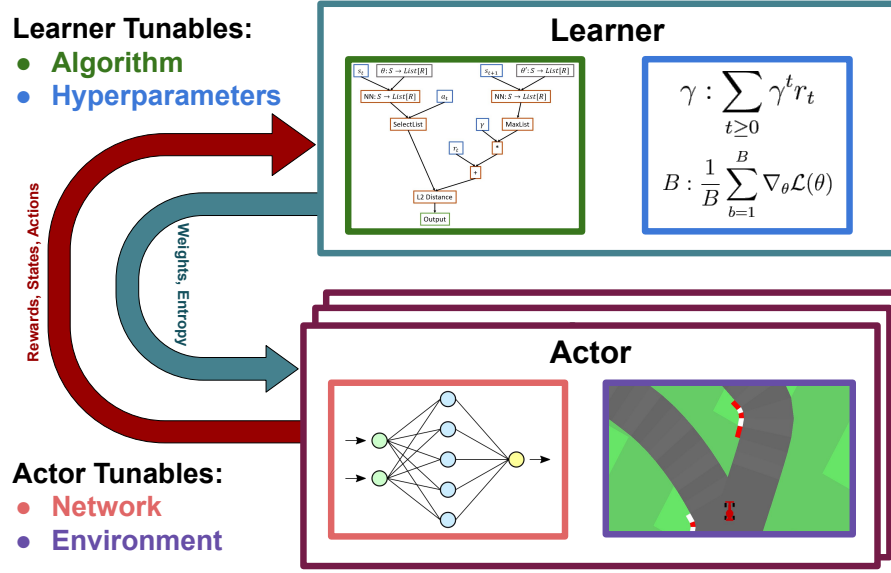


Figure 1: Components, or definitions of ζ , that have been commonly tuned in AutoRL approaches. Most pipelines consist of a learner and actors. The learner possesses tunable algorithms (e.g. Q-learning computation graph by Co-Reyes et al. (2021)) and hyperparameters (e.g.: discount factor γ and batch size B). The actors possess the network with weights, and the environment (e.g. Car-Racing by Brockman et al. (2016)).

preprocessing steps that may be customized per environment. Indeed, one of the very first use successes of deep RL made use of greyscale to simplify the learning problem and to stack consecutive frames to form the observation (Mnih et al., 2013). While such additional processing is not always needed, using raw frames directly can be demanding in terms of computation and memory requirements (Mnih et al., 2013). In addition, a large action space makes it significantly harder for an agent to begin learning; so it is often required for researchers to pick the available actions for an agent, or consider learning them (Farquhar et al., 2020).

Finally, the environments to train on can also be controlled by the designer. We discuss a wide variety of automated environment design methods in Section 4.8.

3.2 Which Algorithm Do We Use?

Once we are able to define an MDP (or POMDP) to solve, the next question is the choice of algorithm. In cases where RL has already demonstrated strong performance, the choice may seem rather simple. For example, when playing a new Atari game, a variant of DQN can be expected to perform well. For a continuous control task from MuJoCo (Todorov et al., 2012), an actor critic algorithm such as SAC (Haarnoja et al., 2018) would likely be a strong baseline. However, even for these standard benchmarks, RL agents are known to be brittle (Henderson et al., 2018; Andrychowicz et al., 2021; Engstrom et al., 2020) and this choice

is not as simple as it seems. For a completely new problem, the challenge is significantly greater and prevents the uptake of RL for real world problems. Without expertise in the field or vast computational resources, many use cases may result in sub-optimal solutions as arbitrary algorithms are used based on success in somewhat unrelated problems.

To tackle the problem of which algorithm to use, there are multiple possible avenues. One could use a learning to learn approach (Andrychowicz et al., 2016; Chen et al., 2017) where a meta-learner learns an agent that can perform well on a set of related tasks. The agent would be trained over a distribution of tasks and learn to recognize the task during rollouts at test time. Such recognition capabilities can be achieved by a Recurrent Neural Network (RNN), for instance, that rolls out a policy depending on its state that would encode the task at hand.

One could learn the objective function itself, where each objective function defines a new algorithm. In the most general form, RL’s objective is to maximize expected cumulative reward $J(\theta; \zeta)$ in a given environment. In the context of deep RL, this objective is not differentiable with respect to model parameters; therefore proxy objectives are used in practice, which have a strong impact on the learning dynamics. Indeed, many advancements in deep RL result from improvements in the objective functions, such as double Q-learning (van Hasselt et al., 2016), distributional value functions (Bellemare et al., 2017) and yet more (Lillicrap et al., 2016; Schulman et al., 2017a; Haarnoja et al., 2018). These algorithms have fundamental differences in the objective functions, which are designed by human experts. Even smaller tweaks to known objective functions can make a big difference, e.g. Munchausen-DQN (Vieillard et al., 2020) and CQL (Kumar et al., 2020b), yet these tweaks require significant theoretical analysis and empirical experiments to validate their effectiveness.

One could also make a categorical choice between existing algorithms based on multiple evaluations. In AutoML, such a choice of algorithm can be automated through algorithm selection (Rice, 1976). In algorithm selection, a meta-learning model is used to decide which algorithm to use for an environment at hand. The so called selector is trained based on past observed performances and features of the environment. While this alleviates the need of expert knowledge, it requires potentially many resources to gather enough performance data to learn a well performing selector.

We discuss works related to learning algorithms in RL in Section 4.7.

3.3 What about Architectures?

Many of the large breakthroughs in machine learning have come through the introduction of new architectures (Krizhevsky et al., 2012; He et al., 2016; Vaswani et al., 2017). To automate this discovery, the field of *Neural Architecture Search* (NAS) (Elsken et al., 2019; Lindauer & Hutter, 2020) has become an active area of research over the past few years. In contrast to supervised learning, very little attention has been paid to the design of neural architectures in RL. For tasks from proprioceptive states, it is common to use two or three hidden layer feedforward MLPs, while many works learning from pixels still make use of the convolutional neural network (CNN) architecture used in the original DQN paper, known as “Nature CNN”. More recently, it has become commonplace to make use of the network proposed in the IMPALA paper (Espeholt et al., 2018), which is now referred to as “IMPALA-CNN”. While

the IMPALA-CNN has been shown to be a stronger architecture for vision and generalization (Cobbe et al., 2020, 2019), there has been little research into alternatives, although some have focused on using attention modules for policies (Parisotto et al., 2020; Tang et al., 2020; Zambaldi et al., 2019).

Along with IMPALA-CNN, there is evidence that deeper and denser networks, use of different nonlinearities, as well as normalizers, such as Batch Normalization, can improve current methods across a suite of manipulation and locomotion tasks (Sinha et al., 2020; Song et al., 2020), even for the MLP setting. Kumar et al. (2020a) further expanded upon the downside of underparameterization for value-based methods. In general, there remains little conceptual understanding (and uptake) on architectural design choices and their benefits in the RL domain. While Cobbe et al. (2020, 2019) have shown *overparameterization* and batch normalization (Ioffe & Szegedy, 2015) effects in RL generalization, it is unclear whether they can be explained by supervised learning theories, i.e. *implicit regularization* (Neyshabur, 2017; Neyshabur et al., 2015), Neural Tangent Kernels (Jacot et al., 2018; Arora et al., 2019), complexity measures (Neyshabur et al., 2019) and landscape smoothness (Santurkar et al., 2018).

We discuss works seeking to address neural architectures in RL in a variety of sections, given that it can be addressed using many different approaches.

3.4 Last but not Least: What about Hyperparameters?

Having defined the task and selected (or learned) an algorithm and architecture, the last remaining challenge is selecting hyperparameters. The most widely studied area of AutoRL is the sensitivity of RL algorithms to hyperparameters. Indeed, in one of the best-known studies, Henderson et al. (2018) found that many of the most successful recent algorithms were brittle with respect to hyperparameters, implementation, or even seed, while Islam et al. (2017) noted that it is challenging to compare benchmark algorithms from different papers given the impact of hyperparameters on performance.

One of the better understood hyperparameters is the discount factor γ , which determines the time-scale of the return. Prokhorov and Wunsch (1997) as well as Bertsekas and Tsitsiklis (1996) found that lower discount factors led to faster convergence, with the potential risk of leading to myopic policies. Singh and Dayan (1996) explored the manner in which TD learning is sensitive to the choice of its step size and eligibility trace parameters.

Looking at specific algorithms, Andrychowicz et al. (2021) conducted an extensive investigation into design choices for on-policy actor critic algorithms. They found significant differences in performance across loss functions, architectures and even initialization schemes, with significant dependence between these choices. Obando-Ceron and Castro (2020) also explored design choices for off-policy RL, highlighting the differing performance for MSE vs. Huber loss functions, while also assessing the importance of n-step returns, which Fedus et al. (2020) and Rowland et al. (2020) also studied. Bas-Serrano et al. (2021) showed that the performance improved by ensuring the convexity in the Q-learning using logistic Bellmann error function. Furthermore, Liu et al. (2021b) showed that the choice of regularizer can also significantly impact performance.

Finally, beyond the well-flagged hyperparameters, there are even significant *code level* implementation details. Henderson et al. (2018) identified this and showed that different

codebases for the *same algorithm* produced markedly different results. Furthermore, Engstrom et al. (2020) investigated implementation details in popular policy gradient algorithms (PPO, Schulman et al. (2017a) and TRPO Schulman et al. (2015)), where details such as reward normalization were found to play a crucial role in RL performance. With this area being the most studied component of AutoRL, we discuss various different solution approaches to the hyperparameter optimization problem in Sections 4.1 - 4.6.

4. Methods for Automating Reinforcement Learning

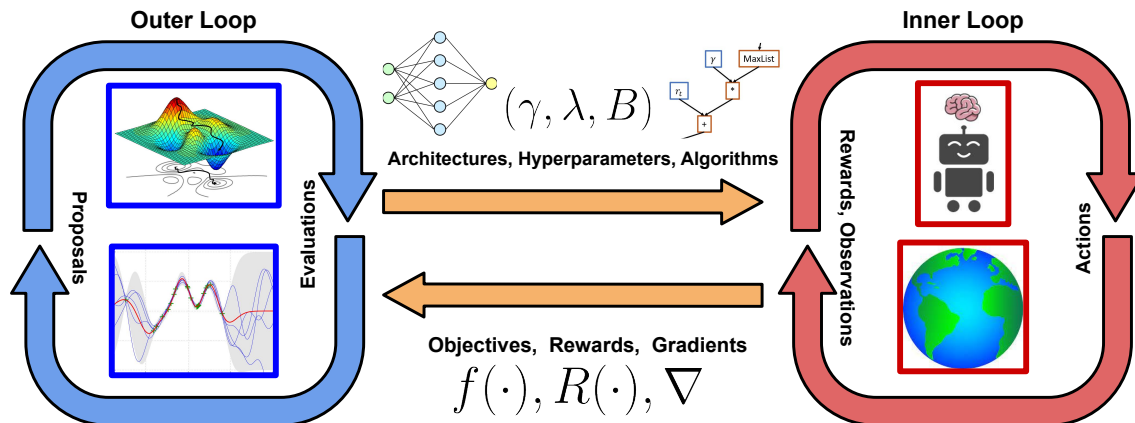


Figure 2: Most approaches can be organized in terms of an outer loop and inner loop, where the outer loop sends specifications, such as architecture specification, hyperparameters, and algorithms, while the inner loop sends back objectives, rewards, and gradients. Images from (Pérez-Cruz et al., 2013; Co-Reyes et al., 2021; Guo, 2020).

In this section, we survey methods for AutoRL, spanning a wide range of communities and encompassing a broad array of techniques. In general, most methods can be conveniently organized in terms of a combination of an *inner loop*, which consists of a standard RL pipeline, and an *outer loop*, which optimizes the agent configuration. Each loop can be optimized via either blackbox optimization or gradient-based methods, although the combination of gradients for the outer loop and blackbox for the inner loop blackbox is not possible, as the inner loop blackbox setting would make gradients unavailable. This is shown in Table 2 and Figure 2.

	Benefits	Downsides
Blackbox	Flexible/No assumptions on pipeline	Can be sample-inefficient
Gradient	Scalable and sample-efficient	Inflexible/Requires differentiable pipelines

Table 2: Comparison between gradient-based and blackbox approaches.

We summarize the taxonomy of AutoRL methods along broad classes (which often overlap) in Table 3. Each has its own pros and cons, as there are inevitably trade-offs, such as sample vs. compute efficiency. The scope for each method is also vastly different, from tuning a single hyperparameter, to learning a reward function, or an entire algorithm from scratch. In each subsection we first discuss related methods before proposing open problems.

Table 3: A high level summary of each class of AutoRL algorithms. In each case, the properties are a generalization, and specific algorithms in each class may vary.

Class	Algorithm properties	What is automated?
Random/Grid Search (4.1)	††† ■ ⇒ ✓	hyperparameters, architecture, algorithm
Bayesian Optimization (4.2)	††† ■ ⇒ ✓	hyperparameters, architecture, algorithm
Evolutionary Approaches (4.3)	††† ■ ⇒ ✓	hyperparameters, architecture, algorithm
Population Based Training (4.4)	††† ■ ⇒ ✓	hyperparameters, architecture
Meta-Gradients (4.5)	† ∇ → ●	hyperparameters
Blackbox Online Tuning (4.6)	† ■ → ✓	hyperparameters
Learning Algorithms (4.7)	††† ■ ⇒ ●	algorithm
Environment Design (4.8)	††† ■ ⇒ ●	environment

† only uses a single trial, ††† requires multiple trials

∇ requires differentiable variables, ■ works with non-differentiable hyperparameters

⇒ parallelizable → not parallelizable

✓ works for any RL algorithm, ● works for only some classes of RL algorithms,

4.1 Random/Grid Search Driven Approaches

We begin by discussing the most simple methods: Random Search (Bergstra & Bengio, 2012) and Grid Search (Hutter et al., 2019). As the names imply, Random Search randomly samples hyperparameter configurations from the search space and Grid Search divides the search space into fixed grid points which are evaluated. Due to their simplicity, Random Search and Grid Search can be used to select a list of hyperparameters², exhaustively evaluate all of them and pick the best configuration, making them very general approaches. Indeed, Grid Search is still the most commonly used method in RL, featuring in the vast majority of cases where hyperparameters are tuned, but should not be considered as the most efficient approach.

These classical approaches do not take the potential non-stationarity of the optimization problem (recall Section 2.2) into account. We describe the issue below, using Figure 3. Assume we use these procedures to *minimize* the loss of an RL algorithm that has two continuous hyperparameters ζ_0 and ζ_1 (see Figure 3). We evaluate 9 hyperparameter settings in parallel. At $t = 0$ (First Column of Figure 3), we observe the performance of all settings as indicated by the blue shaded areas. It is clear that changes in ζ_0 result in little difference in

2. As mentioned in Table 3, these approaches are applicable to architectures and algorithms as well, but they are usually only applied to hyperparameters. They are applied to architectures in the form of selecting, e.g., number of layers of the network or the width of a layer, but we include such basic architectural choices under hyperparameters.

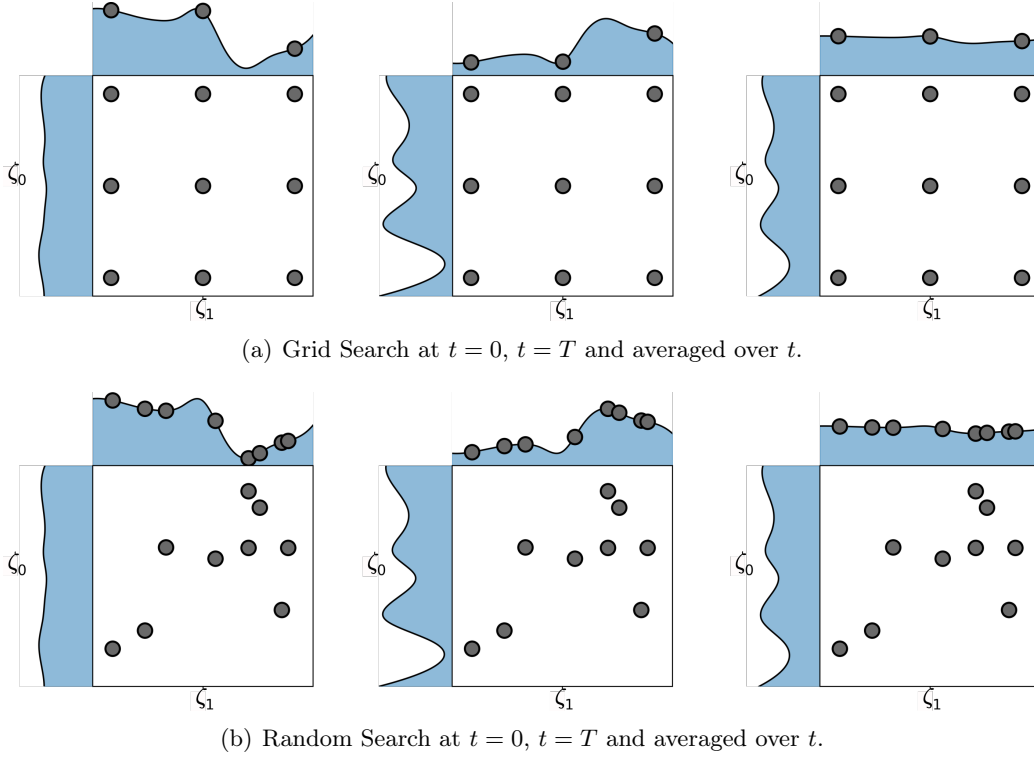


Figure 3: The non-stationarity of the AutoRL problem poses new challenges for classical (hyperparameter) optimization methods. Generally, grid and random search keep the hyperparameters ζ_0 and ζ_1 fixed throughout a run. If the loss landscape changes during the run (see difference between leftmost and middle images) these methods optimize the average performance over time (right most images). Circles represent hyperparameters that are sampled at the beginning of the optimization procedure and the blue shaded area depicts the RL agent’s loss. This figure is based on a figure for the stationary case by Bergstra and Bengio (2012).

the agents performance, whereas changes in ζ_1 result in large performance differences. While random search is likely to observe the performance of 9 unique values per hyperparameter, grid search only observes 3. At $t = T$ (Middle Column of Figure 3), we observe that the loss landscape has shifted and that now both hyperparameters have an impact on the final performance. Furthermore, while in the early phase of the optimization procedure, large values of ζ_1 were beneficial, now smaller values are preferable. Looking at the loss averaged over the whole optimization procedure (Last Column of Figure 3) we can see that this view, although often used with static configuration approaches, abstracts away a lot of information. For example, both approaches would view ζ_1 as much less important than ζ_0 even though it had an overall larger impact during the whole optimization procedure. At $t = 0$, low values for ζ_1 resulted in bad performance whereas at $t = T$, large values resulted in bad performance. If we now average the performance over time, it appears to have little to no impact. Similarly, looking only at the final performance hides a lot of valuable information

and can lead to sub-optimal hyperparameter configurations at different stages of the run. Thus, these methods might be insufficient in cases where changes in hyperparameters are required during the run to achieve the best performance.

A common way to improve the performance of Random Search is with Hyperband (Li et al., 2017), a bandit-based configuration evaluation for hyperparameter optimization. It focuses on speeding up Random Search through adaptive resource allocation and early-stopping. The hyperparameter optimization task is considered as a pure-exploration non-stochastic infinite-armed bandit problem where a predefined resource like iterations, data samples, or features is allocated to randomly sampled configurations. In particular, Hyperband uses Successive Halving (Jamieson & Talwalkar, 2016) which allocates a budget to a set of hyperparameter configurations. This is done uniformly, and after this budget is depleted, half of the configurations are rejected based on performance. The top 50% are kept and trained further with twice the budget. This process is repeated until only one configuration remains. Zhang et al. (2021) used Random Search and Hyperband for tuning hyperparameters of their MBRL algorithm. Furthermore, Zhang et al. (2021) analyzed the correlation of configuration performance across the considered budgets, and based on low correlations, they moved from static to dynamic configuration methods.

Open Problems: The key drawback of random/grid search approaches is being unable to leverage the information regarding promising regions of the hyperparameter search space for making informed decisions. During the optimization, this information becomes clearer as more and more hyperparameter configurations are tried out. However, as these approaches solely focus on exploration and do not exploit this information, they typically scale poorly as the search space increases in size.

4.2 Bayesian Optimization

The next set of approaches involved are those which inherently have a notion of sequential decision making. Bayesian Optimization (BO, Mockus (1974), Jones et al. (1998), Brochu et al. (2010)) is one of the most popular approaches to date, used for industrial applications (Golovin et al., 2017; Balandat et al., 2020; Perrone et al., 2021) and a variety of scientific experimentation (Frazier & Wang, 2015; Hernández-Lobato et al., 2017; Li et al., 2018; Griffiths & Hernández-Lobato, 2020; Tran et al., 2021; van Bueren et al., 2021). For RL applications, one of the most prominent uses of BO was for tuning AlphaGo’s hyperparameters, which include its core Monte Carlo Tree Search (MCTS) (Browne et al., 2012) hyperparameters and time-control settings. This led to an improvement of AlphaGo’s win-rate from 50% to 66.5% in self-play games (Chen et al., 2018). In Figure 4, we demonstrate the general concept of Bayesian Optimization in the RL case.

Because of the fairly large optimization overhead, standard BO methods require expensive black-box evaluations, such as training an ML algorithm to the end to observe the accuracy. This way of training is time-consuming and costly because each set up may take hours and days to run. An alternative choice to the standard BO for tuning RL hyperparameters is leveraging different fidelities (Cutler et al., 2014; Kandasamy et al., 2016), such as with different number of seeds and epochs. Particularly, recent works have attempted to exploit internal information readily available from RL applications for improving the optimization, which we describe below.

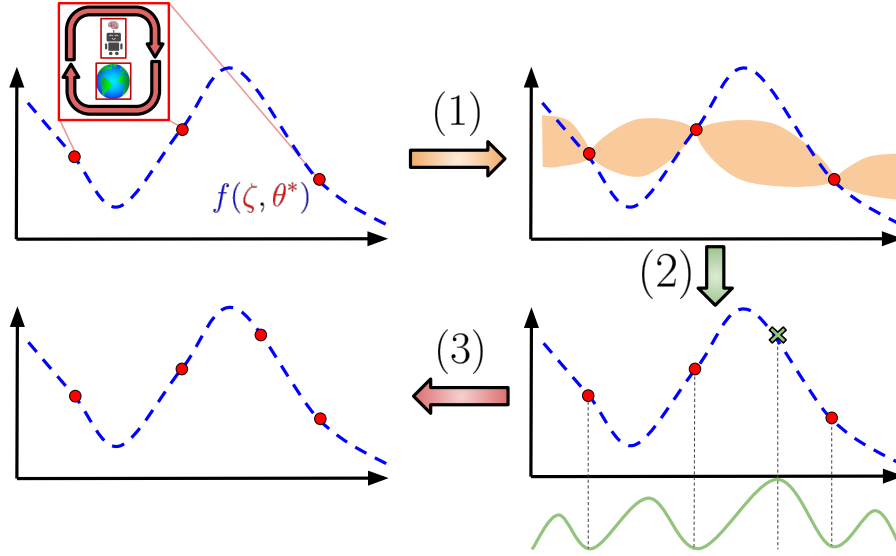


Figure 4: Bayesian Optimization, which consists of 3 main steps. (1): A regressor (commonly a Gaussian Process) is used to construct uncertainty estimates on the blackbox function $f(\cdot)$ given previous evaluation data. (2): An acquisition function is constructed from the regressor, which represents the explore-exploit tradeoff on f . (3): The argmax of the acquisition function is used for the next trial.

BOIL (Nguyen et al., 2020) enhances tuning performance by modelling the training curves, providing a signal to guide search. It transforms the whole training curve into a numeric score to represent high vs low-performing curves. Then, BOIL introduces a data augmentation technique leveraging intermediate information from the training curve to inform the underlying GP model. The algorithm not only selects a hyperparameter setting to evaluate, but also how many epochs it should evaluate. Thus, BOIL makes it possible to run a larger number of cheap (but high-utility) experiments, when cost-ignorant algorithms would only be able to run a few expensive ones, resulting in greater sample-efficiency than traditional BO approaches when tuning deep RL agents.

It is also possible to exploit *external* knowledge of the maximum achievable return, i.e. knowing $\max_{\tau} \sum_{t \geq 0} \gamma^t r_t$ to improve hyperparameter tuning in RL. This optimum value is available in advance for some RL tasks, such as the maximum reward (when $\gamma = 1$) being 200 in CartPole. To utilize such knowledge, Nguyen and Osborne (2020) proposed to (i) transform the surrogate model and (ii) select the next point using the optimum value. They showed that exploiting this external information can improve the optimization.

In addition, Hertel et al. (2020) employed Successive Halving (Jamieson & Talwalkar, 2016), Random Search and BO and concluded that Bayesian Optimization with a noise robust acquisition function is the best choice for hyperparameter optimization in RL tasks. Finally, Lu et al. (2021) showed it was possible to improve the performance of agents trained with offline RL when tuning hyperparameters using BO (Wan et al., 2021).

Open Problems: BO-based approaches usually perform static tuning, which may not be the most effective for RL. While there are BO approaches (Parker-Holder et al., 2020a) that take the temporal nature of the optimization, especially relevant for RL, into account, these are scarce to the best of our knowledge.

4.3 Evolutionary Approaches

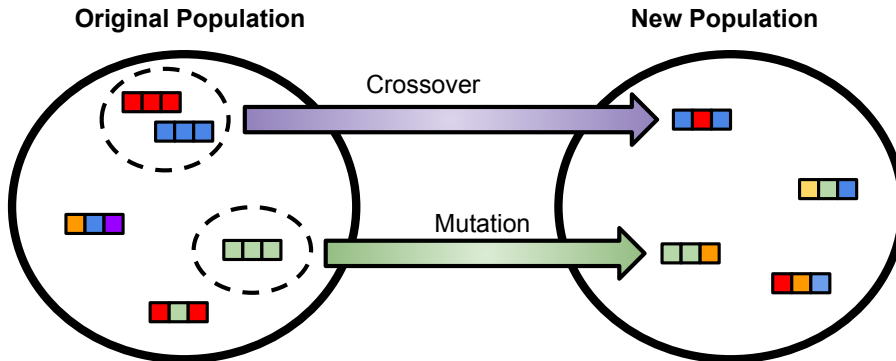


Figure 5: Most evolutionary algorithms consist of updating entire populations, usually by mechanisms such as crossover (between multiple genomes) or mutation (on a single genome).

Evolutionary approaches are widely used for various optimization tasks in different fields. These may have different ways of representing the tasks and mechanisms to mutate, recombine, evaluate and select parameters. Such mechanisms are represented in Figure 5.

While many in the deep RL community are familiar with Evolution strategies (ES, Rechenberg (1973)), a specific kind of evolutionary approach that can be used in lieu of an RL algorithm to optimize policies (Such et al., 2018; Lehman et al., 2018; Chrabaszcz et al., 2018), there remains little cross pollination with the broader evolutionary computation community. One particular subfield relevant for AutoRL is neuroevolution (Stanley et al., 2019), which has been used to evolve both weights and architectures, inspired by biological brains. In particular, the NEAT algorithm was shown to effectively evolve architectures for Pole Balancing in the early 2000s (Stanley & Miikkulainen, 2002), predating the surge of interest in deep RL. NEAT was made more expressive with the extension to HyperNEAT (Stanley et al., 2009), which was evaluated in a robotic control task in the original paper. Since then, NEAT and HyperNEAT have been evaluated in a series of control problems (Lee et al., 2013; Gomez et al., 2006; Clune et al., 2009; Risi & Stanley, 2013), even training agents to play Atari games prior to the seminal DQN paper (Hausknecht et al., 2014). More recently WANNs (Gaier & Ha, 2019) showed it was possible to use NEAT to solve RL tasks by only evolving network topology, using a single randomly initialized weight parameter.

Evolutionary methods has also been used to search for the hyperparameters of RL algorithms. Eriksson et al. (2003) used a real-number Genetic Algorithm (GA, Michalewicz (2013)), which encodes the hyperparameters of the RL algorithm via genes in every individual

of the population, to tune the hyperparameters of SARSA(λ), applying the approach to control a mobile robot. Cardenoso Fernandez and Caarls (2018) used GAs to tune the hyperparameters of RL algorithms in simple settings and achieved good performance by combining with automatic restarting strategies (Fukunaga, 1998) to escape from local minima. Similarly, Sehgal et al. (2019) also showed that GAs can be applied to improve the performance of DDPG with Hindsight Experience Replay (Andrychowicz et al., 2017) by tuning hyperparameter configurations. Ashraf et al. (2021) used a Whale Optimization Algorithm (WOA, Mirjalili and Lewis (2016)), which is inspired by the hunting strategies of humpback whales, to optimize the hyperparameters of DDPG in various RL tasks in order to improve the performance.

Open Problems: One of the key challenges of evolutionary approaches is their inefficiency, often requiring thousands of CPU cores to achieve strong results. While this may be possible for well-equipped industrial labs, it renders many methods impractical for small to medium sized groups and in many practical applications. Furthermore, there remain very few cases of large-scale evolutionary approaches being applied to both hyperparameters (ζ) and neural network parameters (θ), although recent efforts such as ES-ENAS (Song et al., 2021) have attempted to do so by combining different evolutionary algorithms.

4.4 Population Based Training

In this section we focus on a specific type of evolutionary algorithm, known as *Population Based Training* (PBT, Jaderberg et al. (2017)). While PBT inherits ideas from many evolutionary approaches (Spears, 1995; Bäck, 1998; Gloger, 2004; Clune et al., 2008), it refers to a *specific class of methods* which have been particularly successful in RL. PBT seeks to replicate how a human would observe experiments; it trains multiple agents in parallel and periodically replaces weaker agents with copies of stronger ones. Taking inspiration from Lamarckian Evolutionary Algorithms (Whitley et al., 1994), where parameters are inherited whilst hyperparameters are evolved, PBT seeks to “exploit” stronger agent weights, while “exploring” the hyperparameter space, typically through random perturbations. The benefit of this procedure is that it is possible to explore the hyperparameter space with the same wall clock time as a single training run, given access to parallel computational resources.

Another key benefit of PBT is the ability to learn hyperparameter *schedules*, which were shown in the original paper to be particularly effective in RL, likely due to the non-stationarity of the problem (see: Section 2.2). As such, PBT has had a prominent role in many high profile RL publications (Schmitt et al., 2018; Liu et al., 2019b, 2021a; Espeholt et al., 2018; Jaderberg et al., 2019; Team et al., 2021; Zhang et al., 2021).

In the following we give a simplified view on how PBT-like approaches are able to produce hyperparameter schedules. For this we consider a dynamic version of random search: a version that resamples the hyperparameters after a fixed time interval (see Figure 6). Assume we use these procedures to *minimize* the loss of an RL algorithm that has two continuous hyperparameters ζ_0 and ζ_1 , as in Figure 3. With the dynamic variant of random search however, we change the hyperparameter settings on the fly. In this example, changing the hyperparameters on the fly allows to find better performing hyperparameter schedules than keeping the hyperparameters fixed throughout the run. Although taking the non-stationarity of the optimization problem into account can result in better performing agents, it poses

interesting new challenges for the field of AutoRL. PBT-like and evolutionary approaches are a natural way of handling the non-stationarity, although they might require far too many resources in cases where hyperparameters need not be changed on the fly.

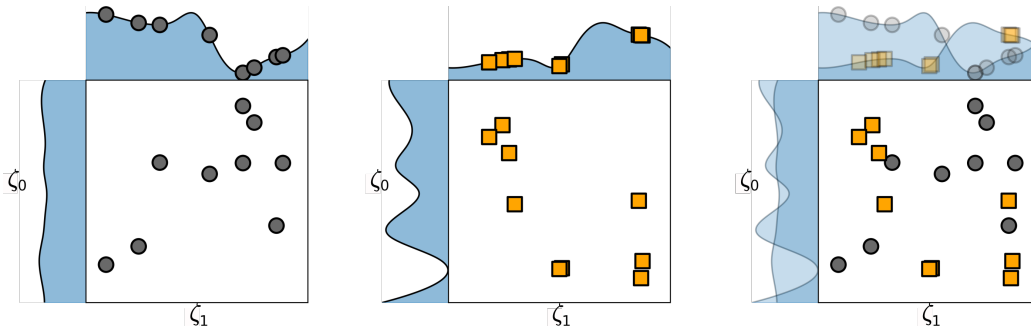


Figure 6: Dynamic random search at $t = 0$ (first column), $t = T$ (second column) and averaged over t . Dynamic random search resamples the hyperparameters ζ_0 and ζ_1 after a fixed time interval T . Circles represent hyperparameters that are sampled at the beginning ($t = 0$) of the optimization procedure, orange squares hyperparameters that were sampled at $t = T$ and the blue shaded area depicts the RL agent’s loss. This figure is based on Figure 1.1 from Hutter et al. (2019).

In recent times, there has been a series of additional improvements over PBT-style algorithms. Franke et al. (2021) proposed SEARL and showed it is possible to share experience amongst agents in an off-policy setting, leading to significant efficiency gains. Zhang et al. (2021) proposed PBT-BT which included a backtracking component to the exploit step of PBT, and evaluated the approach on a challenging MBRL setting. Finally, Dalibard and Jaderberg (2021) addressed the greediness of the exploitation phase of PBT, and showed that higher long term performance could be achieved by maintaining sub-populations, and using a metric based on expected improvement.

Open Problems: A disadvantage of PBT-style methods is the relative data inefficiency; thus, future work may consider approaches to share data across trials. This will be particularly important when increasing the search space beyond a handful of hyperparameters as typically tuned with PBT. In addition, the population size is currently a meta-parameter which has a significant impact on the results; so far there has been very little research understanding how the efficacy of PBT works when this changes.

4.5 Meta-Gradients for Online Tuning

Meta-gradients provide an alternative approach to dealing with the non-stationarity of RL hyperparameters. The meta-gradient formulation is inspired by meta-learning methods, such as MAML (Finn et al., 2017), which optimize both an inner and outer loop with *gradients*. In particular, meta-gradient methods specify a subset of their (differentiable) hyperparameters to be meta-parameters η , e.g., bootstrapping, discount factor and learning rate. In the inner loop, the agent is optimized with a fixed η , taking gradient steps to minimize a (typically fixed) loss function. In the outer loop, η is optimized by taking gradient steps to minimize

an outer loss function. Each specific choice of the inner and outer loss function defines a new meta-gradient algorithm.

In the original meta-gradient paper, Xu et al. (2018), used IMPALA (Espeholt et al., 2018) and set $\eta = \{\lambda, \gamma\}$, the bootstrapping hyperparameter and discount factor. When evaluated on the full suite of Atari games, the meta-gradient version improved over the baseline agent by between 30% and 80% depending on the evaluation protocol used. This work was extended to all differentiable IMPALA hyperparameters with *Self-Tuning Actor-Critic* (STAC, Zahavy et al. (2020)). STAC introduced a new loss function to handle varying hyperparameters, which allowed it to further boost performance on the same set of Atari games, as well as robotic benchmarks. In addition, Zahavy et al. (2020) also introduced a means to integrate meta-gradients with auxiliary tasks, producing STACX, which saw further gains. Interestingly, the agents learned non-trivial hyperparameter schedules which could not have been tuned by hand as they were not smoothly varying or static schedules usually used in manual tuning. More recently, Flennerhag et al. (2021) proposed *Bootstrapped Meta-Learning*, which first bootstraps a target from the meta-learner, then seeks to match it in a meaningful space, making it possible to extend the meta-learning horizon. This results in state-of-the-art performance for model free agents on the Atari benchmark, by tuning multiple hyperparameters on the fly.

Meta-gradients have also been used to discover auxiliary tasks (Veeriah et al., 2019), discover options (Veeriah et al., 2021) and learn RL objectives online, demonstrating strong asymptotic performance (Xu et al., 2020). Importantly, (Xu et al., 2020) showed that it was more effective to meta-learn the *target* rather than the full update rule, with the FRODO algorithm capable of producing strong asymptotic performance. Finally, in the field of NAS, differentiable architecture search can also be viewed as a meta-gradient approach. The DARTS algorithm (Liu et al., 2019a) and its successors have become widely popular as well in the NAS community, due the effective use of gradient-based search. Recently this approach has been shown to be effective in RL, finding effective architectures in challenging environments (Miao et al., 2021; Akinola et al., 2021).

Open Problems: Meta-gradient methods have two well-known weaknesses. First, they typically rely on their meta-parameters being initialized well, which itself is a hyperparameter optimization problem. In addition, current meta-gradient methods cannot tune non-differentiable hyperparameters, e.g., the choice of optimizer or the activation function. Nonetheless, they remain one of the most efficient approaches, and offer the potential to improve upon existing strong algorithms with known hyperparameters.

4.6 Blackbox Online Tuning

The strength of both PBT and meta-gradients is the ability to adapt hyperparameters on the fly. However, these are not the only approaches to do so. Indeed, a variety of other methods have been considered, from blackbox methods to online learning inspired approaches. This section focuses on single agent approaches to adapt on the fly in settings where the hyperparameters are not (necessarily) differentiable.

Adaptive methods for selecting hyperparameters have been prominent since the 1990s. Sutton and Singh (1994) proposed three alternative methods for adaptive weighting schemes in TD algorithms. Kearns and Singh (2000) derived upper bounds on the error of temporal-

difference algorithms, and used these bounds to derive schedules for λ . Downey and Sanner (2010) used Bayesian Model Averaging to select the λ bootstrapping hyperparameter for TD methods. More recently, White and White (2016) proposed λ -greedy to adapt λ as a function of the state and achieve an approximately optimal bias-variance trade-off. Paul et al. (2019) proposed HOOF which uses random search with off policy data to periodically select new hyperparameters for policy gradient algorithms.

Several algorithms make use of bandits to adapt hyperparameters. In a distributed setting, Schaul et al. (2020) proposed to adapt several behavioral hyperparameters, such as the degree of stochasticity of an agent, using a notion of learning progress as feedback. This idea inspired Agent57 (Badia et al., 2020) which adaptively selects from several exploration policies to become the first algorithm to achieve human level performance on all 57 games in the Arcade Learning Environment (Bellemare et al., 2012). Other methods have had success using bandits to select the degree of exploration (Ball et al., 2020), the degree of optimism for off policy methods (Moskovitz et al., 2021) or the amount of diversity to add to a population of agents (Parker-Holder et al., 2020b). Finally, Riquelme et al. (2019) considered adaptively switching between Temporal Difference (TD) learning and Monte Carlo (MC) policy evaluation using learned confidence intervals that detect biases of TD estimates.

Open Problems: One of the challenges of these approaches is the limited scope for the search space, since the bandit algorithm must be able to explore all arms. In addition, most bandit algorithms assume the arms to be independent which may lead to decreased efficiency by removing information which is known to the algorithm designer.

4.7 Learning Reinforcement Learning Algorithms

Initial approaches to learning RL algorithms employed the learning to learn formulation. Wang et al. (2016) and Duan et al. (2016), both, use a meta-learner that updates the weight of an agent equipped with an RNN to learn over a distribution of interrelated RL tasks. The former’s main interest was in structured task distributions (e.g., dependent bandits) while the latter focussed on unstructured task distributions (e.g., uniformly distributed bandit problems and random MDPs). Wang et al. (2016) even showed generalization, to some extent, beyond the exact training distribution encountered. Related to these, Rakelly et al. (2019) introduced PEARL, which adapts to new tasks by performing inference over a latent context variable on which the policy is conditioned. They use Variational Autoencoders (VAEs) (Kingma & Welling, 2014) to perform such inference. Zintgraf et al. (2020) introduced variBAD, which uses meta-learning to utilise knowledge obtained in related tasks and perform approximate inference in unknown environments to approximate Bayes-optimal behaviour. They also used VAEs perform such inference but used an RNN as the encoder.

Recently however, there has been increased interest in learning to learn or Meta-RL, which aims to automate the design of RL loss functions. A key insight is that a loss function can be viewed as a parameterizable object that can be learned from data. Instead of using a fixed loss function $\mathcal{L}(\theta)$, one can construct a family of loss functions $\mathcal{L}(\theta; \zeta)$ parameterized by ζ , and seek to maximize the expected reward $J(\theta; \zeta)$ via optimizing the surrogate loss $\mathcal{L}(\theta; \zeta)$. In what follows, we separate ζ into two cases: 1) neural loss functions where ζ encodes neural network parameters, and 2) symbolic loss functions where ζ encodes computational graphs.

Neural loss functions: In this case, the loss function is a neural network with parameters ζ which may be optimized via ES or gradient based methods. For example, in Evolved Policy Gradient (Houthoofd et al., 2018), the inner loop uses gradient descent to optimize the agent’s policy against a loss function provided by the outer loop. The policy’s performance is used by the outer loop to evolve the loss parameterization, using ES.

Gradient based methods are closely related to meta-gradient methods, as they use second-order derivatives to optimize ζ . Bechtle et al. (2020) described a general framework for meta learning with learned loss functions. Most meta-gradient RL algorithms, as mentioned in Section 4.5, start with a human designed loss function $\mathcal{L}(\cdot)$ and modify it with parameterization $\mathcal{L}(\theta; \zeta)$ to allow inner loop and outer loop procedures. In the inner loop, gradient descent via $\nabla_{\theta} \mathcal{L}(\theta; \zeta)$ obtains $\theta^*(\zeta)$, which can be viewed as a function of ζ . In the outer loop, the quality of ζ is then measured by $\mathcal{L}(\theta^*(\zeta); \zeta)$, and we can optimize ζ via gradient descent using $\nabla_{\zeta} \mathcal{L}(\theta^*(\zeta); \zeta)$. This approach requires computing second-order information, i.e. $\nabla_{\zeta} \nabla_{\theta}$, although usually only Hessian-vector products are needed for the pipeline, which are readily available in popular autodifferentiation libraries (Jax (Bradbury et al., 2018), Tensorflow (Abadi et al., 2015), Pytorch (Paszke et al., 2019)).

Examples which employ the above technique include MetaGenRL (Kirsch et al., 2020), which is an extension to the DDPG actor-critic framework where the critic is trained to minimize the TD-error as usual. Meta-learning is applied to the policy update. In the original DDPG, an additional policy parameter ϕ is trained to maximize the value function $Q_{\theta}(s_t, \pi_{\phi}(s_t))$. In MetaGenRL, this is used as the outer loss $Q_{\theta}(s_t, \pi_{\phi^*(\zeta)}(s_t))$, and the inner loss $\mathcal{L}(\phi; \zeta)$ is modeled as an LSTM.

In Learned Policy Gradient (LPG) (Oh et al., 2020), instead of using a neural meta loss function end-to-end, an LSTM network is used to provide target policy $\hat{\pi}$ and target value \hat{y} . The meta loss and the task loss are defined manually. Oh et al. (2020) show that a learned update rule can be transferred between qualitatively different tasks.

Symbolic loss functions: In this case, the loss function is represented as a symbolic expression consisting of predefined primitives, akin to genetic programming. Alet et al. (2020) used a Domain Specific Language (DSL) to represent a curiosity module as a directed acyclic graph (DAG). The curiosity module provides intrinsic rewards, which are added to the loss function and can be optimized by PPO. The search space contains 52,000 valid programs and they are evaluated exhaustively with pruning techniques, such as training in a cheap environment and predicting algorithm performance ("meta-meta-RL"). Co-Reyes et al. (2021) proposed a DSL to represent the entire loss function as a DAG, and this loss function is used to train value-based agents. Unlike Alet et al. (2020), the DAG is optimized using an evolutionary algorithm called Regularized Evolution (Real et al., 2019).

Finally, regarding the categorical choice of an algorithm for RL, Laroche and Féraud (2018a) used Algorithm Selection for RL where, given an episodic task and a portfolio of off-policy RL algorithms, a UCB bandit-style meta-algorithm selects which RL algorithm is in control during the next episode so as to maximize the expected return. They evaluated their approach, among others, on an Atari game, where it improved the performance by a wide margin.

Open Problems: In general, it is difficult to understand analytical properties of neural loss functions. Developing tools to empirically study these loss functions becomes crucial

for explaining why they work and for understanding their generalization capabilities. For symbolic loss functions, the search space (of all possible graphs) and the search algorithm (e.g., regularized evolution) play a fundamental role, yet it is far from clear what the optimal design choices are.

4.8 Environment Design

Environment design is an important component for automating the learning in RL agents. From curriculum learning (Jiang et al., 2021b; Eimer et al., 2021b; Klink et al., 2020; Matiisen et al., 2020; Sukhbaatar et al., 2018) to synthetic environment learning (Ferreira et al., 2021) and generation (Volz et al., 2018) to combining curriculum learning with environment generation (Bontrager & Togelius, 2020; Wang et al., 2019, 2020; Dennis et al., 2020), the objective here is to speed up the learning for the RL agents through environment design.

We organize algorithms performing Automated Environment Design according to the component of the environment (assumed to be a POMDP as defined in Section 2) that they try to automatically learn. This organization can also be seen in Figure 7.

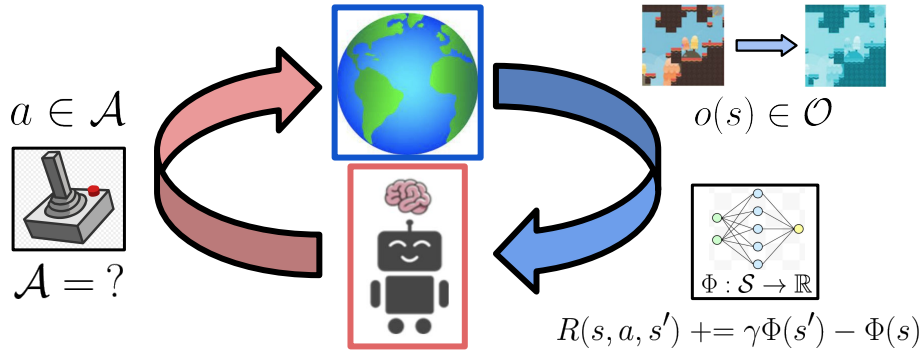


Figure 7: Representation of a typical policy + environment feedback loop, with controllable components such as the reward function R from (Ng et al., 1999), action space \mathcal{A} , and observation space \mathcal{O} from (Raileanu et al., 2020).

Reward function, R : Zheng et al. (2018) presented a bi-level optimization approach that learns reward shaping for policy gradient algorithms using a parameterized intrinsic reward function. In an inner loop, the parameters of the agent are updated using gradient descent to increase the sum of intrinsic and extrinsic rewards, while in the outer loop, the parameters of the intrinsic reward are updated using gradient descent to increase only the extrinsic rewards. Hu et al. (2020) also presented a bi-level optimization approach which they term BiPaRS (and its variants). They use a PPO (Schulman et al., 2017b) agent in the inner loop. Furthermore, they use meta-gradients with respect to the (state-action dependent) parameters of *user-defined* reward shaping functions to learn helpful reward functions in the outer loop. Zou et al. (2019) proposed to meta-learn a potential function (Ng et al., 1999) prior over a distribution of tasks. Inspired by MAML (Finn et al., 2017), they try to adapt the meta-learned prior towards the optimal shaping function (which they derive

to be equal to the optimal state-value function V). Konidaris and Barto (2006) introduced a function that preserves value information between tasks and acts as the agent’s internal shaping reward. The input to this function is the part of the state space whose meaning does *not* change across tasks. This function can be used as the initial estimate for newly observed states and is further refined based on parts of the state space whose meaning *does* change across tasks. Snel and Whiteson (2010) used an evolutionary feature selection method and showed that this method chooses representations that are suitable for shaping and value functions. Their algorithm can find a shaping function in multi-task RL without pre-specifying a separate representation. Marthi (2007) proposed automatically learning a shaped reward and a decomposed reward. Given a set of state and temporal abstractions, they create an abstracted MDP over the original MDP and learn the reward shaping using collected reward samples based on a mathematical formulation they derive.

Faust et al. (2019) investigate the effect of learning a multi-objective intrinsic reward over several RL algorithms and benchmarks with an evolutionary search. The results show that a) the utility of automated reward search correlates with the difficulty of the task, b) using simple sparse task objectives (e.g. distance travelled in MuJoCo tasks) as a fitness function leads close to identical results to using the default yet complex hand-tuned MuJoCo rewards, and c) reward search is more likely to produce better policies than the HP search on a fixed training budget and with reasonable hyperparameters.

Action Space, \mathcal{A} : Simplifying an environment’s action space can make training significantly easier and faster. The two main approaches used to accomplish this are repeating single actions in order to reduce the number of overall decision points or to construct a new action space entirely, composed of combinations of basic actions as macro actions or options. While handcrafting has been common in action space augmentation, Sharma et al. (2017) learned the number of repetitions for a given action alongside the action selection. Biedenkapp et al. (2021) presented an extension of the idea by conditioning the amount of repetition on the predicted action itself. In automatic macro action discovery, Farahani and Mozayani (2019) showed that it is possible to combine actions into suitable macro actions by defining sub-goals to be reached in the environment; this is achieved by partitioning its transition graph. Options are similar to macro actions, but instead of executing a macro action once, each option has its own intra-option policy that is followed until a termination function defers back to the agent (Sutton et al., 1999b). Bacon et al. (2017) jointly learned both a policy across these options as well as the options themselves. Mankowitz et al. (2018) extended the idea to also learn options that are robust to model misspecification.

Observation Space, \mathcal{O} : Raileanu et al. (2020) proposed using a UCB bandit to select an image transformation (e.g. crop, rotate, flip) and applying it to the observations. The augmented and original observations are passed to a regularized actor-critic agent which uses them to learn a policy and value function which are invariant to the transformation.

Multiple Components, Unsupervised: We discuss here approaches that change multiple components in the environment or the whole environment itself. Most notable here are curriculum learning approaches that usually modify the state space, S , and the initial state distribution, ρ . As a result of modifying S , they naturally also change the P and R since these are functions with S a component of their domains. We begin with unsupervised

methods seeking a generally robust agent, before moving to supervised approaches which typically have a target goal or task.

Wang et al. (2019) as well as Wang et al. (2020) proposed POET that generates new environments according to an environment encoding. The environments are automatically generated, either with random mutations (Wang et al., 2019) or if the new environments create a significantly different ranking of existing agents (Wang et al., 2020). These methods of generating new environments are assumed to create a diversity of environments on which to train agents in a curriculum. Lee et al. (2020) applied the principle to controlling quadrupedal robots and found the robustness to increase significantly.

Dennis et al. (2020) proposed PAIRED that also automatically generates new environments to create a curriculum. They used a fixed environment encoding. In contrast to Wang et al. (2019, 2020), environments are chosen to maximize *regret*, defined as the difference in performance between the protagonist agent and an additional *antagonist* agent. This means the adversary is encouraged to propose the simplest environments the protagonist cannot currently solve, while provides theoretical guarantees that (at equilibrium) the protagonist follows a minimax regret strategy. Extending PAIRED, Gur et al. (2021) proposed Compositional Design of Environments (CoDE) for compositional tasks. CoDE’s environment generative model builds a series of compositional tasks and environments tailored to the RL agent’s skill level and makes use of a population of agents, making it possible to train agents to navigate the web. Extending the theoretical framework from PAIRED in a different direction, Jiang et al. (2021a) showed that rather than learn to *generate* new environments, it is also effective to *curate* randomly sampled ones using *Prioritized Level Replay* (PLR, Jiang et al. (2021b)). This approach maintains the theoretical properties of PAIRED while demonstrating stronger empirical performance.

Bontrager and Togelius (2020) also employed an environment generator (in addition to human created environments) and an actor-critic agent which work both cooperatively and adversarially to create a curriculum for the agent by selecting environments minimizing the agent’s expected value.

Multiple Components, Supervised: If the agent’s goal is solving a specific task instead of being generally more robust, it can be supported by continually progressing a simple version of the task towards this goal in a curriculum (Narvekar et al., 2020). Progression is usually tied to how well the agent currently performs in order to keep the environment difficulty at an appropriate level. A well-known example of this is OpenAI et al. (2019) who showed it is possible to use a robot hand to solve the Rubik’s cube, by starting from an almost solved cube and gradually increasing the starting position complexity of both hand and cube as soon as the agent can solve the current state sufficiently well. Klink et al. (2020) applied the same principle to several physics simulation tasks, using value estimations as the progression criterion. Value estimation approaches in general have been successful for RL because their approximation of an environment’s challenge level is cheap to compute (Jiang et al., 2015; Zhang et al., 2020; Eimer et al., 2021b). They are an important class in the starting state curriculum generation taxonomy proposed by Wöhlke et al. (2020). Student-teacher curriculum learning approaches can also create new task variations, e.g. by using GANs, although they only gradually increase the complexity of their distribution as the agent improves during training (Florensa et al., 2018; Matiisen et al., 2020; Turchetta et al.,

2020). We can even induce a difficulty curve into environments that are immutable by using Self-Play to challenge agents with ever more difficult opponents (da Silva et al., 2019). A canonical approach is *Asymmetric Self-Play* (ASP, Sukhbaatar et al. (2018)) which proposes to use two agents: “Alice”, who proposes new tasks by doing a sequence of actions and “Bob” who must undo or repeat them. ASP was also shown to be highly effective for challenging robotic manipulation tasks (OpenAI et al., 2021). Finally AMIGo (Campero et al., 2021) and APT-Gen Fang et al. (2021) both consider settings with a fixed task, whereby the goal becomes incrementally harder as the student becomes increasingly capable.

Ferreira et al. (2021) proposed a method that learns a given target environment’s transition and reward functions in order to train agents more efficiently. They framed this as a bi-level optimization problem and optimized the learnt environment (an NN) in an outer loop to maximize the reward of the agent in the inner loop. They showed that their *synthetic environments* can not only serve as a more efficient proxy for expensive target environments, but that training on them can also reduce the number of training steps.

Open Problems: There are many different approaches for environment design and it is unclear which of them leads to the biggest gains in performance. This raises the possibility of: a) employing several of these methods in a single approach and studying the impact on performance and to what extent the gains are complementary; and b) evaluating the approaches on a shared benchmark. Unfortunately, there is currently also a lack of unified frameworks and shared benchmarks. To further progress towards fully automated progression through environments, more efforts like Romac et al. (2021) would be helpful in encouraging closer cooperation and better comparability.

4.9 Hybrid Approaches

Inevitably some methods do not fall into a single category. Indeed, many methods seek to exploit the strengths of different approaches, which we refer to as a *hybrid* method. In this section we define these hybrid methods as those which use more than one class of approaches from Table 3.

BOHB (Falkner et al., 2018) combined Hyperband with BO to determine how many configurations to evaluate with which budget, but it replaces the random selection of configurations at the beginning of each Hyperband iteration with BO, where the model is trained on the configurations that were evaluated so far. BOHB can also efficiently and effectively take advantage of parallel resources. BOHB was used to optimize the hyperparameters of PPO on the cartpole swing-up task from Gym and the problem of RNA design from (Runge et al., 2019).

DEHB (Awad et al., 2021) combined Hyperband with Differential Evolution (DE) to optimize the hyperparameters of the PPO algorithm 5x faster than random search (see Figure 9 in the paper) on an AutoRL task and up to three orders of magnitudes on other hyperparameter optimization tasks. Chiang et al. (2019) combined evolutionary search with reward shaping to automatically select a reward function and neural architecture for navigation task. They learn a more robust policy and a hyperparameter configuration which generalizes better to unseen environments.

Jaderberg et al. (2019) achieved human-level performance in the game Quake III Arena in Capture the Flag mode, using only pixels and game points scored as input. To do this,

their *FTW* agent learned reward shaping coefficients and hyperparameters jointly in an outer optimization loop. They use a bi-level optimization process with PBT, with the inner loop optimizing an IMPALA (Espeholt et al., 2018) RL agent. The outer loop is evolutionary and maintains a population of such independent RL agents which are trained concurrently from thousands of parallel matches on randomly generated environments. Each agent learns its own internal reward signal and rich representation of the world. More recently, another large-scale project saw the use of environment design, through a form of guided domain randomization, and PBT to produce “generally capable” agents in a large simulation environment (Team et al., 2021). This work attempted to achieve a more open-ended system, whereby an agent could learn to play a wide variety of games, resulting in multiple innovations, such as generational training which allowed agents to transfer behaviors across different reward functions in a PBT setup.

The Population Based Bandits (PB2 Parker-Holder et al. (2020a)) approach seeks to combine ideas from both PBT and BO. It formulates the explore step of PBT as a batch GP-bandit optimization problem and uses an upper confidence bound (UCB) acquisition function to select new configurations. In a series of RL problems it was shown to be more sample efficient than PBT, but remains untested in larger problems or with more than a handful of hyperparameters. In addition, PB2 was recently extended to deal with mixed input hyperparameters (continuous and categorical) (Parker-Holder et al., 2021), but there has been very little work exploring kernel choice, improving the time-varying mechanism or further extending, for example, to architectures.

Open Problems: In addition to the open problems for each of the individual sub-sections above, hybrid approaches face the additional open problems of how best to combine the individual approaches. Since the compute requirement of combining many methods and searching for the best combination among these could be extremely large, hybridizing approaches would require being efficiently able to prune the search space of such combinations.

5. Future Directions

In this section, we highlight a few specific areas which we believe will be particularly fruitful avenues for future work.

In this survey we emphasized the success of methods for AutoRL that dynamically adapt configurations during training. However, to the best of our knowledge, the non-stationarity of hyperparameters of many modern state-of-the-art algorithms has not been studied extensively. Thus, it is often not clear which hyperparameters need to be optimized dynamically and which are best optimized statically. Furthermore, it remains largely an open question if the impact of hyperparameters remains the same across environments or if different hyperparameters are important for different tasks (Eimer et al., 2021a), and why that may be the case. Methods to analyze such effects have so far only been proposed for static configuration procedures (Hutter et al., 2014; Fawcett & Hoos, 2016; Biedenkapp et al., 2017, 2018; van Rijn & Hutter, 2018) and have not yet found wide-spread use in RL.

Classical hyperparameter optimization (Hutter et al., 2019) for (un-)supervised learning considers only individual datasets when searching for well performing configurations. Similarly, when optimizing the hyperparameters of an RL agent commonly only individual environments are considered. In fact, nearly all of the discussed optimization methods

throughout this paper consider only individual environments. Given the sensitivity of RL agents discussed throughout this paper (Henderson et al., 2018; Andrychowicz et al., 2021; Engstrom et al., 2020), it is to be expected that the discovered settings are not transferable to other environments. Recently however there is increasing interest in training RL agents that are capable of handling multiple (homogeneous) environments. While agents have typically used single configurations across all Atari games (Mnih et al., 2013), it remains a challenge to find robust configurations that work in a variety of settings (Eimer et al., 2021a). AutoRL approaches that tune RL agents across environments fall into the class of algorithm configuration (Hutter et al., 2009) methods, which seek to find better parameters to improve general algorithm performance. Such methods are capable of finding well performing and robust hyperparameters for a set of environments (Eggenberger et al., 2019). Recently, evaluation protocols were proposed that consider the performance of RL algorithms across a set of environments (Jordan et al., 2020; Patterson et al., 2021), which may prove useful for future work in this space.

Related to the problem of algorithm configuration, algorithm selection (Rice, 1976) can be used to choose which RL algorithm to use for learning (Laroche & Féraud, 2018b). To the best of our knowledge, so far no AutoRL approach has explored the intersection of algorithm selection and algorithm configuration known as per-instance algorithm configuration (PIAC, Xu et al. (2010), Kadioglu et al. (2010)). In this framework, a selector can choose a configuration from a portfolio of well performing configurations and decides which of these to use for the environment at hand.

One important area for research is to provide a more rigorous understanding of the impact of design choices on performance. If we can understand how each component interacts with others then we can either select more amenable combinations or design search spaces to account for this dependency. This could come from empirical investigations or theoretical analysis. Indeed, recent works such as Fedus et al. (2020), Obando-Ceron and Castro (2020) and Andrychowicz et al. (2021) have provided foundations in this area, but significant work remains to be done. Furthermore, hyperparameter importance methods and analysis tools from the AutoML community (Hutter et al., 2014; Fawcett & Hoos, 2016; Biedenkapp et al., 2017, 2018; van Rijn & Hutter, 2018) have not yet been explored in AutoRL. Increasing focus in this area is likely to have profound knock-on effects on other areas of RL, especially AutoRL.

Another crucial future direction is clear benchmarks for evaluating AutoRL methods. Many works thus far have considered tuning components of a baseline method, typically on continuous control tasks from OpenAI Gym (Brockman et al., 2016) or discrete environments from the Arcade Learning Environment (Bellemare et al., 2012). However, there is increasing emphasis on using environments that test generalization. Whiteson et al. (2009) were one of the first to propose testing agents on distributions of environments, with a popular modern benchmark being OpenAI Procgen (Cobbe et al., 2020). Indeed, this environment has been used in AutoRL (Miao et al., 2021; Parker-Holder et al., 2021). Other procedurally generated environments include MiniGrid (Chevalier-Boisvert et al., 2018), NetHack (Küttler et al., 2020), MiniHack (Samvelyan et al., 2021), Griddly (Bamford et al., 2020) or MineRL (Guss et al., 2019). CARL (Benjamins et al., 2021) provides similar environment complexity, but instead of using procedural generation the environment distribution is defined via context features like floor friction. In addition, it may be fruitful to consider AutoRL in more targeted,

compositional tasks. Yu et al. (2019) introduce Meta-World, a benchmark that proposes 50 distinct robotic manipulation tasks and their variations to enable such learning. Wang et al. (2021) is another complex benchmark that also proposes a meta-distribution for RL agents that may be used to perform meta-RL to determine an underlying latent causal structure. Rajan and Hutter (2019) as well as Osband et al. (2020) provide simple environments with such a latent causal structure that may be used to perform similar experiments at a much lower cost, however at the expense of the complexity of the environments. Learning over such distributions can not only make RL agents robust to variation but also allow them to perform few-shot learning on a distribution of environments. Indeed it remains understudied to consider AutoRL for generalization (Song et al., 2019), where it becomes a challenge to define an appropriate task for the outer loop.

In addition to the discussion so far, the majority of the work in this survey addresses *single agent* RL. However, many real-world systems are in fact inherently multi-agent (Foerster, 2018). Consider, for example, self-driving cars which need to cooperate with others to safely drive on the road. When using RL in this type of problem, there is an additional challenge of how to parameterize the different agents: whether to train in a centralized or decentralized manner, while also designing reward functions and algorithms to capture the impact of individual agent actions.

Another recent area of research is *offline* RL, where agents must generalize to an online simulator or real world environment from a static dataset of experiences. Research in this space remains nascent, however, it already contains a large diversity of methods, while also introducing new challenges. For example, it is challenging to get real-world policy returns for an AutoRL algorithm, so often we must make use of off policy evaluation (Precup et al., 2000). It is possible that in this setting there may be scope to use more “traditional” AutoML methods, or it may require completely new approaches.

6. Conclusion

This paper has introduced AutoRL by discussing a wide variety of methods to automate the RL training pipeline. Indeed, unlike supervised learning, which is usually an open-loop one-step process, RL is a complete closed-loop *system*. As such, it is likely each of the components discussed has an influence on others, and if we want to train our agents end-to-end as part of a broader system, it ultimately will require a holistic solution. The challenge is compounded in RL since evaluations in RL are almost always necessarily stochastic and (potentially much more) noisy than in supervised learning, due to various sources (e.g. policy, environment), which can be a challenge for any form of automatic tuning. However, we have presented a variety of promising directions in this survey that can help overcome the challenge and which will likely provide improvements in the coming years. It is evident that AutoRL is maturing as a field and exciting possibilities lay ahead.

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