Pythia: A prototype artificial agent for designing optimal gravitational-wave follow-up campaigns

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Abstract

Joint observations in electromagnetic and gravitational waves shed light on the physics of objects and surrounding environments with extreme gravity that are otherwise unreachable via siloed observations in each messenger. However, such detections remain challenging due to the rapid and faint nature of counterparts. Protocols for discovery and inference still rely on human experts manually inspecting survey alert streams and intuiting optimal usage of limited follow-up resources. Strategizing an optimal follow-up program requires adaptive sequential decision-making given evolving light curve data that maximizes a global objective despite incomplete information and is robust to stochasticity introduced by detectors/observing conditions. We design a novel reinforcement learning agent that executes such a design for the goal of maximizing follow-up photometry for the true kilonova among several contaminant transient light curves from the Zwicky Transient Facility. It achieves $3\times$ higher accuracy compared to a random strategy and comes close to human-level performance. We suggest that more complex agents (e.g. using deep Q networks or policy gradient algorithms) could perform at par or surpass human experts. Agents like these could pave the way for machine-directed software infrastructure to efficiently respond to next generation detectors, for conducting science inference and optimally planning expensive follow-up observations, scalably and with demonstrable performance guarantees.

1 Introduction

The inspiral and subsequent merger of compact objects emits gravitational waves (GWs) that can be detected by ground-based interferometers like LIGO [LSC et al., 2015], Virgo [Acernese et al., 2014], and Kagra [Akutsu et al., 2021] (also the International Gravitational-wave Network; IGWN). If at least one of the binary components is a neutron star (NS), these phenomena may have analogs in electromagnetic (EM) waves with signatures spanning the EM spectrum, from gamma rays to radio

Machine Learning and the Physical Sciences Workshop, NeurIPS 2023.

waves. Kilonovae (KNe) are ultraviolet, optical, near-infrared transients that arise due to rapid neutron capture (*r*-process) nucleosynthesis in the merger ejecta [Lattimer and Schramm, 1974, Symbalisty and Schramm, 1982, Li and Paczyński, 1998]. They are robust counterparts to most binary neutron star (BNS) and many neutron-star black hole (NSBH) mergers [Metzger et al., 2010]. Their light curves and spectra provide the opportunity to probe the ejecta and processes driving nucleosynthesis in it [Kasen et al., 2017, Drout et al., 2017, Kasliwal et al., 2017], and hypermassive/supramassive NS formation scenarios to place independent constraints on the NS equation of state (EoS) [Bauswein et al., 2017, Radice et al., 2018]. However, they are quite elusive because they are faint (M$\sim$ -16 mag in optical) and short-lived ($\lesssim$1 week) [Bulla, 2019].

When the IGWN detects a signal from a compact binary coalescence, they issue a General Coordinates Network (GCN) notice to the astronomy community, along with some GW derived inference, like source sky localization and distance[1]. Depending on the orientation of the system, satellites could detect a gamma-ray burst (GRB) powered by the merger and help reduce the search area by crossmatching credible regions. In fact, several GRB afterglow target-of-opportunity (ToO) searches [Singer et al., 2015, Ahumada et al., 2022] have paved the way for GW ToO campaigns [Kasliwal et al., 2020]. Transients that are temporally and spatially coincident with the GW event are assembled. The vast majority of contaminants in this list are supernovae, cataclysmic variables (CVs), and unassociated GRB afterglows. Especially at early phases, these can be difficult to distinguish from KNe. Human experts manually examine the candidate light curves together with additional information, like host galaxies/environment, preliminary fits to theoretical models, and perform additional follow-up to obtain better characterization, and hopefully identify the real event. This step can occur at late hours via oral/written electronic communication and is the one of the main sources of inefficiency in GW counterpart searches.

While key aspects of this protocol have been successful at identifying novel and elusive fast transients like Fast Blue Optical Transients [Ho et al., 2022, 2021, 2020] and GRB afterglows [Andreoni et al., 2021], it has struggled at identifying KNe. This is because these discoveries were only possible when the light curve was sufficiently resolved to allow early estimates for e.g. decline rate. For the vast majority of KNe, there are too few photometric points to reveal any signature characteristics. In fact, post-mortem archival searches have not revealed new KNe [Andreoni et al., 2020]. This indicates that additional real-time follow-up is crucial for identification. At the same time, candidates requiring follow-up far exceed available resources. In practice, especially for KNe at or close to detection limits, human-directed follow-up strategies can be no better than guesswork.

The situation appears daunting as we begin IGWN's current observing run (O4). Owing to the increased sensitivity from its previous run (O3), the network is projected to discover $\sim 10\times$ more BNS/NSBH mergers than O3 [Abbott et al., 2018]. The associated sky localizations are expected to improve, but not by much, leaving the effective sky footprint needing to be searched nearly the same. Moreover, only a fraction of BNS mergers are likely to be accompanied by a detectable GRB as with GW170817 [Mandhai et al., 2018], which was key in the rapid identification of AT2017gfo, the first, and so far only, kilonova associated with a GW signal discovered [Coulter et al., 2017, Smartt et al., 2017]. The search for KNe using current human-centered protocols is ill-suited to handle the increased volume and will continue resulting in inefficiencies and lost opportunities of both human and scientific resources.

In this paper, we demonstrate using a toy RL agent that the KN follow-up problem can be addressed using artificial intelligence (AI). Given N transient light curves from Zwicky Transient Facility (ZTF), one of which is a KN and the rest are contaminants, the agent must maximize an additional follow-up photometry (300s exposure in ZTF g, r or i) allocated to the true KN each night for 6 nights. Our agent belongs to the class of ORACLEs [Sravan et al., 2020, 2021].

2 `Pythia`: a KN photometric follow-up agent

2.1 Problem Statement

Our agent is presented N transient light curves from ZTF, one of which is the KN and the rest are contaminants, chosen randomly from a list of supernovae and unassociated GRB afterglows. The agent observes the candidates on day 1. On days 2 through 7 it assigns one additional photometry

[1] `https://emfollow.docs.ligo.org/userguide/`

Algorithm 1 SARSA and TD(0) target

Initialize w to small random weights
Set $\epsilon_0 = 1$
for k = 1, M **do** ▷ For each episode
  $\epsilon \leftarrow \epsilon_0 / k^n$
  Initialize s_1
  for t = 1, horizon **do**
    With probability ϵ select random action a_t
    otherwise select $a_t = \max_a \hat{Q}(s_t, a_t; \hat{w})$
    Execute action and observe reward r_t and next state s_{t+1} from environment
    With probability ϵ select random action a_{t+1}
    otherwise select $a_{t+1} = \max_a \hat{Q}(s_{t+1}, a_{t+1}; \hat{w})$
    Set $\Delta\hat{w} \leftarrow [r_t + \gamma\hat{Q}(s_{t+1}, a_{t+1}; \hat{w}) - \hat{Q}(s_t, a_t; \hat{w})]\nabla_w \hat{Q}(s_t, a_t; \hat{w})$
      ▷ Loss is MSE between TD(0) target (substitute for Q^*) and current Q
    Update $\hat{w} \leftarrow \hat{w} + \alpha\Delta\hat{w}$ ▷ α is using Adam
  end for
end for

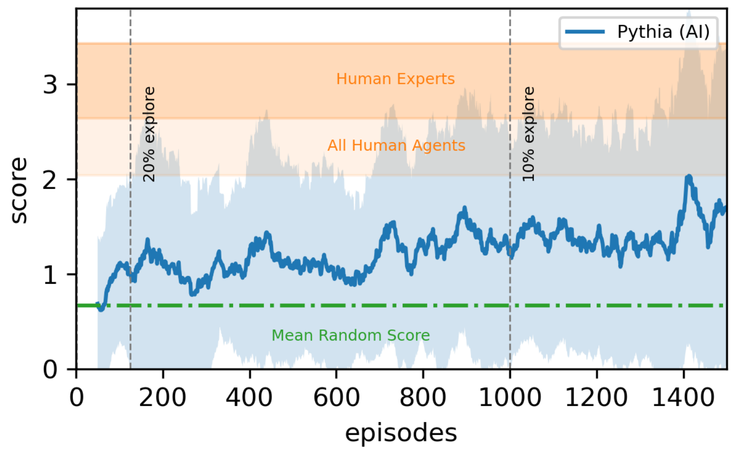

Figure 1: Learning curve of our KN follow-up agent `Pythia` (blue). Our agent achieves $> 3.5\times$ higher score than a random agent during training. The score variance (shaded blue region) is computed using a moving average with a length of 50 episodes. The mean random score is 6/9. Human references are show as orange shaded regions.

point with ZTF in g, r, or i using a deep 300s exposure to one of the events. The agent gets a reward 1 if the follow-up is assigned to the KN, and 0 otherwise. The objective is to learn a policy to maximizes the number of follow-up assigned to the true KN. The maximum achievable score is 6. A random agent will achieve an expected score of $6/N$.

2.2 RL Algorithm

We learn the optimal behavior policy using SARSA. SARSA is a simple on-policy learning algorithm, i.e. samples from the policy are used to update Q (see Algorithm 1). We parametrize $Q = x(s, a)^T w$, where $x(s, a)$ is the state-action feature representation and w is a set of linear weights to be learned. We choose a TD(0) target, i.e. $r_t + \gamma\hat{Q}(s_{t+1}, a_{t+1}; \hat{w})$, where $\hat{Q}$ is the running estimate. The policy is ϵ-greedy: with probability ϵ the agent chooses a random action and otherwise chooses $\max_a \hat{Q}(s_t, a_t; \hat{w})$, the action with the maximum $\hat{Q}$-value. If the learning rate α_t satisfies the Robbins-Munro sequence and $\epsilon \rightarrow 0$ as $i \rightarrow \infty$ the agent is Greedy in the Limit of Infinite Exploration (GLIE) and is a sufficient condition for convergence in SARSA, where n is a hyperparameter that controls how fast the agent becomes greedy. To ensure sample efficiency and propagate TD updates faster, we reuse episodes m times, where we set $m = 5$.

Table 1: AI and human agent performance

Agent	Score	Fraction KNe
Pythia	1.84	0.81
Non-expert 1	2.04	0.54
Non-expert 2	3.15	0.86
Expert 1	2.64	0.76
Expert 2	2.74	0.78
Expert 3	2.94	0.72
Expert 4	3.43	0.90

Our agent learns online in a simulated environment, i.e. all our light curves are artificially generated. Additional follow-up photometry decided by the agent are simulated as follows. We estimate the distribution of forecast photometry given an action using 2-D Gaussian Process regression on the observed light curve. To compute *state-action* features, $x(s, a)$, we convert the observed ZTF light curves and forecast photometry given action a to a tiled $3 \times \sqrt{N} \times \sqrt{N}$ image that we pass to a convolutional autoencoder (CAE). This choice is important because the agent's decisions need to be invariant to the order of the events. CAEs are appropriate because the convolution operation makes them translation invariant. We choose $x(s, a)$ to be the penultimate layer in the Xception network [Chollet, 2016]. This choice precludes us from having to train a custom encoder using state-action pairs derived from a preset policy, which could potentially bias Q estimates. Note that this two-step learning issue (one for state-action features and the other for Q) can be avoided avoided using deep Q-networks [Mnih et al., 2013]. The observed photometry (*next state*) given an *action* is simulated using 2-D Gaussian Process regression using either the full ZTF or theoretical model light curves for SNe and GRB afterglows/KNe, respectively. Then, uncertainties and limits are applied in a similar way to the generation of the training dataset.

Our choice of linear VFA was motivated by the fact that the triad of non-linear function approximators, off-policy learning (like Q-learning), and bootstrapping (as in Temporal-difference learning) can cause the Q function to diverge [Tsitsiklis and Van Roy, 1997]. Though recent works have made significant progress to address this issue (e.g. prioritized reply [Schaul et al., 2015], asynchronous methods [Mnih et al., 2016], dueling DQN targets [Wang et al., 2016]), we adopt linear VFA and SARSA for our toy implementation to assess the feasibility of RL approaches to solve the KN follow-up problem and disambiguate limitations from convergence issues. Linear VFA in SARSA is guaranteed to converge to within a constant factor of the optimal behavior policy under minor assumptions [discussed above, see also Tsitsiklis and Van Roy, 1997]. This attribute makes it suitable for our pilot investigation where we are interesting exploring the suitability of RL approaches to solve the KN follow-up problem and providing useful benchmarks on the same. An issue may be that the choice of linear VFA as hypothesis function class may not be a sufficiently rich representation of the true Q function. This does indeed appear to be the case as we discuss later.

3 Results

We refer to our AI agent as `Pythia`.

We train `Pythia` for $N = 9$ events. We perform a grid search for the hyperparameters $\gamma = 1.0$, 0.5, 0.1, $n = 1$, 2, 3, and $\alpha = 0.1$, 0.01, 0.001, 0.0001. Figure 1 shows the learning curve of our trained agent, smoothed using a moving average with length = 50 episodes. Here $\gamma = 0.5$, $n = 3$, and $\alpha = 0.01$. `Pythia` achieves $> 3.5\times$ higher score than a random agent during training. It is $3\times$ better than random during testing.

3.1 Human benchmark

Due to the absence of ground truth in RL problems (the true optimal Q in our case) it is important to compare against strong benchmarks to assess the quality of learned policies. Here we use benchmarks provided by astronomers as a stronger point of reference than a random policy.

We solicited the aid of six volunteer astronomers to solve our KN follow-up problem. Similar to `Pythia` they completed a training and testing phase, the former with as many episodes are they chose and the latter with 100 episodes. During both phases, we recorded their choices and decision times. Finally, we asked them to self-identify as experts and non-experts in KN searches and provide a short description of their strategies. We list the comparison of the performance of all agents in Table 1. Score is the average number of photometry allocated to the true KN. Fraction KNe denotes the fraction of episodes in which the true KN received at least one follow-up. The scores for human agents are shown in orange in Figure 1. All human agents surpassed `Pythia`. Interestingly, `Pythia` performed well in the fraction of KNe allocated at least one follow-up observation even though it was not the follow-up objective.

4 Conclusions

In this paper we develop the first AI agent capable of strategizing a sequential transient follow-up program. Using a simple behavior policy (linear VFA) our agent demonstrates that the problem is learnable by machines and comes close to human performance. However, the agent is quite greedy in its decisions (the score does not improve much with time) suggesting that the agent's hypothesis function is an insufficient representation of the optimal behavior policy. More complex agents (e.g. using deep Q networks or policy gradient algorithms) could help bridge the gap with human experts. This could really help streamline KN search efforts. In the development of such agents it would also be useful to employ graph neural networks to represent the light curves as this is a more natural choice to ensure learning order invariant policies than the convolutional neural networks used here.

In order to assist in realistic searches, our framework would need to accommodate variable number of events (candidates are continuously eliminated due to information from other sources), a comprehensive state (e.g. low latency data from IGWN) and action space (more than one photometric point or spectroscopic follow-up, etc along with consideration of observing costs), and return for physics models (e.g. ejecta mass, inclination angle). In fact, for optimizing physics constraints in real-time, RL agents are the only solution. Finally, trained agents would need to be deployed into existing frameworks (e.g. SkyPortal or REFITT) to iteratively execute observing plans and ingest observations.

Acknowledgments and Disclosure of Funding

We thank the experts from the GROWTH team who helped provide benchmarks reported here. This research was partly completed on Expanse at the San Diego Supercomputer Center at UC San Diego (Accelerate ACCESS Award# AST200029). N. Sravan is grateful for support from the National Science Foundation award AST-2307374. N. Sravan, M. J. Graham, and M. W. Coughlin were supported by the National Science Foundation award PHY-211799. M. J. Graham acknowledges support from the National Science Foundation with grant number AST-2034437. M. W. Coughlin acknowledges support from the National Science Foundation with grant number PHY-2308862. S. Anand acknowledges support from the National Science Foundation GROWTH PIRE grant No. 1545949.

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