Unsupervised Resource Allocation with Graph Neural Networks

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Abstract

We present an approach for maximizing a global utility function by learning how to allocate resources in an unsupervised way. We expect interactions between allocation targets to be important and therefore propose to learn the reward structure for near-optimal allocation policies with a GNN. By relaxing the resource constraint, we can employ gradient-based optimization in contrast to more standard evolutionary algorithms. Our algorithm is motivated by a problem in modern astronomy, where one needs to select—based on limited initial information—among 10^9 galaxies those whose detailed measurement will lead to optimal inference of the composition of the universe. Our technique presents a way of flexibly learning an allocation strategy by only requiring forward simulators for the physics of interest and the measurement process. We anticipate that our technique will also find applications in a range of allocation problems from social science studies to customer satisfaction surveys and exploration strategies of autonomous agents.

1 Resource Allocation for Observational Studies

We consider a problem that frequently arises in observational sciences as well as the training of autonomous agents. Due to resource limitations, not every desirable action is admissible, leading to the problem of finding a strategy that makes best use of the available resources. We are particularly interested in a scenario where many individual actions need to be performed before their combined utility can be determined. In such a scenario it should be beneficial to learn not just which actions have high reward but also how interactions between possible actions influence the outcome.

As a concrete example, modern astronomical observations fall into two groups. So-called surveys cover wide areas of the sky without any specific selection of celestial objects. On the other hand, targeted observations often draw from prior surveys to select specific objects for detailed characterization. Telescope facilities for targeted studies are rare and expensive to operate. Access to them is severely limited and competitively allocated based on the perceived merit of the proposed scientific study. After decades of astronomical sky surveys, *some* information is available for hundreds of millions of celestial objects (such as their position on the sky and their brightness), but detailed information can only be acquired for a much smaller subset. Based on what is already known of these objects, astronomers need to decide which of them merit further study (see Figure 1 for a schema of the problem). The situation resembles that of an organization whose management wants to incentivize beneficial user behavior through an intervention aimed at specific users; or of an autonomous agent

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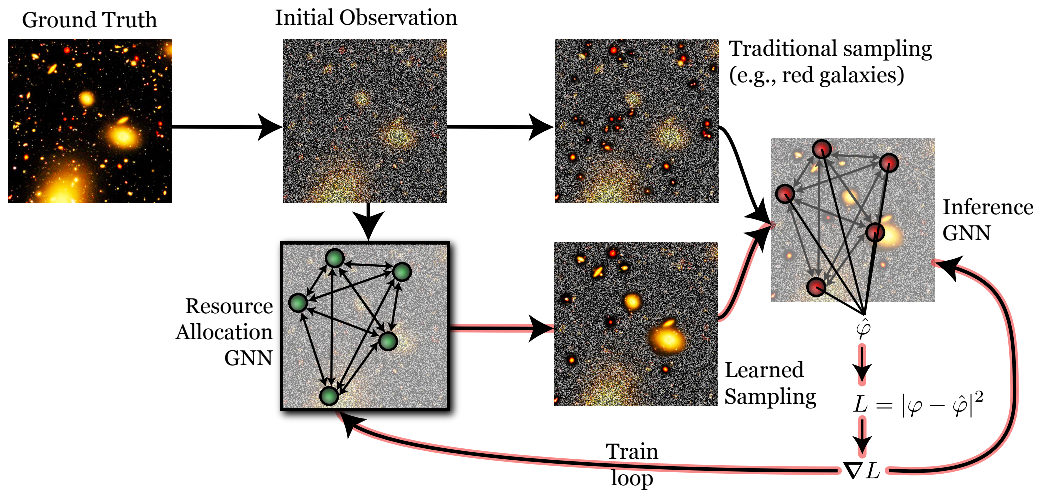

Figure 1: Schema of the proposed technique applied to an astronomical dataset. Given initial (noisy) information, *GNN*$_1$ proposes how the distribute observing resources over all galaxies, after which *GNN*$_2$ predicts a more accurate posterior estimate of a global variable φ of scientific interest. The accuracy of this prediction is used to update both GNNs to better allocate resources. A traditional allocation method is shown only for comparison (see Section 3.3).

that has a "foggy" view of its surroundings and only enough sensory bandwidth to explore a few possible options before having to move on.

We are interested in finding a policy for taking actions in an unknown environment $M \in \mathcal{M}$, described as a Markov Decision Process (MDP), $M = (\mathcal{S}, \mathcal{A}, \mathcal{P}, \mathcal{R}, H)$, where $\mathcal{S}$ is the set of possible states, $\mathcal{A}$ the set of actions, and $\mathcal{P}$ the set of transition probabilities from state s to state t by means of action a, $\mathbb{P}(t \mid s, a)$, resulting in the reward $r(s, a) \sim \mathcal{R}$. The horizon H describes how many actions can be taken and reflects the resource limitations. In contrast to problems in scheduling and control, our problem is not sequential and can thus be described as finding the policy

$$\pi^* = \operatorname{argmax}_\pi U(s_H^\pi) \tag{1}$$

for some domain-specific utility function U. Note that U depends only on the final state s_H^π after all H actions have been taken according to policy π, but not on the ordering of the actions.

For observational sciences, the state set is given by all possible study subjects $\mathbf{v}_i \in \mathbb{R}^{n_v}$, $i = 1 \dots N$, more precisely what we know about them. Possible actions are restricted to allocating an available resource to observe a subject i, which amounts to advancing our knowledge from a prior $p(\mathbf{v}_i)$ to a posterior $p(\mathbf{v}_i \mid a_i = \text{observe } i)$. The set of observed subjects $\mathcal{O}^\pi = \{i : a_i = \text{observe } i\}$ has cardinality H. The final state is thus given by $s_H^\pi = \{p(\mathbf{v}_i)\}_{i \notin \mathcal{O}^\pi} \cup \{p(\mathbf{v}_i \mid i \text{ observed})\}_{i \in \mathcal{O}^\pi}$. The utility is then usually the inverse variance of the posterior of parameter φ for some hypothesized model of the process under study, based on the collection of observations,

$$U(s_H^\pi) = \text{var}^{-1}\left[p(\varphi \mid s_H^\pi)\right]. \tag{2}$$

The non-sequential nature of this problem allows a substantial simplification. Because any action amounts to observing one $i \in \{1, \dots, N\}$, the reward r can be expressed on per-subject basis: $r(s, a = \text{observe } i) = r(i \mid \mathcal{O})$, i.e. the reward of adding i to $\mathcal{O}$. We seek to determine the reward for every possible subject such that the final set $\mathcal{O}$ maximizes U. We propose to parameterize $r(i \mid \mathcal{O})$ as a Graph Neural Network (GNN) $r_\theta(\{\mathbf{v}_i\})$ to exploit possible relations between subjects in forming the optimal set $\mathcal{O}$. GNNs, as defined in [1], are neural networks that accept as input or output an arbitrary graph (defined as a set of nodes and edges) or a scalar variable. A GNN can be thought of as the generalized version of an Interaction Network (INs) [2], using inductive biases motivated from physics. Early work on GNNs include [3; 4; 5]. The optimal policy can be determined by rank-ordering $r_\theta(\{\mathbf{v}_i\})$ and selecting the highest-ranked H subjects. The advantage of this approach lies in avoiding black-box optimization (by e.g. evolutionary algorithms) usually employed for finding solutions to Equation 1 [6; 7]. Instead, we can utilize novel approaches of black-box back-propagation [8; 9] or perturbed optimization [10] for combinatorical problems.

We can further relax the strict set assignment $i \in \mathcal{O}$ and interpret the prediction of the GNN as the *amount* of allocated resources for each subject, e.g. observing time, so that $\sum_i r_\theta(\{\mathbf{v}_i\}) = H$. This redefinition allows us to put the sum constraint into the loss function. If a non-zero minimum allocation is required for any improvement in U (as is often the case in practice), the network predictions will naturally approximate the previous case of a small number of subjects being observed. We continue to employ gradient-based optimization to learn the resource allocation with a GNN and replace the black-box relaxation hyper-parameter in [8; 10] with a variable feasibility penalty on H, increasing it until the constraint is satisfied within acceptable bounds.

2 Context & Related Work

The main contributions of our proposal are two-fold. First, by gradually transitioning from an unconstrained problem to a constrained problem, it should be easier for the GNN to first learn which samples are relevant for maximizing the utility, and then to adjust to the resource limitations — all within the same gradient-based architecture. Second, whereas traditional approaches often rely on manually defined reward functions based on heuristics, we learn a reward function from scratch with the help of a second GNN and forward simulations of the parameter(s) of interest. This flexibility should allow for further improvements in the allocation strategy. Furthermore, performing symbolic regression on the GNN [11; 12] can lead to generalizable formulations of interaction terms that reveal which nodes of the subject network need to be maintained under resource limitations. Providing such a form of model interpretability is very important to the astronomical community for their adoption of any proposed technique.

Resource allocation through Reinforcement Learning (RL) is a rich problem space that spans a wide range of activities and domains. These include control of and communication between autonomous agents (e.g., self-driving cars), assignment of tasks and resources to nodes in grid computing, communication across wireless networks, as well as selecting study subjects in the observational sciences [13; 14; 15; 16]. Topically most similar to our work, [7] optimized the observation schedule for a large astronomical survey with an evolutionary algorithm.

GNNs in particular have been used in prior work for learning policies. The "NerveNet" model [17] uses message passing between different body parts to determine a generalizable policy for agent movement. The "policy-GNN" [18] uses similar principles to our proposed architecture, using GNNs to select the next node in a graph, but considers meta-learning for traditional GNN classification algorithms rather than resource allocation, and cannot be reconfigured to our problem. It also assumes iterative sampling, whereas for our astronomical problem one needs to select the samples at once, based on limited information about the graph. Additional examples of GNNs used for resource allocation include [19; 20], which were applied to resources on a wireless network and focus on the edges of a GNN, whereas we use the edges merely as a way of factoring in interactions between potential subjects.

3 Methodology & Experimental Protocol

We motivate our experiment in Section 3.1 by a real-world problem from current astronomical research. In Section 3.2, we give a detailed definition of our GNN variant, with a full list of hyperparameters, and the algorithm to train it. In Section 3.3, we define how we will perform the experiments, the metric for success, as well as the comparison to existing allocation policies.

3.1 Case Study

Motivated by a challenging problem for large-scale astronomical surveys of the coming years, we focus on the following case study: the selection of celestial objects, usually called "targets", to improve our knowledge of the make-up of the universe. In particular, we will look at the measurement of $O(10^9)$ distant galaxies, for which very accurate positions on the sky (x_1, x_2) are known, but their distances d and masses m are known only to within 10-30%. For precise cosmological studies, all four features, $\mathbf{v} = (x_1, x_2, d, \log m)$, need to be known accurately, the distance to within $\approx 0.1\%$. As astronomers are able to perform targeted observations for $O(10^7)$ galaxies [21], we need to decide which galaxies should be further studied with a more accurate instrument. The final utility from Equation 2 will be given by the inverse variance on a single parameter $\varphi = \Omega_m$, the fraction

Algorithm 1 Pseudocode for learning a strategy of allocating a finite amount of resources H over a large set of study subjects. The goal is to advance from a prior (noisy) to a posterior (accurate) state so that the parameter of interest φ can be optimally inferred.

procedure LEARNOPTIMALOBSERVATIONSTRATEGY
    $\theta_1 \leftarrow$ Kaiming initialization
    $\theta_2 \leftarrow$ Kaiming initialization
    $\lambda \leftarrow$ learning rate
    $H \leftarrow$ total resource allocation
    $(\tau, \delta\tau, \eta) \leftarrow (0, 0.1H^{-2}, 0.001H)$
    $\alpha \leftarrow$ sparsity coefficient
    repeat
        $\varphi \sim p(\varphi)$ ▷ parameter of simulated environment
        $\{\mathbf{v}_i\} \sim$ simulator(φ) ▷ simulated subject catalog, arbitrary cardinality
        for all $i = 1 \dots |\{\mathbf{v}_i\}|$ **do**
            $\epsilon \sim \mathcal{N}(0, \Sigma_{\text{prior}})$
            $\mathbf{v}'_i \leftarrow \mathbf{v}_i + \epsilon$ ▷ simulated prior state
        $\{r_i\} \leftarrow GNN_1(\{\mathbf{v}'_i\}; \theta_1)$ ▷ resource allocation
        for all $i = 1 \dots |\{\mathbf{v}_i\}|$ **do**
            $\epsilon \sim \mathcal{N}\left(0, \Sigma_{\text{posterior}}(r_i)\right)$
            $\mathbf{v}''_i \leftarrow \mathbf{v}_i + \epsilon$ ▷ simulated posterior state
        $\hat{\varphi} \leftarrow GNN_2(\{\mathbf{v}''_i\}; \theta_2)$ ▷ parameter estimation
        $L \leftarrow (\hat{\varphi} - \varphi)^2 + \tau \left(\sum_i r_i - H\right)^2 + \alpha \sum_i r_i$ ▷ regression and regularization losses
        $(\theta_1, \theta_2) \leftarrow (\theta_1, \theta_2) - \lambda \cdot \nabla_\theta L$
        if $|\sum_i r_i - H| > \eta$ **then** ▷ allocation feasibility
            $\tau \leftarrow \tau + \delta\tau$
    until L has stabilized
return GNN_1, the optimized survey scheduler; GNN_2, the optimized inference statistic

of the total energy density in the universe in the form of matter (as opposed to e.g. radiation).[1] Broadly speaking, increasing Ω_m increases the amount of spatial clustering of galaxies throughout the universe. Thus, knowing their precise 3D positions and masses allows to recover Ω_m.

3.2 Architecture & Algorithm

We propose to combine two independent GNNs: GNN_1 encodes the reward, or rather: the resource allocation for every target in a simulated universe [23], as a set-to-set mapping. GNN_2 seeks to estimate the cosmological parameter of the simulated universe, thereby emulating the posterior inference step of Equation 2 as a set-to-scalar mapping. The second GNN is a fast proxy for a scientific analysis, which traditionally would take days or months to complete, and resembles the function of the value network in [24]. We point out that the training of GNN_1 is unsupervised as it is never shown a predefined optimal target set. Our approach is visually depicted in Figure 1.

Our GNN models take the form of the message-passing network variant with a single message-passing step. Using notation from [1], we denote multi-layer perceptrons (MLPs) by $\phi : \mathbb{R}^{(\cdot)} \to \mathbb{R}^{(\cdot)}$, $GNN_1 \equiv (\phi_1^e, \phi_1^v)$, which maps from set to set, is defined by two MLPs: $\phi_1^e : \mathbb{R}^{n_v+n_v} \to \mathbb{R}^{n_e}$, and $\phi_1^v : \mathbb{R}^{n_v+n_e} \to \mathbb{R}^1$; with operations $\mathbf{e}_{1,ij} = \phi_1^e(\mathbf{v}_i, \mathbf{v}_j)$, and the resource allocation $r_i = \phi_1^v\left(\mathbf{v}_i, \sum_{j \in \text{edges}_i} \mathbf{e}_{1,ij}\right)$. Then, $GNN_2 \equiv (\phi_2^e, \phi_2^v, \phi_2^u)$, a GNN from set to scalar, is defined by three different MLPs: $\phi_2^e : \mathbb{R}^{n_v+n_v} \to \mathbb{R}^{n_e}$, $\phi_2^v : \mathbb{R}^{n_v+n_e} \to \mathbb{R}^{n_h}$, and $\phi_2^u : \mathbb{R}^{n_h} \to \mathbb{R}$, with operations $\mathbf{e}_{2,ij} = \phi_2^e(\mathbf{v}_i, \mathbf{v}_j)$, $\mathbf{h}_i = \phi_2^v\left(\mathbf{v}_i, \sum_{j \in \text{edges}_i} \mathbf{e}_{2,ij}\right)$, $\hat{\varphi} = \phi_2^u\left(\frac{1}{n}\sum_i \mathbf{h}_i\right)$. Here, $n = |\{\mathbf{v}_i\}|$, n_v is the fixed number of features for each (input) node, n_e is a hyperparameter for the number of features for each (learned) message $\mathbf{e}_{1,ij}, \mathbf{e}_{2,ij}$, and n_h is a hyperparameter for the number of latent features for each (learned) latent node $\mathbf{h}_i$. We will define edges$_i$ based on a simple Euclidean distance cutoff, with the distance set as a hyperparameter. These GNNs are to be trained using the procedure defined in Algorithm 1.

[1] The interested reader can find more information about cosmology in [22].

3.3 Experiments to perform

Mimicking the general conditions of a follow-up study with a spectrograph instrument at one of the world's largest telescopes, we standardize all four features to the range of $[0, 1]$, and set the prior variances as $\Sigma_{\mathrm{prior}}(\mathbf{v}_i) = \mathrm{Diag}(0, 0, 0.1, 0.25)$. The posterior variance dependents on the amount of resources r_i spent on target i as well as its mass and distance because more massive nearby galaxies are brighter and thus easier to observe in general:

$$\Sigma_{\mathrm{posterior}} = \begin{cases} \Sigma_{\mathrm{prior}} & \text{if } r_i < r_{\min}(d, \log m) \\ \mathrm{Diag}\left(0, 0, 0.001, 0.1\right) & \text{else.} \end{cases} \tag{3}$$

The minimum resource requirement reflects that observations below a certain threshold are practically useless or impossible to perform; it is typically determined by the scientific study itself. We will adopt $\bar{r}_{\min}/H = 10^{-7}$. Its presence is also meant to ensure that the allocations are sparse. As long as $r_{\min}$ is small, the presence of solution polytopes should be tolerable during training. If not, or if the allocations remain insufficiently sparse, we will add a ℓ_1 penalty term to the loss function, whose strength is treated as a hyperparameter.

For realistic surveys, the outcome depends only weakly on the exact value of H, with practical influences, such as weather, likely to play a more important role. Consequently, we have some flexibility η in the total allocation and will set $\eta/H = 10^{-3}$. As this target might be easier to meet, we will experiment with a fixed τ instead of a variable one, and treat its value again as a hyperparameter.

We will do a coarse hyperparameter search over internal architectures of the MLPs for both GNNs: specifically, a grid search over models with between 2 to 5 hidden layers, and 10 to 1000 hidden nodes. This MLP architecture will be the same for all MLPs, and use ReLU activations. The latent dimensions n_e and n_h will also be searched in the same space from 10 to 1000, independently of the hidden layer search.

We are interested if our allocation strategy with GNNs produces better cosmological results than traditional methods. Therefore, we will make a comparison with two alternatives: 1) We will employ the strategy commonly used in astronomy of uniform random selection among galaxies above a certain mass or brightness threshold [21]; 2) We will adapt the evolutionary algorithm from [7] to maximize Equation 2 by varying the importance of a fixed set of well-motivated but predefined feature functions for policy proposals. We define the metric for success as $\mathrm{var}^{-1}[\hat{\varphi} - \varphi_{\mathrm{test}}]$, where $\hat{\varphi}$ is computed for 50 test simulations with some $\varphi_{\mathrm{test}} \sim p(\varphi)$.

We are also interested in realistic applicability of this technique. Therefore, we will measure the generalizability of this method to a slightly different simulator than the one used during training, and introduce biases in the data not seen in the training set, to determine if the learned observational strategy still produces better results than traditional methods.

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