Abstract

In supervised learning, we fit a single statistical model to a given data set, assuming that the data is associated with a singular task, which yields well-tuned models for specific use, but does not adapt well to new contexts. By contrast, in meta-learning, the data is associated with numerous tasks, and we seek a model that may perform well on all tasks simultaneously, in pursuit of greater generalization. One challenge in meta-learning is how to exploit relationships between tasks and classes, which is overlooked by commonly used random or cyclic passes through data. In this work, we propose actively selecting samples on which to train by discerning covariates inside and between meta-training sets. Specifically, we cast the problem of selecting a sample from a number of meta-training sets as either a multi-armed bandit or a Markov Decision Process (MDP), depending on how one encapsulates correlation across tasks. We develop scheduling schemes based on Upper Confidence Bound (UCB), Gittins Index and tabular Markov Decision Problems (MDPs) solved with linear programming, where the reward is the scaled statistical accuracy to ensure it is a time-invariant function of state and action. Across a variety of experimental contexts, we observe significant reductions in sample complexity of active selection scheme relative to cyclic or i.i.d. sampling, demonstrating the merit of exploiting covariates in practice.

1 Introduction

In supervised learning, we learn to map features to targets by minimizing a statistical loss averaged over samples from an unknown distribution which is typically associated with a singular task (Learned-Miller 2011). When this map is a universal function approximator, i.e., a deep neural network (DNN), this framework has yielded successes across a variety of applications (Yin et al. 2017; Gopalakrishnan et al. 2017; Du et al. 2017; Pan et al. 2012). However, its successes have been limited when data is comprised of several qualitatively different regimes, or tasks. To enhance adaptivity to disparate tasks, meta-learning seeks to obtain model parameters along the Pareto frontier of the minimizer of many training objectives simultaneously (Andrychowicz et al. 2016), and has gained attention for overcoming data starvation issues in robotics and physical systems (Finn, Abbeel, and Levine 2017).

Existing approaches, however, offer little guidance about how to select samples on which to train to enable fast convergence, and instead operate via cyclic or random sampling. Doing so is appropriate when disparate tasks are statistically independent. However, in many contexts such as meteorology (Racah et al. 2017), computer vision, and robotics (Finn, Abbeel, and Levine 2017), significant relationships between tasks exist. We are then faced with the question of how to incorporate such relationships into the training of a meta-model. In this work, we do so via active sample selection during training meta-models. This active sample selection is executed according to correlation within and across tasks via multi-armed bandits (MAB) (Lattimore and Szepesvári 2020) and Markov Decision Processes (MDPs) (Puterman 2014) based schedulers, which yields substantial gains in sample efficiency across a variety of experimental settings.

Before continuing, a few historical remarks are in order. Augmenting DNN training to improve adaptivity has received substantial interest over the years. Transfer learning relaxes the independent and identically distributed (i.i.d.) hypothesis on data, and seeks to transform a model good for one task to another (domain adaptation) (Tian et al. 2018; Dai et al. 2007), i.e., transfer an understanding of Spanish to Italian (Dai et al. 2007). Generative modeling, by contrast, directly estimates the data distribution in order to output new examples that plausibly could have been drawn from the original data, similar in spirit to bootstrapping. Recent advances in parameterizing these models using deep neural network, have enabled scalable modeling of complex, high-dimensional data (Shorten and Khoshgoftaar 2019). Both approaches are effective for transferring from one task to another, but it is unclear how to employ these approaches when seeking generalization across many tasks, unless the generative/covariance model co-evolves with data drift, which may cause instability (Radford, Metz, and Chintala 2015).

By contrast, meta-learning seeks to learn attributes of a problem class which are common to many distinct domains, and has been observed to improve adaptability via explicitly optimizing their few-shot generalization across a set of meta-training tasks (Wang et al. 2019). Importantly, doing so enables learning of a new task with as little as a single example (Yu et al. 2018; Yin et al. 2019). Meta-learning algorithms can be framed in terms of a cost that ties together many training sub-tasks simultaneously, with, for instance,
Figure 1: Our scheduler selects which samples from training subsets to execute task-specific updates to ensure the meta-model’s performance improves as rapidly as possible as quantified by meta-training subsets’ contribution to the meta-model’s validation accuracy. Doing so requires a novel definition of the reward in multi-armed bandits or MDPs.

recurrent or attention-based models, or an otherwise two-stage objective (Liu and Vicente 2019); the inner cost defines performance on a single task, and the outer multi-objective tethers performance across tasks. Doing so results in procedures that experimentally have yielded substantial gains in terms of DNN adaptation and generalization to new tasks (Rajeswaran et al. 2019).

The aforementioned works, as well as other meta-learning objectives, operate under the assumption that training samples are i.i.d. to justify sampling cyclically or randomly. This assumption is invalid for settings involving drift or latent relationships between classes, such as training an NLP system for both Spanish and Italian (Peters, Ruder, and Smith 2019), image classification of animals from a common genus (Wang et al. 2018), or systems identification problems arising in ground robotics when traversing prairie and forest floor (Koppel et al. 2016; Chiuso and Pillonetto 2019). Thus, in this work, we propose to build a scheduler on top of the meta-learner (Figure 1) to exploit relationships between meta-training data subsets to allocate samples judiciously.

To do so, we incorporate ideas from active learning (Cohn, Ghahramani, and Jordan 1996), specifically, selecting a given meta-learning training subset, according to either a multi-armed bandit (Auer, Cesa-Bianchi, and Fischer 2002a) or a Markov decision process (MDP) (Bellman 1957). Which technique is appropriate depends on whether the statistical accuracy of one task is allowed to be correlated with another. In either case, the state is the weights of a meta-learning model, the arm (action) is the index of the specific training task or class label, and the reward is the statistical accuracy of the meta-model on a validation set multiplied by a scaling factor to ensure the reward is stationary. Moreover, regret of a given arm is the scaled average long-run validation accuracy on that meta-training subset.

Experimentally, we observe the merit of bandit selections when we employ the Upper Confidence Bound (UCB) or Gittins Index, and MDP policies based upon a linear programming solver (De Farias and Van Roy 2003) for meta-training DNNs. In particular, we obtain orders of magnitude improvement in sample complexity when employing our sample selection schemes relative to cyclic or random sampling (Table 1) for training feedforward multilayer DNNs and convolutional variants on MNIST (Lecun et al. 1998), the real world Extreme Weather dataset (Racah et al. 2017), and a meta-learning variant of CIFAR100 (Krizhevsky 2012). On top of sample efficiency gains, the order of sample selection experimentally can fundamentally improve the limit points to which the meta-model converges.

2 Elements of Meta-Learning

In supervised learning, we seek to build a predictor \( f_w : \mathcal{X} \rightarrow \mathcal{Y} \) which maps feature vectors \( x \in \mathcal{X} \) to target variables \( y \in \mathcal{Y} \) by minimizing a loss function \( \ell : \mathbb{R}^p \times \mathcal{X} \times \mathcal{Y} \rightarrow \mathbb{R} \). Here \( w \in \mathbb{R}^p \) denotes the parameters of the statistical model (such as a feedforward or convolutional neural network). The loss \( \ell \) quantifies the difference between candidate prediction \( f_w(x) \) at an input vector \( x \in \mathcal{X} \) and a target variable \( y \in \mathcal{Y} \), and is small when \( f_w(x) \) and \( y \) are close. For concreteness and clarity, we focus on the case of multi-class classification, an instance of supervised learning, although the ideas developed in this work are also applicable to unsupervised and reinforcement learning. Thus, the space of target variables is of the form \( \mathcal{Y} = \{1, \ldots, C\} \), where \( C \) is the number of classes. In this context, we wish to compute the parameters that minimize the statistical loss over \( w \in \mathbb{R}^p \),

\[
w^* = \arg\min_w \mathbb{E}_{x,y}[\ell(f_w(x), y)]
\]

where the expectation is over \( \mathbb{P}(x,y) \). In practice, one is given a batch of data \( D = \{(x_1, y_1), \ldots, (x_N, y_N)\} \), which may be associated with any number \( N \) of unknown distributions \( \{\mathbb{P}^i(x,y)\}_{i=1}^N \) colloquially referred to as tasks. In particular, we have access to \( N \) distinct training subsets \( D_i = \{x_{u}, y_{u}\}_{u=1}^{n_i} \) whose union is \( D \), and we would like to find a model that simultaneously performs well on each:

\[
w^* = \arg\min_{w \in \mathbb{R}^p} \sum_{i=1}^{N} \ell(f_w(x_u), y_u) \quad \text{for } i = 1, \ldots, N
\]

We consider that each meta-learning sample subset \( D^i \) is split into a training and a validation set, i.e., \( D^i = D^i_{tr} \cup D^i_{val} \) with \( |D^i_{tr}| = n_i \) and that the training subsets \( D^i_{tr} \) for all \( i \) are used for training within tasks, whereas the validation set is used across tasks. Moreover, we denote \( D_{val} = \cup_i D^i_{val} \) and \( D_{tr} = \cup_i D^i_{tr} \).

Then, we hypothesize that the statistical model \( f_{w} \) depends on a vector of hyperparameters \( \lambda \in \mathbb{R}^d \), such as the regularizer, the radius of a pooling step in a convolutional neural network, or other architectural considerations. One way to pose the problem of meta-learning

\( ^{1}\)For disambiguation, we denote samples of \( D^i \) as \( \{x_{u}, y_{u}\} \) for \( u = 1, \ldots, n_i \). Moreover, we denote \( n_i \) as the number of training examples available for task \( i \). Throughout, to further alleviate notation, we suppress the dependence of example \( \{x_{u}, y_{u}\} \) on class \( c \), and instead leave this dependence implicit.

Table 1: Relative sample efficiency gain compared to baseline cyclic sampling on different experiments.
where $h$ is again some cost, possibly equal to $\ell$, which is small when $f_{w_\lambda}(x_u)$ and $y_u$ are close. This formulation yields models $f_{w_\lambda}$ which both perform well on individual tasks $i$ as quantified by $H^i(w_{\lambda})$ and across tasks through seeking to minimize $L^i(w_{\lambda})$ for all $i = 1, \ldots, N$ simultaneously. That is, model selection of $f_{w_\lambda}$ according to (2) at the inner-stage (the constraint evaluation) is decoupled across tasks, whereas at the outer stage, the objective is coupled by hyperparameters $\lambda$. For connections to bilevel optimization, see (Franceschi et al. 2018; Likhosherstov et al. 2020).

Given that computing the simultaneous minimizer of a number of different non-convex functions is intractable, one may hypothesize that the universal quantifier over task $i$ in (2) may be replaced by the sum-costs

$$L(w_{\lambda}) = \sum_{i=1}^{N} L^{i}(w_{\lambda}), \quad H(w_{\lambda}) = \sum_{i=1}^{N} H^{i}(w_{\lambda}), \quad (3)$$

which presupposes that tasks and classes are statistically independent. Then, because exactly solving the inner optimization problem, i.e., the constraint in (2), is both intractable numerically when $f_{w_\lambda}$ is a neural network (as the problem becomes non-convex) and may lead to solutions that over-prioritize a singular task (over fit), one may consider the computational approximation of (2) as (Finn, Abbeel, and Levine 2017)

$$\min_{\lambda} L^{\lambda}(w_{\lambda}) \quad \text{s.t.} \quad w_{\lambda} = w_{\lambda} - \eta \nabla H(w_{\lambda}). \quad (4)$$

Note that the $\text{argmin}$ in the constraint of (2) been substituted in (4) by the fact that we seek model parameters close to the fixed point of the gradient of the task-specific objective $H^{i}(w_{\lambda})$ (Finn, Abbeel, and Levine 2017), while also minimizing the cost $L$ which is defined across tasks. The spirit of (4) is that we seek model parameters that perform well after a few gradient steps on an unseen task, whereas (1) yields solutions that perform well on average observing a number of samples from a common distribution. Prevaling practice in meta-learning is built upon assuming statistical independence between tasks and classes, i.e., writing $H = \sum_{i=1}^{N} H^{i}$, which permits grouping the inner and outer expectations – see (Fallah, Mokhtari, and Ozdaglar 2020).

**Main Results** In this work, we move beyond the hypothesis that tasks and classes are independent by considering a generalization of (4); rather than focusing on the aggregate task-specific cost $H(w_{\lambda})$, we retain the task-specific model fitness in the constraint $H^{i}(w_{\lambda})$

$$\min_{\lambda} L^{\lambda}(w_{\lambda}) \quad \text{s.t.} \quad w_{\lambda} = w_{\lambda} - \eta \nabla H^{i}(w_{\lambda}), i = 1, \ldots, N, \quad (5)$$

which instead reveals the question of how to compute a point at the intersection of a set of $N$ constraints for each of $C$ classes when the satisfaction of one constraint influences another. In this work, we focus on sequential approaches to addressing this question, inspired by active learning (Cohn, Ghahramani, and Jordan 1996; Settles 2011). In particular, we develop techniques to select which among the $N$ different tasks and $C$ different classes one should execute a training step at any given time such that the overall meta-learning performance $L(w_{\lambda})$ is optimized expeditiously. Doing so yields significant gains in sample efficiency of training meta-learners across a variety of experimental contexts, as we demonstrate in Sec. 4 – see Table 1. Next, we shift to the technical development of bandits and MDPs to this end.

### 3 Active Sample Selection

In meta-learning (5), there are two intertwined challenges. First, to enforce the constraint, one requires access to training examples $(x^{i}_{u}, y^{i}_{u})$ for each task $i$ and class $c$ in order to evaluate the gradient of the different task-specific objectives $H^{i}(w_{\lambda})$ with respect to model parameters $w_{\lambda}$ for fixed hyperparameters $\lambda$. With access to $(x^{i}_{u}, y^{i}_{u})$ for each task, a stochastic gradient update with step-size $\delta > 0$ is performed:

$$w_{t+1} = w_{t} - \delta \nabla \sum_{u=1}^{B} h(f_{w_{t}}(x^{i}_{u}), y^{i}_{u}) \quad (6)$$

where $1 \leq B \leq n$ is some mini-batch size, which makes (6) a stochastic gradient step (for $B < n$), and we have suppressed dependence on $\lambda$ for succinctness. Existing approaches proceed to execute training steps on all tasks $i$ and classes cyclically, meaning there are $t = N$ total updates of the form (6) – see (Andrychowicz et al. 2016; Finn, Abbeel, and Levine 2017). Then, we conduct a stochastic gradient update of step-size $\eta > 0$ with respect to the meta-model:

$$\lambda_{k+1} = \lambda_{k} - \eta \sum_{(x_u,y_u) \in D_{val}} \nabla \lambda \ell(f_{w_{\lambda}}(x_u), y_u), \quad (7)$$

For simplicity, we consider that $B$ samples are chosen from validation set $D_{val}$ to execute a meta-model update in (7).
Any sequential selection strategy for $\theta$ served sequentially, under the setting that the underlying (Lattimore and Szepesvári 2020). Since rewards are obtained by a player (scheduler) selecting one among $S$ available arms, where the indicator $\mathbb{1}$ is 1 when the model $f_{\theta}$ classifies training example $(x_u, y_u)$ correctly and null otherwise. Observe, however, that as the model $w$ and hyperparameters $\lambda$ evolve during training, the reward will drift as the validation accuracy improves, which invalidates the stationarity hypothesis (that the distribution in $\mathbb{S}$ is stationary) underlying the guarantees of UCB and Gittins indices.

To ameliorate this issue, we use the fact that the convergence rate of SGD and its first-order variants (such as Adam) on non-convex problems exhibit a $O(1/\sqrt{t})$ convergence rate to a first-order stationary point in terms of attenuation of the gradient norm (Bottou, Curtis, and Nocedal 2018). Section 3.1 Multi-armed Bandits Scheduling of Subsets

Multi-armed bandits (MAB) encapsulates the setting where we seek to exploit covariates within a task, e.g., how one class is correlated with another. In MAB, at each time $t$, a player (scheduler) selects one among $S$ available arms, denoted as $\theta_t \in \{1, \ldots, S\}$ (subsequently we abbreviate $\{1, \ldots, S\} := [S]$), after which a reward $r_t(\theta_t)$ is revealed (Lattimore and Szepesvári 2020). Since rewards are observed sequentially, under the setting that the underlying generating process of the rewards is stationary, the optimal selection is the one that performs best-in-hindsight, i.e., $\theta^* = \text{argmax}_{\theta \in \Theta} R(\theta) := \mathbb{E}(r_t(\theta))$. The performance of any sequential selection strategy for $\theta_t$ may be quantified as the expected sub-optimality, or regret $R_T$, defined as,

$$R_T = \mathbb{E}\{T \cdot r_t(\theta^*) - \sum_{t=1}^{T} r_t(\theta_t)\}.$$ (8)

Strategies whose time-average regret approaches null, $R_T/T \to 0$ as the time horizon $T$ becomes large are called no-regret. We consider two widely-used MAB no-regret algorithms, the Upper-Confidence Bound (UCB) (Lai and Robbins 1985) and Gittins Indices (Gittins 1979; Glazebrook and Weber 2011), due to both their simplicity and that they operate upon fairly different principles. Before shifting to describing how $\theta_t$ is selected for these algorithms, we identify how the structural attributes of MABs are well-suited to active sampling for meta-models.

In meta-learning, for multi-class classification with $C^t$ classes for task $i$, the $S$ different possible arms are the $\cup_i [C^i]$, and the arm $\theta_t$ pulled at a given time $t$ is the class $c_t$, meaning that one executes a SGD step associated with class $c_t$. An open question is then how to define the reward $r_t(\theta)$. One possibility is the statistical accuracy on the validation set $D_{val}$:

$$\tilde{r}_t(\theta) = \frac{1}{|D_{val}|} \sum_{(x_u, y_u) \in D_{val}} \mathbb{1}[f_{\theta}(x_u) = y_u],$$ (9)

where the indicator $\mathbb{1}$ is 1 when the model $f_{\theta}$ classifies training example $(x_u, y_u)$ correctly and null otherwise. Observe, however, that as the model $w$ and hyperparameters $\lambda$ evolve during training, the reward will drift as the validation accuracy improves, which invalidates the stationarity hypothesis (that the distribution in $\mathbb{S}$ is stationary) underlying the guarantees of UCB and Gittins indices.

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Figure 2: Scaled $\sqrt{t} \times$ (validation error) on MNIST is nearly constant for each class (state) as a function of within-task training index $t$. Thus, via the approximate relationship between the rate of attenuation of the expected gradient of the meta-training objective $\mathbb{E}[\|w_t L(w_t)\|]$ and validation error $e(t)$ during within-task training, we can define a reward $r(t) = 1 - \sqrt{t}e(t)$ which is time-invariant, and hence satisfies the conditions required for a valid bandit formulation in the sense that the distribution in $\mathbb{S}$ is stationary.

One way of going beyond statistical independence between tasks in the updates is by using second-order information (Im, Jiang, and Verma 2019; Song et al. 2019; Park and Oliva 2019); however, when computing the Hessian of the Lagrangian of $\mathbb{C}$, its statistical properties are only locally (not globally) informative due to non-convexity – see (Nocedal and Wright 2006). Instead, we directly exploit dependencies both within and between tasks. While related ideas have been proposed for how to weight the gradient of the meta-objective $L(w)$ in (Cai et al. 2020; Simon et al. 2020; Nicholas et al. 2020), none have augmented the update rule both within a task and across tasks.

To do so, we estimate dependencies both within each task and dependencies across different tasks as respectively a multi-armed bandit (MAB) or a Markov Decision Problem (MDP). Before proceeding to defining their specific use in modeling dependencies to more effectively schedule which task one should perform an inner-loop update at a given time, we present the generic procedure for concreteness as Algorithm 1 which is depicted graphically in Figure 1. It involves a MAB/MDP scheduler followed by the within-task and cross-task SGD optimization. Next, we define in detail the Scheduler called in Algorithm 1.

Algorithm 2: UCB Scheduler

Result: Batch $B$
Input: Time index $t$
Initialization: Upper Bound $U = 2$; Exploration factor $\xi > 1$; $V_{\theta, D^i}$: number of visits to subset $D^i$, until time $t$; Use initial model to train on each $D^i$ with first batch of samples $\{x_u, y_u\}_{u=1}^B$ independently to obtain $r_0(D^i)$; $V_0(D^i) = 1, \forall i \in [N]$

At time $t$:

$$\tilde{\mu}_{t-1, D^i} = \frac{1}{V_{t-1, D^i}} \sum_{\tau=0}^{t-1} r_{\tau}(\theta_{\tau}) \mathbb{1}\{\theta_{\tau} = D^i\}, \forall i \in [N]$$

$$\theta_t = \text{argmax}_{D^i}\{\tilde{\mu}_{t-1, D^i} + U \sqrt{\frac{\log t}{V_{t-1, D^i}}}\}$$

$$V_{t, D^i} = \sum_{\tau=0}^{t} \mathbb{1}\{\theta_{\tau} = D^i\}, \forall i \in [N]$$

$$B = \{x_u, y_u\}_{u=(t-1)B+1}^t$$

The expected sub-optimality, or regret $R_T$, defined as,
Algorithm 3: Gittins Index Scheduler

Result: Batch $B$
Input: Time index $t$;
Initial: Compute Gittins Indices $v^i$ of $D^i$ using Algorithm 4 in Appendix B

At time $t$:
\[ \theta_t = \arg \max_{\lambda} D, v^i(y^i_{t+1} - B + 1) \]
\[ B = \{ x_u, y_u \}_{u \in \{ t+1 \}}^B \]

4.3]. Then, based on the hypothesis that the rates of attenuation of the gradient norm $E[\|\nabla_w L(w)\|]$ and the statistical error $\epsilon_t = 1 - \hat{r}_t(\theta)$ are comparable, $\sqrt{\epsilon_t}$ should be constant during training. Thus, we define the reward as
\[
 r_t(\theta) = 1 - \sqrt{1 - \hat{r}_t(\theta)} \tag{10}
\]

Figure 2 shows the errors of some classes in a sample meta-training subset over the first 120 training steps in our MNIST experiment (elaborated upon in Section 4). Observe that $\sqrt{\epsilon_t}$ of each state is approximately a constant over time, which provides evidence to support our hypothesis, and thus substantiates our choice of reward for linking class selection among performance on training subsets $H^i(w)$ with the meta-learning validation objective $L(w)$ [cf. [3]]. The values of $\sqrt{\epsilon_t}$ may increase for larger $t$ since the model parameters may settle to the local minima and the error saturates. This is not a problem, however, as later selections influence regret less due to the accumulating sum over time in regret [5]. This decrease in importance of later decisions may further be enforced through discounting that arises in UCB, Gittins Indices, and MDPs as described next.

Upper Confidence Bound Upper Confidence Bound (UCB) operates upon the principle of optimism in the face of uncertainty. Specifically, we initialize the model associated with task $i$ via a single iteration of [5] on $(x_t^i, y_t^i)$. Then, we count the number of times $\theta = \theta_t$ has been chosen at time $t$ as $V_{t,\theta}$ for each $\theta \in [C]$, i.e., $V_{t,\theta} = \sum_{\tau=1}^t \mathbb{1} \{ \theta_{\tau} = \theta \}$ and its associated average reward:
\[
 \mu_{t,\theta} = \frac{1}{V_{t,\theta}} \sum_{\tau=1}^t r_{\tau}(\theta_{\tau}) \mathbb{1} \{ \theta_{\tau} = \theta \}
\]

Then, UCB selection operates via calibrated perturbation from the sample mean of the reward $\mu_{t,\theta}$ as
\[
 \theta_{t+1} = \arg \max_{\theta} \mu_{t,\theta} + U \left( \frac{\xi \log t}{V_{t,\theta}} \right)
\]

where $\xi$ and $U$ are constants that encourage exploration. This procedure is repeated for $B - 1$ total steps, and achieves regret that is logarithmic in the total number of steps $B$, which is precisely the within-task mini-batch size — see [Lai and Robbins 1985]. We set the exploration factor $U = 2$. For each hyperparameter update of $\lambda$, a batch of $B$ samples are selected from $D_{val}$ according to those classes from $\cup_i[C^i]$ which maximize the upper-confidence bound as determined by Algorithm 2. Then, these samples are used to update the hyperparameters $\lambda$ w.r.t. the validation loss in [7].

Algorithm 4: MDP Scheduler

Result: Batch $B$
Input: Time index $t$;
Initial: Compute Value vectors $V(s)$ solving LP [15]
At time $t$:
\[
 s = (y^i_t B + 1, y^i_{t+1} B + 1, \ldots, y^i_{t+1} B + 1) \]
\[
 a = \arg \max_{\gamma \in [N]} (r(s, i) + \sum_{s'} \gamma P(s, s') V(s'))
\]
\[
 B = \{ x_u, y_u \}_{u \in \{ t+1 \}}^B
\]

Gittins Index UCB is a frequentist (non-Bayesian) strategy: it does not construct any distributional model for how to select $\theta_t$. Next we consider a Bayesian approach based upon Gittins Index, which may also be shown to be no regret (Gittins and Dempster 1979). It has the additional merit that it exploits the Markovian dependencies between states by the transition matrix structure. Proceeding with its technical development necessitates a distributional model among states. For task $i$, we construct the count-based measure:
\[
 P_{c_{c'}} = \frac{\text{number of jumps from label } c \text{ to } c'}{\text{number of examples with label } c} \tag{11}
\]
This count-based construction of the transition matrix between classes in $D^i$ has precedent in Bayesian filtering [Krishnamurthy 2016]. Gittins index is then defined as
\[
 v^i(\theta) = \max_{\tau > 0} \frac{\mathbb{E} \left[ \sum_{\tau=0}^\tau \beta^\tau r_{\tau}(\theta_{\tau}) \mathbb{1} \{ \theta_{\tau} = \theta \} \right]}{\mathbb{E} \left[ \sum_{\tau=0}^\tau \beta^\tau \mathbb{1} \{ \theta_{\tau} = \theta \} \right]} \tag{12}
\]

where $\tau$ is a measurable stopping time. Here $v^i(\theta)$ is called Gittins index associated with reward $r(\theta)$ at state $\theta$, and the expectation $\mathbb{E}$ is computed with respect to the distribution $P_{c_{c'}}$ over labels $[C^i]$ for a fixed $i$. We define the Gittins index identically as (12) for each meta-training subset $i$ as $v^i(\theta)$.

The Gittins Index Theorem establishes that a selection is optimal, i.e., no regret [3], if and only if it always selects the bandit with highest Gittins Index at each iteration. Gittins Index scheduler is shown in Algorithm 3.
of classes valued consisting of the meta-learning scheduler policy. The state space $S$ and Van Roy (2003). We proceed to formulate this LP for the capable [cf. (11)] is via linear programming (LP) (De Farias

The optimal policy is time-homogeneous, i.e., assigns a fixed action $a$ to any state $s$ independent of time $t$ for $H = \infty$. One way to obtain the optimal policy for tabular settings, i.e., when the state and action spaces are discrete and of moderate cardinality, when the transition matrix is available [cf. (11)] is via linear programming (LP) (De Farias and Van Roy 2003). We proceed to formulate this LP for the meta-learning scheduler policy. The state space $S$ is vector-valued consisting of the $N$-fold Cartesian product of the set of classes $[C] \times \cdots \times [C]$, the aggregate transition model is the $N$-fold Kronecker product of task-specific transition matrix

$P^i = I^1 \otimes I^2 \otimes \cdots \otimes I^N$. The Kronecker product ensures the dimensionality consistency between state space $S$ and the transition model $P^i$. The action determines which meta-training subset should be chosen at the next training time-slots. Moreover, the reward is given as the validation accuracy (10), as in the beginning of Sec. 3.1, except now we reinterpret the reward as being not only a function of the selected class but also the meta-learning subset $D^i$ as well, i.e., $r(\theta) = r(s, i)$. This is the additional expressive power of MDPs over Gittins Index. In MDPs, the reward for the same state changes when different arms are played, which exploits both within and cross-task correlation. Then, we formulate an LP to solve for the optimal value $V(s)$:

$$\min \sum_s V(s), s.t. V(s) \geq r(s, i) + \sum_{s'} \gamma P^i(s, s') V(s')$$  \hspace{1cm} (15)$$

for $\forall s, i$. The optimal policy is computed by equation (14), where $V(s')$ is obtained from the optimal solution in LP (15). The MDP scheduler is shown in Algorithm 4. With our various active selection schemes defined, we shift to establishing their experimental merits for improving the training of meta-models across a variety of problem contexts.

4 Experiment

We experiment the proposed MAB/MDP scheduler on three datasets with either explicit or inexplicit sample dependencies within and cross tasks. Across all experiments, we observe significant relative sample efficiency gain compared to basic cyclic sampling, demonstrating the merit of exploiting covariates in practice.

Digit Recognition We first evaluate the performance of the schedulers on MNIST handwritten digits (LeCun 1998) – MNIST forms the validation set $D_{val}$, and the task-specific subsets are the related Optical Recognition (Xu, Krzyzak, and Suen 1992) and Semeion Handwritten Digit data sets (Buscema 1998) – see Appendix C for additional details.
In cross-task \( L_{w_f} \), we select multinomial logistic as the loss \( l \), and in task specific \( H_f(w_f) \), cross-entropy is selected as \( lss^i \) (Murphy [2012]). The specific model \( f_{w_f} \) is a four-layer fully-connected neural network with 300 nodes per layer, and the hyperparameters \( \lambda \) concatenates the inner objective’s (the constraint in (5)) learning rate and the initialization \( w^i \). We use Adam (Kingma and Ba [2014]) with decaying learning rate as outer objective optimizer.

To evaluate the performance, we vary the batch size \( B \in \{1, 20, 100\} \). We compare UCB (Algorithm 2), Gittins Index (Algorithm 3), and cyclic sampling from all subsets, where one simply passes through rows of training data one after another. Results are given in Figure 3. Because there are no strong inner dependencies between examples in MNIST dataset, Gittins index algorithm does not exhibit significant gains compared to UCB. However, both active schedulers outperform the cyclic sampling: to obtain test accuracy 80%, Gittins index requires 40 samples as compared with 53 for UCB sampling and 1300 for cyclic from test data.

Meta-CIFAR-100 The CIFAR-100 dataset is an image dataset containing 100 classes with 600 images each (Krizhevsky [2009]). We construct 4 task-specific meta-training subsets: each task is associated with a superclass, that is, we form meta-training subsets consisting entirely of a single superclass. This defines a classification problem associated with those classes within it – see Appendix C.

We use cross entropy as both the inner and outer loss functions and employ a four-layer CNNs with strided convolutions and 64 filters per layer. The hyperparameters are the same as in the Digit Recognition – see Appendix C.

Figure 4 shows the result of using Gittins Index and UCB compared with cyclic sampling. Note the significant improvements in sample efficiency and the superior limit point to which the model converges when using active selection as compared with cyclic passes through task-specific samples. Moreover, Gittins index outperforms UCB, which is evidence that inherent correlation in the class and task structure is more pronounced for this setting. To achieve 40% accuracy, Gittins Index scheduler requires 1400 samples, while UCB requires 2000 samples and cyclic scheduler needs 5000 samples, meaning they are respectively \(2.57\times\) and \(1.50\times\) more efficient than cyclic sampling.

Extreme Weather Gittins index, as compared to UCB, employs the Markovian transition matrix [cf. (11)] to select the next sample (12), and thus leverages dependencies between classes. In principle, the merit of modeling correlations may be greater when the order of the data has physical meaning. This is not obvious in the case for Meta CIFAR-100 and Digit Recognition. To further investigate the merit of exploiting covariates between samples, we focus on an instance arising in meteorology, as the physical meaning of ordering is inherent due to, e.g., the water cycle.

Data Preparation We consider the Extreme Weather Dataset (Racah et al. [2017]). Training data consists of image patterns of various features and the bounding boxes (prescribed regions) on the images label a specific extreme weather type (considered as class). We use various bounding boxes with different features to construct the meta training, validation and test sets – see Appendix C for details.

Result Our results are summarized in Table 2 and Figure 5.

| Schedulers | U850 | TMQ | U850 | V850 | VBOV | Z100 |
|------------|-----|-----|------|------|------|------|
| MDP        | 0.901 | 0.873 | 0.917 | 0.870 | 0.704 | 0.842 |
| Gittins Index | 0.904 | 0.850 | 0.925 | 0.825 | 0.735 | 0.797 |
| UCB        | 0.673 | 0.689 | 0.684 | 0.641 | 0.609 | 0.619 |
| Cyclic     | 0.352 | 0.043 | 0.304 | 0.480 | 0.392 | 0.448 |

Table 2: Overall Test Classification Accuracy on Various Features using Different Schedulers. MDP and Gittins Index Schedulers outperform UCB and cyclic scheduling.

Figure 5: Evolution of multi-Classification accuracy when using various features. MDP and Gittins Index Schedulers outperform UCB and cyclic scheduling.

We departed from prior works on meta-learning that presume independence between tasks by directly considering within and across-task correlation. We proposed a module to select samples according to their contribution to meta-model validation accuracy, which yielded significant sample efficiency gains across a variety of domains as compared to cyclic passes through data. Rigorously analyzing these sample efficiency gains is the subject of future work.

5 Conclusion
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In the supplementary material, we provide additional details regarding the construction of meta-learning tasks and evaluations, the associated data sets, and quantities constructed toward these ends.

A Determine Sample Dependencies in Meta-training Subsets Using Chi-squared Test

First, we focus on the statistical validation of the transition matrices constructed as (11) for the various data sets. These transition matrices are essential to the constructing Gittins Index (12) and the policy associated with an MDPs (15). Our goal here is to determine whether the constructed transition matrices provide evidence that classes and tasks exhibit any significant correlation effects.

To do so, we use the Pearson’s Chi-Squared to determine whether there is a statistically significant difference between the expected frequencies and the observed frequencies at the 95% confident level, i.e., p value of 0.05. The null hypothesis is samples are i.i.d. in each subset. If the statistical test rejects the null hypothesis, i.e., p-value $\leq 0.05$, Gittins Index or MDPs are justified for scheduling. Under independence, the rows of the constructed Markov chain induced by the transition matrix $P_{cc'}$ are identical for a fixed $D_{tr}$. Table 3 shows the p-values of meta-training subsets in MNIST and meta CIFAR-100 experiments. The p-values of subsets in Extreme Weather experiment are all nearly 0.

| Subset 1 | Subset 2 | Subset 3 | Subset 4 | Subset 5 |
|----------|----------|----------|----------|----------|
| p-value  | $4.36 \times 10^{-7}$ | 0.0314 | 0.00836 | $2.33 \times 10^{-16}$ | $1.20 \times 10^{-9}$ |

(a) Digit Subsets

| Subset 1 | Subset 2 | Subset 3 | Subset 4 | Subset 5 |
|----------|----------|----------|----------|----------|
| p-value  | 0.0302 | 0.00986 | 0.00215 | 0.00351 |

(b) Meta CIFAR-100

Table 3: p-values of meta-training subsets in MNIST and Meta CIFAR-100. p-values for the Extreme Weather data set are identically near null, and the transition matrix is diagonally dominant – see Appendix D.

Algorithm 5: Compute Gittins Indices of States in Meta Training Subsets

Result: Gittins Indices $v^i$

State (label) space $Y = \{1, ..., C\}$

N meta training subsets $\{D_i\}_{i=1}^N$, $D_i = \{x_u, y_u\}_{u=1}^\hat{n}$

Transition Matrices of each subset $P_i$, $i = 1, ..., N$

Discount factor $\beta$

for $i = 1, ..., N$ do

Fit the first sample of each label in $D_i$ into the initial model independently and get the reward vector $r_i = [r_i^1, ..., r_i^C]$

end

for $i = 1, ..., N$ do

Compute gittins index $v^i$ of each subset $D_i$:

Initialization:

state $\alpha_1 = \arg\max_{\alpha \in Y} r_{i\alpha}^1$

$v^i(\alpha_1) = r_{i\alpha_1}^1$

for $l = 2, ..., C$ do

$C(\alpha_l) = \{\alpha_1, ..., \alpha_{l-1}\}$, $S(\alpha_l) = Y \setminus C(\alpha_l)$

$Q_{a,b}^l = \begin{cases} P_{ab}^i & \text{for } b \in C(\alpha_l) \\ 0 & \text{otherwise} \end{cases}$ \quad $\forall a, b \in Y$

$d^{(l)} = [I - \beta Q^{(l)}]^{-1} r^i$, $b^{(l)} = [I - \beta Q^{(l)}]^{-1} 1$

choose $\alpha_l = \arg\max_{\alpha \in S(\alpha_l)} \frac{d^{(l)}}{b^{(l)}}$

$v^i(\alpha_l) = \frac{d^{(l)}}{b_{\alpha_l}^{(l)}}$

end

end
This provides substantial evidence across the different data domains that classes and tasks exhibit Markovian dependence, which is evidence that exploiting correlation effects may be useful for scheduling.

B Largest-remaining-index Algorithm for Gittins Index in Meta Learning

We use largest-remaining-index algorithm to compute the Gittins Index of each state (class) in each meta-learning subset $i$. We elaborate upon how this procedure works next. Suppose the state space for a given subset is $\mathcal{Y} = \{1, ..., C\}$. First step is to identify state (class) $\alpha_1$ with the highest Gittins index:

$$\alpha_1 = \arg\max_{\alpha \in \mathcal{Y}} r^i_\alpha, \; v^i(\alpha_1) = r^i_{\alpha_1}$$

Next step is the recursion to find state $\alpha_l$ with $l$th largest Gittins index. Define continuation set as $C(\alpha_l) = \{\alpha_1, ..., \alpha_{l-1}\}$ and stopping set as $S_l(\alpha_l) = \mathcal{Y}\backslash C(\alpha_l)$. Then state $\alpha_l$ and its associated Gittins Index can be computed using a matrix $Q \in \mathbb{R}^{C \times C}$ and two vectors $d,b \in \mathbb{R}^C$, which are shown in detail in Algorithm $\[5\]$. This procedure is then used in the Gittins Index based scheduler summarized in Algorithm $\[3\].

C Additional Details of Experiments

We elaborate upon the meta-learning problem formulation in terms of data preparation and allocation, parameter selection, loss function specification, etc. for the experimental results presented in Section 4. These points are collated into Table 4 for convenience.

| Meta-training subsets | Within-task loss | Cross-task loss | Neural set | Hyperparameters |
|-----------------------|------------------|-----------------|------------|----------------|
| Digit Recognition     | 2 subsets from Semeion Dataset | Cross-entropy | Multinomial logistic | DNN initial weights $w$ and biases $b$ Within-task objective learning rate |
|                       | 3 subsets from Opt. Recognition Dataset | Cross-entropy | 4-layer fully connected DNN 300 nodes per layer | |
| Meta CIFAR-100        | 4 subsets from superclasses | Cross-entropy | Cross-entropy | DNN initial weights $w$ and biases $b$ Within-task objective learning rate |
|                       | aquatic mammals, medium-sized mammals, small mammals, insect | 4-layer CNNs with strided convolutions 64 filters per layer | |
| Extreme Weather       | 5 subsets from first 5 bounding boxes | Cross-entropy | Cross-entropy | DNN initial weights $w$ and biases $b$ Within-task objective learning rate |
|                       | each subset contains different 5 features | 4-layer CNNs with strided convolutions 64 filters per layer | |
|                       | 500 samples per subset | | |

Table 4: Experimental setup: data description, parameter selection, architecture specification, loss functions, meta-model definition.

C.1 Digit Recognition

We construct $N = 5$ meta-training subsets with 1400 samples per set. Two are selected from Semeion dataset, and the data from the other three sets are from Optical Recognition Dataset. We construct a common validation set with size 1400 from the two datasets above to evaluate the performance after each hyper iteration. The performance of this procedure is evaluated on a test set comprised of 60000 samples from MNIST dataset. The size of digit images from Optical Recognition dataset and Semeion dataset is different from the size of MNIST images. So we resize the training and validation image to 28 × 28 in order to ensure images have compatible dimensionality.

C.2 Meta CIFAR-100

The CIFAR-100 dataset is an image dataset containing 100 classes with 600 images each (Krizhevsky 2009). There are 500 training images and 100 testing images per class. The 100 classes are grouped into 20 superclasses, each of which contains classes. Each image comes with a “fine” label (the class to which it belongs) and a “coarse” label (the superclass to which it belongs). We construct the task-specific subsets where each task is associated with a superclass, that is, we form data sets consisting entirely of a single superclass, which defines a classification problem associated with those classes within it. Superclasses consist of “aquatic mammals”, “medium-sized mammals”, “small mammals” and “insect.” Then, we use the superclass “large carnivores” as the cross-task validation set. This construction we call Meta-CIFAR-100.

C.3 Extreme Weather

We consider the Extreme Weather Dataset (Racah et al. 2017), where samples from both climate simulations and re-analysis are considered. The reanalysis samples are generated by assimilating observations into a climate model. Ground truth labeling of various events is obtained via multivariate threshold based criteria implemented in TECA, and manual labeling by experts (Racah et al. 2017). Training data consists of image patterns, where several relevant spatial variables are stacked together over a prescribed region (called bounding box) that bounds a type of weather event, which is considered as ground truth label. The dimension of the bounding box is based domain knowledge of events observed in the real world. There are 1460 example images (4 per day, 365 days in the year) arranged in time order for each year’s dataset. We only used 2005’s dataset for the experiment.
Each image has 16 channels corresponding to 16 features. Each channel is 768 x 1152 corresponding to one measurement per 25 square km on earth.

We first build the Meta training subsets. For each image, there are up to 15 bounding boxes, where each box indicates a prescribed region in the image that bounds a type of extreme weather event. We used these bounding boxes to split the dataset into different subsets of meta-training set. The first box of each image forms the first subset, the second boxes form the second subset, and so on. Only the first 5 boxes of each image are used, so in total we have 5 different tasks. In order to better differentiate tasks, each subset uses different 5 among 16 features and the features used in each subset are not identical. The first five bounding boxes forms the 5 subsets with 500 images each, another 50 images with all bounding boxes and 5 features are used for validation and other images with all bounding boxes with only one feature are used for testing. Because of the spatial dimension of climate events vary significantly and the spatial resolution of source data is non-uniform, the bounding boxes are resized to 32 x 32.

D Additional Result of Extreme Weather Experiment

We present a sample transition matrix of the task-specific data subset via (11) below:

\[
\begin{bmatrix}
0.721 & 0.256 & 0.020 & 0.003 \\
0.052 & 0.901 & 0.033 & 0.014 \\
0.004 & 0.037 & 0.939 & 0.020 \\
0.000 & 0.017 & 0.454 & 0.529 \\
\end{bmatrix}
\]

The transition matrix is diagonal-dominant which means that the examples in the dataset are highly correlated. The same type of weather event or its neighbor type of event are likely to happen after one type of extreme weather happens. Combining this structure of likelihood with reward vectors obtained, which are the initial validation accuracy, the Gittins Index reflects the relative “importance” of each state in each arm during the training process. Following the Gittins Index policy we can find the optimal stopping time on one meta-training set and the next dataset the ML model should learn.

Table 5 displays the summary of examples used in each meta training subset to train the ML model using different schedulers, and feature U850 in test set. Observe that for MDP and Gittins Index scheduler, each meta-training subset contributes to training different types of weather events while training set 4 is rarely scheduled, which indicates that it contributes little towards validation performance for any of type of events. This filtering out of irrelevant information makes training the meta-learner more efficient. The overall classification accuracy for each weather type at the end of training is summarized in Table 6. Since the schedulers select more samples labeled as Tropical Cyclone and Extratropic Cyclone, the classification accuracy on these weather types are higher in general.

| Subset | Trop. Depression | Trop. Cyclone | Extratropic Cyclone | Atmo. River |
|--------|-----------------|---------------|---------------------|------------|
| Subset 1 | 140             | 0             | 0                   | 0          |
| Subset 2 | 10              | 3190          | 0                   | 0          |
| Subset 3 | 230             | 0             | 1150                | 0          |
| Subset 4 | 0               | 0             | 20                  | 0          |
| Subset 5 | 0               | 0             | 0                   | 260        |

(a) MDP Scheduler

| Subset | Trop. Depression | Trop. Cyclone | Extratropic Cyclone | Atmo. River |
|--------|-----------------|---------------|---------------------|------------|
| Subset 1 | 440             | 20            | 0                   | 0          |
| Subset 2 | 0               | 1870          | 0                   | 0          |
| Subset 3 | 0               | 10            | 2450                | 0          |
| Subset 4 | 0               | 10            | 0                   | 0          |
| Subset 5 | 0               | 0             | 0                   | 210        |

(b) Gittins Index Scheduler

| Subset | Trop. Depression | Trop. Cyclone | Extratropic Cyclone | Atmo. River |
|--------|-----------------|---------------|---------------------|------------|
| Subset 1 | 120             | 850           | 180                 | 0          |
| Subset 2 | 170             | 650           | 180                 | 0          |
| Subset 3 | 90              | 430           | 490                 | 0          |
| Subset 4 | 90              | 140           | 670                 | 100        |
| Subset 5 | 40              | 90            | 700                 | 100        |

(c) UCB Scheduler

Table 5: Summary of Examples used in Meta-training subsets, each subset uses different 5 features. The test set uses feature U850. By exploiting correlation, samples associated with certain classes and tasks are significantly down-sampled.

|        | Trop. Depression | Trop. Cyclone | Extratropic Cyclone | Atmo. River |
|--------|-----------------|---------------|---------------------|------------|
| MDP    | 0.789           | 0.961         | 0.947               | 0.658      |
| Gittins Index | 0.421       | 0.836         | 0.963               | 0.395      |
| UCB    | 0.368           | 0.698         | 0.788               | 0.421      |

Table 6: Test Classification Accuracy of each Weather Type using Feature U850