Learning to learn by gradient descent as a discrete-time finite-horizon MDP

A thesis submitted by Matthew Stachyra

in partial fulfillment of the requirements for the degree of Master of Science in Computer Science

Tufts University

December 2023

Advisor: Jivko Sinapov

Thank you to my parents for supporting me. In their own words, they don't care what I am working on as long as I enjoy it. Perhaps that's for the best.

Thank you to Daniel Fuenmayor for being the first person to believe in my thesis. You indulged my ideas before they took shape, and gave me the confidence to shape them.

Thank you to Michael Joseph for your eternal skepticism.

/noindent Meta-learning, often referred to as "learning to learn," is a paradigm within machine learning that focuses on developing models that generalize knowledge across tasks. Such a model learns across tasks as it learns within tasks, enabling the model to adapt quickly to new, unseen tasks. A model for a new task can be generated with near-optimal parameters in no or very few training steps. Meta-learning in machine learning is desirable in cases where there is limited data for a task or when a model needs to learn efficiently within few data samples. This thesis investigates whether Meta-learning can be cast as Reinforcement learning (RL) problem for non-RL tasks. RL applied to Meta-learning has included hyperparameter search for neural architectures and meta-policies in RL task domains (Meta-Reinforcement Learning). RL has not been used to train models (parameter search) for non-RL tasks in the Meta-learning paradigm. This thesis asks: can Meta-learning be formulated as a sequential task? And if Meta-learning can be formulated as a sequential task, can Meta-learning be a discretetime finite-horizon MDP solved by deep RL? Reinforcement Meta-Learning (REML) is proposed to formulate the Meta-learning task as composing neural networks layer by layer for sampled tasks with a shared parameter space across tasks. REML is evaluated according to the protocol proposed by Finn et al (2018) as used for the Model-agonistic meta-learning (MAML) algorithm. REML is first tested on regression tasks as a series of varying sinusoidal curves. Performance is evaluated looking at loss per step (convergence speed) for a model constructed by REML as compared to a model trained from scratch. REML is also tested on a few-shot learning task where it is given 5 and 10 samples and tested after 0, 1, and 10 gradient steps. Future work is to continue testing REML on classification and reinforcement learning tasks, and expanding the action space of REML to decide hyperparameters in addition to parameters.

Chapter 1

Introduction

A deep learning model of a target function is always constrained by available data in the target domain. Few data examples limits the ability of the model to represent the target function at unknown points. Trying to learn under this constraint is known as few shot learning. One paradigm applied to manage this constraint is meta-learning or "learning to learn". This thesis contributes a new meta-learning algorithm. We are using the definition of meta-learning as proposed initially by Thrun et al in 1998: an algorithm is learning to learn if its performance at each task (where there is more than 1 task, more than 1 performance measure, and more than 1 training experience) is expected to improve with the number of tasks and training experiences on these tasks. The new meta-learning algorithm is Reinforcement Meta-Learning (REML), which casts learning to learn as a parameterized markov decision process.

REML is composed of a supervisory agent in a system with the models it generates for provided tasks in a domain. The supervisory agent is implemented with reinforcement learning with a parameterized action space, and the models are implemented as deep neural networks in the environment of the meta-learner agent. The supervisory agent composes and trains the models layer by layer for each task. In this way the reinforcement learning meta-learner is responsible for both hyperparameters and parameters.

This is to my knowledge the first work to use reinforcement learning as the meta-learner in a model agnostic manner akin to MAML (model agnostic meta-learning) proposed by Finn et al 2018. Other works at the intersection of reinforcement learning and meta-learning include RL-driven hyperparam-

eter search (i.e., neural architecture search) and meta-reinforcement learning, where both the inner and outer loops are RL agents. The performance of REML will be evaluated for regression, classification, and reinforcement learning tasks on the same benchmarks as the MAML (Model agnostic meta-learning) paper by Finn et al 2018. As time allows, or as future work, I will investigate certain convenient properties inherent to this design. One of these may be robustness to learning on unrelated tasks, relative to offline trained tasks. I hypothesize that because layers in REML are composed individually, they have a more expressive quality in their availability to be sequenced in different combinations. This is as opposed to a single initial set of policy parameters adapted for each task, as is in MAML.

The research questions this work seeks to answer are: (1) can REML enable fast learning for new tasks?, (2) can REML be model agnostic and perform for regression, classification, and reinforcement learning?, and (3) is REML robust to unrelated tasks at meta test time?

To answer these research questions, preliminary questions answered are: (1) how to design a neural network using reinforcement learning?, (2) how to train a neural network using reinforcement learning?, (3) how to transfer learning across tasks using reinforcement learning?, and (4) how to enable meta-learning with reinforcement learning as the meta-learner?

Chapter 2

Related work

The REML algorithm proposed in this thesis is deep reinforcement learning for meta-learning. Related work includes the research where reinforcement learning is applied to meta-learning, and more generally, popular meta-learning algorithms in recent years. REML is unlike most meta-learning research in its use of RL as the meta-learning agent, rather than adapting a meta-learning agent to RL. Algorithms that have used RL as the meta-learning agent are typically limited to RL tasks (CITE). REML is unique in adapting parameters with RL for non-RL tasks. For this reason, REML is Reinforcement Meta-Learning and not Meta Reinforcement Learning.

RL² is perhaps the most similar work to REML in that it frames the learning process as the RL agent's objective [1]. It frames learning a new algorithm as a reinforcement learning problem. The difference is that the new algorithm learned is limited to reinforcement learning tasks, hence the work is called RL².

REML has parallels to neural architecture search (NAS) in searching a space for a configuration to build a neural network with. The difference is that the configuration is hyperparameters in NAS versus parameters in REML. Neural architecture search with reinforcement learning is a specific method similar its use of in the use of an RL learner to generate networks where the loss of these generated networks is the reward signal to the RL learner [2]. The authors represent the model description as a variable length string that is generated by an RNN.

Model Agnostic Meta-Learning (MAML) shares with REML the ability to generalize to different learning tasks including regression, classification, and reinforcement learning [3]. A notable difference is MAML uses a single set of parameters that it adapts to new tasks and calculates the Hessian to update the global parameters with information on how these parameters changed for each new task. The intent was to enable the architecture to adapt with few gradient steps, to multiple tasks.

- 2.1 Title section 2.1
- 2.1.1 If needed
- 2.1.2 If needed
- 2.2 Title section 2.2
- 2.2.1 If needed
- 2.2.2 If needed
- 2.3 Title section 2.3
- 2.3.1 If needed
- 2.3.2 If needed

Chapter 3

Background

3.1 Artificial Neural Networks

Artificial neural networks (ANNs) are non-linear computational models that approximate a target function $f: \mathbb{R}^n \to \mathbb{R}^m$, where n and m are integers [4]. Given a set $X = \{(\mathbf{x}_1, \mathbf{y}_1), \dots, (\mathbf{x}_N, \mathbf{y}_N)\} \subset \mathbb{R}^n \times \mathbb{R}^m$ of input-output pairs of size N the model is trained to approximate f such that $f(\mathbf{x}_i) = \mathbf{y}_i \forall i \in \{1, 2, \dots, N\}$. By the Universal Approximation theorem, a neural network's approximation of a continuous function is theoretically guaranteed to be as precise as it needs to be given the network has at least one hidden layer with some finite number of nodes [5].

3.1.1 Starting from linear regression

Consider the problem of predicting the value of one or more continuous target variables $\mathbf{t} \subset \mathbb{R}^m$ provided a D-dimensional vector \mathbf{x}_n of input variables, or what is called regression. Given a set consisting of N observation and value pairs $\{(\mathbf{x}_n, \mathbf{t}_n)\}_{n=1}^N$, the objective is to predict the value for any input vector \mathbf{x}_n such that it is as as close as possible to the provided target value \mathbf{t}_n .

One approach is linear regression, or a linear combination over the components of an input pattern \mathbf{x}_n

$$y(\mathbf{x}_n, \mathbf{w}) = w_0 + w_1 x_1 + \ldots + w_D x_D \tag{3.1}$$

where \mathbf{x}_n has D dimensions, $\mathbf{x}_n = (x_1, \dots, x_D)^T$ and $w \in \mathbb{R}^{D+1}$ represents the parameters of the function, $w = (w_0, \dots, w_D)$ and D is extended to D+1

for the bias weight w_0 .

As is, this regression function is limited to being a linear function over the input vector \mathbf{x}_n . Non-linear basis functions ϕ on the input variables make the function $y(\mathbf{x}_n, \mathbf{w})$ non-linear for an input \mathbf{x}_n :

$$y(\mathbf{x}_n, \mathbf{w}) = w_0 + \sum_{i=1}^{D} w_i \phi_i(x_i)$$
(3.2)

This equation can be simplified further if we define a useful basis function for the bias $\phi_0(\mathbf{x}) = 1$ such that

$$y(\mathbf{x}_n, \mathbf{w}) = \sum_{i=0}^{D} w_i \phi_i(x_i)$$
(3.3)

Despite producing non linear outputs over the input \mathbf{x} this is *linear regression* because it is linear with respect to \mathbf{w} .

3.1.2 Constructing neural networks

Basic ANNs can be seen as an extension to linear regression where the basis functions become parameterized. The basis functions continue to be non-linear functions over the linear combination of the input, but now the output of the basis function is dependent on the learned coefficients $\{w_j\}$. In this construction, basis functions are known as *activation* functions h in the context of neural networks.

We start by rewriting equation 1.2 as a linear combinations over the input variables to produce a or the activation.

$$a = \sum_{i=1}^{D} w_i x_i + w_0 \phi(x_i)$$
 (3.4)

The value a is transformed using a non-linear activation function h. This transformation produces z and is referred to as a *hidden unit*.

$$z = h\left(a\right) \tag{3.5}$$

The coefficients $\{w_j\}$ parameterizing this non-linear transformation are referred to as a *layer*.

An ANN has a minimum of two layers - an input layer and output layer. However, ANNs are not limited to 2 layers. ANNs can have l many layers where $l \in [2, +\infty)$. Networks with > 2 layers are referred to as deep neural networks. For the purposes of the background, we will continue with the simple 2-layer case to establish preliminaries.

The input layer operates on an input (x_1, \ldots, x_D) to produce activations $a_j = (a_1, \ldots, a_M)$, where M denotes the number of parameters $\{w_j\}$ in the input layer. The parameters for the input layer are represented with a superscript (1) and the parameters for the output layer will be represented with a superscript (2).

$$a_j = \sum_{i=1}^{D} w_{ji}^{(1)} x_i + w_{j0}^{(1)}$$
(3.6)

The activations are passed through a non-linear activation h

$$z_j = h\left(a_j\right) \tag{3.7}$$

The output layer then transforms the hidden units z_j to produce output unit activations a_k where $k \in (1, ..., K)$ and K is the number of outputs expected for this problem (i.e., appropriate to the target variable \mathbf{t}_i for \mathbf{x}_i).

$$a_k = \sum_{j=1}^{M} w_{kj}^{(2)} z_j + w_{k0}^{(2)}$$
(3.8)

The activation a_k is transformed by a different non-linear activation function that is appropriate for K. Here this activation function is represented as σ . A common choice of activation function h for non-output layers is the rectified linear unit $h(a) = \min(0, a)$. A common choice of activation function for σ is the sigmoid function $\sigma(a) = \frac{1}{1+e^{-a}}$ for classification problems and the identity $y_k = a_k$ for simple regression problems. We now present the equation for a feed-forward pass through a 2-layer ANN.

$$y_k(\mathbf{x}_n, \mathbf{w}) = \sigma \left(\sum_{j=1}^M w_{kj}^{(2)} h \left(\sum_{i=1}^D w_{ji}^{(1)} + w_{j0}^{(1)} \phi(x_i) \right) + w_{k0}^{(2)} \right)$$
(3.9)

A neural network then is a non-linear function over an input $\mathbf{x_n}$ to an output y_k that seeks to approximate $\mathbf{t_n}$ and is controlled by a set of adaptable parameters \mathbf{w} .

3.1.3 Training a neural network

The goal of learning for a neural network is to optimize the parameters of the network such that the loss function $E(X, \mathbf{w})$ takes the lowest value. Continuing with the previous example for regression, we look at the sum-of-squares error function

$$E(X, \mathbf{w}) = \frac{1}{2} \sum_{n=1}^{N} ||y(\mathbf{x}_n, \mathbf{w}) - \mathbf{t}_n||^2$$
(3.10)

There is typically not an analytical solution and iterative procedures are used to minimize the loss function E. The steps taken are

$$\mathbf{w}^{(\tau+1)} = \mathbf{w}^{(\tau)} + \Delta \mathbf{w}^{(\tau)} \tag{3.11}$$

where τ is the iteration step. An approach for the weight update step with $\Delta \mathbf{w}^{(\tau)}$ is to use the gradient of $E(X, \mathbf{w})$ with respect to the parameters \mathbf{w} . The weights are updated in the direction of steepest error function decrease or in the $-\nabla E(X, \mathbf{w})$ direction.

$$\mathbf{w}^{(\tau+1)} = \mathbf{w}^{(\tau)} + \alpha \nabla E\left(X, \mathbf{w}^{(\tau)}\right) \tag{3.12}$$

where $\alpha > 0$ is the learning rate controlling the size of update step taken. This iterative procedure is called *gradient descent optimization* [6].

3.1.4 Error function derivatives

The gradient $\nabla E(X, \mathbf{w})$ is calculated with respect to every $w \in \mathbf{w}$, for all $\mathbf{x}_n \in X$.

We start with one input pattern $\mathbf{x_n}$ and rewrite the error function as

$$E_n = \frac{1}{2} (y(\mathbf{x_n}, \mathbf{w}) - \mathbf{t_n})^2$$

$$= \frac{1}{2} \sum_{j=1} (w_{kj} z_j - t_{nk})^2$$
(3.13)

The calculation starts with the gradient of E_n with respect to each w_{kj} in the output layer (2) then continues backwards to layer (1) for w_{ji} . This method can extend to l-layer networks where l = (1, ..., L) and $L \subseteq \mathbb{R}$.

Observe that

$$\frac{\partial E_n}{\partial w_{kj}} = \frac{\partial E_n}{\partial a_k} \frac{\partial a_k}{\partial w_{kj}} \tag{3.14}$$

We start by calculating the partial derivative of E_n with respect to the activation a_k . Recall that $a_k = \sum_k w_{kj} z_j$. By the chain rule:

$$\frac{\partial E_n}{\partial a_k} = (h(a_k) - t_{nk})h'(a_k)
= h'(a_k)(\hat{y}_n - t_{nk})$$
(3.15)

We introduce a new notation to call this partial derivative an error

$$\delta_k \equiv \frac{\partial E_n}{\partial a_k} \tag{3.16}$$

Next we calculate the partial derivate of a_k with respect to w_{kj}

$$\frac{\partial a_k}{\partial w_{kj}} = \frac{\partial}{\partial w_{kj}} \left(\sum_k w_{kj} z_k \right)$$

$$= z_k$$
(3.17)

With which we can write

$$\frac{\partial E_n}{\partial w_{kj}} = \delta_k z_k \tag{3.18}$$

The procedure will continue in the same way for the remainder of the layers and their units, where we calculate the errors δ for the units in the layer and multiply error of that unit by its activation z. For layer (1) (input layer) we need to calculate

$$\frac{\partial E_n}{\partial w_{ji}} = \frac{\partial E_n}{\partial a_j} \frac{\partial a_j}{\partial w_{ji}} \tag{3.19}$$

starting with δ_j or $\frac{\partial E_n}{\partial a_j}$. Observe that

$$\frac{\partial E_n}{\partial a_j} = \sum_k \frac{\partial E_n}{\partial a_k} \frac{\partial a_k}{\partial a_j} \tag{3.20}$$

where k is the number of outputs (here, k=1 for the continued regression example).

We calculated $\frac{\partial E_n}{\partial a_k}$ above. Continue with

$$\frac{\partial a_k}{\partial a_j} = \frac{\partial}{\partial a_j} \left(\sum_k w_{kj} h(a_j) \right)
= h'(a_j) w_{kj}$$
(3.21)

We can finish calculating the error δ_j for equation 1.18

$$\frac{\partial E_n}{\partial a_k} \frac{\partial a_k}{\partial a_j} = h'(a_k)(\hat{y}_n - t_{nk})h'(a_j)w_{kj}$$

$$= \frac{\partial E_n}{\partial a_j}$$

$$= \delta_j$$
(3.22)

Thus we obtain the backpropagation formula

$$\delta_j = h'(a_j) \sum_k w_{kj} \delta_k \tag{3.23}$$

where the error for a unit j is the result of backpropagating the errors in the units later in the network.

Calculating the gradient is backpropgating the errors. As we have seen, this procedure begins with a forward propagation of the input vectors x_n to calculate the activations of all units. Then, it involves calculating the errors δ_k in the output layer. Using δ_k we can calculate δ_j for the hidden units in previous layers. With all errors δ , the gradient is calculated by multiplying the error by the activations a transformed by their non-linear function h where h(a) = z.

3.1.5 Recurrent Neural Networks

ANNs can be constructed as directed graphs, formally defined as G = (V, E) where V is the set of vertices $\{v_1, \ldots, v_n\}$ and E is the set of edges $\{(u, v) \mid u, v \in V\}$. We show neural networks are directed because the edges are a set of ordered

pairs. In comparison, an undirected graph would have edges $\{\{u,v\} \mid u,v \in V\}$. In terms appropriate to neural networks, V corresponds to our hidden units $\{z\}$ and output units and E corresponds to the parameters $\{w\}$.

The 2-layer network we constructed above was a directed acyclic graph. G is acyclic if $\forall v \in V$, there does not exist a cycle containing v. This means that for $\forall (u, v) \in E, u \neq v$.

ANNs can contain cycles however. A type of ANN that contains cycles is a recurrent neural network (RNN) [6]. An RNN is recurrent in that information persists in the network by being passed from one forward propagation step to the next. This ability to incorporate past network data makes RNNs useful for simulating dynamical systems.

RNNs model past network data as \mathbf{h}_t or the hidden state

$$\mathbf{h}_t = f_h(\mathbf{x}_t, \mathbf{h}_{t-1}) \tag{3.24}$$

$$\mathbf{y}_t = f_o(\mathbf{h}_t) \tag{3.25}$$

where f_h is a transition function parameterized by θ_h and f_o is an output function parameterized by θ_o [7]. The transition function can be a non-linear function such as the rectified linear unit or the sigmoid function.

Datasets used with RNNs may include T_n many input patterns $\mathbf{x}^{(n)}$ where $T_n \in \mathbb{R}$ is the number of timesteps for which there is data for the datapoint

$$\left\{ \left(\mathbf{x}_{1}^{(n)}, \mathbf{y}_{1}^{(n)} \right), \dots, \left(\mathbf{x}_{Tn}^{(n)}, \mathbf{y}_{Tn}^{(n)} \right) \right\}_{n=1}^{N}$$
 (3.26)

The cost function is

$$E(\theta) = \frac{1}{N} \sum_{n=1}^{N} \sum_{t=1}^{T} d(\mathbf{y}_{t}^{(n)}, f_{o}(\mathbf{h}_{t}^{(n)}))$$
(3.27)

where θ is the parameters of the network, and $d(\mathbf{a}, \mathbf{b})$ is the divergence measure such as Euclidean distance used in the above sum of squares error.

The parameters θ are updated with a variant of backpropagation that works with sequential data called *backpropagation through time (BPTT)* [8]. This method "unrolls" the RNN into each a computational graph one time step

at a time. This unrolled RNN is equivalent to a deep neural network where the same parameters re-appear throughout the network per timestep. Backpropagation through time sums the gradient with respect to each parameter for all times the parameter appears in the network.

RNNs are prone to challenges during training including exploding gradient and vanishing gradient. During training with BPTT the gradients can become very large (i.e., exploding) or very small (i.e., vanishing). Calculating the errors involves multiplying the errors from later layers by the activations in earlier layers as defined above. RNNs can have long sequences in the unrolled network, meaning many multiplication operations over the gradients. Multiplying large or small numbers many times will lead to very large numbers and very small numbers, respectively.

A large gradient will cause large weight updates in the gradient update step, such as in gradient descent optimization, which will make training unstable. A small gradient will cause negligent or no weight updates such that no learning happens and hidden unit activation trend to 0. These activations are called *dead neurons* where "neuron" is another word for a hidden unit.

3.1.6 Long Short-Term Memory Networks

An extension of the RNN is the Long Short-Term Memory Network (LSTM), intended to address the exploding and vanishing gradient problems or "error back-flow problems" [9]. LSTMs introduce additional calculations called "gates" within the cells of an RNN. These gates control how much information is retained or discarded in each timestep. Each cell has state C_t and the gates responsible for modifying C_t across T_n for (x_{1n}, \ldots, x_{Tn}) .

The forget gate controls the amount of information retained from the previous unit h_{t-1} and the input x_t to include in this state C_t

$$f_t = \sigma(W_f \cdot [h_{t-1}, x_t] + b_f)$$
 (3.28)

where W_f is a weight matrix and b_f is the bias term. The sigmoid is used as it outputs a value in [0,1], with 0 meaning to discard all previous network data and 1 meaning to keep all previous network data.

The *input gate* controls the amount of information to be included from the input x_t

$$i_t = \sigma(W_i \cdot [h_{t-1}, x_t] + b_i)$$
 (3.29)

where W_i is the weight matrix and b_i is the bias term for this gate, respectively.

The output of the forget gate and input gate are composed as a proposal vector that would be added element-wise to C_t .

$$\widetilde{C}_t = \tanh\left(W_C \cdot [h_{t-1}, x_t] + b_C\right) \tag{3.30}$$

where \widetilde{C}_t holds the amount of information to include from x_t and h_{t-1} . The tanh function is the hyperbolic tangent function $\frac{e^{2x}-1}{e^{2x}+1}$. It is used to transform x to a value within [-1,1] that results in more stable gradient calculations.

The cell state C_t is the sum of the two values we have constructed: some amount of the previous state C_{t-1} and some amount of the proposed \widetilde{C}_t .

$$C_t = f_t * C_{t-1} + i_t * \widetilde{C}_t \tag{3.31}$$

The final calculation what to output - the new hidden state h_t . The cell calculates how much of the new cell state C_t to output for this timesteep.

$$o_t = \sigma(W_o \cdot [h_{t-1}, x_t] + b_o)$$
 (3.32)

$$h_t = o_t * \tanh(C_t) \tag{3.33}$$

3.2 Reinforcement Learning

An agent exhibiting reinforcement learning (RL) learns from interacting with an environment. The environment is represented in terms of states it can take on based on the agent's actions. This environment gives the agent a numerical reward signal based on the state-action pair. The agent continues to take actions within the environment, trying to maximize its cumulative reward.

In reinforcement learning, the learning objective of the agent then is to learn a policy π , a map from each state $s \in S$ and action $a \in A_s$ to the probability of $\pi(a|s)$ of taking action a in state s that maximizes cumulative reward over timesteps t.

Reinforcement learning is considered a distinct type of learning to supervised learning and unsupervised learning. The learning considered thus far has been supervised learning or learning from labeled examples where the ground truth is known. In this supervised context, the agent or model is given the answer after it acts. The model's task is instead to learn from labeled data such that it can generalize or approximate to unseen examples where a label does not exist. RL is not supervised learning because no answer is ever provided to the agent; the agent needs to discover its' own answer. RL is also not unsupervised learning, where the objective is to find patterns in unlabeled data; while the agent may build a model of the environment it interacts with as a kind of pattern recognition, the objective of RL is to maximize the numerical reward signal rather than to discover hidden structure.

A reason reinforcement learning is used over supervised learning is the answer may not be known for a sufficiently complex task. Another reason is its often impractical to provided a full set of representative examples of all states the agent may experience.

3.2.1 Markov Decision Processes

Consider an agent that interacts with the environment over timesteps $t \in \mathbb{R}_{\geq 0}$. For each timestep $t = 0, 1, 2, \ldots$ the agent is in a state $s \in S$ where it can take an action $a \in A_s$ and receive the reward signal r_{t+1} as it transitions from state $s = s_t$ to state $s' = s_{t+1}$. This sequence would look something like

$$S_0, A_0, R_1, S_1, A_1, R_2, \dots$$
 (3.34)

The state is the information the agent has about the environment. It is based on this state that the agent takes an action and enters a new state – and this process of taking an action from a state to a new state repeats. Therefore, the state needs to encode information that allows a decision in the context of how the agent is doing doing in the environment.

This information is more than the immediate sensations provided by the environment but must include relevant information about the sequence thus far (i.e., the history) of the agent's interactions with the environment. A state is said to be *Markov* if it encodes all previous states' information as

relevant to take the next action in the current state.

In other words, $\forall s \in S$, s incorporates information (history) of the sequence to the current state. The probability of the next state s_{t+1} only depends on s_t and a_s . The past history of states and action transitions is not needed. This condition is the *Markov property*.

When a state is Markov, it has complete information on the dynamics of the environment

$$p(s', r|s, a) = P\{R_{t+1} = r, S_{t+1} = s' \mid S_t, A_t\}$$
(3.35)

where the probability of the environment continuing to state s' depends only on this state s_t and action a_t . For this to be true, $\forall s \in S$, s has a history of all sequences possible from that state.

RL problems that have the Markov property can be modelled as Markov Decision Processes (MDP) [10]. A markov decision process (MDP) is represented as a 4-tuple (S, A, P_a, R_a) where

- S is the set of states or state space
- $A = \{A_s \mid s \in S\}$ is the set of actions or action space
- P is $P_a(s,s') = P(s_{t+1} = s'|s,a)$ or transition function
- $R_a(s,s') = \{r \mid r \in \mathbb{R}\}\$ is the reward upon transition from state s to state s' or reward function

The goal of the agent is to maximize the reward signal over timesteps t where $t \in T$, $T \subseteq \mathbb{R}$. The reward value $r_t \in \mathbb{R}$ is rewarded by the environment to the agent every timestep. This accumulated value is called the *return*.

$$G_t = R_{t+1} + R_{t+2} + R_{t+3} + \ldots + R_T \tag{3.36}$$

This equation for the return works if the time horizon of the agent's experience is finite. This is the case when experience have a termination condition that concludes the agent's trajectory. A learning experience that ends with a finite T is called an *episode* as in *episodic learning*. This type of learning fits tasks that have a natural endpoint, such as a car parking itself in a valid

spot. A learning experience without a boundary like this is called a *continuing task*. However, if $T = \infty$ then the return could be infinite.

Another problem with the above formulation for return is it provides equal weighting to all rewards. A $discount\ factor$ is often added to the calculation to produce a finite sum

$$G_t = R_{t+1} + \gamma R_{t+2} + \gamma^2 R_{t+3} + \dots + \gamma^{T-1} R_T$$
(3.37)

$$=\sum_{k=0}^{\infty} \gamma^k R_{t+k+1} \tag{3.38}$$

where the discount factor γ is typically a number between 0 and 1. The addition of a discount factor transforms the reward contribution to the return such that a reward k time steps into the future is only worth γ^{k-1} as much. The reward is in this sense "discounted".

Values closer to 0 will make the agent "myopic" in the sense the agent only takes into account the immediate reward and zeroes all subsequent rewards after s_{t+1} . In this configuration, the agent learns only from the next action it takes and is unable to learn sequences of actions that lead to some future state.

Values closer to 1, on the other hand, increasingly weigh future actions further in the trajectory. A value of 1, as discussed above, would mean each action is weighed equally; therefore, values closer to 1 such 0.95 or 0.90 provide more weight to actions near T.

The discount factor is tuned to reach a balance between a focus on near-term rewards and longer-term rewards. It helps address the problem of temporal credit assignment or the difficulty attributing credit to past action(s) for an observed return. Part of the challenge is the delay from the timestep t an action a_t is taken at and when the return is calculated T. In other words, the environment may pass through multiple timesteps before the effect of an action is observed. The problem can be framed as figuring out the influence of each action on the return. Using a discount factor spreads the credit across timesteps as a measure of the reward and how far into the future actions are from the current timestep.

3.2.2 Value Functions

As an agent interacts within its environment taking actions, the agent needs a way to decide what next action a_t to take in its state s_t . The value is decided in terms of the expected return discussed above.

There are two kinds of functions to approximate value depending on whether the input is the state s_t or the state-action pair (s_t, a_t) .

The value of a state is

$$v_{\pi}(s) = \mathbb{E}_{\pi}[G_t|S_t = s] = \mathbb{E}\left[\sum_{k=0}^{\infty} \gamma_k R_{t+k+1w}|S_t = s\right]$$
 (3.39)

where $\mathbb{E}[\cdot]$ is the expected value of a random variable provided the agent follows policy π at timestep t.

- 3.2.3 Policy Gradient Methods
- 3.2.4 PPO
- 3.2.5 Recurrent Policy

3.3 Meta-Learning

Meta-learning or "learning to learn" is a general framework of using information learned from one task for future tasks. One definition extends the idea of reuse for future tasks by specifying that performance on future tasks should improve with each task learned [11]. Another definition...

3.3.1 Few shot learning

Chapter 4

Method

4.1 Preliminaries

We define a discrete-time and finite-horizon Markov decision process (MDP) as a tuple $\mathcal{M} = \{\mathcal{S}, \mathcal{A}, P_a, R_a, \gamma\}$, where \mathcal{S} is the set of states or state space, $\mathcal{A} = \{\mathcal{A}_s \mid s \in S\}$ is the set of actions or action space, P is $P_a(s,s') = P(s_{t+1} = s' | s, a)$ or transition function, $R_a(s,s') = \{r \mid r \in \mathbb{R}\}$ is the reward upon transition from state s to state s' or reward function, $\gamma \in [0,1]$ is the discount factor. The objective is to maximize the discounted expected return $G = \mathbb{E}_{\tau}[\sum_{t=0}^{T} \gamma^t r(s_t, a_t)]$ where τ represents the trajectory of state-action pairs $\tau = (s_0, a_0, r_0, s_1, \ldots)$.

4.2 Formulation

REML casts "learning to learn" as an RL problem. The task given to REML is to learn regression algorithms, provided labeled regression datasets. The learning process across the set of datasets is represented as a discrete-time and finite-horizon MDP.

Each regression algorithm begins as a different regression dataset. Each regression dataset is provided as a task to REML. Such a task \mathcal{T} is defined as a dataset comprising N samples of input-output pairs represented by (x_i, y_i) , where x_i and y_i are real numbers. Each task is randomly sampled from a distribution, and the set of all tasks is represented as \mathcal{D} . Specifically, each task \mathcal{T}_i is defined as $\mathcal{T}_i = \{(x_{i1}, y_{i1}), (x_{i2}, y_{i2}), \dots, (x_{iN}, y_{iN})\}$, where

 $i=1,2,\ldots,M$, and M is the total number of tasks. Additionally, for the purpose of evaluation, one task, denoted as \mathcal{E} , is chosen at random and left out. The set of such tasks then is

$$\mathcal{D} = \{\mathcal{T}_1, \mathcal{T}_2, \dots, \mathcal{T}_{M-1}\}$$
 and $\mathcal{E} = \mathcal{T}_M$

Each task \mathcal{T} is solved by approximation with a neural network N. REML constructs each N from neural network layers it sequences and trains from a pre-initialized pool of layers \mathcal{L} . This layer pool \mathcal{L} consists of M input layers $\{\mathcal{I}_1, \mathcal{I}_2, \ldots, \mathcal{I}_M\}$, M output layers $\{\mathcal{O}_1, \mathcal{O}_2, \ldots, \mathcal{O}_M\}$, and a pre-defined number of hidden layers that is M times the depth of the composed network. Each input layer \mathcal{I}_i is associated with a specific task \mathcal{T}_i , and each output layer \mathcal{O}_i corresponds to the output of the network for task \mathcal{T}_i . This layer pool \mathcal{L} can be represented as

$$\mathcal{L} = \{\mathcal{I}_1, \mathcal{I}_2, \dots, \mathcal{I}_M, \mathcal{H}_1, \mathcal{H}_2, \dots, \mathcal{H}_K, \mathcal{O}_1, \mathcal{O}_2, \dots, \mathcal{O}_M\}$$

where \mathcal{H}_k represents the k-th hidden layer, and K is the total number of hidden layers in the network. Each type of layer in \mathcal{L} (i.e., \mathcal{I} , \mathcal{H} , and \mathcal{O}) has the same dimension for all tasks $\mathcal{T} \in \mathcal{D}$. Different sets of task \mathcal{D} would have different dimensions for layer in the pool.

Training starts with sampling training tasks \mathcal{T} and initializing N with an input layer \mathcal{I} and output layer \mathcal{O} from \mathcal{L} . Training consists of episodes where an episode terminates when the sequenced network N reaches a pre-defined depth. Each step, REML selects a layer from \mathcal{L} to sequence in N based on the state $s \in \mathcal{S}$. The state s is composed of information characterizing the task \mathcal{T} , the magnitude of outputs from N as a max absolute value of outputs seen for the task, the sequence of layers represented as indices within \mathcal{L} . The reward is the negative mean square error loss (MSE loss) signal of N after N is tested on a batch of data from task \mathcal{T} . At the end of an episode, layers are trained with the Adam optimizer [12]. A treatment of the negative mean squared loss error (MSE loss) is the reward signal. The trained layer copies are then updated in the layer pool \mathcal{L} . The idea is that knowledge acquired by REML is held by these updated layers in \mathcal{L} with the policy serving as a map to rebuild a network it has made perform for the task or a related task in the past.

4.3 Policy Representation

The policy is represented as either a recurrent policy with a Long short-term memory (LSTM) network or a non-recurrent policy with a Multi-layer perceptron (MLP) network. An MLP is a feed-forward ANN without cycles that has multiple hidden layers. An LSTM is an MLP with cycles or recurrent connections that allow the architecture to use information from previous states observed in the network. These recurrent connections are composed of selective memory cells which learn if and how to incorporate past states' data. This mechanism enables the network to capture long-term dependencies in sequential data.

An LSTM was chosen for the recurrent policy to capture the patterns in the sequence of layers chosen by REML for a task. In this formulation, the sequence of layers chosen by REML are sequential data. The layers or paramemeters in a neural network are not interchangeable without changing the approximation. Therefore, the sequence of the selected layers by REML is as important as the layers that are chosen.

4.4 Policy Optimization

With the formulation as an RL problem, the policy can be optimized with RL algorithms. REML uses the Proximal policy optimization (PPO) algorithm with both MLP and LSTM policies, for reasons noted above [13]. PPO was selected as it works with a discrete action space and was designed with training stability in mind. PPO clips updates calculated from a rollout of batch data such that the new policy is never too different from the old policy after a step. Stability was a priority given the policy would be trained across multiple different tasks and it would be possible for the policy to anchor to a particular task in a particular epoch, skewing the performance to that task.

4.5 Learning Signal

The learning signal or reward function R_a is the negative MSE loss. The MSE loss captures "how good" the last few actions REML made are by assessing the performance of N on task \mathcal{T} . It is a highly interpretable metric

with direct correlation to network performance as it is the measure of network performance. The loss is made negative because the objective of the "outer" network (REML) is to maximize a reward though the objective of the "inner" network N (sequenced by REML) is to minimize a loss.

The negative MSE loss was min-max scaled after it was observed to lead to unstable training at times. Across epochs, different tasks would dip in their performance after it seemed REML converged for that task. In addition, this performance dip coincided with a drift in output values across tasks. The networks would anchor to one task (dataset) within an epoch and the other networks would output values in magnitude closer to the much smaller or larger target values for the anchored task.

Further testing showed that the Adam optimizer was responsible for a disproportionate degree of task performance in terms of MSE loss. MSE loss data per step per task per epoch showed that REML would choose different layers in different sequences and N would acheive the same, or in some cases better, MSE loss for the batch. Though the sequenced N or "inner network" performed well, the "outer network" REML wasn't learning effectively because it was choosing different layers with the same results.

By design, the Adam optimizer was to train the layers selected by REML for N; however, the intention was a balance in what Adam optimized in a sequenced network and in the network sequenced by REML REML was to learn from Adam in terms of what sequence of layers (what sequence of actions) produced the highest return for the task. This finding was addressed by introducing a discount factor (to credit poor initial layers by REML and discredit Adam's training of poor layers) and to reduce the amount of gradient steps taken by the Adam optimizer in an episode (to credit the sequence of actions more).

The discount factor scales an episode's return by "how bad" the initial 2 layers (the input layer and the output layer) are in N. "Bad" here is defined in terms of the loss after the first 2 actions relative to the max loss observed for the task. As N's loss approaches the max observed loss, the scale factor is smaller and the return is smaller. The effect is that the return would be lower for an episode with the same final loss (the same performance N) if N contains "bad" layers. A lower return in this case would reduce the influence

of Adam on the learning signal to REML by crediting those actions that lead to high initial loss, and making REML less likely to choose them again. The reward is shaped to instruct REML to choose layers in a sequence that has the lowest MSE loss.

The purpose of the discount factor was to assign more credit to earlier actions (i.e., the first couple layers sequenced by REML) and to discredit high reward values that began as very high loss values tempered by the Adam optimizer being very effective.

4.6 Algorithm

Algorithm 1 Reinforcement Meta-learning

```
Input: \alpha, \beta: learning rate hyperparameters
Input: p(\mathcal{T}): distribution over tasks t
Input: \mathcal{L}: set of layers l
Input: f_{\theta_o}: policy \theta_o
Initialize all l \in \mathcal{L} with \theta_i
Sample training tasks \mathcal{T}_i from p(\mathcal{T})
for all \mathcal{T}_i do
     Initialize network N
     while not done do
           Sample batch \{\mathbf{x}^{(j)}, \mathbf{y}^{(j)}\} from \mathcal{T}_i
           Pass \{\mathbf{x}^{(j)}, \mathbf{y}^{(j)}\} through N to get next state s_k
           Get next layer l_k \in L via f_{\theta_o}(s_k)
           Expand \theta_i with l_k's \theta
           Evaluate \mathcal{L}_{\theta_o} for chosen f_o
           Evaluate \mathcal{L}_{\theta_i} for chosen f_i
           \theta_o \leftarrow \theta_o + \alpha \nabla \mathcal{L}_{\theta_o}
           \theta_i \leftarrow \theta_i + \beta \nabla \mathcal{L}_{\theta_i}
     end while
end for
```

4.7 Implementation

REML was implemented using Pytorch for the layer pool and functions as part of the the constructed networks N. Stablebaselines3 was used for policy with its open-source implementations of deep RL algorithms [14], [15]. Stablebaselines3 was developed by researchers with the intent to provide reliable baselines given recent findings that deep RL results are hard to reproduce. It ws found that the same RL algorithms produce different results depending on seed and other minor choices made in the implementation [16]. In fact, these differences were found to be greater in some cases than the differences between deep RL algorithms [17]. Stablebaselines3 benchmarks their implementations on common environments used in research and compares theirs to other implementations. Environments used in thesis are custom and created by the author using Gymnasium [18].

Computations were carried out using the Tufts University High Performance Cluster (HPC) with available gpu for batch jobs running about 15 hours for the regression tasks across 10 runs of 30 epochs and 7 tasks.

Evaluation data was captured and analyzed using Tensorboard and Weights & Biases (wandb) [19], [20]. Plots were generated using matplotlib with scienceplots [21], [22].

Chapter 5

Evaluation

The following research questions guided evaluation of REML:

- Can REML transfer knowledge from tasks it has learned to new tasks?
- How well does this model adapt to new tasks while retaining previously learned knowledge (does REML generalize without catastrophic forgetting)?
- Can REML generate models that learn near-optimal parameters from few examples for unseen tasks (can it do few-shot learning)?

These questions are evaluated in the context of a non-RL task with regression. REML is evaluated using varying sinusoidal curves, following the protocol proposed by Finn, Abbeel, and Levine for Model Agnostic Meta-learning (MAML) [3]. Sine curves have an inherent periodicity for the meta-learner to learn across tasks.

5.1 Sinusoidal curve regression

The testbed is defined as a distribution of sine curves that vary in amplitude and phase shift. The amplitude is chosen from [0.1, 5.0] and phase shift is chosen from [0, pi]. Each task is a dataset with 100 values linearly spaced within [-5, 5]. Batches of size 32 and 64 are tested and compared with learning rates of 0.005 and 0.01.

The layer pool \mathcal{L} for this regression task is composed of linear layers with 40

nodes. Layers are initialized with Xavier Glorot initialization to minimize the chance of exploding or vanishing gradients, particularly in the recurrent policy case. Xavier Glorot initialization initializes the parameters with the aim to keep variance of activations similar across layers [23]. The max depth of each constructed N is 5 with 3 hidden layers. The activation function between hidden layers is the ReLU to introduce non-linearity in the approximation. The activation function for the output layer is just the identity function given this is regression. Leaky ReLU was tested with different alpha values but it generally slowed down convergence and there was no need without any observed irregularies in gradients. The hyperparameters for N are set ahead of time as the task is parameter search not hyperparameter search.

The Adam optimizer is used to train each N at the end of an episode over 10 gradient steps [12]. Such a small number of gradient steps is chosen to train for the few-shot learning task where k is no more than 10. Fewer gradient steps with Adam also overcome the challenge discussed in the Method where Adam would compensate for REML's errors and train a "bad" sequence of layers to the same or better MSE loss performance than a sequence of layers observed with lower MSE loss without any gradient steps.

The MLP policy and LSTM policies tested with PPO are neural networks with 64 nodes per layer with 2 layers, as defined by the benchmark implementation provided by Stablebaselines3 [15]. The default hyperparameters for the PPO implementation are used. The policy takes 2048 steps before making an update to the parameters with a batch size of 64. The learning rate is 0.0003 with a discount factor is 0.9.

Training performance is evaluated over epochs, averaged over 10 runs. An epoch is here defined as one pass through the tasks. Each task is trained in episodes where an episode terminates when the constructed N has reached 5 layers. This may be more than 5 steps if REML continutes to make errors; in the case of errors, no layer is added to N and REML receives a penalty. The below metrics are gathered per epoch, by task.

- \bullet cumulative MSE loss of N
- cumulative reward to REML

• cumulative errors made by REML

Meta-learning performance is evaluated for a task held out at the start of training. REML is asked to construct an N for this unseen task. Sample efficiency is evaluated comparing training performance over 100 gradient steps for an N from REML and a baseline network trained from scratch. The layers in the baseline network are likewise initialized with the Xavier transform like the layers in \mathcal{L} . Few-shot learning is evaluated using k=5 and k=10 sample datapoints in continuation with the protocol proposed by Finn et al.

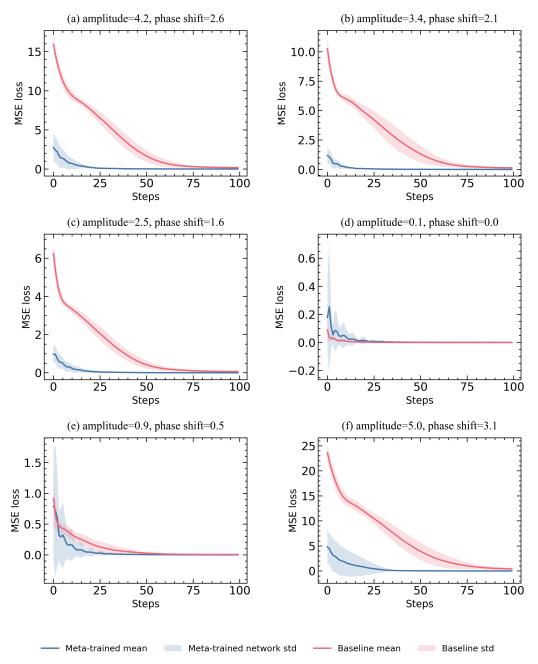


Figure (5.1) This is a comprehensive caption describing the key aspects of the figure. It should convey essential information for understanding the visual content.

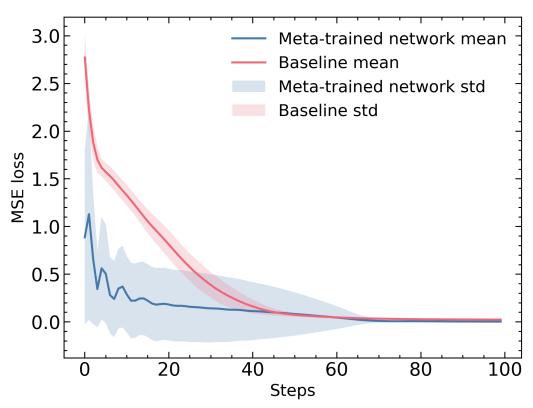


Figure (5.2) This is a comprehensive caption describing the key aspects of the figure. It should convey essential information for understanding the visual content.

Chapter 6

Discussion

Bibliography

- [1] Y. Duan, J. Schulman, X. Chen, P. L. Bartlett, I. Sutskever, and P. Abbeel, "Rl2: Fast reinforcement learning via slow reinforcement learning," arXiv preprint arXiv:1611.02779, 2016.
- [2] B. Zoph and Q. V. Le, "Neural architecture search with reinforcement learning," arXiv preprint arXiv:1611.01578, 2016.
- [3] C. Finn, P. Abbeel, and S. Levine, "Model-agnostic meta-learning for fast adaptation of deep networks," in *International conference on machine learning*, PMLR, 2017, pp. 1126–1135.
- [4] C. M. Bishop and N. M. Nasrabadi, *Pattern recognition and machine learning*. Springer, 2006, vol. 4.
- [5] K. Hornik, M. Stinchcombe, and H. White, "Multilayer feedforward networks are universal approximators," *Neural networks*, vol. 2, no. 5, pp. 359–366, 1989.
- [6] D. E. Rumelhart, G. E. Hinton, and R. J. Williams, "Learning representations by back-propagating errors," nature, vol. 323, no. 6088, pp. 533–536, 1986.
- [7] R. Pascanu, C. Gulcehre, K. Cho, and Y. Bengio, "How to construct deep recurrent neural networks," arXiv preprint arXiv:1312.6026, 2013.
- [8] P. J. Werbos, "Backpropagation through time: What it does and how to do it," *Proceedings of the IEEE*, vol. 78, no. 10, pp. 1550–1560, 1990.
- [9] S. Hochreiter and J. Schmidhuber, "Long short-term memory," *Neural computation*, vol. 9, no. 8, pp. 1735–1780, 1997.
- [10] R. Bellman, "A markovian decision process," *Journal of mathematics* and mechanics, pp. 679–684, 1957.

- [11] S. Thrun and L. Pratt, "Learning to learn: Introduction and overview," in *Learning to learn*, Springer, 1998, pp. 3–17.
- [12] D. P. Kingma and J. Ba, "Adam: A method for stochastic optimization," arXiv preprint arXiv:1412.6980, 2014.
- [13] J. Schulman, F. Wolski, P. Dhariwal, A. Radford, and O. Klimov, "Proximal policy optimization algorithms," arXiv preprint arXiv:1707.06347, 2017.
- [14] A. Paszke, S. Gross, F. Massa, et al., "Pytorch: An imperative style, high-performance deep learning library," in Advances in Neural Information Processing Systems 32, Curran Associates, Inc., 2019, pp. 8024-8035. [Online]. Available: http://papers.neurips.cc/paper/9015-pytorch-an-imperative-style-high-performance-deep-learning-library.pdf.
- [15] A. Raffin, A. Hill, A. Gleave, A. Kanervisto, M. Ernestus, and N. Dormann, "Stable-baselines3: Reliable reinforcement learning implementations," *The Journal of Machine Learning Research*, vol. 22, no. 1, pp. 12348–12355, 2021.
- [16] P. Henderson, R. Islam, P. Bachman, J. Pineau, D. Precup, and D. Meger, "Deep reinforcement learning that matters," in *Proceedings of the AAAI conference on artificial intelligence*, vol. 32, 2018.
- [17] L. Engstrom, A. Ilyas, S. Santurkar, et al., "Implementation matters in deep policy gradients: A case study on ppo and trpo," arXiv preprint arXiv:2005.12729, 2020.
- [18] M. Towers, J. K. Terry, A. Kwiatkowski, et al., Gymnasium, Mar. 2023. DOI: 10.5281/zenodo.8127026. [Online]. Available: https://zenodo.org/record/8127025 (visited on 07/08/2023).
- [19] Martín Abadi, Ashish Agarwal, Paul Barham, et al., TensorFlow: Large-scale machine learning on heterogeneous systems, Software available from tensorflow.org, 2015. [Online]. Available: https://www.tensorflow.org/.
- [20] L. Biewald, Experiment tracking with weights and biases, Software available from wandb.com, 2020. [Online]. Available: https://www.wandb.com/.

- [21] J. D. Hunter, "Matplotlib: A 2d graphics environment," Computing in Science & Engineering, vol. 9, no. 3, pp. 90–95, 2007. DOI: 10.1109/MCSE.2007.55.
- [22] J. D. Garrett, "garrettj403/SciencePlots," version 1.0.9, Sep. 2021. DOI: 10.5281/zenodo.4106649. [Online]. Available: http://doi.org/10.5281/zenodo.4106649.
- [23] X. Glorot and Y. Bengio, "Understanding the difficulty of training deep feedforward neural networks," in *Proceedings of the thirteenth international conference on artificial intelligence and statistics*, JMLR Workshop and Conference Proceedings, 2010, pp. 249–256.