Online hyperparameter optimization by real-time recurrent learning

Daniel Jiwoong Im 1 Cristina Savin 1 Kyunghyun Cho 1

Abstract

Conventional hyperparameter optimization methods are computationally intensive and hard to generalize to scenarios that require dynamically adapting hyperparameters, such as lifelong learning. Here, we propose an online hyperparameter optimization algorithm that is asymptotically exact and computationally tractable, both theoretically and practically. Our framework takes advantage of the analogy between hyperparameter optimization and parameter learning in recurrent neural networks (RNNs). It adapts a well-studied family of online learning algorithms for RNNs to tune hyperparameters and network parameters simultaneously, without repeatedly rolling out iterative optimization. This procedure yields systematically better generalization performance compared to standard methods, at a fraction of wallclock time.

1. Introduction

The success of training complex machine learning models critically depends on good choices for hyperparameters that control the learning process. These hyperparameters can specify the speed of learning as well as model complexity, for instance, by setting learning rates, momentum, and weight decay coefficients. Oftentimes, finding the best hyperparameters requires not only extensive resources, but also human supervision.

Well-known procedures, such as random search and Bayesian hyperparameter optimization, require fully training many models to identify the setting that leads to the best validation loss (Bergstra & Bengio, 2012; Snoek et al., 2012). While popular for cases when the number of hyperparameters is small, these methods easily break down when the number of hyperparameters increases. Alternative gradient-based hyperparameter optimization methods take a two level approach (often referred to as the ‘inner’ and the ‘outer loop’). The outer loop finds potential candidates for the hyperparameters, while the inner loop is used for model training. These methods also require unrolling the full learning dynamics to compute the long-term consequences that perturbation of the hyperparameters has on the parameters (Luketina et al., 2016; Lorraine & Duvenaud, 2018; Metz et al., 2019). This inner loop of fully training the parameters of the model for each outer loop hyperparameter update makes existing methods computationally expensive and inherently offline. It is unclear how to adapt these ideas to nonstationary environments, as required by advanced ML applications, e.g. lifelong learning (German et al., 2019; Richard et al., 2020). Moreover, while these type of approaches can be scaled to high-dimensional hyperparameter spaces (Lorraine & Duvenaud, 2018), they can also suffer from stability issues (Metz et al., 2019), making them non-trivial to apply in practice. In short, we are still missing robust and scalable procedures for online hyperparameter optimization.

We propose an alternative class of online hyperparameter optimization (OHO) algorithm that update hyperparameters in parallel to training the parameters of the model. At the core of our framework is the observation that hyperparameter optimization entails a form of temporal credit assignment, akin to the computational challenges of training recurrent neural networks (RNN). Drawing on this similarity allows us to adapt real-time recurrent learning (RTRL) (Williams & Zipser, 1989), an online alternative to backprop through time (BPTT), for the purpose of online hyperparameter optimization.

We empirically show that our joint optimization of parameters and hyperparameters yields systematically better generalization performance compared to standard methods. These improvements are accompanied sometimes with a substantial reduction in overall computational cost. We characterize the behavior of our algorithm in response to various meta-parameter choices and to dynamic changes in hyperparameters. OHO can rapidly recover from adversarial perturbations to the hyperparameters. We also find that OHO with layerwise hyperparameters provides a natural trade-off between a flexible hyperparameter configuration and computational cost. In general, our framework opens a door to a new line of research, that is, real-time hyperparameter learning.

Equal contribution 1 New York University. Correspondence to: Daniel Jiwoong Im <ji641@nyu.edu>.

Preprint under review
2. Background

2.1. Iterative optimization

A standard technique for training large-scale machine learning models, such as deep neural networks (DNN), is stochastic optimization. In general, this takes the form of parameters changing as a function of the the data and the previous parameters, iteratively updating until convergence:

\[
\theta_{t+1} = g(\theta_t, B_r; \phi),
\]

where \( \theta \) denotes the parameters of the model, \( g \) is the update rule reflecting the learning objectives, \( \phi \) denotes the hyperparameters, and \( B_r \) is the random subset of training data (the minibatch) at iteration \( r \).

As a representative example, when training a DNN \( \theta \) where \( \phi \) denotes the parameters of the model, \( g \) is the update rule, \( B_r \) is the random subset of training data, and \( \Gamma \) is the influence matrix, dynamically updates as

\[
\Gamma_r = D_r \Gamma_{r-1} + G_{r-1},
\]

where \( D_r = \frac{\partial h}{\partial \theta_{r-1}} \) and \( G_r = \frac{\partial h}{\partial \phi_{r-1}} \). In this way, the complexity of learning no longer depends on the temporal horizon. However, this comes at the cost of memory requirements \( O(|\phi||h_t|) \), which makes RTRL rarely used in ML practice.

2.2. Recurrent neural networks

An RNN is a time series model. At each time step \( t = \{1 \cdots T\} \), it updates the memory state \( h_t \) and generates the output \( o_{t+1} \) given the input \( x_t \):

\[
(h_{t+1}, o_{t+1}) = r(h_t, x_t; \phi),
\]

where the recurrent function \( r \) is parametrized by \( \phi \).

Learning this model involves optimizing the total loss over \( T \) steps with respect to \( \phi \) by gradient descent. BPTT is typically used to calculate the gradient by unrolling the network dynamics and backward differentiating through the chain rule:

\[
\nabla_{\phi}L = \sum_{t=1}^{T} \left( \sum_{s \geq t+1} \frac{\partial L_s}{\partial h_{t+1}} \frac{\partial h_{t+1}}{\partial h_t} + \frac{\partial L_t}{\partial h_t} \right) \frac{\partial h_t}{\partial \phi},
\]

where \( L_t \) is the instantaneous loss at time \( t \), and the double summation indexes all losses and all the applications of the parameters. Because the time complexity for BPTT grows with respect to \( T \), it can be challenging to compute the gradient using BPTT when the temporal horizon is lengthy. In practice, this is mitigated by truncating the computational graph (‘truncated BPTT’).

2.3. Real-time learning recurrent

RTRL (Williams & Zipser, 1989) is an online alternative to BPTT, which –instead of rolling out the network dynamics– stores a set of summary statistics of the network dynamics that are themselves updated online as new inputs come in. To keep updates causal, it uses a forward view of the derivatives, instead of backward differentiation, with the gradient computed as

\[
\nabla_{\phi}L = \sum_{t=1}^{T} \frac{\partial L_{t+1}}{\partial h_t} \frac{\partial h_t}{\partial \phi} + \frac{\partial L_t}{\partial \phi}.
\]

The Jacobian \( \Gamma_r = \frac{\partial h}{\partial \phi} \) (also referred to as the influence matrix), dynamically updates as

\[
\Gamma_r = D_r \Gamma_{r-1} + G_{r-1},
\]

where \( D_r = \frac{\partial h}{\partial \theta_{r-1}} \) and \( G_r = \frac{\partial h}{\partial \phi_{r-1}} \). In this way, the complexity of learning no longer depends on the temporal horizon. However, this comes at the cost of memory requirements \( O(|\phi||h_t|) \), which makes RTRL rarely used in ML practice.

3. Learning as a recurrent neural network

Both RNN parameter learning and hyperparameter optimization need to take into account long-term consequences of (hyper-)parameter changes on a loss. This justifies considering an analogy between the recurrent form of parameter learning (Eq. 1) and RNN dynamics (Eq. 3).

Mapping SGD to a recurrent network. To establish the analogy, consider the following mapping:

parameters \( \theta_r \) → state \( h_t \)

batch \( B_r \) → input \( x_t \)

update rule \( g(\cdot) \) → recurrent function \( r(\cdot) \)

hyper-parameters \( \phi \) → parameters \( \phi \).

Parameters \( \theta_r \) and recurrent network state \( h_t \) both evolve via recurrent dynamics, \( g(\cdot) \) and \( r(\cdot) \), respectively. These dynamics are each parametrized by hyper-parameters \( \phi \) and parameters \( \phi \). The inputs \( x_t \) in the RNN correspond to the minibatches of data \( B_r \) in the optimizer, and the outputs \( o_t \) to \( \{f(x; \theta_r) | x \in B_r\} \), respectively. In short, we interpret a full model training process as a single forward propagation of a sequence of minibatches in an RNN.

Mapping the validation loss to the RNN training loss. The same analogy can be made for the training objectives. We associate the per-step loss of the recurrent network to the hyperparameter optimization objective:

\[
L(\theta_r, \phi_r; D_{val}) = \frac{1}{|D_{val}|} \sum_{(x,y) \in D_{val}} l(y, f(x; \theta_r(\phi_r))),
\]
with $l$ is the per-example loss function, with $\varphi = \{\alpha, \lambda\}$ the set of tune-able hyperparameters, which in our concrete example corresponds to learning rate $\alpha$ and regularizer $\lambda$. The hyperparameter optimization objective is calculated over the validation dataset $D_{\text{val}}$. The total loss over a full training run is $L_{\text{Total}} = \sum_{\tau=1}^{\infty} L(\theta_{\tau}, \varphi_{\tau}; D_{\text{val}})$, where there are multiple parameter updates within a run. We use $\infty$ to emphasize that the number of epochs is often not determined a priori.

Both the hyperparameter optimization objective and the update rule, Eq. 2, contain the per-example loss $l$. The former updates the parameters of RNN using $D_{\text{val}}$, while the latter updates the state of RNN using training batch $B_{\tau}$. This meta-optimization loss function is commonly used for hyperparameter optimization in practice (Bengio, 2000; Pedregosa, 2016). Nevertheless, the mapping from the optimizer to RNN and the mapping from the validation loss to RNN training objective is novel and enables us to treat the whole hyperparameter optimization process as an instance of RNN training.

4. Online hyperparameter optimization

With our analogies in place, we are ready to construct our online hyperparameter optimization (OHO) algorithm. We adapt the hyperparameters at each time step, such that both the parameters and hyperparameters are jointly optimized in a single training process (Fig. 1).

To achieve this, we update the parameters using training data and update the hyperparameters using validation data. Then, the update rules for $\theta$ and $\varphi$ are:

$$\begin{align*}
\theta_{\tau+1} &= \theta_{\tau} - \alpha_{\tau} \Delta \theta_{\tau} + \alpha_{\tau} w(\theta_{\tau}, \lambda_{\tau}) \\
\varphi_{\tau+1} &= \varphi_{\tau} - \eta \Delta \varphi_{\tau},
\end{align*}$$

(5)

where $\Delta \theta_{\text{val}}$ is a descent step with respect to training or validation data, respectively, and $w(\theta_{\tau}, \lambda_{\tau})$ is a regularization function. We can use any differentiable stochastic optimizer, such as RMSProp and ADAM, to compute the descent direction $\Delta$. Without the loss of generality, from now on, we use SGD to compute the $\Delta$ and use weight decay penalty as a regularizer for the rest of the paper. Expanding $\Delta(\varphi_{\tau}; D_{\text{val}})$ in Eq. 6, we have

$$\begin{align*}
\Delta_{\text{val}}(\varphi_{\tau}) &= \nabla_{\varphi} L_{\text{val}}(\theta_{\tau+1}, \varphi_{\tau}) \\
&= \nabla_{\varphi} L_{\text{val}}(\theta_{\tau} - \alpha_{\tau} \Delta \theta_{\tau} - w(\theta_{\tau}, \lambda_{\tau}), \varphi_{\tau}).
\end{align*}$$

(7)

The gradient of hyperparameters depends on $\varphi_{0} \cdots \varphi_{\tau}$ at iteration $\tau$. We apply RTRL to compute this gradient in an online fashion. Let us re-write the gradient expression of RTRL in Eq. 4 taking into account our mappings,

$$\nabla_{\varphi} L_{\text{val}} = \sum_{\tau=1}^{T} \frac{\partial L_{\text{val}}}{\partial \theta_{\tau+1}} \left( \frac{\partial \theta_{\tau+1}}{\partial \theta_{\tau}} + \frac{\partial \theta_{\tau+1}}{\partial \varphi_{\tau}} \right)_{\tau+1} \nabla_{\varphi_{\tau}} \Gamma_{\tau+1}$$

(8)

Generally, meta-optimization involves computing the gradient through a gradient, as shown in Eq. 7. This causes the temporal derivative to contain the Hessian matrix,

$$\frac{\partial \theta_{\tau+1}}{\partial \theta_{\tau}} = I - \alpha_{\tau} H_{\tau} - 2\alpha_{\tau} \lambda_{\tau},$$

where $H_{\tau} = \mathbb{E}_{L}[\nabla_{\theta}^{2} L]$ is the Hessian of the minibatch loss with respect to the parameters. Then, we plug $\frac{\partial \theta_{\tau+1}}{\partial \theta_{\tau}}$ into the influence matrix’s recursive formula,

$$\Gamma_{\tau+1} = (I - \alpha_{\tau} H_{\tau} - 2\alpha_{\tau} \lambda_{\tau}) \Gamma_{\tau} + G_{\tau}.$$  

(9)

By approximating the Hessian-vector product using the finite difference method,$^1$ we compute the gradient $\frac{\partial L_{\text{val}}}{\partial \alpha_{\tau}}$ in linear time. The formulation shows that the influence matrix is composed of all the relevant parts of the learning history and is updated online as new data come in. In other words, it accumulates the long-term influence of all the previous applications of the hyperparameters $\varphi$ on the parameters $\theta$. Overall RTRL is more efficient than truncated BPTT for hyperparameter optimization, in both computation and memory complexity. First, RTRL greatly reduces the computational cost since the influence matrix formulation circumvents the explicit unrolling of temporal dependencies. Our approach is intrinsically online, while BPTT is strictly an offline algorithm (although it can sometimes be loosely approximated to mimic online methods, see (Lorraine & Duvenaud, 2018)). Moreover, the standard memory challenge of training RNNs with RTRL does not apply in the case of hyperparameter optimization, as the number of hyperparameters is in general much smaller than the number of parameters. For example, one popular choice of $\varphi$ is to just include a global learning rate and some regularization coefficients.

4.1. Gradient computation

Since we frame hyperparameter optimization as RNN training, one might reasonably wonder about the fundamental issues of vanishing and exploding gradients (Hochreiter et al., 2001) in this setup. Gradients do not vanish, because the SGD update in Eq. 2 is additive. This resembles RNN architectures such as long- short-term memory (LSTM; Hochreiter & Schmidhuber, 1997) and gated recurrent units (GRU; See https://justindomke.wordpress.com/2009/01/17/hessian-vector-products/ for details.)
Because the influence matrix $\Gamma_{r+1}$ is defined recursively, the gradient of the validation loss with respect to $\varphi$ contains the product of Hessians:

$$\nabla_{\varphi} L_{\text{val}} = \left( G_r, - \sum_{i=0}^{r} \left( \prod_{j=i+1}^{r} (1 - \alpha_j H_j - 2\alpha_j \lambda_j) \right) G_i \right),$$

where $\langle \cdot, \cdot \rangle$ denotes an inner product. $G_i$ and $H_j$ are the gradient and Hessian of the loss $L(\theta_r)$ at iteration $i$ and $j$, respectively. The product of the Hessians can lead to gradient explosion, especially when consecutive gradients are correlated (Metz et al., 2019). It remains unclear whether the gradient explosion is an issue for RTRL (or, more generally, forward-differentiation based optimization). We study this in our experiments.

5. Related work

Optimizing hyperparameters based on a validation loss has been tackled from various stances. Here, we provide a brief overview of state-of-the-art approaches to hyperparameter optimization.

**Random search.** For small hyperparameter spaces, grid or manual search methods are often used to tune hyperparameters. For a moderate number of hyperparameters, random search can find hyperparameters that are as good or better than those obtained via grid search, at a fraction of its computation time (Bengio, 2000; Bergstra & Bengio, 2012; Bergstra et al., 2011).

**Bayesian optimization approaches.** Bayesian optimization (BO) is a smarter way to search for the next hyperparameter candidate (Snoek et al., 2012; 2015; Eriksson et al., 2019) by explicitly keeping track of uncertainty. BO iteratively updates the posterior distribution of the hyperparameters and assigns a score to each hyperparameter based on it. Because evaluation of hyperparameter candidates must largely be done sequentially, the overall computational

**Gradient-based approaches.** Hyperparameter optimization with approximate gradient (HOAG) is an alternative technique that iteratively updates the hyperparameters following the gradient of the validation loss. HOAG approximates the gradient using an implicit equation with respect to the hyperparameters (Pedregosa, 2016). This work was extended to DNNs with stochastic optimization settings by Lorraine & Duvenaud (2018). In contrast to our approach, which uses the chain rule to compute the exact gradient online, this approach exploits the implicit function theorem and inverse Hessian approximations. While the hyperparameter updates appear online in form, the method requires the network parameters to be nearly at a stable point. In other words, the network needs to be fully trained at each step.

Metz et al. (2019) attempt to overcome the difficulties of backpropagation through an unrolled optimization process by using a surrogate loss, based on variational and evolutionary strategies. Although their method addresses the exploding gradient problem, it still truncates backpropagation, which introduces a bias in the gradient estimate. In contrast, our method naturally addresses both issues: It is unbiased by algorithm design, and the gradients are empirically stable, as will be shown in Experiment 6.5.

**Forward differentiation approaches.** One potential disadvantage of our approach is that the memory complexity grows with the number of hyperparameters. There are however several approximate variants of RTRL that can be used to address this issue. As an example, unbiased online recurrent optimization (UORO) reduces the memory complexity of RTRL from quadratic to linear (Tallec & Ollivier, 2017). UORO uses rank-1 approximation of the influence matrix and can be extended to rank-k approximation (Mujika et al., 2018). Although UORO gives an unbiased estimate of the gradient, it is known to have high variance, which may slow down or impair training (Cooijmans & Martens, 2019; Marshall et al., 2020). It remains an open question whether these more scalable alternatives to RTRL are also applicable for online hyperparameter optimization.

6. Experiments

We conduct empirical studies to assess the proposed algorithm’s performance and computational cost. We compare them to widely used hyperparameter optimization methods, on standard learning problems such as MNIST and CIFAR10 classification. To better understand the properties of OHO, we examine hyperparameter dynamics during training and how they are affected by various meta-hyperparameter settings. We explore layerwise hyperparameter sharing as a...
Online hyperparameter optimization by real-time recurrent learning

6.1. Performance

We compare OHO against hyperparameter optimization by uniform random search and Bayesian optimization, in terms of the number of training runs and the computation time required to achieve a predefined level of generalization performance (test loss ≤ 0.3, see Fig. 2). We vary the optimizer \( g \) (Eq. 1) by considering five commonly used learning rate schedulers: 1) SGD with fixed learning rate (‘Fixed’), 2) Adam, 3) SGD with step-wise learning rate annealing (‘Step’), 4) exponential decay (‘Exp’), and 5) cosine (‘Cosine’) schedulers (Loshchilov & Hutter, 2017). We optimize the learning rate and weight decay coefficient. Additionally, we tune step size, decay rate, and momentum coefficients for Step, Exp, and Adam, respectively. In our experiments, we find that OHO usually takes a single run to find a good solution. The single training run takes approximately 12× longer than training the network once without OHO, and yet, the other hyperparameter algorithms require multiple training of neural network to reach the same level of performance. Overall OHO ends up significantly faster at finding a good solution in terms of total wall-clock time (Fig. 2, bottom row).

For each method, we measure the final test loss distribution obtained for various initial learning rates and weight decay coefficients. For both MNIST and CIFAR10, our procedure, which dynamically tunes the learning rate and degree of regularization during model learning, results in better generalization performance and much smaller variance compared to other optimization methods (Fig. 3, ‘global OHO’). This demonstrates the robustness of OHO to the initialization of hyperparameters and makes it unnecessary to train multiple models in order to find good hyperparameters. These results also suggest that there may be a systematic advantage in jointly optimizing parameters and hyperparameters.
We find that the layerwise OHO test loss (green curves) is generally lower than that of global OHO (purple curves) across runs with different initial learning rates, we observe that learning rates tend to cluster according to their layers regardless of the starting points, and their values are layer-specific (Fig. 4). This suggests that layerwise grouping of the hyperparameters may be an appropriate thing to do in such models.

We analyze the performance and computational speed trade-off of layerwise OHO with coarser hyperparameter grouping schemes. If we define one hyperparameter set as the learning rates for the weight and bias, together with the L2 regularization weights, then global OHO has one set, while layerwise OHO has as many sets as there are layers in the network (6 for MNIST and 62 for CIFAR10). We can then interpolate between these extremes. Specifically, for \( k \) hyperparameter sets, we partition the network layers into \( k \) neighboring groups, each with their own hyperparameter set (Fig. 5).

For example, for \( k = 2 \), the 6-layer network trained on MNIST would be partitioned into top 3 and bottom 3 layers, with 2 separate hyperparameter sets. For each configuration, we ran OHO optimization 10 times with different random initializations. As shown in Fig. 5, the average performance improves as the number of hyperparameter sets increases, while the variance shrinks. In contrast, the wallclock time increases with the number of hyperparameter sets. This demonstrates a clear trade-off between the flexibility of the learning dynamics (and subsequently generalization performance) and computational cost, which argues for selecting the richest hyperparameter grouping scheme possible given a certain computational budget.

### 6.3. Response to hyperparameter perturbations

Due to its online nature, the OHO algorithm lends itself to being used for non-stationary problems, for instance when input statistics or task objectives change over time. Here we emulate such a scenario by perturbing the hyperparameters directly under a static learning scenario, and track the evolution of (meta-)learning in response to these perturbations. In particular, we initialize the learning rates to a fixed value (0.1) and then reset them to a higher value (0.2) at various points during CIFAR10 training (Fig. 6A). We observe that the learning rates decrease rapidly early on and that after being reset, they drop almost immediately back to the value before the perturbation. This illustrates the resilience and rapid response of OHO against learning rate corruption which reflects sudden change in an environment. We further compare the performance of OHO to the setting where the learning rate is fixed after re-initialization. Figure 6B shows the test losses for fixed (dashed line) and OHO (solid line). We find that the dynamic optimization of hyperparameters leads to systematically better performance.

In the next set of experiments we reset the weight decay coefficient to zero at various epochs: 30, 50, 90, 180, and...
Figure 7. Sensitivity analysis on CIFAR10. A) The comparison of learning when the outer-gradient $\frac{\partial L_D}{\partial \phi}$ is subject to training vs validation dataset. B) The performance when using 100, 500, and 1000 validation batch sizes.

Figure 8. Test loss as a function of learning time, when the influence get reset to zero at every 1, 100, and 1000 steps; ‘no reset’ corresponds to standard infinite-horizon global OHO.

270. The results are similar, with the weight decay coefficients quickly adapting back to their previous values (Fig. 6C and D). The test loss fluctuates less for continually optimized OHO, relative to the fixed hyperparameters setting. Altogether, these results suggest that joint optimization of parameters and hyperparameters is more robust to fluctuations in a learning environment.

6.4. Long-term dependencies in learning and their effects on hyperparameters

Past work has suggested that the temporal horizon for the outer-loop learning influences both performance and the stability of hyperparameter optimization (Metz et al., 2019). In our case, the influence matrix is computed recursively over the entire learning episode and there is no strict notion of a horizon. We can however control the extent of temporal dependencies by resetting the influence matrix at a predefined interval (effectively forgetting all previous experience). We compare such resetting against our regular infinite-horizon procedure (global-OHO; see Fig. 8). We find that both the average test loss and its variance decrease as we reset less frequently; ultimately global OHO performs the best. Thus, we conclude it is important to take into account past learning dynamics for improving generalization performance.

6.5. Sensitivity analysis for meta-hyperparameters.

In order to better understand how OHO works in practice, we explore its sensitivity to meta-hyperparameter choices: the validation dataset, initial learning rates, and meta learning rates.

Validation dataset. We explore the gradient of the meta-optimization objective $\nabla_{\phi} L_{\text{val}}$ in Eq. 8, where the outer gradient $\frac{\partial L_D}{\partial \phi}$ is computed with respect to the validation dataset $D_{\text{val}}$. To show the importance of having a separate validation loss for the outer loop optimization, we replace the validation dataset with the training dataset, and find that it yields to systematically worse generalization performance (Fig. 7B). Expectedly, hyperparameters overfit to the training loss when using the training dataset, but not when using the validation dataset. When using the validation dataset, OHO prevents overfitting by shrinking the learning rates and increasing the weight regularization over time. In other words, OHO early-stops on its own.

In some practical applications it may prove computationally cumbersome to use the full validation dataset. We experiment using a random subset of validation set to compute the outer gradient while varying the validation minibatch size: 100, 500, and 1,000. Unsurprisingly we find that bigger is better (Fig. 7C): the test loss is lowest for the largest size considered, while the test loss for the smallest (100) minibatch size is on par with the step-wise learning rate scheduler. The performance gradually changes as we vary the size, which allows us to make trade-off between computational cost and the final performance.

Meta learning rates and initial hyper-parameters. To deploy OHO in practice, one needs to choose a meta learning rate and the initial hyperparameters. We investigate the sensitivity of OHO to these choices in order to inform users on what may be a sensible range for each meta-hyperparameter. We define the sensible range to be the region where training vs validation dataset. When using the validation dataset, OHO prevents overfitting by shrinking the learning rates and increasing the weight regularization over time. In other words, OHO early-stops on its own.

In some practical applications it may prove computationally cumbersome to use the full validation dataset. We experiment using a random subset of validation set to compute the outer gradient while varying the validation minibatch size: 100, 500, and 1,000. Unsurprisingly we find that bigger is better (Fig. 7C): the test loss is lowest for the largest size considered, while the test loss for the smallest (100) minibatch size is on par with the step-wise learning rate scheduler. The performance gradually changes as we vary the size, which allows us to make trade-off between computational cost and the final performance.

To deploy OHO in practice, one needs to choose a meta learning rate and the initial hyperparameters. We investigate the sensitivity of OHO to these choices in order to inform users on what may be a sensible range for each meta-hyperparameter. We define the sensible range to be the region where training is stable. We consider learning to be stable when the gradients are well-defined along the entire learning trajectory, in which computing the gradient hinges upon the product of Hessians induced by the recursion in the influence matrix. In sum, sensible meta-hyperparameters should keep the norm of the influence matrix bounded throughout the training.
We visualize the evolution of the norms of the influence matrices for the learning rates, $\|\frac{\partial \theta (\tau)}{\partial \alpha}\|^2_F$, and weight decay coefficients, $\|\frac{\partial \theta (\tau)}{\partial \lambda}\|^2_F$, for different meta learning rates and initial learning rates (Fig. 9A, B). The norm is numerical ill-conditioned (blows up) with large meta learning rates ($> 1e^{-4}$) at the end stage of training, but is smooth with smaller meta learning rates. Recall that the OHO-optimized learning rates decrease during training to avoid overfitting. Later in training this eventually leads to a regime where the meta learning rate is larger than the learning rate. Some elements of the scaled gradient can then become greater than the corresponding learning rate $\alpha^{t-1}_i < \epsilon |\nabla_\alpha L(\theta)|^2$, causing instability. The ideal meta learning rate should thus be small.

We further investigate the norm of influence matrix during training. We train multiple models with different initialization of hyperparameters while fixing the meta learning rate to $5 \times 10^{-5}$. We find that the norm rarely explodes in practice (Fig. 10 A, B). The norms plateau as training converges, but they do not explode. We observe similar results for the norm of the Hessian matrix $\|\frac{\partial^2 \theta (\tau)}{\partial \alpha^2}\|^2_F$ as well.

In order to understand why the norm of influence matrix is stable along the trajectory, we look into exploding gradient phenomena. As we discussed in Section 4.1, exploding gradients likely happen when a series of gradients are correlated. We compute the moving average and standard deviation of gradient correlations with the window size of 100 updates (a single epoch). The mean correlation very rapidly approaches zero, with the standard deviation also decreasing as training progresses (Fig. 10C). The gradients only correlate at the beginning of training but quickly decorrelate as learning continues. This causes the norm of the influence matrix to plateau and prevents the gradients from exploding.

7. Discussion

Truly online hyperparameter optimization remains an open problem in machine learning. In this paper, we presented a novel hyperparameter optimization algorithm, OHO, which takes advantage of online temporal credit assignment in RNNs to jointly optimize parameters and hyperparameters based on minibatches of training and validation data. This procedure leads to robust learning, with better generalization performance than competing offline hyperparameter optimization procedures. It is also competitive in terms of total wallclock time.

The dynamic interaction between parameter and hyperparameter optimization was found to not only improve test performance but to also reduce variability across runs. Beyond automatic shrinking of learning rates that avoids overfitting, OHO quickly adapts the hyperparameters to compensate for sudden changes, such as perturbations of the hyperparameters and allows the learning process to reliably find better models.

The online nature of OHO updates makes it widely applicable to both stationary and nonstationary learning problems. We expect the same set of benefits to apply to problems such as life-long learning (German et al., 2019; Richard et al., 2020), or policy learning in deep reinforcement learning (Padakandla et al., 2019; Xie et al., 2020; Igl et al., 2020), in which the statistics of data and learning objectives change over time. Up to now, it has been virtually impossible to do automated hyperparameter tuning in such challenging learning settings. OHO on the other hand may prove to be a key steppingstone for achieving robust automated hyperparameter optimization in these domains.

In machine learning, an enormous amount of time and energy is spent on hyperparameter tuning. Out of the box, RTRL-based OHO is already quite efficient, with memory requirement that is linear in the number of parameters and outer-loop gradients computation having a similar cost to that of computing inner gradients. This covers many practical use cases of meta-optimization. We believe that OHO and related ideas can dramatically reduce the burden of tuning hyperparameters and becoming a core component of future off-the-shelf deep learning packages.
References

Bengio, Y. Gradient-based optimization of hyperparameters. *Journal of Big Data*, 12:1889–1900, 2000.

Bergstra, J. and Bengio, Y. Random search for hyperparameter optimization. *Journal of Machine Learning*, 13:281–305, 2012.

Bergstra, J., Bardenet, R., Bengio, Y., and Kegl, B. Algorithms for hyper-parameter optimization. In *NeurIPS*, 2011.

Chung, J., Gulcehre, C., Cho, K., and Bengio, Y. Empirical evaluation of gated recurrent neural networks on sequence modeling. *arXiv preprint arXiv:1412.3555*, 2014.

Cooijmans, T. and Martens, J. On the variance of unbiased online recurrent optimization. In *arXiv preprint arXiv:1902.02405*, 2019.

Eriksson, D., Pearce, M., Gardner, J. R., Turner, R., and Poloczek, M. Scalable global optimization via local bayesian optimization. In *NeurIPS*, 2019.

German, I., Ronald, K., Partc, J. L., Christopher, K., and Stefan, W. Continual lifelong learning with neural networks: A review. *Neural Networks*, 113:54–71, 2019.

He, K., Zhang, X., Ren, S., and Sun, J. Deep residual learning for image recognition. In *CVPR*, pp. 770–778, 2016.

Hochreiter, S. and Schmidhuber, J. Long short-term memory. *Neural computation*, 9(8):1735–1780, 1997.

Hochreiter, S., Bengio, Y., Frasconi, P., Schmidhuber, J., et al. Gradient flow in recurrent nets: the difficulty of learning long-term dependencies, 2001.

Igl, M., Farquhar, G., Luketina, J., Boehmer, W., and White, S. The impact of non-stationarity on generalisation in deep reinforcement learning. In *arXiv preprint arXiv:2006.05826*, 2020.

Kingma, D. P. and Ba, J. L. Adam: A method for stochastic optimization. In *International Conference on Learning Representation*, 2015.

Krizhevsky, A., Hinton, G., et al. Learning multiple layers of features from tiny images. 2009.

Langley, P. Crafting papers on machine learning. In Langley, P. (ed.), *Proceedings of the 17th International Conference on Machine Learning* (ICML 2000), pp. 1207–1216, Stanford, CA, 2000. Morgan Kaufmann.

LeCun, Y., Bottou, L., Bengio, Y., and Haffner, P. Gradient-based learning applied to document recognition. *Proceedings of the IEEE*, 86(11):2278–2324, 1998.

Lorraine, J. and Duvenaud, D. Stochastic hyperparameter optimization through hypernetworks. In *arXiv preprint arXiv:1802.09419*, 2018.

Loshchilov, I. and Hutter, F. Sgdr: stochastic gradient descent with warm restarts. In *International Conference on Learning Representation*, 2017.

Luketina, J., Berglund, M., Greff, K., and Raiko, T. Scalable gradient-based tuning of continuous regularization hyperparameters. In *International conference on machine learning*, pp. 2952–2960. PMLR, 2016.

Marschall, O., Cho, K., and Savin, C. A unified framework of online learning algorithms for training recurrent neural networks. *Journal of Machine Learning*, 21:1–34, 2020.

Metz, L., Maheswaranathan, N., Nixon, J., Freeman, C. D., and Sohl-Dickstein, J. Understanding and correcting pathologies in the training of learned optimizers. In *Proceedings of the 36th International Conference on Machine Learning* (ICML 2019), 2019.

Mujika, A., Meier, F., and Steger, A. Approximating real-time recurrent learning with random kronecker factors. In *NeurIPS*, 2018.

Padakandla, S., J, P. K., and Bhatnagar, S. Reinforcement learning in non-stationary environments. In *arXiv preprint arXiv:1905.03970*, 2019.

Pedregosa, F. Hyperparameter optimization with approximate gradient. In *ICML*, 2016.

Richard, K., Cseke, B., Klushyn, A., Smagt, P. v. d., and Günnemann, S. Continual learning with bayesian neural networks for non-stationary data. In *International Conference on Learning Representation*, 2020.

Shorten, C. and Khoshgoftaar, T. M. A survey on image data augmentation for deep learning. *Journal of Big Data*, 6, 2019.

Snoek, J., Larochelle, H., and Adams, R. P. Practical bayesian optimization of machine learning algorithms. In *NeurIPS*, 2012.

Snoek, J., Rippel, O., Swersky, K., Kiros, R., Satish, N., Sundaram, N., Prabha, M. M. A. P., and Adams, R. P. Scalable bayesian optimization using deep neural networks. In *ICML*, 2015.

Tallec, C. and Ollivier, Y. Unbiased online recurrent optimization. In *arXiv preprint arXiv:1702.05043*, 2017.

Tieleman, T. and Hinton, G. Lecture 6.5 - rmsprop, courses: Neural networks for machine learning. In *Technical report*, 2012.
Williams, R. J. and Zipser, D. A learning algorithm for continually running fully recurrent neural networks. *Neural Computation*, 1:270–280, 1989.

Xie, A., Harrison, J., and Finn, C. Deep reinforcement learning amidst lifelong non-stationarity. In *arXiv preprint arXiv:2006.10701*, 2020.