HOT SWAPPING FOR ONLINE ADAPTATION OF OPTIMIZATION HYPERPARAMETERS

Kevin M. Bache & Padhraic Smyth
Department of Computer Science
University of California, Irvine
Irvine, CA 92697, USA
{kmbache,smyth}@ics.uci.edu

Dennis DeCoste
Machine Learning Group
eBay Research Labs
San Jose, CA 95125, USA
ddecoste@ebay.com

ABSTRACT

We describe a general framework for online adaptation of optimization hyperparameters by ‘hot swapping’ their values during learning. We investigate this approach in the context of adaptive learning rate selection using an explore-exploit strategy from the multi-armed bandit literature. Experiments on a benchmark neural network show that the hot swapping approach leads to consistently better solutions compared to well-known alternatives such as AdaDelta and stochastic gradient with exhaustive hyperparameter search.

1 INTRODUCTION

In this paper, we introduce a new stochastic gradient method with adaptive learning rate selection based on the insight that optimization hyperparameters may be freely ‘hot swapped’ in the middle of the learning process.

Where existing adaptive learning rate algorithms are based on running curvature estimates of the local loss surface (Schaul et al., 2012; Zeiler, 2012), we present a procedure which recasts learning rate selection as an explore-exploit problem which can be addressed using existing solutions to multi-armed bandit problems. This method is straightforward to implement, retains the runtime characteristics and memory footprint of stochastic gradient, and outperforms existing methods on a common benchmark task.

2 ALGORITHM

The basis of the proposed algorithm is the observation that optimization hyperparameters such as learning rate and momentum may be freely ‘hot swapped’ during optimization runs. This is in contrast to model hyperparameters, such as hidden layer size or unit type, which cannot be changed so easily during learning. This approach can also be contrasted to traditional hyperparameter search strategies such as grid search, random search, or Bayesian optimization which set optimization hyperparameters in an outer loop and treat learning as an inner loop (Bergstra and Bengio, 2012; Snoek et al., 2012).

Instead, we propose to observe the optimization process under a variety of hyperparameter settings and to preferentially continue to use those settings which have performed best in the past. We do this...
by maintaining a meta-model of hyperparameter performance. The general hot swapped optimization procedure is defined in algorithm 1.

Many meta-models may work well for this task, but in this work we cast the problem of learning rate selection into an explore-exploit framework and choose a discounted upper confidence bound (DUCB) model for hyper-parameter selection. In brief, we seek an algorithm that ‘explores’ the space of possible learning rates—in order to learn which ones perform best on the given problem—while reserving most of its time to ‘exploit’ the best performing rates—by repeatedly using them to update model parameters. The upper confidence bound algorithm is a common choice for tackling explore-exploit problems, and its discounted form achieves the optimal regret bound up to a logarithmic factor for rapidly shifting reward distributions (Garivier and Moulines, 2008).

The procedure for hot swapped optimization with a DUCB model is listed in algorithm 2 with the full details given in algorithm 3. We assume that we have a finite set of learning rates to select from, \(\alpha \equiv \{\alpha_1, ..., \alpha_K\}\), a positive objective function to be minimized \(f(\tilde{\theta}; B)\), along with its gradient \(g(\tilde{\theta}; B)\), both of which can be evaluated at a point in parameter space \(\tilde{\theta}\) for a given data batch \(B\).

We define the ‘reward’ granted to a given learning rate \(\alpha_k\) as \(r = \log(f(\tilde{\theta}_0; B)) - \log(f(\tilde{\theta}_k; B))\), where \(\tilde{\theta}_0\) represents the (non-hyper) parameters at the beginning of the current iteration and \(\tilde{\theta}_k \equiv \tilde{\theta}_0 - \alpha_k g(\tilde{\theta}_0; B)\) represents the parameters obtained by choosing learning rate \(\alpha_k\). We use a logarithmic scaling of the rewards which treats multiplicative reductions of the objective function \(f\) as equally valuable, a useful feature given the exponential slowdown of optimization progress which is often observed in practice. The \(\alpha\) value chosen at each step is selected by the DUCB algorithm in the usual way (see the function \texttt{GETDUCBSUGGESTEDINDEX} in algorithm 3 for details).

The DUCB model will periodically seek to explore different learning rates as the optimization procedure progresses. This introduces the potential to take catastrophically large steps which could discard progress made up to the current time. To prevent this, we perform a line search across learning rates to find the best learning rate value for each minibatch. The line search starts from the learning rate proposed by the DUCB algorithm and decreases through the other available learning rates until it finds one which lowers the current minibatch’s objective function value below the value it held before the current update. Because the line search is only performed on the current minibatch of data, it still takes linear time in batch size and problem dimension, just like simple SGD.

In practice, these two processes work well together. The line search prevents the bandit algorithm’s tendency to explore catastrophically large step sizes, while the bandit algorithm’s carefully chosen initial step sizes reduce the number of minibatch objective function evaluations from the large number required by a vanilla minibatch line search to a much smaller quantity.

3 Initial Results

We test the efficacy of this procedure on a neural network based on the MNIST dataset. MNIST is comprised of 60,000 28x28 pixel black and white images of handwritten digits. The task is to classify each image as a number ‘0’ through ‘9’.

We show results from fully connected feed-forward network with 50 sigmoidal units in the first hidden layer, 300 sigmoidal hidden units in the second hidden layer, and a final 10-way softmax output. We trained on the first 50,000 images of the training set.

We perform an exhaustive search of SGD hyperparameters for comparison. We consider all combinations of the following parameters: initial learning rates in \(\alpha_0 \in \{1.0, 0.3, 0.1, 0.03, 0.01, 0.003\}\), per-epoch learning rate multipliers of \(\eta \in \{0.99, 0.995, 1.0\}\), momentum coefficients \(\mu \in \{0.0, 0.5, 0.7, 0.9\}\) and batch sizes \(\in \{64, 128, 256, 512, 1024\}\) for a total of 360 SGD settings.

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1 Minibatch line search is not without precedent (Ngiam et al. 2011; Roux et al. 2012), though it has received little direct attention in the past.

2 This experiment was conducted using Theano, PyLearn2, and a cluster of computers with NVIDIA GRID K520 GPUs.
We also compare against AdaDelta, another widely used adaptive learning rate algorithm, using the hyperparameters described in [Zeiler (2012)] for MNIST: \( \epsilon = 10^{-6} \) and decay rate factor of 0.95 across batch sizes \( \in \{64, 128, 256, 512, 1024\} \).

Finally, we tested hot swapped optimization with a DUCB step size model and batch sizes \( \in \{64, 128, 256, 512, 1024\} \).

We ran each algorithm for 500 epochs using three random weight initializations. Figure 1 shows the spread of training and test performances of all 380 algorithms after 200 and 500 training epochs. Each dot represents the median performance of a single set of hyperparameters with error bars indicating min and max performance across initializations. The best performing algorithms will be in the bottom left. At convergence, all 15 hot swap DUCB algorithms (red) achieve the lowest training objective (negative log likelihood) of every other algorithm tested (green and blue).

Furthermore, while test performance isn’t the direct target of an optimization process—test performance is also heavily linked to regularization quality, a factor to which optimization algorithms are agnostic—the DUCB algorithm obtained the lowest median test error rate across all of its variations (1.85% vs 1.97% for AdaDelta and 2.35% for SGD) and the best single test performance overall (1.63% error rate), despite the fact that SGD instantiations outnumbered hot swapped DUCB instantiations by a factor of 75:1.

The performance of SGD algorithms vary widely across hyperparameter settings. The AdaDelta algorithms consistently exhibit performance in the top 30% of the SGD algorithms, through as with hot swapped DUCB, they vary across batch size.

Figure 1: Best viewed in color. Training objective (training set negative log likelihood) and test performance (test set misclassification rate) for various algorithms on MNIST 784-500-300-10 with sigmoidal units. Each dot represents one algorithm with one set of hyperparameters. The best performing algorithms are in the bottom left. The only parameter varied for DUCB and AdaDelta are batch size. SGD algorithms were varied across initial learning rate, learning rate decrease schedule, momentum and batch size. Error bars represent performance of a single algorithm and hyperparameter set across 3 random weight initializations. All 15 instantiations of the hot swap DUCB achieve better training likelihood than all 1125 other algorithms we compare against.

Figure 2 gives a direct comparison of training time vs. various measures of performance for one instantiation each of the five DUCB hot swapping algorithms (one for each batch size), the five

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4It’s worth noting that batch size is the one significant hyperparameter for the hot swapping DUCB algorithm. It is similar in this regard to other adaptive learning rate methods such as AdaDelta and No More Pesky Learning Rates.
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Figure 2: Best viewed in color. Performance of hot swapping with DUCB model, AdaDelta, and the two best-performing SGD algorithms (out of a total of 1080) on MNIST 784-500-300-10 with sigmoidal units.

AdaDelta algorithms, and the two best-performing SGD algorithms (chosen retrospectively out of a total of 1080 SGD algorithms; ‘best performing’ measured in final training objective and test misclassification).

The top plot in figure 2 shows test error rate vs. wall clock time. Despite the fact that DUCB hot swapping with a batch size of 64 takes the most time per iteration, it makes sufficient progress in each step that by 1000 seconds into the training run it has attained the best test error of any algorithm we tested. The second plot shows training objective over time (training set negative log likelihood), with all of the DUCB algorithms making significant training progress well after the SGD and AdaDelta algorithms have plateaued and finding lower optima. The third plot suggests that the DUCB algorithms naturally learn to decrease their learning rates as they near local optima. The fourth plot shows a running average of gradient norms over time, with the DUCB algorithms all finding flatter optima than competing algorithms.

On other problems in which we have tested the hot swapping DUCB procedure, we have observed similarly strong training performance with greater variation on test performance that we observed here. This suggests that the hot swapped DUCB procedure is a strong optimization algorithm that requires similarly strong regularization not to overfit.

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5 A single iteration of DUCB hot swapping takes between 1.6 and 3.6 times as long as a comparable iteration of SGD or AdaDelta because it performs several line search iterations per step. However, it makes considerably greater progress per iteration than SGD and continues to do so well after SGD and AdaDelta have plateaued, converging to better optima than the existing algorithms. For additional details on the relative timing of each method, see [Appendix 1: Timing].

6 The AdaDelta algorithms are not included in the learning rate plots because AdaDelta maintains a different learning rate for each parameter.
4 CONCLUSION

We have introduced a new adaptive learning rate algorithm for stochastic gradient that is built to hot swap an optimization hyperparameter over the course of a learning run. Preliminary results indicate that the proposed method consistently outperforms competing methods on several measures.

Numerous extensions of this basic procedure are possible, including using different meta-models, swapping new optimization or regularization hyper parameters, swapping multiple parameters at once, and reducing the frequency of line search to speed performance. We are currently working to test this and other hot swapping procedures on a wide variety of problems.

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APPENDIX 1: TIMING

This section contains details of the relative timings of SGD, AdaDelta, and the hot swapped DUCB algorithm for the model detailed in section 3.

DUCB tends to require more line search iterations per step as it nears a local optima, meaning that it takes less time per minibatch earlier in the optimization process and more time per minibatch later in the optimization process. This effect is significantly mitigated with larger batch sizes as they exhibit less variance across minibatches. This helps the DUCB model to predict which step size will perform optimally for a given problem, which limits the number of line search iterations required per minibatch and yields epoch timings that are closer to SGD and AdaDelta.

Overall, hot swapped DUCB takes between 1.6 and 3.6 times as long per minibatch as SGD and AdaDelta, however it makes more progress per iteration than either of these competing algorithms and converges to better optima (see figure 2 and the discussion in section 3).

| Batch Size: | SGD | AdaDelta | DUCB, epoch 100 | DUCB, epoch 300 | DUCB, epoch 500 |
|-------------|-----|----------|-----------------|-----------------|-----------------|
| 64:         | 11.9| 12.1     | 30.1            | 40.2            | 42.4            |
| 128:        | 13.0| 13.2     | 20.3            | 38.8            | 43.7            |
| 256:        | 16.8| 16.7     | 26.4            | 39.7            | 49.2            |
| 512:        | 24.7| 25.5     | 37.9            | 38.2            | 56.2            |
| 1024:       | 39.2| 40.8     | 60.2            | 60.4            | 63.3            |

Table 1: Milliseconds per minibatch for SGD, AdaDelta, and the hot swapped DUCB algorithm. Timing varies over the course of the optimization run for the hot swapped DUCB algorithm, and so its average timing is listed after 100, 300, and 500 epochs.

| Batch Size: | SGD | AdaDelta | Seconds per Epoch |
|-------------|-----|----------|-------------------|
| 64:         | 9.3 | 9.4      | 23.5              |
| 128:        | 5.1 | 5.2      | 7.9               |
| 256:        | 3.3 | 3.3      | 5.2               |
| 512:        | 2.4 | 2.5      | 3.7               |
| 1024:       | 1.9 | 2.0      | 3.0               |

Table 2: Seconds per epoch for SGD, AdaDelta, and the hot swapped DUCB algorithm. Timing varies over the course of the optimization run for the hot swapped DUCB algorithm, and so its average timing is listed after 100, 300, and 500 epochs.
APPENDIX 2: FULL ALGORITHM DESCRIPTION

Algorithm 1 General hot swapped optimization

Require: $\theta$, the parameters to be optimized, $X$, a dataset which may be broken into batches denoted $B$, $f(\theta; X)$ the objective function to be optimized, $A$, a set of optimization hyperparameter values to consider, $M$, some model of optimization hyperparameter performance, $U(\theta; B, \alpha)$, an update step for the parameters $\theta$ given a batch of data points and optimization hyperparameter value, a convergence criteria

1: while not converged do
2: $B \leftarrow$ a new batch of data
3: $\alpha \leftarrow$ the best optimization hyperparameters $\alpha \in A$ as judged by $M$
4: $\theta \leftarrow U(\theta; B, \alpha)$
5: $M$ observes performance of $\alpha$
6: end while

Algorithm 2 Hot Swapped Stochastic Optimization with DUCB model

Require: $\theta, f, g, \bar{\alpha}$ array, a dataset, convergence criteria

1: maxIndex $\leftarrow$ maximum index in the $\alpha$ array
2: rewards $\leftarrow$ array of 0s of same length as $\bar{\alpha}$
3: counts $\leftarrow$ array of 0s of same length as $\bar{\alpha}$
4: $t \leftarrow -1$
5: while not converged do
6: $t \leftarrow t + 1$
7: $B \leftarrow$ new batch of data
8: $startIndex \leftarrow$ INITIALALPHAINDEX(rewards, counts, $t$, maxIndex)
9: $\theta \leftarrow$ BACKTRACKINGLINESEARCHWITHREWARDS($f, g, B, \theta, \bar{\alpha}, startIndex$)
10: end while
Algorithm 3 DUCB Helper Functions

1: function INITIAL_ALPHA_INDEX(rewards, counts, t, maxIndex)
2:     if $t < \text{maxIndex}$ then return $t$
3:     else return GET_DUCB_INDEX(rewards, counts)
4: end function
5:
6: function GET_DUCB_INDEX(rewards, counts)
7:     rewards ← $\gamma \ast \text{rewards}$
8:     counts ← $\gamma \ast \text{counts}$
9:     means ← rewards / counts
10:     $n \leftarrow \text{sum(counts)}$
11:     confIntervals ← $\sqrt{\text{exploreConst} \ast \log(n) / \text{counts}}$
12:     ucs ← means + confIntervals
13:     return arg max(ucbs)
14: end function
15:
16: function TRACKING_LINE_SEARCH_WITH_REWARDS(f, g, B, $\vec{\theta}$, $\vec{\alpha}$, startIndex)
17:     maxIndex ← the maximum index in the $\vec{\alpha}$ array
18:     $f_{\text{start}} \leftarrow f(\vec{\theta}; B)$
19:     $f_{\text{current}} \leftarrow f_{\text{start}}$
20:     $f_{\text{best}} \leftarrow f_{\text{start}}$
21:     $\alpha_{\text{best}} \leftarrow \text{startIndex}$
22:     haveFoundBetterThanStart ← False
23:     for all index ← startIndex : maxIndex do
24:         $f_{\text{prev}} \leftarrow f_{\text{current}}$
25:         $\alpha \leftarrow \alpha[i\text{ndex}]$
26:         $f_{\text{current}} \leftarrow \text{OBJECTIVE_AT_ALPHA}(\vec{\theta}, f, g, B, \alpha)$
27:         GRANT_REWARD(index, rewards, counts, $f_{\text{start}}$, $f_{\text{current}}$)
28:         if $f_{\text{current}} < f_{\text{best}}$ then
29:             $f_{\text{best}} \leftarrow f_{\text{current}}$
30:             $\alpha_{\text{best}} \leftarrow \alpha$
31:             haveFoundBetterThanStart ← True
32:         end if
33:         if haveFoundBetterThanStart and $f_{\text{current}} > f_{\text{prev}}$ then
34:             Break Loop
35:         end if
36:     end for
37:     $\vec{\theta} \leftarrow \vec{\theta} - \alpha_{\text{best}} g(\vec{\theta}; B)$ return $\vec{\theta}$
38: end function
39:
40: function OBJECTIVE_AT_ALPHA($\vec{\theta}, f, g, B, \alpha$) return $f(\vec{\theta} - \alpha g(\vec{\theta}; B); B)$
41: end function
42:
43: function GRANT_REWARD(index, rewards, counts, $f_{\text{start}}$, $f_{\text{current}}$)
44:     rewards[index] ← rewards[index] + log($f_{\text{start}}$) − log($f_{\text{current}}$)
45:     counts[index] ← counts[index] + 1
46: end function