Deep Q-Networks for Accelerating the Training of Deep Neural Networks

Jie Fu∗ Zichuan Lin† Miao Liu‡ Nicholas Leonard§ Jiashi Feng¶ Tat-Seng Chua∥

Abstract

We present a novel method, called QAN, for improving the generalization ability of a deep neural network (DNN). It achieves this by feeding the weights of the DNN during training into a deep Q-network (DQN) as its states. The actions of the DQN modify different hyperparameters during training. The reward function of this DQN is designed to learn policies to accelerate the training of that DNN. Empirically, this acceleration leads to better generalization performance of the DNN. Compared to other similar works, QAN is thousands of times faster as it takes into account the characteristics of DNNs’ training. To the best of our knowledge, QAN is the first practical solution to speeding up the training of a DNN using a DQN on real-world benchmark datasets. The code can be downloaded from https://github.com/bigaidream-projects/qan

1 Introduction

The motivation for this work is founded on the proof [4] that deep networks trained by a stochastic gradient method with fewer iterations have a better generalization ability. A natural question arises: how can we accelerate the training of deep networks in practice? In this paper, we achieve this by tuning two unusual hyperparameters at every iteration: mini-batch selecting and learning rates scheduling.

The contributions of this paper are as follows:

• We propose a practical framework based on DQNs to improve modern deep neural networks’ generalization performance by accelerating their training.

∗National University of Singapore, homepage: http://bigaidream.github.io/
†Tsinghua University, Beijing
‡Massachusetts Institute of Technology, homepage: http://www.mit.edu/~miaoliu/
§Element Inc., New York City, homepage: https://github.com/nicholas-leonard
¶National University of Singapore, homepage: https://sites.google.com/site/jshfeng/
∥National University of Singapore, homepage: http://www.comp.nus.edu.sg/~chuats/

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• We demonstrate how to use a DQN to optimize learning rates of a DNN during training. We also propose to use a DQN to select mini-batches for a DNN during training. These two new methods only require a limited “black box” interface to deep models, allowing us to tune very sophisticated, state-of-the-art deep networks without having to look under the hood.

• A regressor is added to each layer of the deep nets whose hyperparameters are being optimized. This regressor can speed up the overall hyperparameter optimization process.

2 Related Work

A pseudo-Bayesian neural network is used to tune a few hyperparameters of another deep neural network in [14]. The authors add a Bayesian linear regressor to the last hidden layer of a deep net, marginalizing only the output weights of the net while using a point estimate for the remaining parameters. The hyperparameters of this pseudo-Bayesian net are tuned by another Gaussian process based Bayesian optimizer.

For tuning learning rates, the most similar work is [3], where a DQN has been proposed to control one hyperparameter. However, the states require careful hand-construction of features and can only be used to tune learning rates. Furthermore, their method cannot handle stochastic settings and needs at least 150,000 episode for training DQNs, which is totally impractical. In contrast, our methods only needs 20 episodes for DQNs on MNIST dataset and can deal with stochastic situations.

As for mini-batch selection, the authors in [10] study how to choose samples for a mini-batch. Their rank-based approach relies on the assumption that ranks (defined by the entropy of training samples during training) of losses over samples change slowly over time, which seems not hold in larger datasets [10]. Also based on the entropy of training samples, self-paced learning methods[7] are, however, usually coupled with the original optimization problems and, as far as we know, there is no work successfully applying self-paced learning to deep nets training [1].

3 Deep Q-Networks (DQNs)

Reinforcement learning algorithms are designed to train an agent to perform a task within an environment. The goal of a reinforcement learning agent is to maximize its expected total reward by learning an optimal policy (mapping from states to actions). At each time step \( t \), the agent observes a state \( s_t \in \mathcal{S} \) (in fact we set \( s_t = w_t \)), selects an action \( a_t \in \mathcal{A} \), and receives a reward \( r_{t+1} \), following the agent’s decision it observes the next state \( s_{t+1} \). Markov Decision Process (MDP) property is assumed for the environment here. That is given the current state \( s_t \) and action \( a_t \), the probability of arriving at the next...
state $s_{t+1}$ and receiving reward $r_{t+1}$ does not depend on any of the previous states or actions. The accumulative return at time $t$ is given by $R_{t+1} = r_{t+1} + \sum_{t'=t}^{T-1} \gamma^{t'-t} r_{t'}$, where $T$ is the termination time step, also called the number of episodes\(^1\). The action-value function $Q^\pi(s, a) : (S, A) \rightarrow \mathbb{R}$ measures the expected return after observing state $s_t$ and taking an action under a policy $\pi : \mathcal{S} \rightarrow \mathcal{A}$. The optimal action-value function $Q^*(s, a) = \max_{\pi} Q^\pi(s, a)$ obeys the well-known Bellman equation,

$$Q^*(s_t, a_t) = \mathbb{E}[r_{t+1} + \gamma \max_{a'} Q^*(s_{t+1}, a') | s_t = s, a_t = a].$$ (1)

At each time step the estimate $\hat{y}_t$ is defined as $\hat{y}_t = Q_t(s_t, a_t)$ and the target $y_t$ is given by $y_t = r_{t+1} + \gamma \max_{a'} Q_t(s_{t+1}, a')$. The update is based on the difference between $\hat{y}_t$ and $y_t$.

The DQN method\(^2\) approximates the optimal Q-function with a DNN. We denote it as $Q(s; \theta) : \mathbb{R}^{|S|} \rightarrow \mathbb{R}^{|A|}$ to emphasize that this DQN is parameterized by the weights $\theta$. It tries to minimize the expected Temporal Difference (TD) error of the optimal Bellman equation: $E_{s_t, a_t, r_t, s_{t+1}} \| Q_{\theta}(s_t, a_t) - y_t \|_2^2$, where

$$y_t = \begin{cases} r_{t+1} + \mathbf{1}_{t \neq T-1} (\gamma \max_{a'} [Q(s_{t+1}; \theta)]_{a'}) & a = a_t \\ [Q(s_t; \theta)]_a & a \neq a_t \end{cases}. \quad (2)$$

DQN represents a state by a sequence of history features.

4 Generic Design for Tuning Hyperparameters

4.1 Weights as States

In this paper, the states fed into a DQN are defined by the learned weights of a DNN during training. This is different from \(^3\), where state features are manually crafted by the author. This not only avoids the troublesome feature engineering procedure, but also enables us to tune more types of hyperparameters besides learning rates. For example, as we demonstrate later, the states are also useful for selecting mini-batches.

Because the current best performing DNN type for supervised tasks is convolutional neural networks (CNNs), we focus on tuning the hyperparameters of CNNs. More specifically, the states are defined by the weights of those convolutional layers during training. Also because of this change\(^3\), different from \(^12\), we only employ a standard MLP in the DQN.

\(^1\)In this paper, one episode is defined as one entire training of the DNN from random weights till convergence. This definition is the same as meta-iteration defined in other hyperparameter papers, such as \(^11\).

\(^2\)Note that weights $\theta$ are used to parameterize the DQN, whereas weights $w$ denote the parameters of the DNN being tuned.

\(^3\)To some extent, we put the CNN outside the DQN.
4.2 Fixing Weights by Adding Regressors

Unfortunately, due to the global update mechanism of back-propagation, the positions of filters will be changed spontaneously after every episode. To force the filters to appear at the same positions at every episode, we add a regressor to every layer: \[ L_{\text{regressor}}(W_{\text{current}}, W_{\text{last}}) = \frac{1}{2} \| W_{\text{current}} - W_{\text{last}} \|^2, \]
where \( W_{\text{current}} \) are the parameters at current iteration and \( W_{\text{past}} \) are the parameters copied from last episode after convergence.

By fixing the weights of a CNN, we have two main added benefits. The first benefit is that the repeated training processes of the CNN can be accelerated. Obviously, if we only gradually change some hyperparameters, the training trajectories of the CNN should not differ significantly between episodes. Therefore, this regressor will provide more information to the training of the CNN from the previous episodes.

The second byproduct is that the number of states can be decreased dramatically, which is crucial for its scalability. This is due to the locality assumed by a convolutional operation, which leads to filters of a convolutional layer being relatively independent from each other. In other words, a small subset of filters is representative of all the others. This is quite different from the states used by Atari games [12], where the global state representations are needed. Fewer states help accelerate the training of DQNs, because there are fewer parameters to optimize, which will become more clear when we discuss the experiments.

4.3 Reward Function

The reward function is defined to ensure that the DQN learns a policy to find the optimal objective value in the fewest number of time steps. We define the reward function, similar to [3], as:

\[ r(f, s'_t) = \frac{1}{f(s'_t) - f_{\text{lower}}}, \quad f(s'_t) > f_{\text{lower}} \forall s'_t \]

(3)

where \( f_{\text{lower}} \) is a predefined lower-bound constant of the training loss, \( s'_t \) is the weights of convolutional layers of the CNN during training, and \( f \) is the training loss function.

5 DQN Actions for Specific Tasks

We need to determine the suitable actions for tuning learning rates and mini-batch selection.

5.1 Tuning Learning Rates

The training of a DNN with \( n \) free parameters can be formulated as the problem of minimizing a function \( f : \mathbb{R}^n \to \mathbb{R} \). Following the tradition of [10, 5], we define a loss function \( \psi : \mathbb{R}^n \to \mathbb{R} \) for each training sample; the distribution of training
samples then induces a distribution over function $D$, and the overall function $f$ we aim to optimize is the expectation of this distribution:

$$f(w) := \mathbb{E}_{\psi \sim D}[\psi(w)].$$

(4)

The commonly used procedure to optimize $f$ is to iteratively adjust $w_t$ (the weight vector at time step $t$) using gradient information obtained on a mini-batch of size $b$. More specifically, at each time step $t$ and for a given $w_t \in \mathbb{R}^n$, a mini-batch $\{\psi_{i=1}^b\} \sim D^b$ is selected to compute $\nabla f_t(w_t)$, where $f_t(w_t) = \frac{1}{b} \sum_{i=1}^b \psi_i(w_t)$.

In this work, the stochastic setting is assumed, as it is currently the most efficient to train deep models on large datasets. We also assume that we are preparing training samples for a classification task. The SGD is not robust in that its performance is heavily dependent on how learning rates are tuned over time [13].

The SGD procedure then becomes a natural extension of the Gradient Descent (GD) to stochastic optimization of $f$ as follows:

$$w_{t+1} = w_t - \eta_t \nabla f_t(w_t),$$

(5)

where $\eta_t$ is a learning rate. It has been shown in [10] that not only the selection of the update of $w_t$ given $\nabla f_t(w_t)$ is crucial, but the selection of the mini-batch $\{\psi_{i=1}^b\} \sim D^b$ used to compute $\nabla f_t(w_t)$ also greatly contributes to the overall performance.

It has been shown in [11] that the optimal learning rates schedule starts by taking large steps and then takes smaller step sizes in the following iterations. Thus in order to tune the learning rate of the CNN, we design three actions: increasing the $\eta_t$ by 0.05, decreasing $\eta_t$ by 0.05 and remaining the same.

5.2 Tuning Mini-Batch Selection

Training samples are not equally valuable in terms of the contribution to the generalization performance [9]. The next natural question is how can we squeeze the training data efficiently and effectively? Self-paced learning [8] has a similar flavor to active learning, which chooses a sample to learn from at each iteration, based on the entropy during training. Active learning approaches differ in their sample selection criteria. However, entropy is a kind of low-level information in the sense that it changes rapidly over training.

In this paper, we consider the information associate with labels as the selection criteria, which is more close to curriculum learning [2, 7]. Specifically, DQN will decide which categories of training samples should be included in one mini-batch. Different from [7], where they encourage diverse examples within a mini-batch, we do not hard-code such prior knowledge. Take image classification task for example. Maybe in the early stage of training, it might be better to put cats and dogs into the mini-batches more frequently; but later it would be better to put dogs, cars and trucks into mini-batches more often.
The actions of the DQN are associated with distinct categories. One problem remains: DQN can only take one action at a time. Suppose we are solving a classification problem with 3 categories \{c_1, c_2, c_3\}. A naïve solution is to simply use one-hot coding approach to define 8 distinct actions. Actually the number of needed actions grows exponentially with the number of classes. This is impractical even for handling 10 categories, which needs to define 1024 actions.

To solve this problem, we use a First-In-First-Out Queue to act as a buffer for the actions. For example if the buffer size is 5, then at every iteration the DQN will take an action and put it into the buffer. Initially, DQN has to fill the buffer with 5 actions (categories), which implies in the first 5 iterations the DQN will have no control over the CNN. After this “burn-in” phase, DQN will update this buffer with a new action.

Suppose again that we are dealing with a classification task with 3 categories \{c_1, c_2, c_3\}, and the actions in the buffer are \{c_1, c_1, c_3, c_3, c_1\}. Then the mini-batch will consist of 60% training samples from category 1 and 40% training samples from category 3.

6 Experiments
In this section, we empirically demonstrate how a DQN can accelerate a CNN and thus improve its test accuracy. All the experiments are done on the MNIST dataset with 20,000 training and 10,000 testing samples. MNIST dataset is a popular computer vision classification benchmark with 10 categories. The CNN we consider here consists of 2 convolutional layers, with the first having 16 and the second having 256 filters. Only the 16 filters of the first convolutional layer are used as the states for DQNs. Reducing the number of states this way allows the DQN to converge extremely fast in practice. Above these, we add 2 fully-connected layers with 256 and 128 neurons respectively. All the non-linear functions are \textit{Tanh}. The original learning rate is set to 0.05 in all experiments.

6.1 Tuning Learning Rates
We test that the DQN learns useful learning rates scheduling. We do not intend to compare it to other adaptive learning rate schedulers.

The mini-batch size is set to 10 and the number of epochs is 20. After training the DQN for 20 episodes, the final testing accuracy obtained by a CNN tuned by that DQN is 98.02%, whereas the baseline CNN’s testing accuracy is 97%. From Figure 1 we can also observe that the convergence rate of the CNN tuned by a DQN is much faster than the baseline CNN.

6.2 Tuning Mini-Batch Selection
Here we test whether the selection of training samples makes the training algorithms converge faster.
The mini-batch size is set to 128, the buffer size is 10 and the number of epochs is 40. It should be noted that other state-of-the-art results on MNIST dataset usually set the mini-batch size to a very small value, such as 10. Actually we tried 10 and 32 as the mini-batch sizes, but the improvements were not significant. However, increasing the mini-batch size is more than a pedantic trick, as doing so could utilize the parallel computing resources more effectively [6].

As shown in Figure 2, after training the DQN for 20 episodes, the final testing accuracy of a CNN with adaptive mini-batches selected by a DQN is 92.97%, whereas the baseline CNN's testing accuracy is 91.97%. Figure 2 also shows that a CNN with adaptive mini-batch selection performs consistently better than the baseline CNN at every epoch.

7 Conclusion and Discussion

In this paper, we proposed a scalable framework, called QAN, based on DQNs to improve modern deep neural networks' generalization performance on real-world benchmark datasets by accelerating their training. We demonstrated how to use a DQN to optimize learning rates of a DNN during training. We also showed how to use a DQN to select mini-batches for a DNN during training.

It has been shown that [15] lower layer features are relatively easy to transfer.
Figure 2: The testing accuracy obtained by a CNN with adaptive mini-batch selected by a DQN on MNIST with 10,000 testing samples.

Because the DQN in our framework only monitors the first convolutional layer, it seems straightforward to study the transferrability of the learned policies of DQNs. For example, we could first train the DQN on a subset of ImageNet and then use these policies to accelerate CNNs on the full dataset of ImageNet. We would also like to investigate the combined effects of using DQNs and other popular adaptive learning rate schedulers together, such as ADADELTA [16].

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