X-TrainCaps: Accelerated Training of Capsule Nets through Lightweight Software Optimizations

Alberto Marchisio¹, Beatrice Bussolino¹,², Alessio Colucci², Muhammad Abdullah Hanif¹, Maurizio Martina², Guido Masera² and Muhammad Shafique¹

¹Technische Universität Wien (TU Wien), Vienna, Austria
²Politecnico di Torino (PoliTo), Turin, Italy
Email: {alberto.marchisio, muhammad.hanif, muhammad.shafique}@tuwien.ac.at
{beatrice.bussolino, alessio.colucci}@studenti.polito.it
{maurizio.martina, guido.masera}@polito.it

Abstract

Convolutional Neural Networks (CNNs) are extensively in use due to their excellent results in various machine learning (ML) tasks like image classification and object detection. Recently, Capsule Networks (CapsNets) have shown improved performances compared to the traditional CNNs, by encoding and preserving spatial relationships between the detected features in a better way. This is achieved through the so-called Capsules (i.e., groups of neurons) that encode both the instantiation probability and the spatial information. However, one of the major hurdles in the wide adoption of CapsNets is its gigantic training time, which is primarily due to the relatively higher complexity of its constituting elements. In this paper, we illustrate how can we devise new optimizations in the training process to achieve fast training of CapsNets, and if such optimizations affect the network accuracy or not. Towards this, we propose a novel framework “X-TrainCaps” that employs lightweight software-level optimizations, including a novel learning rate policy called WarmAdaBatch that jointly performs warm restarts and adaptive batch size, as well as weight sharing for capsule layers to reduce the hardware requirements of CapsNets by removing unused/redundant connections and capsules, while keeping high accuracy through tests of different learning rate policies and batch sizes. We demonstrate that one of the solutions generated by X-TrainCaps framework can achieve 58.6% training time reduction while preserving the accuracy (even 0.9% accuracy improvement), compared to the CapsNet in the original paper by Sabour et al. (2017), while other Pareto-optimal solutions can be leveraged to realize trade-offs between training time and achieved accuracy.

1 Introduction

Recently the development of Deep Neural Networks (DNNs), especially Convolutional Neural Networks (CNNs), has seen a dramatic increase, leading to many different architectures. An important computing challenge is the optimization of CNNs and their hyper-parameters. Most of the fine-tuning optimizations (e.g., choosing the training policy, the learning rate, the optimizer, etc.) are repetitive and time-consuming, because every change must be tested with many epochs of training and repeated many times to have statistical significance. This is significantly worsened by increasing the CNN complexity, which leads to a more demanding compute effort to find the right set of optimizations.

Different methods have been explored in the literature to reduce the training time of CNNs, such as one-cycle policy by Smith (2018), warm restarts by Loshchilov and Hutter (2016), adaptive batch size by De et al. (2016), Goyal et al. (2017), Devarakonda et al. (2017). However, a key limitation of CNNs is: no information on the spatial correlation between detected features is retained. This causes poor network performances in terms of accuracy when the object to be recognized is rotated, has a different orientation, or presents any other geometrical variation. Currently, this problem is solved by training networks on expanded datasets, that include also transformed and modified objects. However, wider datasets lead to much longer training times. Longer training times not only pose
delays in the DNN development cycle, but also make it a complex job for a wide range of developers, requiring super-costly training machines like Nvidia’s DGX-2 or rely on outsourcing to third party cloud services that can compromise privacy and security requirements. Hence, both advanced DNN architectures and fast training techniques are necessary.

Capsule Networks (CapsNets, see Figure 1) aim to solve the limitation of CNNs (w.r.t. preserving the spatial correlation between detection features) by substituting single neurons with so called Capsules (i.e., groups of neurons) and routing by agreement between capsule layers, which provide the ability to encode both the instantiation probability of an object and its instantiation parameters (width, orientation, skew, etc.). However, one of the major hurdles in the adoption of CapsNets is their gigantic training time, which is primarily due to the higher complexity of their constituent elements.

To address this challenge, we present X-TrainCaps, a systematic methodology to employ different optimization methods for significantly reducing the training time and number of parameters of CapsNets, while preserving or improving their accuracy. However, this requires a study of impact of different optimizations (like learning rate policy, batch size adaptation, etc.) on the training time and accuracy of CapsNets. X-TrainCaps provides multiple Pareto-optimal solutions that can be leveraged to trade-off training time reductions with no / tolerable accuracy loss. For instance, in our experimental evaluations, X-TrainCaps provides a solution that can reduce the training time of CapsNets by 58.6% while providing a slight increase in its accuracy (i.e. 0.9%). Another solution provides 15% reduction in the number of parameters of the CapsNet without affecting its accuracy.

Our Novel Contributions:

- Analysis of the CapsNets behavior when different learning rate policies (like one-cycle policy or warm restarts) are applied (Section 3).
- A novel training methodology, X-TrainCaps, which accelerates the training of CapsNets by combining warm restarts, adaptive batch size and weight sharing in an automated flow specialized for the nature of CapsNets like capsule and different capsule layers (Section 4).
- Reduction of redundant parameters via weight sharing and a smaller decoder specialized for CapsNets. This optimization reduces the number of parameters by more than 15% (Sections 4.3 & 4.4).

Before proceeding to the technical sections, we present an overview of CapsNets and the learning rate policies in Section 2 to a level of detail necessary to understand the contributions of this paper.

2 Background and Related Work

2.1 CapsNets

Capsules were introduced by Hinton, Krizhevsky, et al. [2011]. A capsule is a group of neurons that encodes both the instantiation probability of an object and the spatial information. Sabour et al. (2017) and Hinton, Sabour, et al. (2018) introduced two architectures based on capsules, tested on MNIST (LeCun et al. 1998), with better accuracy compared to the state-of-the-art traditional CNNs. The architecture of the CapsNet that we use in our work corresponds to the model of Sabour et al.

1Our methodology may also be beneficial for other complex CNNs, as it enables integration of available open-source optimizations in the DNN training loop.
(2017), as shown in Figure 1. The layers composing the encoder are: an initial convolutional layer (ConvLayer), a PrimaryCaps layer, which transforms the scalars numbers of ConvLayer in vectors, and a DigitCaps layer, which outputs the probabilities of the digits being present in the input image. The encoding network is followed by a decoder, composed by three fully-connected layers, which output the reconstructed image. The loss computed on the reconstructed image (Reconstruction Loss) encourages the capsules of the DigitCaps layer to encode the instantiation parameters of the object.

2.2 Learning Rate Schedules

One-Cycle Policy: This method, proposed by Smith (2015) and Smith (2018), consists of three phases of training. In the first phase, the learning rate is linearly increased from a minimum to a maximum value in an optimal range. In the second phase, the learning rate is symmetrically decreased. In a small fraction of the last steps, the learning rate must be annealed to a very low value. In Equation 1 the formulas of the three parts of one cycle policy are reported: $t_s$ is the training step, $T_s$ is the total number of steps in the training epochs, $l_r_{min}$ and $l_r_{max}$ are the learning rate range boundaries. Saddle points in the loss function slow down the training process, since the gradients in these regions have smaller values. Increasing the learning rate helps to faster traverse the saddle points.

\[
\begin{align*}
\frac{lr}{ts} &= \frac{l_r_{min} + ts \cdot \frac{l_r_{max} - l_r_{min}}{0.45 \cdot T_s}}{0 < ts < 0.45 \cdot T_s} \\
\frac{lr}{ts} &= \frac{l_r_{min} + (ts - 0.9 \cdot T_s) \cdot \frac{l_r_{min} - l_r_{max}}{0.45 \cdot T_s}}{0.45T_s < ts < 0.9T_s} \\
\frac{lr}{ts} &= \frac{l_r_{min} - 9 \cdot \frac{l_r_{min}}{T_s} \cdot (ts - 0.9 \cdot T_s)}{0.9 \cdot T_s < ts < T_s}
\end{align*}
\] (1)

Warm Restarts: Stochastic Gradient Descent with Warm Restarts technique was proposed by Loshchilov and Hutter (2016). The learning rate is initialized to a maximum value and then it is decreased with cosine annealing until reaching the lower bound of a chosen interval. When the learning rate reaches the minimum value, it is set again to the maximum value, realizing a step function. The cosine annealing function which is used is reported in Equation 2. $l_r_{min}$ and $l_r_{max}$ are learning rate range boundaries, $t_s$ is the training step, $T_t$ is the number of training steps for each cycle. When $t_s = T_t$, $t_s$ is set to 0 and the cycle starts again. This process is repeated cyclically during the whole training time. The period of a cycle needs to be properly set to optimize the training time and the accuracy. Increasing step-wise the learning rate emulates a warm restart of the network and encourages the model to step out from possible local minima or saddle points.

\[
l_r = l_r_{min} + \frac{1}{2} \left( l_r_{max} - l_r_{min} \right) \left( 1 + \cos \left( \pi \cdot \frac{t_s}{T_t} \right) \right)
\] (2)

2.3 Adaptive Batch Size

When training a DNN, a small batch size can provide a faster convergence, while a larger batch size allows to have an higher data parallelism and, consequently, high computational efficiency. For this reason, many authors have studied methods to increase the batch size with fixed schedules (Babanezhad et al. (2015), Daneshmand et al. (2016)) or following an adaptive criterion (De et al. (2016), Goyal et al. (2017), Devarakonda et al. (2017)).

3 Analysis of Learning Rate Schedules applied to CapsNets

The techniques described in Section 2 have been tailored for traditional CNNs, to improve their performances in terms of accuracy and training time. This section aims to study whether different learning rate policies and batch size selection are effective when applied for training the CapsNets. Since the traditional neurons of the CNNs are replaced by multidimensional capsules in the CapsNets, the number of parameters (weights and biases) to be trained is huge.

For this purpose, we implemented different state-of-the-art learning rate policies for the training loop of the CapsNet, such that these techniques are enhanced for the capsule structures and relevant parameters of the CapsNet. Figure 2(a) shows the learning rate changes for different techniques and how the accuracy of the CapsNet varies accordingly. More detailed results of our analyses, including the comparisons with the LeNet5, are reported in the Table of Figure 2(b).
From the results of this analysis, we can derive the following key observations:

1. The warm restarts technique is the most promising because it allows to reach the same accuracy (99.366%) as the CapsNet with a fixed learning rate, providing a reduction of 79.31% in the training time.
2. A more extensive training with warm restarts leads to an accuracy improvement of 0.074%.
3. The adaptive batch size shows similar improvements in terms of accuracy (99.41%) and number of training epochs.
4. The first epochs with smaller batch size execute in a longer time.

4 X-TrainCaps: Our Framework to Accelerate the Training of CapsNets

Training a CapsNet consists of a multi-objective optimization problem, because our scope is to maximize the accuracy, while minimizing the training time and the network complexity. The processing flow of our X-TrainCaps framework is shown in Figure 3. Before describing how to integrate different optimizations in an automated training methodology and how to generate the optimized CapsNet at the output (Section 4.5), we present how these optimizations have been applied.
implemented with enhancements for the CapsNets, which is necessary to realize an integrated training methodology.

4.1 Learning Rate Policies for CapsNets

The first parameter analyzed to improve the training process of CapsNets is the learning rate. The optimal learning rate range is evaluated with the range boundaries 0.0001 and 0.001. For our framework, we use the following parameters in these learning rate policies:

- **Fixed learning rate**: 0.001;
- **Exponential decay**: starting value 0.001, decay rate 0.96, decay steps 2000;
  \[ lr = lr_0 \cdot 0.96^{\text{current step}/2000} \]
- **One cycle policy**: lower bound 0.0001, upper bound 0.001, annealing to 10^{-5} in the last 10\% of training steps (see Algorithm 1);
- **Warm restarts**: lower bound 0.0001, upper bound 0.001, cycle length = one epoch (see Algorithm 2).

4.2 Batch Size

To realize adaptive batch size, the batch size is set to 1 for the first three epochs, and then increased every five epochs for three times. In particular, the user can choose a value \( P \) and batch size will assume values \( 2^P, 2^{P+1} \) and \( 2^{P+2} \) (see Algorithm 3).

4.3 Complexity of Decoder

The decoder is an essential component of the CapsNet. Indeed, absence of a decoder results in a lower accuracy of the CapsNet. The outputs of DigitCaps are fed to the decoder: the output of the capsule (a vector) with the highest value is left untouched, while the remaining 9 vectors are set to zero (Figure 4 left). Thus, the decoder receives 10×16 values, where 9×16 are null. Therefore, we optimize the model by using a reduced decoder (Figure 4 right) with only the 1×16 inputs which are linked to the capsule that outputs the highest probability. Overall, the original decoder has 1.4M parameters (weights and biases) while the reduced decoder provides a 5\% reduction, with 1.3M parameters.

4.4 Complexity Reduction through Weight Sharing

Algorithm 4 illustrates how to share the weights between the PrimaryCaps and the DigitCaps layers, by having a single tensor weight in common for all the 8-element vectors inside each 6x6 capsule. Using this method, it is possible to reduce the total number of parameters by more than 15\%, from 8.2 millions to 6.7 millions. However, the accuracy drops by almost 0.3\%, when comparing it to the baseline CapsNet.
4.5 WarmAdaBatch

Among the explored learning rate policies, warm restarts guarantees the most promising in terms of accuracy, while adaptive batch size provides a good trade-off to obtain fast convergence. We propose WarmAdaBatch (see Algorithm 5 learning rate policy to expand the space of the solutions by combining the best of two worlds. For the first three epochs, the batch size is set to 1, then it is increased to 16 for the remaining training time. A first cycle of warm restarts policy is done during the first three epochs, a second one during the remaining training epochs. The learning rate variation of the WarmAdaBatch is shown in Figure 5.

4.6 Optimization Choices

Our framework is able to automatically optimize CapsNets and its training depending on which parameters the user wants to improve: using WarmAdaBatch, the accuracy and the training time are automatically co-optimized. The number of parameters can be reduced, at the cost of some accuracy loss and training time increase, by enabling the weight sharing, along with WarmAdaBatch.

Algorithm 1 One Cycle Policy for CapsNet

1: procedure ONECYCLEPOLICY(lr min, lr max, TotalSteps, T curr)
2: \( t_m \leftarrow 0.45 \times TotalSteps \)
3: \( m \leftarrow \frac{lr_{max} - lr_{min}}{t_m} \)
4: \( m_{ann} \leftarrow \frac{9 \times lr_{min}}{TotalSteps} \)
5: if \( T_{curr} \leq t_m \) then
6: \( lr \leftarrow max + lr_{min} \)
7: else if \( t_m \leq T_{curr} \leq 2t_m \) then
8: \( lr \leftarrow -m(x - 2t_m) + lr_{min} \)
9: else
10: \( lr \leftarrow -m_{ann}(x - 2t_m) + lr_{min} \)
11: end if
12: end procedure

Algorithm 2 Warm Restarts for CapsNet: learning rate is decayed with cosine annealing.

1: procedure WARMRESTARTS(lr min, lr max, T curr, T i)
2: \( lr \leftarrow lr_{min} + \frac{1}{2} (lr_{max} - lr_{min}) \left( 1 + \cos \pi \frac{T_{curr}}{T_i} \right) \) \( \triangleright \) Learning rate update
3: if \( T_{curr} = T_i \) then
4: \( T_{curr} \leftarrow 0 \) \( \triangleright \) Warm Restart after \( T_i \) training steps
5: else
6: \( T_{curr} \leftarrow T_{curr} + 1 \) \( \triangleright \) Current step update
7: end if
8: return \( T_{curr} \)
9: end procedure

Algorithm 3 AdaBatch for CapsNet: Batch Size is increased during training.

1: procedure ADABATCH(P, CurrentEpoch)
2: if \( CurrentEpoch \leq 3 \) then
3: \( \text{BatchSize} \leftarrow 1 \)
4: else if \( 4 \leq CurrentEpoch \leq 8 \) then
5: \( \text{BatchSize} \leftarrow 2^P \)
6: else if \( 9 \leq CurrentEpoch \leq 13 \) then
7: \( \text{BatchSize} \leftarrow 2^{P+1} \)
8: else
9: \( \text{BatchSize} \leftarrow 2^{P+2} \)
10: end if
11: end procedure
Algorithm 4 Weight Sharing for CapsNet, it is applied only in the DigitCaps layer

1: procedure DIGITCAPS(input, BatchSize) ⊢ BatchSize represents the dimension containing the single elements
2:   ⊢ Input size is [BatchSize, 32, 36, 8]
3:   initialize weight ⊢ Weight size is [BatchSize, 32, 1, 10, 16, 8]
4:   initialize bias ⊢ Bias size is [BatchSize, 1, 10, 16, 1]
5:   for Step = 1, 36 do ⊢ We move along the dimension with 36 elements
6:     ⊢ Result size is [bs, 32, 36, 10, 16, 1]
7:       u[Step] ← matrix_multiply(weight[1], input[Step]) ⊢ We use always the same weight, instead of cycling
8:   end for
9:   v ← routing(u, bias) ⊢ Output size is [BatchSize, 1, 10, 16, 1]
10: return v
11: end procedure

Algorithm 5 Our WarmAdaBatch for CapsNet

1: procedure WARMADABATCH(lr_{min}, lr_{max}, MaxEpoch, MaxStep) ⊢ Batch size update
2:  ⊢ Batch size update
3:  for Epoch = 1, MaxEpoch do
4:    Adabatch(4, Epoch) ⊢ Steps in 3 epochs with batch size 1
5:    if Epoch ≤ 3 then
6:      T_i ← 3 * 60000 ⊢ Steps in 3 epochs with batch size 1
7:    else
8:      T_i ← 27 * 3750 ⊢ Steps in 27 epochs with batch size 16
9:    end if
10:  for Step = 1, MaxStep do
11:    T_{curr} ← WarmRestarts(lr_{min}, lr_{max}, T_{curr}, T_i) ⊢ Learning Rate update
12:  end for
13: end for
14: end procedure

5 Evaluation

5.1 Experimental Setup

We developed our framework using PyTorch library (Paszke et al. (2017)), running on two Nvidia GTX 1080 Ti GPUs. We tested it on the MNIST dataset (LeCun et al. (1998)), since the original CapsNet proposed by Sabour et al. (2017) is tailored on it. The dataset is composed of 60000 samples for training and 10000 test samples. After each training epoch, a test is performed. At the beginning of each epoch, the samples for training are randomly shuffled.

5.2 Accuracy Results

Evaluating the learning rate policies: Among the state-of-the art learning policies that we enhanced for CapsNets, warm restarts is the most promising with maximum accuracy improved of 0.074%. CapsNet with warm restarts reaches the maximum accuracy of the baseline (with fixed learning rate) in 6 epochs rather than 29, with a training time reduction of 62.07%.

Evaluating Adaptive batch size: Different combinations of batch sizes in adaptive batch size algorithm have been tested, since the smaller the batch size, the faster the initial convergence. However, large batch sizes lead to slightly higher accuracy after 30 epochs and, most importantly, to a reduced training time. In fact, a CapsNet training epoch with batch size 1 lasts for 7 minutes, while with batch size 128 it lasts for only 28 seconds. Batch size 16 is a good trade off between fast convergence and short training time (i.e., 49sec/epoch). The best results, applying adaptive batch size, are obtained using batch size 1 for the first three epochs and then increasing it to 16 for the remaining part of the training. With this parameter selection, there is a 0.044% accuracy gain with respect to baseline and the maximum accuracy of the baseline is reached in 5 epochs rather than in 29. However, the first three epochs take a longer time (88% longer time) because of the reduced batch
Evaluating WarmAdaBatch: As for the batch, the first cycle of learning rate lasts 3 epochs and the second one 27 epochs. Variation of batch size and learning rate cycles are synchronized. This solution allows to have a 0.088% gain in accuracy with respect to CapsNet baseline implementation, and the baseline maximum accuracy is reached by CapsNet with WarmAdaBatch in 3 epochs against 29. After the first three epochs batch size changes and learning rate is restarted, so there is a drop of accuracy, that however re-converges in a few steps to the highest stable value obtained.

Evaluating Weight Sharing: applying weight sharing to the DigitCaps layer, we are able to achieve a 15% reduction in the number of total parameters, decreasing from 8.2 millions to 6.7 millions. However, this reductions leads also to a decrease in the maximum accuracy, dropping by 0.26%.

5.3 Comparison of different optimization types

We compare the different types of optimizations in terms of accuracy, and also based on the training time to reach the maximum accuracy and the number of parameters. As we can see in Figure 6a, we compare different optimization methods in a 3-dimensional space. This representation provides Pareto-optimal solutions, depending on the optimization goals. We also compare, in Figure 6b, the accuracy and the learning rate evolution in different epochs, for AdaBatch, WarmRestarts and WarmAdaBatch. Among the space of the solutions, we discuss in more details two Pareto-optimal ones, WarmAdaBatch and the combination of WarmAdaBatch and weight sharing, which we call WAB+WS.

WarmAdaBatch: This solution provides the optimal point in terms of accuracy and training time, because it achieves the highest accuracy (99.454%) in the shortest time (2400 seconds). Varying the batch size boosts the accuracy improvements in the first epoch and the restart policy contributes to speed-up the training.

WAB+WS: The standalone weight sharing reduces the number of parameters by 15%. By a combination of it with WarmAdaBatch, the accuracy loss is compensated (99.38% versus 99.366% of the baseline), while training time is shorter than the baseline (7200 seconds versus 8700 seconds) but longer than simple WarmAdaBatch. Our framework chooses this solution if also the number of parameter reduction is selected among the optimization goals.

6 Conclusion

In this paper, we proposed X-TrainCaps, a novel framework to automatically optimize the training of a given CapsNet for accuracy, training time or number of parameters, based on the requirements
needed. We enhanced the different learning policies, for the first time, for accelerating the training of CapsNets. Afterwards, we discussed how an integrated training framework can be developed to find Pareto-optimal solutions, including different new optimizations for fast training like WarmAdaBatch, complexity reduction for the CapsNet decoder, and weight sharing for CapsNets. These solutions not only provide significant reduction in the training time while preserving or improving the accuracy, but also enable a new mechanism to provide trade-off between training time, network complexity, and achieved accuracy. This enables new design points under different user-provided constraints.

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