The Effects of Hyperparameters on SGD Training of Neural Networks

Thomas M. Breuel
Google, Inc.
tmb@google.com

Abstract

The performance of neural network classifiers is determined by a number of hyperparameters, including learning rate, batch size, and depth. A number of attempts have been made to explore these parameters in the literature, and at times, to develop methods for optimizing them. However, exploration of parameter spaces has often been limited. In this note, I report the results of large scale experiments exploring these different parameters and their interactions.

1 Datasets and Libraries

All experiments reported here were carried out using the Torch library [1] and CUDA (some of the experiments have been reproduced on a smaller scale with other libraries). The dataset for all the experiments is MNIST [3, 2].

Characters were deskewed prior to all experiments. Deskewing significantly reduces error rates in nearest neighbor classifiers. Skew corresponds to a simple one-parameter family of linear transformations in feature space and causes decision regions to become highly anisotropic. Without deskewing, differences in performance between different architectures might primarily reduce to their ability to “learn deskewing”. With deskewing, MNIST character classification become more of an instance of a typical classification problem. Prior results on classifying deskewed MNIST data both with neural networks and with other methods are shown in the table below.

2 Logistic vs Softmax Outputs

Multi-Layer Perceptrons (MLPs) used for classification usually attempt to approximate posterior probabilities and use those as their discriminant function. Two common approaches to this are the use of least square regression with logistic output units trained with a least square error measure (“logistic outputs”)
and a softmax output layer (“softmax outputs”). In the limit of infinite amounts of training data, both approaches converge to true posterior probability estimates. Softmax output layers have the property that they are guaranteed to produce a normalized posterior probability distribution across all classes, while least square regression with logistic output units generates independent probability estimates for each class membership without any guarantees that these probabilities sum up to one.

Softmax is often preferred, although there is no obvious theoretical reason why it should yield better discriminant functions or lower classification error for finite training sets. In OCR and speech recognition, some practitioners have observed that logistic outputs yield better posterior probability estimates and better results when combined with probabilistic language models. In addition, when the sum of the posterior probability estimates derived from logistic outputs differs significantly from unity, that is a strong indication that the input lies outside the training set and should be rejected.

Figure 1 shows a scatterplot of test vs training error for a large number of MLPs with one hidden layer at different learning rates, different number of hidden units, and different batch sizes. Such scatterplots show what error rates are achievable by the different architectures, hyperparameter choices, initializations, and order of sample presentations. The lowest points in the vertical direction indicate the lowest test set error achievable by the architecture in this set of experiments. The scatterplot shows that logistic outputs achieve test set error rates of about 1.0% vs 1.1% for softmax outputs. At the same time, logistic outputs never achieve zero percent training set error, while softmax outputs frequently do.

In order to ascertain that the difference in test set error between the two

| Method                              | Test Error | Preprocessing | Reference          |
|-------------------------------------|------------|---------------|--------------------|
| Reduced Set SVM deg 5 polynomial    | 1          | deskewing     | LeCun et al. 1998  |
| SVM deg 4 polynomial                | 1.1        | deskewing     | LeCun et al. 1998  |
| K-nearest-neighbors, L3             | 1.22       | deskewing, noise removal, blurring, 2 pixel shift | Kenneth Wilder, U. Chicago |
| K-nearest-neighbors, L3             | 1.33       | deskewing, noise removal, blurring, 1 pixel shift | Kenneth Wilder, U. Chicago |
| 2-layer NN, 300 HU                  | 1.6        | deskewing     | LeCun et al. 1998  |

Table 1: Other previously reported results on the MNIST database.
Figure 1: Training and test error for MLPs with logistic outputs (blue) and softmax output (red). Note that softmax outputs achieve down to zero percent training error (assigned to an error of 1e-4) but logistic outputs give overall better performance on new training samples.

Figure 2: Learning rate and batch size effects depending on output layer type. This is a scatterplot for all networks that yield test set error rates of less than 1.5%, with color indicating the test set error. Softmax outputs yield the best results for a learning rate that is about an order of magnitude smaller than logistic outputs.
architectures is due to the architectures themselves, it is important to ensure that the space of hyperparameters (learning rates, batch sizes, number of hidden units) has been explored sufficiently. Note that, as Figure 2 shows, the in order to yield low error rates, softmax outputs require learning rates that are about an order of magnitude lower than logistic outputs.

Figure 3 demonstrates that the range of parameters (learning rates, batch sizes) has been explored fully; above learning rates of 1e1, both softmax and logistic output models diverge, and at small learning rates, both fail to learn in a reasonable amount of time.

The fact that logistic outputs yield 10% lower relative error rates on such a simple and widely studied problem and architecture compared to softmax outputs does not prove that “logistic outputs are better than softmax outputs”, but it suggests that it is worth testing both logistic and softmax outputs on any particular problem to see which one yields lower test set error.

3 Batch size Effects

Optimizing the weights of a neural network can be carried out by stochastic gradient descent (updating after each sample) or by full gradient descent (computing a gradient on the parameters from the entire training set). In between
Figure 4: Batch size and learning rate vs. error rate (logistic outputs). See the text for an explanation.

those two extremes is batched gradient descent. In batched gradient descent, we update the parameters of the MLP to reduce the error for a small sample (“batch”) of training samples, typically consisting of between 10 and 1000 samples.

Computationally, using batches instead of individual training samples allows for greater parallelism; each layer of an MLP computes effectively a function like:

\[ y = \sigma(M \cdot x) \]

For simple SGD, \( x \) is some d-dimensional vector, but for batched gradient descent, \( x \) is a \( d \times b \) dimensional matrix, where \( b \) is the batch size. The matrix multiplication \( M \cdot x \) can be evaluated much more efficiently and in parallel than evaluating \( b \) individual matrix-vector products in single-sample updates. In fact, if we use \( b \) processors, we can compute updates for \( b \) samples in roughly the same time as we would otherwise use for a single sample in SGD.

When using batch training, a common convention is to rescale the learning rate \( \lambda \rightarrow \frac{\lambda}{b} \). This means that as we increase the batch size \( b \), we need to scale up the learning rate proportionately. This is the convention we use in these experiments.

Figure 4 shows a scatterplot of trained networks with good test set error vs. batch size and learning rate. There are three apparent limits on performance:

1. At the lower end, we have a soft transition from well performing net-
works to poorly performing networks. The explanation of this is that at low learning rates, the network learns too slowly to reach low test set errors within the limited number of training steps. The reason this soft transition slopes upwards is due to the use of normalized learning rates. Without learning rate normalization, this line would remain horizontal and independent of batch size.

2. At a batch size of 1, there is a maximum learning rate; beyond that learning rate, the stochastic gradient descent optimization diverges. Without batch size normalization of learning rate, this upper limit would exist independent of batch size; due to batch size normalization, this line of divergence slopes upwards, parallel to the soft lower bound on learning rates.

3. There is a third, unexpected, constant limit on the batch-normalized learning rate.

The original single sample learning rate determines the speed of convergence of the stochastic gradient descent algorithm; within its region of convergence, halving the learning rate approximately doubles the time needed to reach a given test set error, since each gradient update represents simply a step towards the minimum along some path. This reasoning also applies for batch updates. The constant upper limit on the batch-normalized learning rate corresponds to a single sample learning rate that decreases proportionally to batch size.

The consequence is that, as long as the maximum usable batch normalized learning rate increases proportionally with batch size, we benefit from parallelization in terms of overall speedup of learning. Once we enter the regime where the upper limit of batch normalized learning rates is independent of batch size, further parallelization does not speed up training.

Without further experimentation, we can only guess at the source of the upper limit on the batch-normalized learning rate. As a simplified model, assume that the limit on the learning rate for single sample updates is due to some subset of the input vectors (e.g., vectors that generate particularly large gradients). For batch sizes that contain, on average, only one of those input vectors, we can continue to use the original learning rate, but once we use a batch size that contains, on average, two of those vectors, we have to cut the learning rate in half in order to keep the magnitude of the update within the range that allows convergence. (In practice, we are not necessarily looking at individual samples but subspaces of the input.) This analysis suggests possible strategies for improving training performance with large batch sizes that will be explored elsewhere.

Regardless of the speed of optimization, we can also ask the question of how the test set error of the final network depends on batch size. This is shown in Figure 5. We see that increasing batch size generally results in worse test set errors for both logistic outputs and softmax outputs. The dependence is somewhat stronger for logistic outputs. In addition, logistic outputs appear to yield networks with a higher variability. Note that the differences in error rates
Figure 5: Test error by batch size for logistic and softmax outputs. Note that logistic output units achieve the lowest error. Also note that for larger batch sizes, the advantage of logistic output units over softmax output units disappears.

in this plot are much smaller than the differences in error rates found in the previous learning rate plots; this plot makes small but significant differences among the very best models visible.

The observations on the relationship between batch sizes and learning rates above also have implications for hyperparameter optimization. In particular, the hyperparameter search at large batch sizes becomes harder because the range of learning rates that yield good networks is considerably smaller than it is at small batch sizes (Figure 6). Batch sizes that are too large therefore not only waste computational resources through parallelism that does not result in a speedup for learning, they may actually make the hyperparameter search harder.

4 Convolutional Layers

The above results were all obtained for non-convolutional networks with a single hidden layer. How do they generalize to convolutional networks? There are, of course, many different kinds of convolutional architectures we could investigate. The simplest architecture places a single convolutional layer at the input of the network.

Not surprisingly, adding a convolutional layer results in significantly lower test set error (0.69% test set error) compared to non-convolutional networks (1% test set error), as seen in Figure 7.

For convolutional networks, we also observe that small batch sizes yield the best test set errors. In fact, large batch sizes never reach comparably low error rates (Figure 8).
Figure 6: At large batch sizes, the range of hyperparameter resulting in good test set errors is considerably smaller than at small batch sizes.

Figure 7: Training error vs test set error for non-convolutional (blue) and convolutional (red) networks.
Figure 8: Test set error by batch size for convolutional networks. Output units are softmax, and the plot shows the best networks across all learning rates and number of convolutional units. Note the significant increase in best achievable error rates with increasing batch size.
5 ReLU Units (Not Convolutional)

Another popular architectural choice is to replace the sigmoidal nonlinearity in hidden layers with rectifying linear units (ReLU). To explore the effects of this on the results, networks were trained with all four combinations of sigmoid/ReLU hidden units and softmax/sigmoid output units. The scatterplot of results is shown in Figure 9.

We see in Figure 9 that softmax outputs achieve zero percent test set error for both kinds of hidden layer nonlinearities. Furthermore, ReLU hidden units outperform sigmoidal hidden units for either kind of output layer. The overall best performing combination was logistic output units with ReLU hidden units, resulting in a test set error of 0.92%.

6 ReLU Units (Convolutional)

The previous results for ReLU units are interesting, given the low test set error rate and low dependence on batch size. It’s interesting to see whether we can reproduce those results for convolutional networks. However, in the case of convolutional networks, we find a significant batch size dependence, and that the difference between sigmoidal and ReLU hidden units is considerably smaller than for non-convolutional networks. Furthermore, some softmax networks also come close in performance (Figure 13).

Figure 9: A comparison of sigmoid and ReLU units at the hidden layer, combined with softmax and logistic outputs.
Figure 10: Dependence of test set error on batch size. We see that for sigmoidal hidden units (blue, cyan), large batch sizes perform considerably worse than small batch sizes. For ReLU hidden units (red, magenta), the dependence is considerably weaker, although smaller batch sizes still seem to have a slight advantage.
Figure 11: Dependence of test set error on the number of hidden units. For sigmoidal hidden units (blue, cyan), there is little improvement of test set error with increasing numbers of hidden units. For ReLU hidden units, there is a strong improvement in test set error with the number of hidden units. The maximum number of hidden units tested was 2000, although it looks like larger numbers of hidden units might result in even better performance.
Figure 12: Error rates (indicated by color) vs batch size, learning rate, and number of hidden units (indicated by circle size). These scatterplots suggest that the parameter ranges for all four conditions were explored fairly completely.

Figure 13: Test error vs. batch size for convolutional networks with ReLU units.
Figure 14: The batch size and learning rate parameter space explored for the comparison of convolutional ReLU and sigmoidal networks.
Deep ReLU Networks

ReLU networks also appear to be highly successful for training deep networks. We explore this architectural variant in these experiments by comparing deep networks with ReLU hidden units and sigmoidal hidden units. We find that the performance of deep networks with sigmoidal units degrades with depth, while deep networks with ReLU networks yield good performance even at large (eight layer) depths (Figure 15). However, increasing depth for ReLU networks does not result in better test set performance. The deterioration of test set error with increasing depth for sigmoidal hidden units is probably due to effects like vanishing gradients, something that ReLU networks do not seem to suffer from to the same degree.

For both types of deep networks, we can ask again how test set error depends on batch size. Figure 16 shows that for both types of deep networks and across a range of hidden layers, the best achievable test set error generally increases with increasing batch size.

Conclusions and Discussion

Machine learning algorithms cannot be totally ordered by performance and there is no single best learning algorithm. Nevertheless, machine learning benchmarks in general, and benchmarks on MNIST in particular, tell us something about how machine learning algorithms compare on typical classification tasks, and what kind of architectural features influence performance significantly. That is, the conclusions we can draw from such benchmarks are not so much about which algorithm is “better”, but rather which algorithmic choices may affect the outcome positively or negatively.

Perhaps the most important result from these benchmarks is how complex the interaction between different architectural features and conditions is; per-
Figure 16: Test set error vs batch size for deep networks with ReLU (red) and sigmoidal (blue) hidden layers. Circle size indicates number of hidden layers. Notice that there is a significant decrease in test set performance with increasing batch size.

Figure 17: Test set error (indicated by color with red being high, blue being low) vs # hidden layers and batch size. Note that deep networks are much more sensitive to large batch sizes during training than shallow networks.
Figure 18: Parameters spaces explored by the deep ReLU and sigmoidal networks. The parameter spaces show that the learning rate parameters were explored sufficiently well for both network types.

performance improvements that can be demonstrated in simple networks do not add up when combined together into the same architecture.

Furthermore, many benchmarks that have been carried out in the literature may have been hampered by limited sets of training conditions. For example, benchmarking logistic vs. softmax outputs at larger batch sizes suggests that there is little difference between the two methods; however, at small batch sizes, logistic outputs significantly outperform softmax outputs on MNIST data (Figure 5). Unless both methods are tested at small batch sizes, the significantly better performance of logistic outputs is not revealed. As a second example, for some architectures, ReLU networks show no batch size dependencies, while other network architectures do show such dependencies.

It is important to remember that the MNIST dataset is not necessarily representative of other classification problems: it has a small number of classes, the prior probability is uniform, the number of training samples is small compared to many other problems, all geometric variability (translations, rotations, skew) has been removed, and the input vectors are binary. Therefore, more important than the results about what works are the result of what unexpectedly doesn’t work well even in such a simple case.

Based on the experiments reported here, we observe:

- For many problems, increasing batch sizes in a parallel implementation results in no speedup in training because the per-sample learning rate needs to be scaled down proportionately to batch size. Furthermore, large batch sizes may intrinsically limit the performance of networks. Finally, hyperparameter optimization may get harder for larger batch sizes, as
the range of feasible learning rates (and other parameters) gets narrower. Therefore, it is a good idea to carry out experiments with single sample updates and small batch sizes.

- Softmax outputs may yield lower training errors than logistic outputs, but often also yield higher test set errors. Therefore, it is a good idea to try both kinds of outputs when training neural networks on different tasks. In doing so, it is important to try a wide range of learning rates, since the optimal learning rates for the two kinds of outputs are different.

- For non-convolutional networks, ReLU hidden layer units perform significantly better than sigmoidal hidden layer units in these experiments; they also show lower batch size dependencies and scale to much larger numbers of hidden units. For convolutional networks, however, these effects were not observed, suggesting that both sigmoidal and ReLU non-linearities should be tried.

- It is much easier to train deep networks using ReLU hidden layers than hidden layers with sigmoidal non-linearities. However, additional depth does not improve test set error for either sigmoidal or ReLU units. For deep networks, we also observed batch size dependencies. In addition, the range of good learning rates shifts and becomes smaller for deeper networks.

Generally, these results suggest the following strategy for training new networks:

- Start with single sample updates, both during initial exploration and hyperparameter search.

- When exploring new problems, compare softmax and logistic outputs, as well as ReLU and sigmoidal hidden units.

- Although deep ReLU networks can be trained, be sure to try shallow ReLU networks as well, and test a wide range of learning rates.

We note that there has been an extensive literature on various improved optimization methods for neural network learning, methods for learning hyperparameters, and benchmarks of MLP performance. It is impossible to do this literature justice in this technical report. However, a few general observations should suffice:

- The methods described in this paper all relied on simple SGD training, yet yield excellent performance compared to other reported results. In particular, optimization or hyperparameter selection methods that yield significantly worse results than those reported here are of questionable utility.

- Generally speaking, hyperparameter optimization for these kinds of problems does not seem to be particularly critical; networks yield similar performance over a broad range of hyperparameters.
Hyperparameter optimization should not optimize for the best expected test set error of the resulting networks, but for the minimal error over a collection of multiple trained models.

References

[1] Ronan Collobert, Samy Bengio, and Johnny Mariéthoz. Torch: a modular machine learning software library. Technical report, IDIAP, 2002.

[2] Daniel Keysers. Comparison and combination of state-of-the-art techniques for handwritten character recognition: topping the mnist benchmark. arXiv preprint arXiv:0710.2231, 2007.

[3] Yann LeCun, Corinna Cortes, and Christopher JC Burges. The mnist database of handwritten digits, 1998.