EFFICIENT PER-EXAMPLE GRADIENT COMPUTATIONS

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ABSTRACT

This technical report describes an efficient technique for computing the norm of the gradient of the loss function for a neural network with respect to its parameters. This gradient norm can be computed efficiently for every example.

1 Introduction

We often want to know the value of the L^2 norm of the gradient of a loss function with respect to the model parameters for every example in a minibatch. This is useful for techniques such as optimization based on importance sampling (Zhao & Zhang, 2014), where examples with large gradient norm should be sampled more frequently. Unfortunately, most differentiation functionality provided by most software frameworks does not support computing gradients with respect to individual examples in a minibatch. This technical report describes an efficient technique for obtaining all of the desired gradient norms when training a standard neural network.

2 Problem Definition

Suppose that we have a neural network containing n layers, with each layer implementing a transformation

$$\boldsymbol{z}^{(i)} = \boldsymbol{h}^{(i-1)\top} \boldsymbol{W}^{(i)}$$
$$\boldsymbol{h}^{(i)} = \phi^{(i)} (\boldsymbol{z}^{(i)}).$$

Here $\boldsymbol{h}^{(i)}$ are the activations of the hidden layers of the neural network. To simplify notation, we refer to the input of the network as $\boldsymbol{h}^{(0)}$. The activation function ϕ may be any differentiable function that does not contain any model parameters (for example, it need not be element-wise). The matrix $\boldsymbol{W}^{(i)}$ is the weight matrix for layer i. To simplify the presentation, we treat the biases for each layer as being an extra column of \boldsymbol{W} , with the ϕ function from the layer below providing a constant input of 1 to this column.

Suppose further that we have a loss function

$$L(\boldsymbol{z}^{(1)},\dots,\boldsymbol{z}^{(n)},\boldsymbol{h}^{(0)},\boldsymbol{y})$$

where y is a vector of targets provided from the training set. Note that L is this a function of the targets and the activations of the neural network, but is not permitted to access the model parameters themselves. The model parameters are accessed only via their influence on z.

Given a minibatch of m examples, define $L^{(j)}$ to be the loss when using example j to provide h^0 and y, and define the total cost C to be the sum of all m of these values.

Our goal is to compute $s^{(i)}$ for $i=1,\ldots,n$, where $s^{(i)}$ is a vector of the sum of squared derivatives, defined by

$$s_j^{(i)} = \sum_{k,l} \left(\frac{\partial}{\partial W_{k,l}^{(i)}} L^{(j)}\right)^2$$

The L^2 norm of the parameter gradient for example j is then given by $\sqrt{\sum_i s_j^{(i)}}$. Other norms, for example, the norm of the gradient for an individual weight matrix, can also be computed easily from the s vectors.

3 NAIVE APPROACH

Back-propagation (the term here refers not so much to the original backpropagation algorithm as to any of the modern general symbolic or automatic differentiation algorithms) allows the computation of $\frac{\partial}{\partial W_{k,l}}C$. The naive approach to computing s is to run back-propagation m times with a minibatch size of 1. This provides the gradient for each example. Each of these per-example gradients may then be summed out explicitly.

4 Proposed method

Let $H^{(i)}$ be a matrix representing a minibatch of values of $h^{(i)}$, with row j of $H^{(i)}$ containing $h^{(i)}$ for example j. Let $Z^{(i)}$ likewise contain a minibatch of $z^{(i)}$ values.

Standard backpropagation values allow us to compute the gradient of C with respect to all of the Z matrices in a single pass. Let $\bar{Z} = \nabla_{Z} C$.

We then have

$$\boldsymbol{s}_{j}^{(i)} = \left(\sum_{k} (\bar{Z}_{j,k}^{(i)})^{2}\right) \left(\sum_{k} (H_{j,k}^{(i-1)})^{2}\right).$$

5 COMPARISON

Suppose that each layer has dimension p. Then the asymptotic number of operations required by back-propagation for computing the parameter gradients is $O(mnp^2)$. The naive method for computing s also uses $O(mnp^2)$ operations. The naive method does not re-use any of the computations used by back-propagation, so it roughly doubles the number of operations. The new proposed method re-uses the computations from back-propagation. It adds only O(mnp) new operations. For large p, the extra cost of using the proposed method is thus negligible. In practice, the difference between the methods is much greater than this asymptotic analysis suggests. The naive method of running back-propagation m times with a minibatch of 1 performs very poorly because back-propagation is most efficient when efficient matrix operation implementations can exploit the parallelism of minibatch operations.

6 EXTENSIONS

Computing s allows other per-example gradient operations. For example, after determining the norm of the gradient for each example, we can modify the original \bar{Z} values, for example, by rescaling each row to satisfy a constraint on the norm of the parameter gradient. After obtaining the new modified Z' we can re-run the final step of backpropagation, to obtain

$$\bar{\boldsymbol{W}}^{(i)'} = \boldsymbol{X}^{(i)\top} \bar{\boldsymbol{Z}}^{(i)'}.$$

REFERENCES

Zhao, Peilin and Zhang, Tong. Stochastic optimization with importance sampling. *arXiv* preprint *arXiv*:1401.2753, 2014.