Exponentially Increasing the Capacity-to-Computation Ratio for Conditional Computation in Deep Learning

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Abstract

Many state-of-the-art results obtained with deep networks are achieved with the largest models that could be trained, and if more computation power was available, we might be able to exploit much larger datasets in order to improve generalization ability. Whereas in learning algorithms such as decision trees the ratio of capacity (e.g., the number of parameters) to computation is very favorable (up to exponentially more parameters than computation), the ratio is essentially 1 for deep neural networks. Conditional computation has been proposed as a way to increase the capacity of a deep neural network without increasing the amount of computation required, by activating some parameters and computation “on-demand”, on a per-example basis. In this note, we propose a novel parametrization of weight matrices in neural networks which has the potential to increase up to exponentially the ratio of the number of parameters to computation. The proposed approach is based on turning on some parameters (weight matrices) when specific bit patterns of hidden unit activations are obtained. In order to better control for the overfitting that might result, we propose a parametrization that is tree-structured, where each node of the tree corresponds to a prefix of a sequence of sign bits, or gating units, associated with hidden units.

1 Conditional Computation for Deep Nets

Deep learning is about learning hierarchically-organized representations, with higher levels corresponding to more abstract concepts automatically learned from data, either in a supervised, unsupervised, semi-supervised way, or via reinforcement learning (Mnih et al., 2013). See Bengio et al. (2013) for a recent review. There have been a number of breakthroughs in the application of deep learning, e.g., in speech (Hinton et al., 2012a) and computer vision (Krizhevsky et al., 2012). Most of these involve deep neural networks that have as much capacity (the number of units and parameters) as possible, given the constraints on training and test time that made these experiments reasonably feasible.

It has recently been reported that bigger models could yield better generalization on a number of datasets (Coates et al., 2011; Hinton et al., 2012b, Krizhevsky et al., 2012; Goodfellow et al., 2013) provided appropriate regularization such as dropout (Hinton et al., 2012b) is used. These experiments however have generally been limited by training time in which the amount of training data that could be exploited.

An important factor in these recent breakthroughs has been the availability of GPUs which have allowed training deep nets at least 10 times faster, often more (Raina et al., 2009). However, whereas the task of recognizing handwritten digits, traffic signs (Ciresan et al., 2012) or faces (?) is solved to the point of achieving roughly human-level performance, this is far from true for other tasks...
such as general object recognition, scene understanding, speech recognition, or natural language understanding, even with GPUs.

If we had 100 or 1000 more computing power that could be harnessed for training, then we could train correspondingly larger models on correspondingly larger datasets, covering more categories, modalities and concepts. This is important, considering that current neural network models are still small in size (especially if we count the number of artificial neurons) compared to biological brains, not even reaching the size of animals such as frogs, and several orders of magnitude less than that of mammals or humans. In this sense, we expect that much larger models are needed to build computers that truly master the visual world, or the world of ideas expressed in language, i.e., to make sense of the world around us at a level comparable to a child.

Moore’s law has practically saturated if one considers only the computing power of a single computing core. Most of the continued growth in computing power comes from parallelization. Unfortunately, despite the impressive progress in recent years (Le et al., 2012; Dean et al., 2012), exploiting large computer clusters to efficiently parallelize the training procedures for deep neural networks remains a challenge. Furthermore, additionally to faster training, in some applications we want faster inference, or test. Thus, the question we need to ask is: besides distributed training, are there other ways to build deep neural networks of much higher capacity without waiting a decade for hardware to evolve to the required level?

Bengio (2013); Bengio et al. (2013a) have proposed the notion of conditional computation for deep learning to answer positively to this question. The idea is to activate only a small fraction of the parameters of the model for any particular examples, and correspondingly reduce the amount of computation to be performed.

Currently, the ratio of the number of parameters to the amount of computation is essentially one in deep nets, i.e., every parameter is touched (usually with a single multiply-add) for each example. In contrast, there are machine learning models, such as decision trees (Breiman et al., 1984), with a much more favorable ratio: with \( N \) computations, a decision tree can actively select \( O(N) \) parameters out of a pool of up to \( O(2^N) \). Unfortunately decision trees suffer from poor statistical properties that prevent them, like many other non-parametric techniques relying only on the smoothness prior, from generalizing in a non-trivial way to regions of input space far from training examples. See Cucker and Grigoriev (1999); Bengio et al. (2010) for a mathematical analysis of the case of decision trees and Bengio (2009) for a longer analysis covering a wider class of learning algorithms, such as Gaussian kernel SVMs and graph-based non-parametric statistical models. On the other hand, there are both theoretical and empirical indications suggesting that deep distributed representations (Bengio, 2009; Pascanu et al., 2014) can benefit from advantageous statistical properties, when the data has been generated by multiple factors organized hierarchically, with the characteristics of each factor being learnable without requiring to see all the configurations of the other factors.

The conditional computation for deep learning as well as this paper is aimed at combining the statistical efficiency of deep learning and the computational efficiency, in terms of ratio of capacity to computation, of algorithms such as decision trees.

With this objective in mind, we propose here a novel way to parametrize deep neural networks (supervised or unsupervised, discriminative or generative) that allows up to exponential increase in the ratio of number of parameters to computation. In other words, we allow exponentially many parameters with respect to the amount of computation. We achieve this by observing that one can exploit bit patterns associated with hidden units in order to selectively activate different weight vectors or weight matrices. Since the number of such bit patterns can grow exponentially in the number of bits considered, this gives us the required rate of growth, controllable by the maximum size of these bit patterns.

### 2 Exponentially Rich Parametrization of a Weight Matrix

Here we consider a single layer consisting of \( p \)-dimensional input vector \( x \) and \( q \)-dimensional output vector \( h \). In a conventional approach, the layer is parametrized with a weight matrix \( W \in \mathbb{R}^{p \times q} \).
and a bias vector $b \in \mathbb{R}^q$, and computes
\[
    h = \phi(W^T x + b),
\]
where $\phi$ is an element-wise nonlinear function. In this case, the number of parameters of a single layer is $O(pq)$, and very often $q = O(p)$ so the number of parameters is $O(p^2)$.

In this note, we propose another way to parametrize a layer of a neural network, where the number of free parameters is $O(2^k p^2)$, where $k$ is a free parameter that controls the trade-off between capacity and computation.

Similarly to the conventional approach, a single layer consists of $x \in \mathbb{R}^p$ and $h \in \mathbb{R}^q$. However, now the weight matrix is not anymore independent of the input variable $x$, but is parametrized using $x$. The basic idea is that $k$ bits will be derived from $x$ from which $O(2^k)$ weight matrices will be defined and used to define the actual weight matrix mapping $x$ to $h$.

Let us first define a binary indicator vector $g \in \mathbb{R}^k$ as a function of the input $x$: $g = g(x)$. The gating function $g$ may be chosen freely as long as it provides hard decisions. One possibility is
\[
    g = (x > \tau)_1, \ldots, k,
\]
where $\tau$ is a predefined scalar threshold. It is also possible to make a stochastic decision such that each $g_i$ is sampled from Bernoulli distribution with its mean $\sigma(U^T x)$, where $U \in \mathbb{R}^{k \times k}$.

Using the binary indicators we obtain each column of the weight matrix $w_j$ ($j = 1, \ldots, p$) as a function of $g$ and $j$, using up to $k$ bits of $g$ (possibly chosen according to $j$) to obtain $w_j$:
\[
    w_j = F_j(S_j(g)),
\]
where $S_j$ is a subset of up to $k$ elements of $g$, and $F_j$ maps this binary $k$-dimensional vector to an $\mathbb{R}^q$ vector of output weights for unit $j$. For example, $F_j$ may simply be a look-up in a table indexed by $j$ and $S_j(g)$, and $S_j(g)$ may simply be the first $k$ bits of $g$, or the set of $k$ consecutive bits of $g$ indexed from $[j/k]$ to $[j/k] + k - 1$.

One can view the above as a generalization of three-way connections found in some models (Memisevic and Hinton, 2010; Sutskever et al., 2011) to $k + 2$-way interactions (between the $k$ gating bits, the input $x_j$ and each output $h_i$). For example, Sutskever et al. (2011) select a different recurrent weight matrix $W_{s_t}$ in a recurrent neural network to go from the current state $h_t$ to the next state $h_{t+1}$ depending on the (integer) input $s_t$.

The parametrization proposed here enables the association of up to $O(2^k)$ weight vectors with unit $j$, triggered by the particular values of the selected $k$ bits of $g$. The number of parameters is therefore $O(2^k pq)$. The required computation depends on $F_j$, but can be as low as the cost of a table look-up, followed by the actual computation for the matrix multiplication, i.e., $O(pq)$. In the next section, we describe one particular strategy of implementing $F_j$ that aims to improve the generalization.

## 3 Regularized Tree-Structured Prefix Sum of Weights

One potential issue with the proposed scheme is that a model may easily overfit to training samples because only a fraction of samples are used to activate/update each of the $2^k$ possible weight vectors. Beside the obvious regularization of choosing small $k$, we propose here an additional device that is inspired by the impressive success of smoothed or interpolated n-grams and back-off models in statistical language modeling (Katz, 1987; Jelinek and Mercer, 1980).

The basic idea is to maintain a set of weight vectors that are indexed by bit sequences of different lengths. Those vectors associated with shorter bit sequences will be updated with more examples, therefore not requiring much regularization. Other weight vectors indexed by the longer bit sequences will see few examples and be used only to make small corrections, as needed by the data.

As for the regularization, we simply add the norms of the weight vectors. Regularization, either L1 or L2 weight decay, will automatically penalize more those that are less often activated, since only when a weight vector is activated does it receive a gradient that may counterbalance the regularizer’s pull towards 0.
We examine here one way to achieve this, based on a binary tree structure where each node corresponds to a prefix of the $k$ bits $b = S_j(g)$. We thereby define $F_j(b)$ as follows:

$$F_j(b) = \sum_{l=0}^{k} T(j, b_{1:l})$$

where $b_{1:l} = (b_1, \ldots, b_l)$ is the prefix of the $l$ first bits of $b$, and $T(j, b_{1:l})$ is a table look-up returning an $\mathbb{R}^q$ weight vector associated with unit $j$ and bit pattern $b_{1:l}$. With the empty sequence, $T(j, ())$ returns the default weight matrix for unit $j$.

It can be understood more intuitively by imagining a binary tree of depth $k + 1$, where each node has a weight matrix. The above procedure traverses the tree from its root to one of the leaves using the bit sequence $b$ and sums over the $j$-th columns of the nodes’ weight matrices to get the weight vector $F_j(b)$.

The computation of $F_j(b)$ involves $O(kq)$ additions per unit instead of being a small constant (a single table look-up), or $O(kpq)$ in total. This is a noticeable but at the same time reasonable overhead over the $O(pq)$ multiply-adds that will be required for the actual matrix multiplication.

In this case, the number of weight vectors associated with a unit $j$ is

$$|\theta| = 1 + \sum_{l=1}^{k} 2^l = 2^{k+1}$$

and the total number of parameters in the layer is $pq2^{k+1}$. However, only $2^k$ of these are actually independent parameters while the others serve to help regularization. This is in contrast to the conventional case of $O(pq)$.

Overall the degrees of freedom to computation ratio has thus increased by $\frac{2^k}{k}$, a rapidly growing function of $k$.

As the number of parameters is much larger in the proposed scheme, it is more efficient to implement the weight decay regularization such that only the selected weight vectors at each update are regularized. However, in this case, we must keep track of the interval $\Delta t = t - t'$ since each weight vector was last updated, where $t$ and $t'$ are the current update step and the last time the weight vector was updated. Next time the weight vector $w_j$ is chosen, we treat the weight vector specially to compensate for the lost $\Delta t$ steps of regularization.

For L2 weight decay, regularization with coefficient $\lambda$ and learning rate $\epsilon$, this simply corresponds to pre-multiplying the weight vector by $(1 - \epsilon\lambda)^{\Delta t}$:

$$w_j \leftarrow w_j(1 - \epsilon\lambda)^{\Delta t}.$$ 

This is performed before the new update is applied to $w_j$. For L1 regularization, this can be done by moving $w_j$ towards 0 by $\epsilon\lambda\Delta t$ but not crossing 0:

$$w_j \leftarrow \text{sign}(w_j) \max(0, |w_j| - \epsilon\lambda\Delta t)$$

4 Credit Assignment for Gating Decisions

One issue raised earlier by Bengio et al. (2013a) is the question of training signal for gating decisions, i.e., the credit assignment for the gating decisions. What is the correct way to update parameters associated with the gating units in order to improve the gating decisions?

One interesting hypothesis is that it may be sufficient to back-prop as usual into the network by ignoring the effect of the gating units $g$ on the choice of the weight vectors $W$. Although the gating decisions themselves are not adapted toward minimizing the training loss in this case, the weight vectors are regardlessly updated according to the objective of training. In other words, as long as the gating units perform a reasonable job of partitioning the input space, it might be good enough to adapt the exponentially many parameters stored in the table $T$.

To test that hypothesis, it would be good to evaluate alternative approaches that provide training signal into the gating units. Here are some alternatives:
1. Following Bengio et al. (2013a) and Mnih and Gregor (2014), estimate a gradient using a variance-reduced variant of REINFORCE, i.e., by reinforcement learning.

2. Following Bengio et al. (2013a), Gregor et al. (2014) and Raiko et al. (2014), estimate a gradient using a heuristic that propagates the gradient on \( g \) (obtained by back-prop of the loss) backwards into the pre-threshold values \( x \).

3. In the spirit of the noisy rectifier approach by Bengio et al. (2013a), compute \( F_j \) as a weighted sum, where the gating units’ activation level modulate the selected weight vector’s magnitude:

\[
F_j(b, x) = \sum_{l=1}^{k} T(j, b_{1...l}) \left( \prod_{i=1}^{l} \left( 1 - \tanh(x_{\pi_i}) \right) \right)^{1/l}
\]

where \( \pi_i \) is the index of bit \( b_i \) in the input vector \( x \), and \( x \) is assumed to be the output of a rectifier, i.e., non-negative. Hence, when a unit is too active, it tends to turn off the weight contributions that it controls (which creates a preference for sparse \( x \)). The outside power normalizes for length of the controlling bit sequence.

5 Conclusion

One of the greatest challenges to expand the scope of applicability and the performance of deep neural networks is our ability to increase their capacity without increasing the required computations too much. The approach proposed in this paper has the potential to achieve up to exponential increases in this ratio, in a controllable way.

Future work is clearly required to validate this proposal experimentally on large enough datasets for which the increased capacity would actually be valuable, such as speech or language datasets with on the order of a billion examples.

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