

Highway Networks

Rupesh Kumar Srivastava
Klaus Greff
Jürgen Schmidhuber

RUPESH@IDSIA.CH
KLAUS@IDSIA.CH
JUERGEN@IDSIA.CH

The Swiss AI Lab IDSIA
Istituto Dalle Molle di Studi sull'Intelligenza Artificiale
Università della Svizzera italiana (USI)
Scuola universitaria professionale della Svizzera italiana (SUPSI)
Galleria 2, 6928 Manno-Lugano, Switzerland

Abstract

There is plenty of theoretical and empirical evidence that depth of neural networks is a crucial ingredient for their success. However, network training becomes more difficult with increasing depth and training of very deep networks remains an open problem. In this extended abstract, we introduce a new architecture designed to ease gradient-based training of very deep networks. We refer to networks with this architecture as highway networks, since they allow unimpeded information flow across several layers on information highways. The architecture is characterized by the use of gating units which learn to regulate the flow of information through a network. Highway networks with hundreds of layers can be trained directly using stochastic gradient descent and with a variety of activation functions, opening up the possibility of studying extremely deep and efficient architectures.

使用门控机制

未受阻的

调节

Note: A full paper extending this study is available at <http://arxiv.org/abs/1507.06228>, with additional references, experiments and analysis.

1. Introduction

Many recent empirical breakthroughs in supervised machine learning have been achieved through the application of deep neural networks. Network depth (referring to the number of successive computation layers) has played perhaps the most important role in these successes. For

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instance, the top-5 image classification accuracy on the 1000-class ImageNet dataset has increased from $\sim 84\%$ (Krizhevsky et al., 2012) to $\sim 95\%$ (Szegedy et al., 2014; Simonyan & Zisserman, 2014) through the use of ensembles of deeper architectures and smaller receptive fields (Ciresan et al., 2011a;b; 2012) in just a few years.

On the theoretical side, it is well known that deep networks can represent certain function classes exponentially more efficiently than shallow ones (e.g. the work of Hästad (1987); Hästad & Goldmann (1991) and recently of Montufar et al. (2014)). As argued by Bengio et al. (2013), the use of deep networks can offer both computational and statistical efficiency for complex tasks.

神经网络的表达能力随层数的增加是指指数上升的。

However, training deeper networks is not as straightforward as simply adding layers. Optimization of deep networks has proven to be considerably more difficult, leading to research on initialization schemes (Glorot & Bengio, 2010; Saxe et al., 2013; He et al., 2015), techniques of training networks in multiple stages (Simonyan & Zisserman, 2014; Romero et al., 2014) or with temporary companion loss functions attached to some of the layers (Szegedy et al., 2014; Lee et al., 2015).

为解决深层网络训练困难而提出的方法

In this extended abstract, we present a novel architecture that enables the optimization of networks with virtually arbitrary depth. This is accomplished through the use of a learned gating mechanism for regulating information flow which is inspired by Long Short Term Memory recurrent neural networks (Hochreiter & Schmidhuber, 1995). Due to this gating mechanism, a neural network can have paths along which information can flow across several layers without attenuation. We call such paths *information highways*, and such networks *highway networks*.

本文 highway network 是受 LSTM 的启发, 通过使用门控机制来调节信息流。通过这个门控机制, 信息可以没有衰减地流经多个层。

In preliminary experiments, we found that highway networks as deep as 900 layers can be optimized using simple Stochastic Gradient Descent (SGD) with momentum. For

实验表明: 100层以内的网络, 优化速度和层数无关,
但传统网络, 随着深度增加, 优化速度会有很大影响。

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up to 100 layers we compare their training behavior to that of traditional networks with normalized initialization (Glorot & Bengio, 2010; He et al., 2015). We show that optimization of highway networks is virtually independent of depth, while for traditional networks it suffers significantly as the number of layers increases. We also show that architectures comparable to those recently presented by Romero et al. (2014) can be directly trained to obtain similar test set accuracy on the CIFAR-10 dataset without the need for a pre-trained teacher network.

1.1. Notation

We use boldface letters for vectors and matrices, and italicized capital letters to denote transformation functions. $\mathbf{0}$ and $\mathbf{1}$ denote vectors of zeros and ones respectively, and \mathbf{I} denotes an identity matrix. The function $\sigma(x)$ is defined as $\sigma(x) = \frac{1}{1+e^{-x}}, x \in \mathbb{R}$.

0, 1, I 代表 0 向量、1 向量, 单位矩阵。

2. Highway Networks

A plain feedforward neural network typically consists of L layers where the l^{th} layer ($l \in \{1, 2, \dots, L\}$) applies a non-linear transform H (parameterized by $\mathbf{W}_{H,l}$) on its input \mathbf{x}_l to produce its output \mathbf{y}_l . Thus, \mathbf{x}_l is the input to the network and \mathbf{y}_L is the network's output. Omitting the layer index and biases for clarity,

普通前馈神经网络:

$$\mathbf{y} = H(\mathbf{x}, \mathbf{W}_H). \quad (1)$$

层数 l 通常是 l 的射变换 + 非线性激活函数
 H is usually an affine transform followed by a non-linear activation function, but in general it may take other forms.

For a highway network, we additionally define two non-linear transforms $T(\mathbf{x}, \mathbf{W}_T)$ and $C(\mathbf{x}, \mathbf{W}_C)$ such that

$$\mathbf{y} = H(\mathbf{x}, \mathbf{W}_H) \cdot T(\mathbf{x}, \mathbf{W}_T) + \mathbf{x} \cdot C(\mathbf{x}, \mathbf{W}_C). \quad (2)$$

We refer to T as the transform gate and C as the carry gate, since they express how much of the output is produced by transforming the input and carrying it, respectively. For simplicity, in this paper we set $C = 1 - T$, giving

本文设定 $C = 1 - T$.

$$\mathbf{y} = H(\mathbf{x}, \mathbf{W}_H) \cdot T(\mathbf{x}, \mathbf{W}_T) + \mathbf{x} \cdot (1 - T(\mathbf{x}, \mathbf{W}_T)). \quad (3)$$

The dimensionality of $\mathbf{x}, \mathbf{y}, H(\mathbf{x}, \mathbf{W}_H)$ and $T(\mathbf{x}, \mathbf{W}_T)$ must be the same for Equation (3) to be valid. Note that this re-parametrization of the layer transformation is much more flexible than Equation (1). In particular, observe that

$$\mathbf{y} = \begin{cases} \mathbf{x}, & \text{if } T(\mathbf{x}, \mathbf{W}_T) = 0, \\ H(\mathbf{x}, \mathbf{W}_H), & \text{if } T(\mathbf{x}, \mathbf{W}_T) = 1. \end{cases} \quad (4)$$

Similarly, for the Jacobian of the layer transform,

$$\frac{d\mathbf{y}}{d\mathbf{x}} = \begin{cases} \mathbf{I}, & \text{if } T(\mathbf{x}, \mathbf{W}_T) = 0, \\ H'(\mathbf{x}, \mathbf{W}_H), & \text{if } T(\mathbf{x}, \mathbf{W}_T) = 1. \end{cases} \quad (5)$$

Thus, depending on the output of the transform gates, a highway layer can smoothly vary its behavior between that of a plain layer and that of a layer which simply passes its inputs through. Just as a plain layer consists of multiple computing units such that the i^{th} unit computes $y_i = H_i(\mathbf{x})$, a highway network consists of multiple blocks such that the i^{th} block computes a block state $H_i(\mathbf{x})$ and transform gate output $T_i(\mathbf{x})$. Finally, it produces the block output $y_i = H_i(\mathbf{x}) * T_i(\mathbf{x}) + x_i * (1 - T_i(\mathbf{x}))$, which is connected to the next layer.

就像普通层包含多个计算单元, 第 i 个单元计算 $y_i = H_i(\mathbf{x})$.

highway network 每层包含多个 block, 第 i 个 block 计算 $H_i(\mathbf{x})$ 和 $T_i(\mathbf{x})$, block 输出 $y_i = H_i(\mathbf{x}) \cdot T_i(\mathbf{x}) + x_i \cdot (1 - T_i(\mathbf{x}))$.

2.1. Constructing Highway Networks

As mentioned earlier, Equation (3) requires that the dimensionality of $\mathbf{x}, \mathbf{y}, H(\mathbf{x}, \mathbf{W}_H)$ and $T(\mathbf{x}, \mathbf{W}_T)$ be the same. In cases when it is desirable to change the size of the representation, one can replace \mathbf{x} with $\tilde{\mathbf{x}}$ obtained by suitably sub-sampling or zero-padding \mathbf{x} . Another alternative is to use a plain layer (without highways) to change dimensionality and then continue with stacking highway layers. This is the alternative we use in this study.

公式 (3) 的 $\mathbf{x}, \mathbf{y}, H(\mathbf{x}), T(\mathbf{x})$ 的维度必须一致才能计算, 那为了改变表达的维度,

我们可以对 \mathbf{x} 进行下采样或者 padding, 也可以使用一些普通层, 然后再使用 highway 层.

老和 highway 层

2.2. Training Deep Highway Networks

For plain deep networks, training with SGD stalls at the beginning unless a specific weight initialization scheme is used such that the variance of the signals during forward and backward propagation is preserved initially (Glorot & Bengio, 2010; He et al., 2015). This initialization depends on the exact functional form of H .

对于普通的深层网络, 要想 SGD 可以工作, 必须采用特定的权重初始化机制, 而且初始化方法取决于 H 的具体形式。

For highway layers, we use the transform gate defined as $T(\mathbf{x}) = \sigma(\mathbf{W}_T^T \mathbf{x} + \mathbf{b}_T)$, where \mathbf{W}_T is the weight matrix and \mathbf{b}_T the bias vector for the transform gates. This suggests a simple initialization scheme which is independent of the nature of H : \mathbf{b}_T can be initialized with a negative value (e.g. -1, -3 etc.) such that the network is initially biased towards carry behavior. This scheme is strongly inspired by the proposal of Gers et al. (1999) to initially bias the gates in a Long Short-Term Memory recurrent network to help bridge long-term temporal dependencies early in learning. Note that $\sigma(x) \in (0, 1), \forall x \in \mathbb{R}$, so the conditions in Equation (4) can never be exactly true.

但通过使用 $T(\mathbf{x})$, 只要初始设置 \mathbf{b}_T 是负值, 就可以让非常深的网络正常训练 (\mathbf{W}_H 均值为 0)

In our experiments, we found that a negative bias initial-

→ \mathbf{b}_T

ization was sufficient for learning to proceed in very deep networks for various zero-mean initial distributions of W_H and different activation functions used by H . This is significant property since in general it may not be possible to find effective initialization schemes for many choices of H .

3. Experiments

3.1. Optimization

Very deep plain networks become difficult to optimize even if using the variance-preserving initialization scheme form (He et al., 2015). To show that highway networks do not suffer from depth in the same way we train run a series of experiments on the MNIST digit classification dataset. We measure the cross entropy error on the training set, to investigate optimization, without conflating them with generalization issues.

We train both plain networks and highway networks with the same architecture and varying depth. The first layer is always a regular fully-connected layer followed by 9, 19, 49, or 99 fully-connected plain or highway layers and a single softmax output layer. The number of units in each layer is kept constant and it is 50 for highways and 71 for plain networks. That way the number of parameters is roughly the same for both. To make the comparison fair we run a random search of 40 runs for both plain and highway networks to find good settings for the hyperparameters. We optimized the initial learning rate, momentum, learning rate decay rate, activation function for H (either *ReLU* or *tanh*) and, for highway networks, the value for the transform gate bias (between -1 and -10). All other weights were initialized following the scheme introduced by (He et al., 2015).

The convergence plots for the best performing networks for each depth can be seen in Figure 1. While for 10 layers plain network show very good performance, their performance significantly degrades as depth increases. Highway networks on the other hand do not seem to suffer from an increase in depth at all. The final result of the 100 layer highway network is about 1 order of magnitude better than the 10 layer one, and is on par with the 10 layer plain network. In fact, we started training a similar 900 layer highway network on CIFAR-100 which is only at 80 epochs as of now, but so far has shown no signs of optimization difficulties. It is also worth pointing out that the highway networks always converge significantly faster than the plain ones.

3.2. Comparison to Fitnets

Deep highway networks are easy to optimize, but are they also beneficial for supervised learning where we are interested in generalization performance on a test set? To

address this question, we compared highway networks to the thin and deep architectures termed *Fitnets* proposed recently by Romero et al. (2014) on the CIFAR-10 dataset augmented with random translations. Results are summarized in Table 1.

Romero et al. (2014) reported that training using plain backpropagation was only possible for maxout networks with depth up to 5 layers when number of parameters was limited to $\sim 250K$ and number of multiplications to $\sim 30M$. Training of deeper networks was only possible through the use of a two-stage training procedure and addition of soft targets produced from a pre-trained shallow teacher network (hint-based training). Similarly it was only possible to train 19-layer networks with a budget of 2.5M parameters using hint-based training.

We found that it was easy to train highway networks with number of parameters and operations comparable to fitnets directly using backpropagation. As shown in Table 1, Highway 1 and Highway 4, which are based on the architecture of Fitnet 1 and Fitnet 4 respectively obtain similar or higher accuracy on the test set. We were also able to train thinner and deeper networks: a 19-layer highway network with $\sim 1.4M$ parameters and a 32-layer highway network with $\sim 1.25M$ parameter both perform similar to the teacher network of Romero et al. (2014).

4. Analysis

In Figure 2 we show some inspections on the inner workings of the best¹ 50 hidden layer fully-connected highway networks trained on MNIST (top row) and CIFAR-100 (bottom row). The first three columns show, for each transform gate, the bias, the mean activity over 10K random samples, and the activity for a single random sample respectively. The block outputs for the same single sample are displayed in the last column.

The transform gate biases of the two networks were initialized to -2 and -4 respectively. It is interesting to note that contrary to our expectations most biases actually decreased further during training. For the CIFAR-100 network the biases increase with depth forming a gradient. Curiously this gradient is inversely correlated with the average activity of the transform gates as seen in the second column. This indicates that the strong negative biases at low depths are not used to shut down the gates, but to make them more selective. This behavior is also suggested by the fact that the transform gate activity for a single example (column 3) is very sparse. This effect is more pronounced for the CIFAR-100 network, but can also be observed to a lesser extent in the MNIST network.

¹obtained via random search over hyperparameters to minimize the best training set error achieved using each configuration

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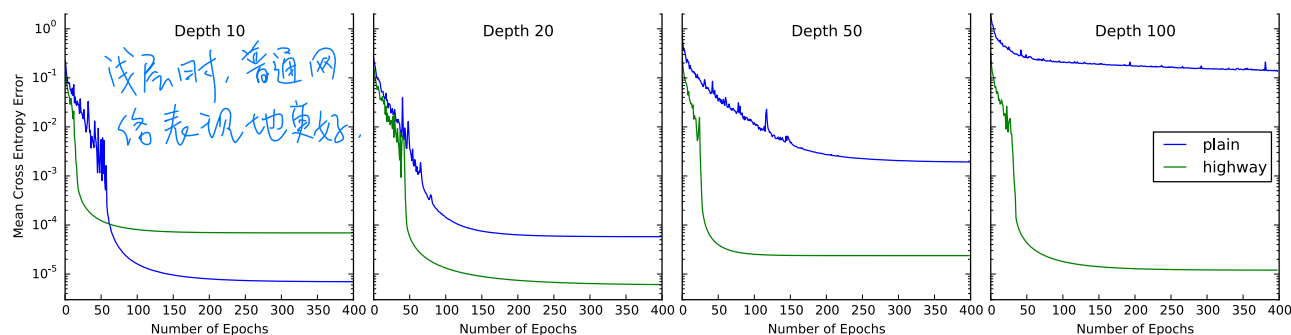


Figure 1. Comparison of optimization of plain networks and highway networks of various depths. All networks were optimized using SGD with momentum. The curves shown are for the best hyperparameter settings obtained for each configuration using a random search. Plain networks become much harder to optimize with increasing depth, while highway networks with up to 100 layers can still be optimized well.

Network	Number of Layers	Number of Parameters	Accuracy
Fitnet Results reported by Romero et al. (2014)			
Teacher	5	~9M	90.18%
Fitnet 1	11	~250K	89.01%
Fitnet 2	11	~862K	91.06%
Fitnet 3	13	~1.6M	91.10%
Fitnet 4	19	~2.5M	91.61%
Highway networks			
Highway 1 (Fitnet 1)	11	~236K	89.18%
Highway 2 (Fitnet 4)	19	~2.3M	92.24%
Highway 3*	19	~1.4M	90.68%
Highway 4*	32	~1.25M	90.34%

Table 1. CIFAR-10 test set accuracy of convolutional highway networks with rectified linear activation and sigmoid gates. For comparison, results reported by Romero et al. (2014) using maxout networks are also shown. Fitnets were trained using a two step training procedure using soft targets from the trained Teacher network, which was trained using backpropagation. We trained all highway networks directly using backpropagation. * indicates networks which were trained only on a set of 40K out of 50K examples in the training set.

The last column of Figure 2 displays the block outputs and clearly visualizes the concept of “information highways”. Most of the outputs stay constant over many layers forming a pattern of stripes. Most of the change in outputs happens in the early layers (≈ 10 for MNIST and ≈ 30 for CIFAR-100). We hypothesize that this difference is due to the higher complexity of the CIFAR-100 dataset.

In summary it is clear that highway networks actually utilize the gating mechanism to pass information almost unchanged through many layers. This mechanism serves not just as a means for easier training, but is also heavily used to route information in a trained network. We observe very selective activity of the transform gates, varying strongly in reaction to the current input patterns.

5. Conclusion

Learning to route information through neural networks has helped to scale up their application to challenging problems by improving credit assignment and making training easier (Srivastava et al., 2015). Even so, training very deep networks has remained difficult, especially without considerably increasing total network size.

Highway networks are novel neural network architectures which enable the training of extremely deep networks using simple SGD. While the traditional plain neural architectures become increasingly difficult to train with increasing network depth (even with variance-preserving initialization), our experiments show that optimization of highway networks is not hampered even as network depth increases to a hundred layers.

The ability to train extremely deep networks opens up the possibility of studying the impact of depth on complex

Fitnet
网络

highway
network

从图2的
最后一列
可以看出:



highway network通过门控机制, 让信息没有衰减地通过很多层.

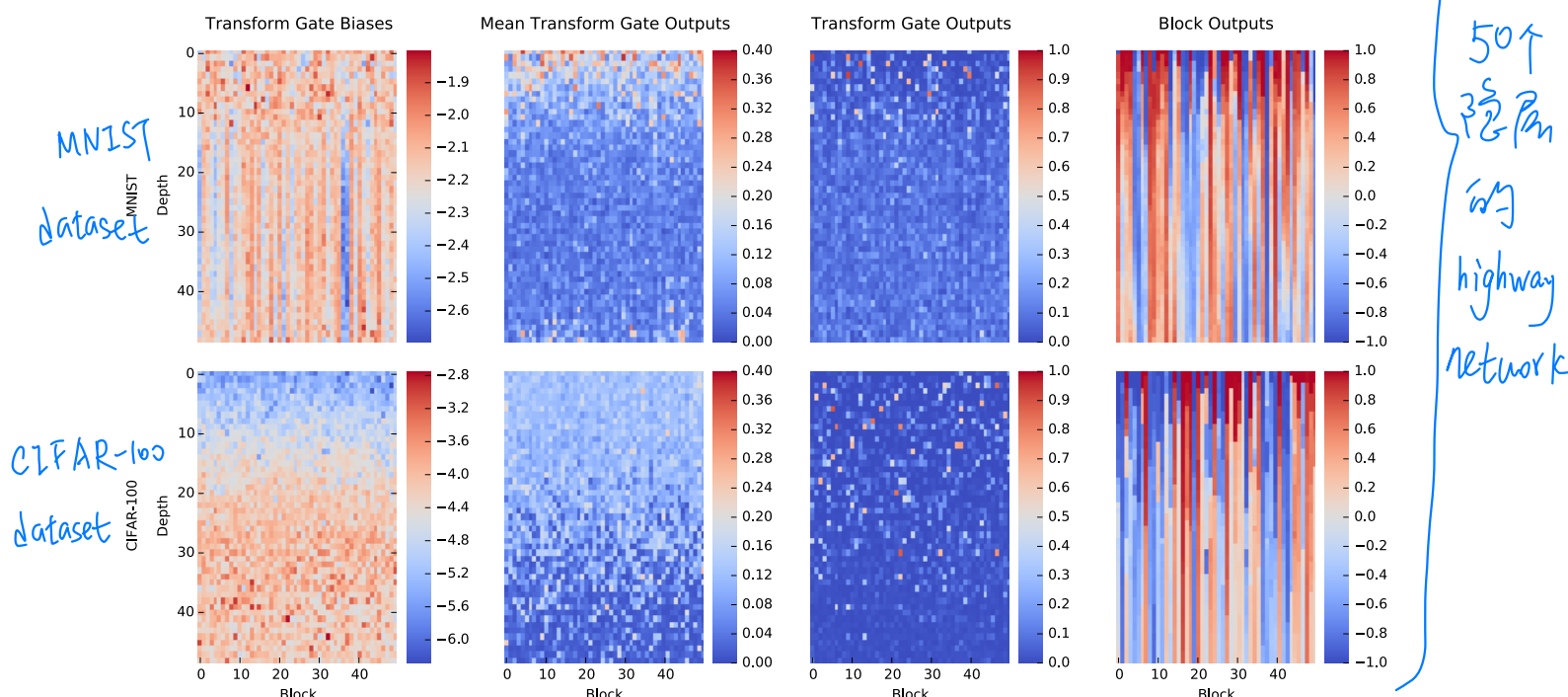


Figure 2. Visualization of certain internals of the blocks in the best 50 hidden layer highway networks trained on MNIST (top row) and CIFAR-100 (bottom row). The first hidden layer is a plain layer which changes the dimensionality of the representation to 50. Each of the 49 highway layers (y-axis) consists of 50 blocks (x-axis). The first column shows the transform gate biases, which were initialized to -2 and -4 respectively. In the second column the mean output of the transform gate over 10,000 training examples is depicted. The third and forth columns show the output of the transform gates and the block outputs for a single random training sample.

problems without restrictions. Various activation functions which may be more suitable for particular problems but for which robust initialization schemes are unavailable can be used in deep highway networks. Future work will also attempt to improve the understanding of learning in highway networks.

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References

Bengio, Yoshua, Courville, Aaron, and Vincent, Pascal. Representation learning: A review and new perspectives. *Pattern Analysis and Machine Intelligence, IEEE Transactions on*, 35(8):1798–1828, 2013. URL http://ieeexplore.ieee.org/xpls/abs_all.jsp?arnumber=6472238.

Ciresan, Dan, Meier, Ueli, Masci, Jonathan, and Schmidhuber, Jürgen. A committee of neural networks for traf-

fic sign classification. In *Neural Networks (IJCNN), The 2011 International Joint Conference on*, pp. 1918–1921. IEEE, 2011a. URL http://ieeexplore.ieee.org/xpls/abs_all.jsp?arnumber=6033458.

Ciresan, Dan, Meier, Ueli, and Schmidhuber, Jürgen. Multi-column deep neural networks for image classification. In *IEEE Conference on Computer Vision and Pattern Recognition*, 2012.

Ciresan, DC, Meier, Ueli, Masci, Jonathan, Gambardella, Luca M, and Schmidhuber, Jürgen. Flexible, high performance convolutional neural networks for image classification. In *IJCAI*, 2011b. URL <http://www.aaai.org/ocs/index.php/IJCAI/IJCAI11/paper/download/3098/3425%0020http://dl.acm.org/citation.cfm?id=2283603>.

Gers, Felix A., Schmidhuber, Jürgen, and Cummins, Fred. Learning to forget: Continual prediction with LSTM. In *ICANN*, volume 2, pp. 850–855, 1999. URL http://ieeexplore.ieee.org/xpls/abs_all.jsp?arnumber=818041.

Glorot, Xavier and Bengio, Yoshua. Understanding the difficulty of training deep feedforward neural networks.

- In *International Conference on Artificial Intelligence and Statistics*, pp. 249–256, 2010. URL http://machinelearning.wustl.edu/mlpapers/paper_files/AISTATS2010_GlorotB10.pdf.
- Håstad, Johan. *Computational limitations of small-depth circuits*. MIT press, 1987. URL <http://dl.acm.org/citation.cfm?id=SERIES9056.27031>.
- Håstad, Johan and Goldmann, Mikael. On the power of small-depth threshold circuits. *Computational Complexity*, 1(2):113–129, 1991. URL <http://link.springer.com/article/10.1007/BF01272517>.
- He, Kaiming, Zhang, Xiangyu, Ren, Shaoqing, and Sun, Jian. Delving deep into rectifiers: Surpassing human-level performance on ImageNet classification. *arXiv:1502.01852 [cs]*, February 2015. URL <http://arxiv.org/abs/1502.01852>.
- Hochreiter, Sepp and Schmidhuber, Jürgen. Long short term memory. Technical Report FKI-207-95, Technische Universität München, München, August 1995. URL <http://citeseerx.ist.psu.edu/viewdoc/summary?doi=10.1.1.51.3117>.
- Krizhevsky, Alex, Sutskever, Ilya, and Hinton, Geoffrey E. Imagenet classification with deep convolutional neural networks. In *Advances in Neural Information Processing Systems*, 2012. URL http://books.nips.cc/papers/files/nips25/NIPS2012_0534.pdf.
- Lee, Chen-Yu, Xie, Saining, Gallagher, Patrick, Zhang, Zhengyou, and Tu, Zhuowen. Deeply-supervised nets. pp. 562–570, 2015. URL <http://jmlr.org/proceedings/papers/v38/lee15a.html>.
- Montufar, Guido F, Pascanu, Razvan, Cho, Kyunghyun, and Bengio, Yoshua. On the number of linear regions of deep neural networks. In *Advances in Neural Information Processing Systems*. 2014. URL <http://papers.nips.cc/paper/5422-on-the-number-of-linear-regions-of-deep-neural-networks.pdf>.
- Romero, Adriana, Ballas, Nicolas, Kahou, Samira Ebrahimi, Chassang, Antoine, Gatta, Carlo, and Bengio, Yoshua. FitNets: Hints for thin deep nets. *arXiv:1412.6550 [cs]*, December 2014. URL <http://arxiv.org/abs/1412.6550>.
- Saxe, Andrew M., McClelland, James L., and Ganguli, Surya. Exact solutions to the nonlinear dynamics of learning in deep linear neural networks. *arXiv:1312.6120 [cond-mat, q-bio, stat]*, December 2013. URL <http://arxiv.org/abs/1312.6120>.
- Simonyan, Karen and Zisserman, Andrew. Very deep convolutional networks for large-scale image recognition. *arXiv:1409.1556 [cs]*, September 2014. URL <http://arxiv.org/abs/1409.1556>.
- Srivastava, Rupesh Kumar, Masci, Jonathan, Gomez, Faustino, and Schmidhuber, Jürgen. Understanding locally competitive networks. In *International Conference on Learning Representations*, 2015. URL <http://arxiv.org/abs/1410.1165>.
- Szegedy, Christian, Liu, Wei, Jia, Yangqing, Sermanet, Pierre, Reed, Scott, Anguelov, Dragomir, Erhan, Dumitru, Vanhoucke, Vincent, and Rabinovich, Andrew. Going deeper with convolutions. *arXiv:1409.4842 [cs]*, September 2014. URL <http://arxiv.org/abs/1409.4842>.