1000+ layers deep neural networks and how to train them

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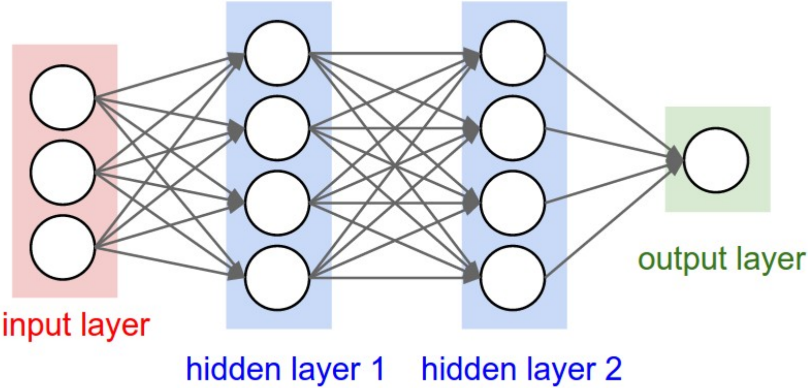
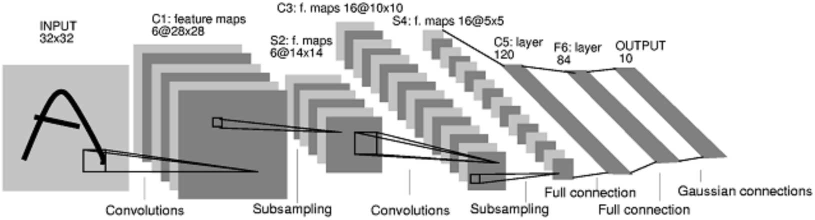
Quickly about neural networks

- Hierarchical ensamble of logistic regressions
- Output of a layer: $z^{i+1} = f(W^i \times z^i)$
- Universality theorem: $\forall F(x) \in C(X)$ exists a finite neural network with one hidden layer that computes approximation of $F(x)$



Convolutions

- $\hat{I}[i,j] = f(\sum_{k=1}^{channels} \sum_{p=-w}^{w} \sum_{q=-w}^{w} I[k, i+p, j+q] w[k,p,q])$
- Example architecture:



Residual networks

ImageNet 2015

Proposed method:

- Insanely deep nets (**152** layers on ImageNet and **1202** layers on CIFAR-10)
- Lower complexity (VGG-19: 19.6×10^9 FLOP[1], ResNet-152: 11.3×10^9 FLOP)
- Faster training
- 1^{st} place in ImageNet classification, ImageNet detection, ImageNet localization, COCO detection, and COCO segmentation

[1] Floating Point Operations

Problems with deep networks

- Vanishing / exploding gradients (better with ReLU)
- Degradation problem: quality drops on deeper nets

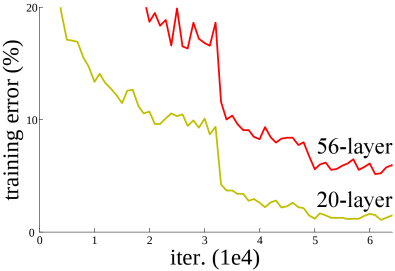


Figure: Training error (left) and test error (right) on CIFAR-10 with 20-layer and 56-layer networks.

- How to build a deeper model from shallow one?

Problems with deep networks

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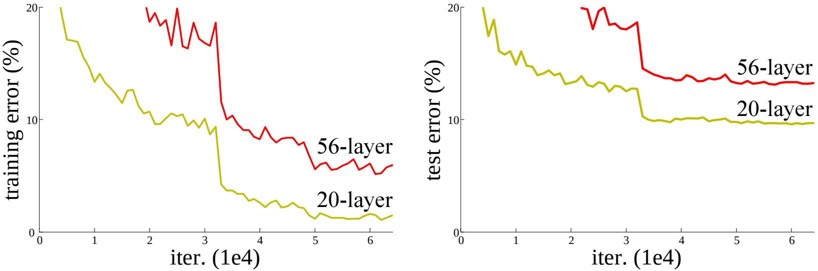


Figure: Training error (left) and test error (right) on CIFAR-10 with 20-layer and 56-layer networks.

- How to build a deeper model from shallow one?
- Add identity layers to the end of a trained net: H(x) = x

Resudual connection

- Very deep nets are unable to represent identity mapping
- Examle with ReLU: $max(x - \infty, 0) + \infty \simeq x$
- **It may be easier to fit** $F(x) = 0$ **and add input to output:** $y = F(x) + x$

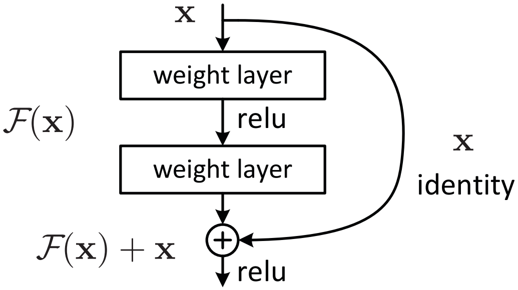
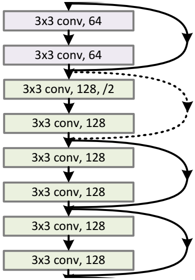


Figure: Residual learning: a building block.

Different dimensions



If input and output dimensions are different, $F(x) + x$ doesn't make sence. Ways to fix it:

- Don't use residual connection
- Add extra zeros at the end of vector x
- Projection shortcut (done by 1x1 convolutions): $y = F(x) + W_p \times x$

Third method shows better results, but brings extra parameters.

Deeper nets

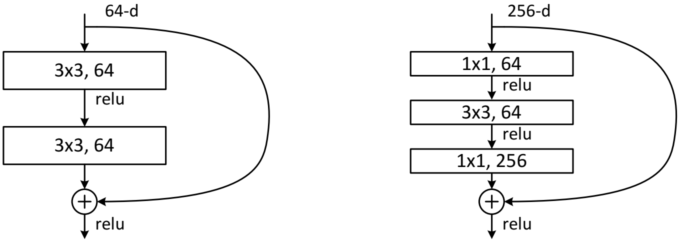


Figure: Left: a building block for ResNet-34. Right: a “bottleneck” building block for ResNet-50/101/152

How to go deeper:

- Reduce number of parameters with botleneck block
- Stack a lot of botleneck blocks
- 152-layer model still has less parameters than VGG-16!
- Important not to use projection shortcut (otherwise time x2)

Experiments

method	top-1 err.	top-5 err.
VGG (ILSVRC'14)	-	8.43
GoogLeNet(ILSVRC'14)	-	7.89
VGG	24.4	7.1
PReLU-net	21.59	5.71
BN-inception	21.99	5.81
ResNet-34[2]	21.84	5.71
ResNet-34[3]	21.53	5.60
ResNet-50	20.74	5.25
ResNet-101	19.87	4.60
ResNet-152	**19.38**	**4.49**

Table: Error rates (%) of **single-model** results on the ImageNet validation set.

[2] Projections when dimension changes

[3] Projections on each shortcut

Experiments

method	top-5 err. (**test**)
VGG(ILSVRC'14)	7.32
GoogLeNet (ILSVRC'14)	6.66
VGG (v5)	6.8
PReLU-net	4.94
BN-inception	4.82
ResNet (ILSVRC'15)	**3.57**

Table: Error rates (%) of **ensembles**. The top-5 error is on the test set of ImageNet and reported by the test server.

Batch normalization

Motivation

- Faster convergence with whitened inputs
- Whitening: $\hat{\mathbf{x}} = Cov[\mathbf{x}]^{-1/2}(\mathbf{x} - E[\mathbf{x}])$
- Normalization: $\hat{x}^{(k)} = \frac{x^{(k)} - E[x^{(k)}]}{\sqrt{Var[x^{(k)}]}}$ for each dimension

Batch normalization

- Covariate shift: changes of input distribution to a learning system

$$L = F(x, \theta)$$

- Internal covariate shift: Extension to the deep network

$$L = F_2(F_1(u, \theta_1), \theta_2) = F_2(x, \theta_2)$$

- Goal: reduce hidden layer activations' covariance shift
- In intermediate layers: $\hat{x}^{(k)} = \frac{x^{(k)} - E[x^{(k)}]}{\sqrt{Var[x^{(k)}]}}$

Problems with batch normalization

1 Computing $E[x]$ and $Var[x]$ is expensive

For each minibatch $\hat{x}^{(k)} = \frac{x^{(k)} - E_{\mathcal{B}}[x^{(k)}]}{\sqrt{Var_{\mathcal{B}}[x^{(k)}]}}$

2 Sigmoids would become almost linear

We want to be able to represent identity mapping

$y^{(k)} = \gamma^{(k)} \hat{x}^{(k)} + \beta^{(k)}$

Algorithm

Inputs: Values of x over a mini-batch $\mathcal{B} = \{x_{1\ldots m}\}$;
Parameters: γ, β
Output: $\{y_i = \mathrm{BN}_{\gamma,\beta}(x_i)\}$

$$\mu_{\mathcal{B}} \leftarrow \frac{1}{m}\sum_{i=1}^{m} x_i \qquad \text{// mini-batch mean}$$

$$\sigma_{\mathcal{B}}^2 \leftarrow \frac{1}{m}\sum_{i=1}^{m}(x_i - \mu_{\mathcal{B}})^2 \qquad \text{// mini-batch variance}$$

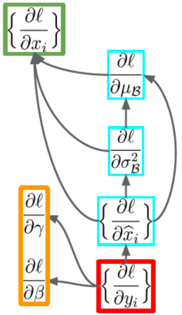
$$\widehat{x}_i \leftarrow \frac{x_i - \mu_{\mathcal{B}}}{\sqrt{\sigma_{\mathcal{B}}^2 + \epsilon}} \qquad \text{// normalize}$$

$$y_i \leftarrow \gamma\widehat{x}_i + \beta \equiv \mathrm{BN}_{\gamma,\beta}(x_i) \qquad \text{// scale and shift}$$

Gradient

Apply chain rule

Note that $\mu_{\mathcal{B}}$ and $\sigma_{\mathcal{B}}^2$ aren't considered to be constants



$$\frac{\partial \ell}{\partial \widehat{x}_i} = \frac{\partial \ell}{\partial y_i} \cdot \gamma$$

$$\frac{\partial \ell}{\partial \sigma_{\mathcal{B}}^2} = \sum_{i=1}^{m} \frac{\partial \ell}{\partial \widehat{x}_i} \cdot (x_i - \mu_{\mathcal{B}}) \cdot \frac{-1}{2} (\sigma_{\mathcal{B}}^2 + \epsilon)^{-3/2}$$

$$\frac{\partial \ell}{\partial \mu_{\mathcal{B}}} = \left(\sum_{i=1}^{m} \frac{\partial \ell}{\partial \widehat{x}_i} \cdot \frac{-1}{\sqrt{\sigma_{\mathcal{B}}^2 + \epsilon}} \right) + \frac{\partial \ell}{\partial \sigma_{\mathcal{B}}^2} \cdot \frac{\sum_{i=1}^{m} -2(x_i - \mu_{\mathcal{B}})}{m}$$

$$\frac{\partial \ell}{\partial x_i} = \frac{\partial \ell}{\partial \widehat{x}_i} \cdot \frac{1}{\sqrt{\sigma_{\mathcal{B}}^2 + \epsilon}} + \frac{\partial \ell}{\partial \sigma_{\mathcal{B}}^2} \cdot \frac{2(x_i - \mu_{\mathcal{B}})}{m} + \frac{\partial \ell}{\partial \mu_{\mathcal{B}}} \cdot \frac{1}{m}$$

$$\frac{\partial \ell}{\partial \gamma} = \sum_{i=1}^{m} \frac{\partial \ell}{\partial y_i} \cdot \widehat{x}_i$$

$$\frac{\partial \ell}{\partial \beta} = \sum_{i=1}^{m} \frac{\partial \ell}{\partial y_i}$$

Inference

Deterministic input-output mapping at test time:

$$\hat{x} = \frac{x - E[x]}{\sqrt{Var[x] + \epsilon}}$$

$$y = \gamma \cdot \hat{x} + \beta$$

$$y = \frac{\gamma}{\sqrt{Var[x] + \epsilon}} \cdot x + (\beta - \frac{\gamma E[x]}{\sqrt{Var[x] + \epsilon}})$$

$E[x]$ and $Var[x]$ are computed over the whole training set
exponential averaging in practice: $E_{i+1} = (1 - \alpha)E_i + \alpha E_{\mathcal{B}}$

Tips

After applying BN:

- Remove biases
- Increase learning rate
- Remove Dropout
- Reduce L_2 weight regularization
- Accelerate learning rate decay
- Shuffle training examples

Covariance shift

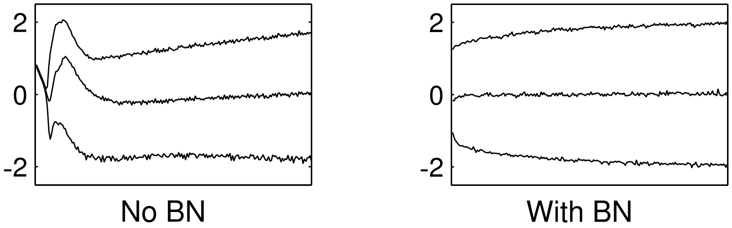
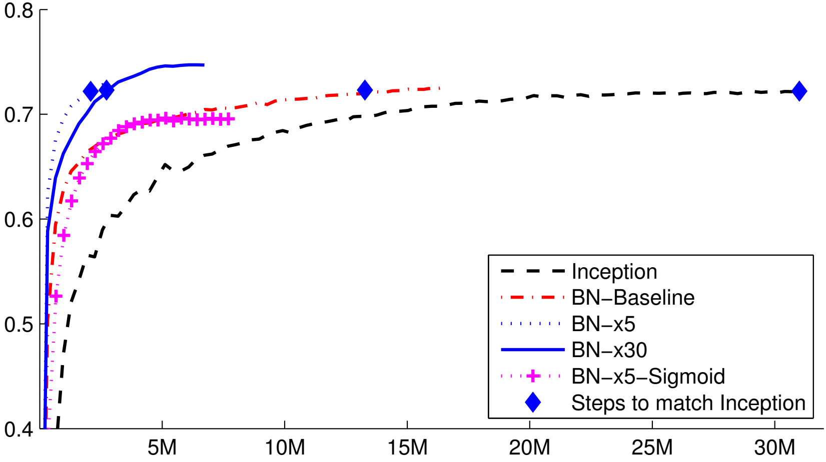


Figure: The evolution of input distributions to a typical sigmoid, over the course of training, shown as $\{15, 50, 85\}$th percentiles.

Learning



Single crop validation accuracy of Inception and its batch-normalized variants, vs. the number of training steps.
(x30 means learning with 30 times larger learning rate)

Experiments

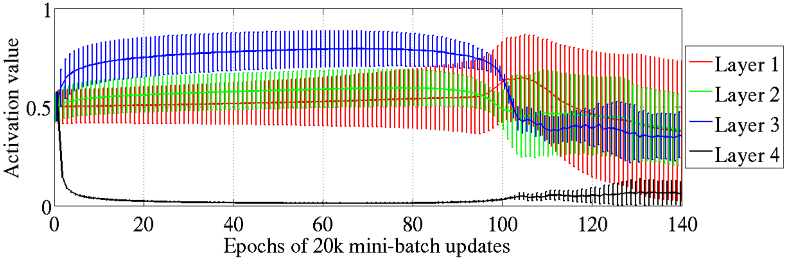
Model	Top-1 error	Top-5 error
GoogLeNet ensemble	-	6.67%
Deep Image low-res	-	7.96%
Deep Image high-res	24.88	7.42%
Deep Image ensemble	-	5.98%
BN-Inception single crop	25.2%	7.82%
BN-Inception multicrop	21.99%	5.82%
BN-Inception ensemble	20.1%	**4.9%***

Figure: *Batch-Normalized Inception comparison with previous state of the art models*

Weight initialization

Motivation of tanh

Activalions' evolution during training:



- After initialization it is better to ignore inputs
- With sigmoid $f(z) = \frac{1}{1+e^{-z}}$
- $f(z) = 0 \Rightarrow z = -\infty$
- Better with $tanh(z) = sh(z)/ch(z) = (e^z - e^{-z})/(e^z + e^{-z})$
- $tanh(z) = 0 \Rightarrow z = 0$

Xavier (Glorot)

Consider $tanh$ activation

- Start in a non-saturated regime
- Avoid vanising gradients

$$z^{i+1} = f(\underbrace{z^i W^i}_{s^i})$$

$$Var[z^i] = Var[x] \prod_{k=0}^{i-1} n_k Var[W^k]$$

$$Var[\frac{\partial L}{\partial s^i}] = Var[\frac{\partial L}{\partial s^d}] \prod_{k=i}^{d} n_{k+1} Var[W^k]$$

Where n_i is a dimension of i-th layer

Xavier (Glorot)

Good initialization:

$$\forall (i,j) \begin{cases} Var[z^i] = Var[z^j] \\ Var[\frac{\partial L}{\partial s^i}] = Var[\frac{\partial L}{\partial s^j}] \end{cases}$$

This is equivalent to

$$\forall i \begin{cases} n_i Var[W^i] = 1 \\ n_{i+1} Var[W^i] = 1 \end{cases}$$

Compromise: $Var[W^i] = \frac{2}{n_i + n_{i+1}}$

$$\boxed{W^i \sim U[-\frac{\sqrt{6}}{\sqrt{n_i + n_{i+1}}}, \frac{\sqrt{6}}{\sqrt{n_i + n_{i+1}}}]}$$

$Var[U(a,b)] = \frac{1}{12}(b-a)^2$

He

If activation is ReLU:

- Not symetric
- Not diferentiable at zero

$$Var[z^i] = Var[x](\prod_{k=0}^{i-1} \frac{1}{2} n_k Var[W^k]) \Rightarrow \frac{1}{2} n_k Var[W^k] \Rightarrow Var[W^k] = \frac{2}{n_k}$$

$$Var[\frac{\partial L}{\partial s^i}] = Var[\frac{\partial L}{\partial s^d}](\prod_{k=i}^{d} \frac{1}{2} n_{k+1} Var[W^k]) \Rightarrow Var[W^k] = \frac{2}{n_{k+1}}$$

It is sufficient to use first:

$$Var[\frac{\partial L}{\partial s^i}] = Var[\frac{\partial L}{\partial s^d}] \prod_{k=1}^{d} \frac{1}{2} n_{k+1} Var[W^k] = \frac{n_2}{n_d} Var[\frac{\partial L}{\partial s^d}]$$

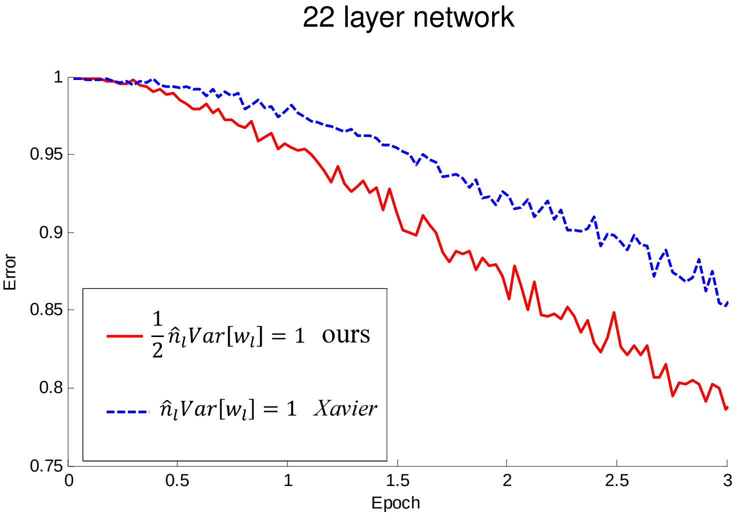
n_2/n_d isn't big for convolution network

$$W^i \sim N(0, \frac{2}{n_i})$$

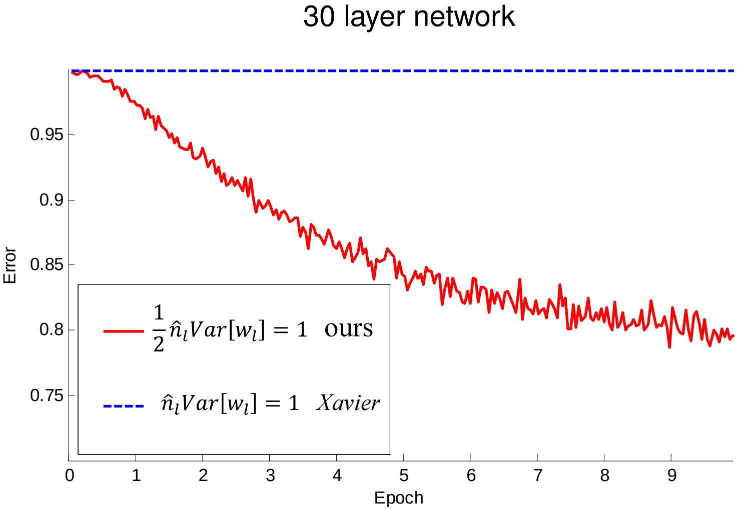
or

$$W^i \sim N(0, \frac{2}{n_{i+1}})$$

Xavier vs He for ReLU



Xavier vs He for ReLU



References

- K. He, X. Zhang, S. Ren, J. Sun. *Deep Residual Learning for Image Recognition*
- S. Ioffe, C. Szegedy. *Batch Normalization: Accelerating Deep Network Training by Reducing Internal Covariate Shift*
- K. He, X. Zhang, S. Ren, J. Sun. *Delving Deep into Rectifiers: Surpassing Human-Level Performance on ImageNet Classification*
- X. Glorot, Y. Bengio. *Understanding the difficulty of training deep feedforward neural networks*

He, Var derivation

$$Var[s^l] = n_l Var[w_l x_l]$$

$$Var[s^l] = n_l Var[w_l] E[x_l^2]$$, if x_l and w_l have zero mean

$$x_l = max(0, s^{l-1})$$

$$E[s^l] = 0$$, if $E[w_l] = 0$

$$E[x_l^2] = \frac{1}{2} Var[s^{l-1}]$$

$$Var[s^i] = \frac{1}{2} n_l Var[w_l] Var[s^{l-1}]$$