#### Normalization Techniques in Training of Deep Neural Networks

Lei Huang (黄雷)

State Key Laboratory of Software Development Environment, Beihang University

Mail:huanglei@nlsde.buaa.edu.cn

August 17<sup>th</sup>, 2017

## Outline

- Introduction to Deep Neural Networks (DNNs)
- Training DNNs: Optimization
- Batch Normalization
- Other Normalization Techniques
- Centered Weight Normalization

## Machine learning

- dataset D={X, Y}
  - Input: X
  - Output: Y
  - Learning: Y=F(X) or P(Y|X)
- Fitting and Generalization
- Types: view of models
  - Non-parametric model
    - $Y=F(X; x_1, x_2...x_n)$
  - Parametric model
    - Y=F(X; θ)







#### Neural network

• Neural network

 $- \operatorname{Y=F}(X) = f_T(f_{T-1}(\dots f_1(X)))$  $- f_i(x) = g(Wx + b)$ 

- Nonlinear activation
  - sigmod
  - Relu







#### Deep neural network

- Why deep?
  - Powerful representation capacity





## Key properties of Deep learning

- End to End learning
  - no distinction between feature extractor and classifier



- "Deep" architectures:
  - Hierarchy of simpler non-linear modules

#### Applications and techniques of DNNs

- Successful applications in a range of domains
  - Speech
  - Computer Vision
  - Natural Language processing
- Main techniques in using deep neural networks networks
  - Design the architecture
    - Module selection and Module connection
    - Loss function
  - Train the model based on optimization
    - Initialize the parameters
    - Search direction in parameters space
    - Learning rate schedule
    - Regularization techniques

• ...

## Outline

- Introduction to Deep Neural Networks (DNNs)
- Training DNNs: Optimization
- Batch Normalization
- Other Normalization Techniques
- Centered Weight Normalization

## **Training of Neural Networks**

 $(1, 0, 0)^T$ 

• Multi-layer perceptron (example)



> 1 Forward calculate y:

$$a^{(1)} = W^{(1)} \cdot x$$
  

$$h^{(1)} = \sigma(a^{(1)})$$
  

$$a^{(2)} = W^{(2)} \cdot h^{(1)}$$
  

$$y = \sigma(a^{(2)})$$

▶ MSE Loss:  $L=(y - \hat{y})^2$ 

> 2 Backward, Calculate  $\frac{dL}{dx}$ :

 $\frac{\mathrm{d}\,\mathrm{L}}{\mathrm{y}} = 2(\mathrm{y} - \widehat{\mathrm{y}})$   $\frac{\mathrm{d}\,\mathrm{L}}{\mathrm{d}a^{(2)}} = \frac{\mathrm{d}\,\mathrm{L}}{\mathrm{d}y} \cdot \sigma(a^{(2)}) \cdot (1 - \sigma(a^{(2)}))$   $\frac{\mathrm{d}\,\mathrm{L}}{\mathrm{d}\,h^{(1)}} = \frac{\mathrm{d}\,\mathrm{L}}{\mathrm{d}a^{(2)}} W^{(2)}$   $\frac{\mathrm{d}\,\mathrm{L}}{a^{(1)}} = \frac{\mathrm{d}\,\mathrm{L}}{\mathrm{d}\,h^{(1)}} \cdot \sigma(a^{(1)}) \cdot (1 - \sigma(a^{(1)}))$   $\frac{\mathrm{d}\,\mathrm{L}}{\mathrm{d}x} = \frac{\mathrm{d}\,\mathrm{L}}{\mathrm{d}a^{(1)}} W^{(1)}$ 

> 3 calculate gradient 
$$\frac{dL}{dW}$$
:

$$\frac{d L}{d W^{(2)}} = \frac{d L}{d a^{(2)}} h^{(1)}$$
$$\frac{d L}{d W^{(1)}} = \frac{d L}{d a^{(1)}} x$$

## **Optimization in Deep Model**

- Goal:  $\theta^* \in \operatorname{argmin}_{\theta} \mathbb{E}_{(x,y) \sim \pi} \left[ -\log p(y \mid x, \theta) \right]$
- Update Iteratively:  $\theta^{(t+1)} \leftarrow \theta^{(t)} \alpha^{(t)} \nabla^{(t)}$
- Challenge:
  - Non-convex and local optimal points
  - Saddle point
  - Severe correlation between dimensions and highly non-isotropic parameter space (ill-shaped)







## First order optimization

• First order stochastic gradient descent (SGD):

The direction of the gradient

$$abla = \mathbb{E}_{\pi} \left[ d\ell / d\theta \right]$$

- Gradient is averaged by the sampled examples
- Disadvantage
  - Over-aggressive steps on ridges
  - Too small steps on plateaus
  - Slow convergence
  - non-robust performance.



Figure 2: zig-zag iteration path for SGD

## **Advanced Optimization**

- Estimate curvature or scale
  - Quadratic optimization
    - Newton or quasi-Newton
      - Inverse of Hessian
    - Natural Gradient
      - Inverse of FIM
  - Estimate the scale
    - AdaGrad
    - Rmsprop
    - Adam

Iteration path of SGD (red) and NGD (green)

- Normalize input/activation
  - Intuition: the landscape of cost w.r.t parameters is controlled by Input/activation L=( $f(x, \theta), y$ )
  - Method: Stabilize the distribution of input/activation
    - Normalize the input explicitly
    - Normalize the input implicitly (constrain weights)

# Some intuitions of normalization for optimization

• How Normalizing activation affect the optimization?

$$-y = w_1 x_1 + w_2 x_2 + b$$
  
 $-L = (y - \hat{y})^2$ 



## Outline

- Introduction to Deep Neural Networks (DNNs)
- Training DNNs: Optimization
- Batch Normalization
- Other Normalization Techniques
- Centered Weight Normalization

## **Batch Normalization--motivation**

• Solving Internal Covariate Shift



- Whitening Input benefits optimization (1998,Lecun, Efficient back-propagation)
  - Centering
  - Decorrelate
  - stretch





#### **Batch Normalization--method**

- Only standardize input: decorrelating is expensive
  - Centering
    Stretch
- How to do it?

$$- \hat{x} = \frac{x - E(x)}{std(x)}$$

#### **Batch Normalization--training**

#### • Forward

**Input:** Values of x over a mini-batch:  $\mathcal{B} = \{x_{1...m}\};$ Parameters to be learned:  $\gamma, \beta$ **Output:**  $\{y_i = BN_{\gamma,\beta}(x_i)\}$  $\mu_{\mathcal{B}} \leftarrow \frac{1}{m} \sum_{i=1}^{m} x_i$ // mini-batch mean  $\sigma_{\mathcal{B}}^2 \leftarrow \frac{1}{m} \sum_{i=1}^m (x_i - \mu_{\mathcal{B}})^2$  // mini-batch variance  $\widehat{x}_i \leftarrow \frac{x_i - \mu_{\mathcal{B}}}{\sqrt{\sigma_{\mathcal{B}}^2 + \epsilon}}$ // normalize  $y_i \leftarrow \gamma \widehat{x}_i + \beta \equiv \mathrm{BN}_{\gamma,\beta}(x_i)$ // scale and shift

#### **Batch Normalization--training**

Backward

$$\begin{split} \frac{\partial \ell}{\partial \hat{x}_{i}} &= \frac{\partial \ell}{\partial y_{i}} \cdot \gamma \\ \frac{\partial \ell}{\partial \sigma_{\mathcal{B}}^{2}} &= \sum_{i=1}^{m} \frac{\partial \ell}{\partial \hat{x}_{i}} \cdot (x_{i} - \mu_{\mathcal{B}}) \cdot \frac{-1}{2} (\sigma_{\mathcal{B}}^{2} + \epsilon)^{-3/2} \\ \frac{\partial \ell}{\partial \mu_{\mathcal{B}}} &= \left( \sum_{i=1}^{m} \frac{\partial \ell}{\partial \hat{x}_{i}} \cdot \frac{-1}{\sqrt{\sigma_{\mathcal{B}}^{2} + \epsilon}} \right) + \frac{\partial \ell}{\partial \sigma_{\mathcal{B}}^{2}} \cdot \frac{\sum_{i=1}^{m} -2(x_{i} - \mu_{\mathcal{B}})}{m} \\ \frac{\partial \ell}{\partial x_{i}} &= \frac{\partial \ell}{\partial \hat{x}_{i}} \cdot \frac{1}{\sqrt{\sigma_{\mathcal{B}}^{2} + \epsilon}} + \frac{\partial \ell}{\partial \sigma_{\mathcal{B}}^{2}} \cdot \frac{2(x_{i} - \mu_{\mathcal{B}})}{m} + \frac{\partial \ell}{\partial \mu_{\mathcal{B}}} \cdot \frac{1}{m} \\ \frac{\partial \ell}{\partial \gamma} &= \sum_{i=1}^{m} \frac{\partial \ell}{\partial y_{i}} \cdot \hat{x}_{i} \\ \frac{\partial \ell}{\partial \beta} &= \sum_{i=1}^{m} \frac{\partial \ell}{\partial y_{i}} \end{split}$$

#### **Batch Normalization--Inference**

• Inference (in paper)

$$E[x] \leftarrow E_{\mathcal{B}}[\mu_{\mathcal{B}}]$$
$$Var[x] \leftarrow \frac{m}{m-1} E_{\mathcal{B}}[\sigma_{\mathcal{B}}^2]$$

- Inference (in practice)
  - Running average
    - $E(x) = \alpha(\mu_B) + (1 \alpha)E(x)$
    - $Var(x) = \alpha(\sigma_B^2) + (1 \alpha)var(x)$

## Batch Normalization—how to use

Convolution layer

- Wrapped as a module
  - Before or after nonlinear?
    - For shallow module, after nonlinear (Layer <11)
    - For deep model, before nonlinear
  - Advantage of before nonlinear
    - For Relu, half activated
    - For sigmod, avoiding saturated region.
  - Advantage of after nonlinear
    - The intuition of whitening





#### Batch Normalization—how to use

• Example:





Residual block (CVPR 2015)

Pre-activation Residual block (ECCV 2016)

#### Batch Normalization—characteristics

- For accelerating training:
  - Weight scale invariant: Not sensitive for weight initialization

BN(Wu) = BN((aW)u)

Adjustable learning rate

$$\frac{\partial BN((aW)u)}{\partial u} = \frac{\partial BN(Wu)}{\partial u}$$
$$\frac{\partial BN((aW)u)}{\partial (aW)} = \frac{1}{a} \cdot \frac{\partial BN(Wu)}{\partial W}$$

- Large learning rate
  - Better conditioning, (1998 Lecun)
- For generalization
  - Stochastic, works like Dropout

#### **Batch Normalization**

 Routine in deep feed forward neural networks, especially for CNNs.

- Weakness
  - Can not be used for online learning
  - Unstable for small mini batch size
  - Used in RNN with caution

#### Batch Normalization– for RNN

- The extra problems need be considered:
  - Where BN should put?

Sequence data

$$\mathbf{h}_t = \phi(\mathbf{W}_h \mathbf{h}_{t-1} + \mathbf{W}_x \mathbf{x}_t)$$

- 2016, ICASSP, Batch Normalized Recurrent Neural Networks
  - How to put BN module

$$\mathbf{h}_t = \phi(BN(\mathbf{W}_h \mathbf{h}_{t-1} + \mathbf{W}_x \mathbf{x}_t))$$

- Sequence data problem
  - Frame-wise normalization
  - Sequence-wise normalization

$$\mathbf{h}_t = \phi(\mathbf{W}_h \mathbf{h}_{t-1} + BN(\mathbf{W}_x \mathbf{x}_t)).$$

## **Batch Normalization for RNN**

2017, ICLR, Recurrent Batch Normalization

 How to put BN module

$$\begin{pmatrix} \tilde{\mathbf{f}}_t \\ \tilde{\mathbf{i}}_t \\ \tilde{\mathbf{o}}_t \\ \tilde{\mathbf{g}}_t \end{pmatrix} = \operatorname{BN}(\mathbf{W}_h \mathbf{h}_{t-1}; \gamma_h, \beta_h) + \operatorname{BN}(\mathbf{W}_x \mathbf{x}_t; \gamma_x, \beta_x) + \mathbf{b}$$
$$\mathbf{c}_t = \sigma(\tilde{\mathbf{f}}_t) \odot \mathbf{c}_{t-1} + \sigma(\tilde{\mathbf{i}}_t) \odot \tanh(\tilde{\mathbf{g}}_t)$$
$$\mathbf{h}_t = \sigma(\tilde{\mathbf{o}}_t) \odot \tanh(\operatorname{BN}(\mathbf{c}_t; \gamma_c, \beta_c))$$

- Sequence data problem
  - T\_max Frame-wise normalization
  - It depends.....

## Outline

- Introduction to Deep Neural Networks (DNNs)
- Training DNNs: Optimization
- Batch Normalization
- Other Normalization Techniques
- Centered Weight Normalization

# Norm-propagation (2016, ICML)

- Target BN's drawback:
  - Can not be used for online learning
  - Unstable for small mini batch size.
- Data independent parametric estimate of mean and variance
  - Normalize input: 0-mean and unit variance
  - Assuming W is orthogonal
  - Derivate the nonlinear dynamic
    - Relu:

**Remark 1.** (*Post-ReLU distribution*) Let  $X \sim \mathcal{N}(0,1)$ and  $Y = \max(0, X)$ . Then  $\mathbb{E}[Y] = \frac{1}{\sqrt{2\pi}}$  and  $\operatorname{var}(Y) = \frac{1}{2}\left(1 - \frac{1}{\pi}\right)$ 

# Layer Normalization (2016, Arxiv)

- Target BN's drawback:
  - Can not be used for online learning
  - Unstable for small mini batch size
  - RNN
- Normalizing each example, over dimensions



#### Natural Neural Network (2015, NIPS)

- How about decorrelate the activations?
- Canonical model(MLP):  $h_i = f_i(W_i h_{i-1} + b_i)$
- Natural neural network

$$h_i = f_i \left( V_i U_{i-1} \left( h_{i-1} - c_i \right) + d_i \right)$$



# Weight Normalization (2016, NIPS)

- Target BN's drawback:
  - Can not be used for online learning
  - Unstable for small mini batch size
  - RNN
- Express weight as new parameters

$$\mathbf{w} = \frac{g}{||\mathbf{v}||}\mathbf{v}$$
  $y = \phi(\mathbf{w} \cdot \mathbf{x} + b).$ 

Decouple direction and length of vectors

#### Reference

- batch normalization accelerating deep network training by reducing internal covariate shift, ICML 2015 (Batch Normalization)
- Normalization Propagation A Parametric Technique for Removing Internal Covariate Shift in Deep Networks, ICML, 2016
- Weight Normalization A Simple Reparameterization to Accelerate Training of Deep Neural Networks, NIPS, 2016
- Layer Normalization, Arxiv:1607.06450, 2016
- Recurrent Batch Normalization, ICLR,2017
- Batch Normalized Recurrent Neural Networks, ICASSP, 2016
- Natural Neural Networks, NIPS, 2015
- Normalizing the normaliziers-comparing and extending network normalization schemes, ICLR, 2017
- Batch Renormalization, Arxiv:1702.03275, 2017
- mean-normalized stochastic gradient for large-scale deep learning, ICASSP 2014
- deep learning made easier by linear transformations in perceptrons, AISTATS 2012

## Outline

- Introduction to Deep Neural Networks (DNNs)
- Training DNNs: Optimization
- Batch Normalization
- Other Normalization Techniques
- Centered Weight Normalization

Centered Weight Normalization in Accelerating Training of Deep Neural Networks

Lei Huang, Xianglong Liu, Yang Liu, Bo Lang, Dacheng Tao International Conference on Computer Vision (ICCV) 2017

## Motivation

- Stable distribution in hidden layer
- Initialization method
  - Random Init (1998, YanLecun)
    - Zero-mean, stable-var
  - Xavier Init (2010, Xavier)

$$W \sim U \Big[ -\frac{\sqrt{6}}{\sqrt{n_j + n_{j+1}}}, \frac{\sqrt{6}}{\sqrt{n_j + n_{j+1}}} \Big]$$

– He Init (2015, He Kaiming)

• 
$$W \sim N\left(0, \sqrt{\frac{2}{n}}\right), n = out * H * W$$

Keep desired characters during training

• Formulation: Constrained optimization problem:

$$\theta^* = \arg\min_{\theta} \mathbb{E}_{(\mathbf{x}, \mathbf{y}) \in D} [\mathcal{L}(\mathbf{y}, f(\mathbf{x}; \theta))]$$
  
s.t.  $\mathbf{w}^T \mathbf{1} = 0 \text{ and } \|\mathbf{w}\| = 1$ 

• Solution by re-parameterization



• Using proxy parameter v:

$$\mathbf{w} = \frac{\mathbf{v} - \frac{1}{d}\mathbf{1}(\mathbf{1}^T\mathbf{v})}{\|\mathbf{v} - \frac{1}{d}\mathbf{1}(\mathbf{1}^T\mathbf{v})\|}$$

Gradient Information:



$$\frac{\partial \mathcal{L}}{\partial \mathbf{v}} = \frac{1}{\|\hat{\mathbf{v}}\|} \left[ \frac{\partial \mathcal{L}}{\partial \mathbf{w}} - \left( \frac{\partial \mathcal{L}}{\partial \mathbf{w}} \mathbf{w} \right) \mathbf{w}^T - \frac{1}{d} \left( \frac{\partial \mathcal{L}}{\partial \mathbf{w}} \mathbf{1} \right) \mathbf{1}^T \right]$$

• Adjustable scale:

$$z = g \frac{\mathbf{v} - \frac{1}{d} \mathbf{1} (\mathbf{1}^T \mathbf{v})}{\|\mathbf{v} - \frac{1}{d} \mathbf{1} (\mathbf{1}^T \mathbf{v})\|})^T \mathbf{h} + b.$$

- Wrapped as module for practitioner:
  - Forward

**Algorithm 1** Forward pass of linear mapping with centered weight normalization.

- 1: Input: the mini-batch input data  $\mathbf{X} \in \mathbb{R}^{d \times m}$  and parameters to be learned:  $\mathbf{g} \in \mathbb{R}^{n \times 1}$ ,  $\mathbf{b} \in \mathbb{R}^{n \times 1}$ ,  $\mathbf{V} \in \mathbb{R}^{d \times n}$ .
- 2: **Output**: pre-activation  $\mathbf{Z} \in \mathbb{R}^{n \times m}$ .
- 3: compute centered weight:  $\hat{\mathbf{V}} = \mathbf{V} \frac{1}{d} \mathbf{1}_d (\mathbf{1}_d^T \mathbf{V}).$
- 4: **for** i = 1 to n **do**
- 5: calculate normalized weight with respect to the *i*-th neuron:  $\mathbf{w}_i = \frac{\hat{\mathbf{v}}_i}{\|\hat{\mathbf{v}}_i\|}$
- 6: end for
- 7: calculate:  $\hat{\mathbf{Z}} = \mathbf{W}^T \mathbf{X}$ .
- 8: calculate pre-activation:  $\mathbf{Z} = (\mathbf{g}\mathbf{1}_m^T) \odot \hat{\mathbf{Z}} + \mathbf{b}\mathbf{1}_m^T$ .

- Wrapped as module for practitioner:
  - Backward

Algorithm 2 Back-propagation pass of linear mapping with centered weight normalization.

- Input: pre-activation derivative {∂L/∂Z} ∈ ℝ<sup>n×m</sup>}. Other auxiliary variables from respective forward pass: Ŷ, W, Ź, X, g.
- 2: Output: the gradients with respect to the inputs {∂L/∂X ∈ ℝ<sup>d×m</sup>} and learnable parameters: ∂L/∂g ∈ ℝ<sup>1×n</sup>, ∂L/∂b ∈ ℝ<sup>1×n</sup>, ∂L/∂V ∈ ℝ<sup>d×n</sup>.
  3: ∂L/∂g = 1<sup>T</sup><sub>m</sub>(∂L/∂Z ⊙ Î)<sup>T</sup>
  4: ∂L/∂b = 1<sup>T</sup><sub>m</sub>∂L<sup>T</sup>/∂Z
  5: ∂L/∂Z = ∂L/∂Z ⊙ (g1<sup>T</sup><sub>m</sub>)
  6: ∂L/∂X = W∂L/∂Z
  7: ∂L/∂W = X∂L<sup>T</sup>/∂Z
  8: for i = 1 to n do
  9: ∂L/∂V<sub>i</sub> = 1/||Ŷ<sub>i</sub>|| (∂L/∂w<sub>i</sub> - (∂L/∂w<sub>i</sub>w<sub>i</sub>)w<sub>i</sub><sup>T</sup> - 1/d(∂L/∂w<sub>i</sub>1d)1<sup>T</sup><sub>d</sub>)
  10: end for

### Discussion

Beneficial Characters for training

 Stabilize the distributions

**Proposition 1.** Let  $z = \mathbf{w}^T \mathbf{h}$ , where  $\mathbf{w}^T \mathbf{1} = 0$  and  $\|\mathbf{w}\| = 1$ . 1. Assume  $\mathbf{h}$  has Gaussian distribution with the mean:  $\mathbb{E}_{\mathbf{h}}[\mathbf{h}] = \mu \mathbf{1}$ , and covariance matrix:  $cov(\mathbf{h}) = \sigma^2 \mathbf{I}$ , where  $\mu \in \mathbb{R}$  and  $\sigma^2 \in \mathbb{R}$ . We have  $\mathbb{E}_{z}[z] = 0$ ,  $var(z) = \sigma^2$ .

Better Conditioning of Hessian

**Proposition 2.** Regarding to the proxy parameter  $\mathbf{v}$ , centered weight normalization makes that the gradient  $\frac{\partial \mathcal{L}}{\partial \mathbf{v}}$  has following properties: (1) zero-mean, i.e.  $\frac{\partial \mathcal{L}}{\partial \mathbf{v}} \cdot \mathbf{1} = 0$ ; (2) orthogonal to the parameters  $\mathbf{w}$ , i.e.  $\frac{\partial \mathcal{L}}{\partial \mathbf{v}} \cdot \mathbf{w} = 0$ .

Regularization in improving performance

- Data set
  - Yale-B
  - SVHN
  - Cifar10, Cifar100
  - ImageNet
- Reproducible experiments and Code: <u>https://github.com/huangleiBuaa/CenteredWN</u>

Ablation study
 YaleB, MLP{128,64,48,48}







• MLP

- SVHN, {128,128,128,128,128}



• MLP

- SVHN, {128,128,128,128,128}



- Cifar10 & Cifar100
  - BN-Inception

	Cifar-10	Cifar-100
Plain	$6.14 \pm 0.04$	25.52 ±0.15
WN	6.18 ±0.34	25.49 ±0.35
WCBN	6.01 ±0.16	24.45 ±0.54

- Residual Network-56 layers.

	Cifar-10	Cifar-100
Plain	7.34 ±0.52	29.38 ±0.14
WN	7.58 ±0.40	29.85 ±0.66
WCBN	6.85 ±0.25	29.23 ±0.14

- ImageNet
  - BN-Inception



Methods	Top-1 error	Top-5 error
plain	30.78	11.14
WN	28.64	9.7
CWN	26.1	8.35

## **Conclusion and Feature work**

#### • Conclusion:

- CWN shows the advantages in accelerating training and better generalization
- CWN module as a optimal module to replace linear module

- Apply CWN module
  - RNNs
  - Reinforcement learning scene

#### Thanks !

