

Not restricted to two layers

Some terminology

2-layer Neural Network

 $\mathbf{s}_1 = W_1 \mathbf{x} + \mathbf{b}_1$ $\mathbf{h} = \max(0, \mathbf{s}_1)$ $\mathbf{s} = W_2 \mathbf{h} + \mathbf{b}_2$





 $\mathbf{h}_1 = \max\{0, \mathbf{e}_1\}$

lapat: x

 $\mathbf{h}_{1} = \max\{0, \mathbf{s}_{1}\}$



Output: a = W.h. + h.

3-layer Neural Network

$$\mathbf{s}_1 = W_1 \mathbf{x} + \mathbf{b}_1$$
 $W_1 \text{ is } m_1 \times m_1$

1st hidden layer activations $ightarrow \mathbf{h}_1 = \max(0, \mathbf{s}_1) \leftarrow$ apply non-linearity via activation fn

 $\mathbf{s}_2 = W_2 \mathbf{h}_1 + \mathbf{b}_2 \quad {}_{W_2 \text{ is } m_2 \times m_1}$

2nd hidden layer activations \rightarrow $h_2 = \max(0, s_2) \leftarrow$ apply non-linearity via activation fn

Output responses $\rightarrow \mathbf{s} = W_3 \mathbf{h}_2 + \mathbf{b}_3$ W_3 is $c \times m_2$



Sometimes referred to as a 2-hidden-layer neural network.





Options for activation functions







Activation function is applied independently to each element of the score vector.

Activation function is generally applied independently to each element of vector.



In modern networks ReLU is the most common activation function.



- m is the number of nodes in the hidden layer.
- No regularization.

Result depends on parameter initialization

Effect of regularization



- m is the number of nodes in the hidden layer.
- No regularization.
- · Different random parameter initialization to previous slide.

$$J(\mathcal{D}, \lambda, \Theta) = \sum_{(\mathbf{x}, y) \in \mathcal{D}} l(\mathbf{x}, y, \Theta) + \lambda R(\Theta)$$

- m = 100 nodes in the hidden layer.
- L₂ regularization.

Do not use size of neural network as a regularizer. Use stronger regularization.



Mini-batch SGD (or variant)

Loop

- 1. Sample a batch of the training data.
- Forward propagate it through the graph and calculate loss/cost.
- 3. Backward propagate to calculate the gradients.
- 4. Update the parameters using the gradient.

Back propagation for 2-layer neural network



For a single labelled training example:

- 1. Forward propagate it through the graph and calculate loss.
- 2. Backward propagate to calculate the gradients.

Gradient Computations for a k-layer neural network



For a single labelled training example:

 In vector notation:
 <u>∂s</u> = W₂
 <u>∂s</u> = W₂

- 1. Forward propagate it through the graph and calculate loss. $\ensuremath{\uparrow}\xspace$ this is straightforward.

Starting point of our demonstration



In Lecture 3 explicitly computed filled in *local Jacobians* and *gradients.*

Backward Pass

Backward Pass



Compute local Jacobian of node ${\bf s}$ w.r.t. its child ${\bf h}$



Compute gradient of J w.r.t. node h





Backward Pass





Backward Pass



Compute local Jacobian of node \mathbf{s}_1 w.r.t. its child \mathbf{b}_1





Backward Pass





Compute gradient of J w.r.t. node W_1



$$\begin{array}{l} \displaystyle \frac{\partial J}{\partial \mathrm{vec}(W_i)} = \frac{\partial J}{\partial h} \frac{\partial s_{ii}}{\partial k} \\ & = \left(g_1 \mathbf{x}^T \ g_2 \mathbf{x}^T \ \cdots \ g_{in} \mathbf{x}^T\right) + \lambda \mathrm{vec}(W_i)^T \quad \leftarrow \mathrm{gradient needed for learning} \\ \mathrm{if we set } \mathbf{g} = \frac{\partial J}{\partial \mathbf{g}_i}. \end{array}$$

Aggregated backward pass for a 2-layer neural network

Compute gradient of J w.r.t. node W_1



Can convert

$$\frac{\partial J}{\operatorname{Vec}(W_1)} = \begin{pmatrix} g_1 \mathbf{x}^T & g_2 \mathbf{x}^T & \cdots & g_m \mathbf{x}^T \end{pmatrix} + 2\lambda \operatorname{vec}(W_1)^T$$

(where $g = \frac{\partial J}{\partial s_i}$) from a vector $(1 \times md)$ back to a 2D matrix $(m \times d)$:

$$\frac{\partial J}{\partial W_1} = \begin{pmatrix} g_1 \mathbf{x}^T \\ g_2 \mathbf{x}^T \\ \vdots \\ g_C \mathbf{x}^T \end{pmatrix} + 2\lambda W_1 = \mathbf{g}^T \mathbf{x}^T + 2\lambda W_1$$

1. Let

$$\mathbf{g} = -\frac{\mathbf{y}^T}{\mathbf{y}^T \mathbf{p}} \left(\mathsf{diag}(\mathbf{p}) - \mathbf{p} \mathbf{p}^T \right)$$

2. Gradient of J w.r.t. second bias vector is the $1\times c$ vector

$$\frac{\partial J}{\partial \mathbf{b}_2} = \mathbf{g}$$

3. Gradient of J w.r.t. second weight matrix W_2 is the $c \times m$ matrix

$$\frac{\partial J}{\partial W_2} = \mathbf{g}^T \mathbf{h}^T + 2\lambda W_2$$

4. Propagate the gradient vector g to the first layers

$$g = gW_2$$

 $g = g \operatorname{diag}(\operatorname{Ind}(s_1 > 0)) \leftarrow \operatorname{assuming ReLu act}$

5. Gradient of J w.r.t. the first bias vector is the $1 \times d$ vector

$$\frac{\partial J}{\partial \mathbf{b}_1} = \mathbf{g}$$

6. Gradient of J w.r.t. the first weight matrix W_1 is the $m \times d$ matrix

$$\frac{\partial J}{\partial W_1} = \mathbf{g}^T \mathbf{x}^T + 2\lambda W_1$$

2-layer scoring function + SOFTMAX + cross-entropy loss + Regularization

- Compute gradients of *l* w.r.t. W₁, W₂, b₁, b₂ for each (x, y) ∈ D^(t):
 - Set all entries in $\frac{\partial L}{\partial \mathbf{b}_1}$, $\frac{\partial L}{\partial \mathbf{b}_2}$, $\frac{\partial L}{\partial W_1}$ and $\frac{\partial L}{\partial W_2}$ to zero.
 - for $(\mathbf{x}, y) \in \mathcal{D}^{(t)}$
 - 1. Let $\mathbf{g} = -\frac{\mathbf{y}^T}{\mathbf{y}^T \mathbf{p}} \left(\operatorname{diag}(\mathbf{p}) \mathbf{p}\mathbf{p}^T \right)$
 - 2. Add gradient of l w.r.t. b_2 computed at (x, y)

$$\frac{\partial L}{\partial \mathbf{b}_2}$$
 += g, $\frac{\partial L}{\partial W_2}$ += g^Th^T

3. Propagate the gradients

$$g = gW_2$$

 $g = g \operatorname{diag}(\operatorname{Ind}(s_1 > 0))$

4. Add gradient of l w.r.t. first layer parameters computed at (x, y)

$$\frac{\partial L}{\partial \mathbf{b}_1}$$
 += g, $\frac{\partial L}{\partial W_1}$ += g^T x^T

- Divide by the number of entries in $\mathcal{D}^{(t)}$:

$$\frac{\partial L}{\partial W_i}$$
 /= $|D^{(t)}|$, $\frac{\partial L}{\partial \mathbf{b}_i}$ /= $|D^{(t)}|$ for $i = 1, 2$

· Add the gradient for the regularization term

$$\frac{\partial J}{\partial W_i} = \frac{\partial L}{\partial W_i} + 2\lambda W_i$$
, $\frac{\partial J}{\partial \mathbf{b}_i} = \frac{\partial L}{\partial \mathbf{b}_i}$ for $i = 1, 2$

Aggregated Backward pass for a k-layer neural network

The gradient computation for one training example (x, y):

Let

$$\mathbf{g} = -\frac{\mathbf{y}^T}{\mathbf{y}^T \mathbf{p}} \left(\mathsf{diag}(\mathbf{p}) - \mathbf{p} \mathbf{p}^T \right)$$

• for $i = k, k - 1, \dots, 1$

1. The gradient of J w.r.t. bias vector b_i

$$\frac{\partial J}{\partial \mathbf{b}_i} = \mathbf{g}$$

2. Gradient of J w.r.t. weight matrix Wi

$$\frac{\partial J}{\partial W_i} = \mathbf{g}^T \mathbf{x}^{(i-1)T} + 2\lambda W_i$$

3. Propagate the gradient vector g to the previous layer (if i > 1)

$$g = gW_i$$

 $g = g \operatorname{diag}(\operatorname{Ind}(s^{(i-1)} > 0))$

- Let x⁽⁰⁾ = x represent the input.
- for $i=1,\ldots,k-1$

$$\mathbf{s}^{(i)} = W_i \mathbf{x}^{(i-1)} + \mathbf{b}_i$$

 $\mathbf{x}^{(i)} = \max \left(0, \mathbf{s}^{(i)}\right)$

· Apply the final linear transformation

$$s^{(k)} = W_k x^{(k-1)} + b_k$$

· Apply SOFTMAX operation to turn final scores into probabilities

$$\mathbf{p} = \frac{\exp(\mathbf{s}^{(k)})}{\mathbf{1}^T \exp(\mathbf{s}^{(k)})}$$

 Apply cross-entropy loss and regularization to measure performance w.r.t. ground truth label y

$$J = -\log(\mathbf{y}^T \mathbf{p}) + \lambda \sum_{i=1}^k ||W_i||^2$$

Assumed ReLu is the activation function at each intermediary layer.

Training Neural Networks a little bit of history

A bit of history

- Perceptron algorithm invented by Frank Rosenblatt (1957).
- Mark 1 Perceptron machine
 First implementation of the perceptron algorithm.
- Machine was connected to camera producing 20 × 20 pixel image and recognized letters.
- · Perceptron classification fn:

 $f(\mathbf{x}; \mathbf{w}) = \begin{cases} 1 & \text{if } \mathbf{w}^T \mathbf{x} + \mathbf{b} > 0 \\ 0 & \text{otherwise} \end{cases}$

 For labelled training example (x, y) (y ∈ {−1, 1}) the Perceptron loss is

$$p_p(\mathbf{x}, y; \mathbf{w}) = \max(0, -y(\mathbf{w}^T \mathbf{x} + b))$$

 Update rule: Use SGD to learn w. If training example (x_i, y_i) is incorrectly classified then

 $\mathbf{w} \leftarrow \mathbf{w} + y_i \mathbf{x}_i$

A bit of history

Learning Internal Representations by Error Propagation, D. Rumelhart, G. Hinton and R. Williams, Parallel Distributed Processing: Explorations in the Microstructure of Cognition, 1986.



First time back-propagation became popular



Adaline a single layer neural network with one output

$$\hat{y} = \mathbf{w}^T \mathbf{x} + b$$

• Loss function: for labelled training example (x, y)

$$l(\mathbf{x}, y, \mathbf{w}) = (y - (\mathbf{w}^T \mathbf{x} + b))^2 = (y - \hat{y})^2$$

Update rule: Use SGD with learning rate η to learn w:

$$\mathbf{w} \leftarrow \mathbf{w} + \eta(y - \hat{y})\mathbf{x}$$

 Extension Madaline: a three-layer, fully connected, feed-forward artificial neural network architecture for classification.

A bit of history

New wave of research in Deep Learning.

- Ability to train networks with many layers.
- Mixture of unsupervised and supervised training.
- Unsupervised: Encoding layers first learnt in stagewise manner using RBMs (restricted Boltzman machines).
- Decode layers using an auto-encoder.
- Supervised: Back-prop used to do final update of weights.



Reducing the Dimensionality of Data with Neural Networks, Hinton and Salakhutdinov, Science, 2006.

 Context-Dependent Pre-trained Deep Neural Networks for Large Vocabulary Speech Recognition, G. Dahl, D. Yu, L. Deng, A. Acero, 2010.



- · Beat the widely established approach of GMM-HMM with a DNN-HMM.
- Improved results on popular datasets by 5.8% and 9.2%.

 ImageNet classification with deep convolutional neural networks A. Krizhevsky, I. Sutskever, G. Hinton, 2012.



- Beat the stagnating established approaches of Handcrafted features + kernel SVM.
- Improved results on ImageNet by ~11%.

Sigmoid

Better understanding of gradient flows during BackProp helped with these breakthroughs Understanding Effect of Activation Functions



- Squashes numbers to range [0,1].
- · Has nice interpretation as a saturating firing rate of a neuron.

Sigmoid $\sigma(x)$ $d\sigma(x)$

$$\sigma(x) = \frac{1}{1 + \exp(-x)}$$

Problems

- 1. Saturated activations kill the gradients.
 - Have a sigmoid activation

s = Wx + b $\mathbf{h} = \sigma(\mathbf{s})$

- Derivative of the sigmoid function is:

$$\frac{\partial h_i}{\partial s_j} = \begin{cases} \frac{\exp(-s_i)}{(1 + \exp(-s_i))^2} & (= \sigma'(s_i)) & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$$

- As

$$\frac{\partial J}{\partial s_i} = \frac{\partial J}{\partial h_i} \frac{\partial h_i}{\partial s_i} = \frac{\partial J}{\partial h_i} \sigma'(s_i)$$

What happens to gradient of J w.r.t. s_i when $|s_i| > 5$?

$$\sigma(x) = \frac{1}{1 + \exp(-\frac{1}{2})}$$

p(-x)

Problems

- 1. Saturated activations kill the gradients.
- 2. Sigmoid outputs are not zero-centered.
 - Have a sigmoid activation

$$s = Wx + T$$

 $h = \sigma(s)$

- Then

$$\frac{\partial J}{\partial \mathbf{w}_i} = \frac{\partial J}{\partial h_i} \frac{\partial h_i}{\partial s_i} \frac{\partial s_i}{\partial \mathbf{w}_i} = \frac{\partial J}{\partial h_i} \sigma'(s_i) \mathbf{x}^T$$

What happens to $\frac{\partial J}{\partial w_i}$ when all entries in x are positive?

Sigmoid

$$\tau(x) = \frac{1}{1 + \exp(-x)}$$

Problems

- 1. Saturated activations kill the gradients.
- 2. Sigmoid outputs are not zero-centered.
 - Have a sigmoid activation

$$s = Wx + b$$
, $h = \sigma(s$

- Then

$$\frac{\partial J}{\partial \mathbf{w}_{i}} = \frac{\partial J}{\partial h_{i}} \frac{\partial h_{i}}{\partial s_{i}} \frac{\partial s_{i}}{\partial \mathbf{w}_{i}} = \frac{\partial J}{\partial h_{i}} \sigma'(s_{i}) \mathbf{x}_{\uparrow}^{T}$$

What happens to $\frac{\partial J}{\partial w_i}$ when all entries in x are positive? \implies entries of $\frac{\partial J}{\partial w_i}$ are either all positive or all negative.

$$\sigma(x) = \frac{1}{1 + \exp(-x)}$$



Sigmoid

Sigmoid

Problems

- 1. Saturated activations kill the gradients.
- 2. Sigmoid outputs are not zero-centered.
 - Have a sigmoid activation

$$s = Wx + b$$
, $h = \sigma(s)$

- Then $\frac{\partial J}{\partial \mathbf{w}_i} = \frac{\partial J}{\partial h_i} \frac{\partial h_i}{\partial \mathbf{s}_i} \frac{\partial s_i}{\partial \mathbf{w}_i} = \frac{\partial J}{\partial \mathbf{w}_i} = \frac{\partial J}{\partial h_i} \frac{\partial h_i}{\partial \mathbf{s}_i} \frac{\partial s_i}{\partial \mathbf{w}_i} = \frac{\partial J}{\partial h_i} \sigma'(s_i) \mathbf{x}^T$

What is $\frac{\partial J}{\partial \mathbf{w}_i}$ when all entries in \mathbf{x} are +tive? (occurs after applying sigmoid) $\implies \text{entries of } \frac{\partial J}{\partial w_i} \text{ are either all positive or all negative.}$ $\implies \text{inefficient zig-zag update paths to find optimal } w_i$

Sigmoid

. disable

maxx (0, x)



Problems

- 1. Saturated activations kill the gradients.
- 2. Sigmoid outputs are not zero-centered.
- 3. exp() is expensive to compute



Properties

- 1. Squashes numbers to range [-1, 1].
- 2. Tanh outputs are zero-centered.
- 3. Saturated activations kill the gradients.

Rectified Linear Unit (ReLu)



$\mathsf{ReLu}(x) = \max(0, x)$

Pros

- 1. Does not saturate for large positive x.
- 2. Very computationally efficient.
- 3. In practice training of a ReLu network converges much faster than one with sigmoid/tanh activation functions.

$\mathsf{ReLu}(x) = \max(0, x)$

Rectified Linear Unit (ReLu)

Problems

- 1. Output is not zero-centered
- 2. Negative inputs result in zero gradients.
 - Have a ReLu activation

$$s = Wx + b$$

 $h = max(0, s)$

- Derivative of the Rel u function is:

$$\frac{\partial h_i}{\partial s_j} = \begin{cases} 1 & \text{if } i = j \& s_j > 0 \\ 0 & \text{otherwise} \end{cases}$$

- Then

$$\frac{\partial J}{\partial s_i} = \frac{\partial J}{\partial h_i} \frac{\partial h_i}{\partial s_i} = \begin{cases} \frac{\partial J}{\partial h_i} & \text{if } s_i > 0\\ 0 & \text{otherwise} \end{cases}$$



Problems

- 1. Output is not zero-centered
- 2. Negative activations have zero gradients and freezes some parameter weights.

As

$$s = Wx + b$$
, $h = max(0, s)$

then

$$\frac{\partial J}{\partial \mathbf{w}_{i}} = \frac{\partial J}{\partial h_{i}} \frac{\partial h_{i}}{\partial s_{i}} \frac{\partial s_{i}}{\partial \mathbf{w}_{i}} = \begin{cases} \frac{\partial J}{\partial h_{i}} \mathbf{x}^{T} & \text{if } s_{i} > 0\\ \mathbf{0} & \text{otherwise} \end{cases}$$

⇒ dead ReLU will never activate

⇒ never update parameter weights.

Exponential Linear Units (ELU)

$$\mathsf{ELU}(x) = \begin{cases} x & \text{if } x > 0\\ \alpha(\exp(x) - 1) & \text{otherwise} \end{cases}$$

Pros & Cons

- 1. All the benefits of ReLu.
- 2. Activations do not die.
- 3. Closer to zero mean outputs.
- 4. Computation requires $\exp()$

[Clevert et al., 2015]



Leaky $\operatorname{ReLu}(x) = \max(.01x, x)$



Pros

- 1. Does not saturate.
- 2. Computationally efficient.
- In practice training of a Leaky ReLu network converges much faster than one with sigmoid/tanh activation functions.
- 4. Activations do not die.

[Mass et al., 2013] [He et al., 2015]

Which Activation Function?

In practice

- Use ReLU.
 - Be careful with your learning rates.
 - Initialize bias vectors to be slightly positive.
- Try out Leaky ReLU / ELU.
- · Try out tanh but don't expect much.
- Don't use sigmoid.

Leaky ReLu



What happens when you initialize each weight matrix entry to zero? (each $W_{i,lm} = 0$)

Initialize with small random numbers

Initialize with small random numbers

 $W_{i,lm} \sim N(w; 0, .01^2)$

Effect of weight initialization & activation function on gradient

What happens in this case?

flow

$$W_{i,lm} \sim N(w; 0, .01^2)$$

What happens in this case?

Works okay for small networks, but can lead to non-homogeneous distributions of activations across the layers of a deep network.

- Initialize a 10-layer network with 500 nodes at each layer.
- Use a tanh activation function at each layer.
- Initialize weights will small random numbers.
- Generate random input data (N(0, 1²)) with d = 500.

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Some activation histograms

Aggregated Backward pass for a k-layer neural network

- All activations become zero at the layers > 2.
- · What happens in the backward pass of the back-prop algorithm?



The gradient computation for one training example (x, y):

Let

$$\mathbf{g} = -\frac{\mathbf{y}^T}{\mathbf{y}^T \mathbf{p}} \left(\operatorname{diag}(\mathbf{p}) - \mathbf{p} \mathbf{p}^T \right)$$

- for $i = k, k 1, \dots, 1$
 - 1. The gradient of J w.r.t. bias vector \mathbf{b}_i

$$\frac{\partial J}{\partial \mathbf{b}_i} = \mathbf{g}$$

2. Gradient of J w.r.t. weight matrix Wi

 $\frac{\partial J}{\partial W_i} = \mathbf{g}^T \mathbf{x}^{(i)T} + 2\lambda W_i$

3. Propagate the gradient vector g to the previous layer (if i > 1)

$$g = gW_i$$

 $g = g \operatorname{diag}(\operatorname{Ind}(s^{(i)} > 0))$

Change the initialization to bigger random numbers

Change the initialization to bigger random numbers

- Initialize a 10-layer network with 500 nodes at each layer.
- Use a tanh activation function at each layer.
- Initialize weights with bigger random numbers: W_{i,lm} ~ N(w; 0, 1²).
- Generate random input data (N(0, 1²)) with d = 500.

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Change the initialization to bigger random numbers

- Almost all neurons completely saturated, either -1 or +1.
- ⇒ Gradients will be all zero
- (Remember the picture of the gradient of tanh.)



Aggregated Backward pass for a k-layer neural network

- The gradient computation for one training example (x, y):
 - Let

$$\mathbf{g} = -\frac{\mathbf{y}^T}{\mathbf{y}^T \mathbf{p}} \left(\mathsf{diag}(\mathbf{p}) - \mathbf{p} \mathbf{p}^T \right)$$

- for $i = k, k 1, \dots, 1$
 - 1. The gradient of J w.r.t. bias vector \mathbf{b}_i

$$\frac{\partial J}{\partial \mathbf{b}_i} = \mathbf{g}$$

2. Gradient of J w.r.t. weight matrix Wi

$$\frac{\partial J}{\partial W_i} = \mathbf{g}^T \mathbf{x}^{(i)T} + 2\lambda W_i$$

3. Propagate the gradient vector g to the previous layer (if i > 1)

 $g = gW_i$ $g = g \operatorname{diag}(\operatorname{tanh}'(s^{(i)}))$

- Initialize a 10-layer network with 500 nodes at each layer.
- Use a tanh activation function at each layer.
- Initialize weights with Xavier initialization: W_{i,lm} ∼ N(w; 0, 1/√500).
- Generate random input data (N(0, 1²)) with d = 500.

- · Initialize a 10-layer network with 500 nodes at each layer.
- Use a tanh activation function at each layer.
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- Generate random input data (N(0, 1²)) with d = 500.



Xavier initialization doesn't work for ReLu activation

- Initialize a 10-layer network with 500 nodes at each layer.
- · Use a ReLu activation function at each layer.
- Initialize weights with Xavier initialization: W_{i,lm} ∼ N(w; 0, 1/√500).
- Generate random input data (N(0, 1²)) with d = 500.



Proper Initialization an active area of research

- Understanding the difficulty of training deep feedforward neural networks by Glorot and Bengio, 2010
- Exact solutions to the nonlinear dynamics of learning in deep linear neural networks by Saxe et al, 2013
- Random walk initialization for training very deep feedforward networks by Sussillo and Abbott, 2014
- Delving deep into rectifiers: Surpassing human-level performance on ImageNet classification by He et al., 2015
- Data-dependent Initializations of Convolutional Neural Networks by Krähenbühl et al., 2015
- · All you need is a good init, Mishkin and Matas, 2015

- Want unit Gaussian activations at each layer? Just make them unit Guassian!
- · Idea introduced in:

Batch Normalization: Accelerating Deep Network Training by Reducing Internal Covariate Shift, S. loffe, C. Szegedy, arXiv 2015.

- Consider activations at some layer for a batch: s₁^(j), s₂^(j)..., s_n^(j)
- · To make each dimension unit gaussian, apply:

$$\hat{\mathbf{s}}_i^{(j)} = \mathsf{diag}(\sigma_1, \dots, \sigma_m)^{-1} \left(\mathbf{s}_i^{(j)} - \boldsymbol{\mu} \right)$$

where

$$\boldsymbol{\mu} = \frac{1}{n} \sum_{i=1}^{n} \mathbf{s}_{i}^{(j)}, \quad \sigma_{p}^{2} = \frac{1}{n} \sum_{i=1}^{n} (s_{i}^{(j)}, p - \mu_{p})^{2}$$

Batch Normalization

Batch Normalization: Scale & shift range

- Usually apply normalization after the fully connected layer before non-linearity.
- Therefore for a k-layer network have
 - for i = 1, ..., k 1for $(\mathbf{x}^{(i-1)}, y) \in \mathcal{D} \leftarrow Apply ith linear transformation to batch$

Lessening the effect of initialization: Batch normalization

$$\mathbf{s}^{(i)} = W_i \mathbf{x}^{(i-1)} + \mathbf{b}_i$$

end Compute batch mean and variances of *i*th layer:

$$\mu = \frac{1}{|\mathcal{D}|} \sum_{\mathbf{s}^{(i)} \in \mathcal{D}} \mathbf{s}^{(i)}, \quad \sigma_j^2 = \frac{1}{|\mathcal{D}|} \sum_{\mathbf{s}^{(i)} \in \mathcal{D}} \left(\mathbf{s}_j^{(i)} - \mu_j \right)^2 \text{ for } j = 1, \dots, m_i$$

for $(\mathbf{s}^{(i)}, y) \in \mathcal{D} \leftarrow$ Apply BN and activation function

$$\begin{split} \hat{\mathbf{s}}^{(i)} &= \mathsf{BatchNormalise}(\mathbf{s}^{(i)}, \boldsymbol{\mu}, \sigma_1, \dots, \sigma_{m_i}) \\ \mathbf{x}^{(i)} &= \max\left(0, \hat{\mathbf{s}}^{(i)}\right) \end{split}$$

end

- Apply final linear transformation: $s^{(k)} = W_k x^{(k-1)} + \mathbf{b}_k$

· Can also allow the network to squash and shift the range

$$\hat{\mathbf{s}}^{(i)} = \gamma^{(i)}\hat{\mathbf{s}}^{(i)} + \beta^{(i)}$$

of the $\hat{\mathbf{s}}^{(i)}$'s at each layer.

- Can learn the $\gamma^{(i)}{}^{\rm s}$ and $\beta^{(i)}{}^{\rm s}$ and add them as parameters of the network.
- · To keep things simple this added complexity is often omitted.

- · Improves gradient flow through the network.
- · Reduces the strong dependence on initialization.
- ⇒ learn deeper networks more reliably.
- · Allows higher learning rates.
- · Acts as a form of regularization.

If training a deep network, you should use Batch Normalization.

- · At test time do not have a batch.
- Instead fixed empirical mean and variances of activations at each level are used.
- These quantities estimated during training (with running averages).

Computational Graph for a BN layer

Back-Prop for a Batch Normalization layer.



· Compute the mean and variance for the scores in the batch:

$$\mu_b = \frac{1}{n} \sum_{i=1}^{n} \mathbf{s}_i, \quad v_{b,j} = \frac{1}{n} \sum_{i=1}^{n} (s_{i,j} - \mu_{b,j})^2$$

where $\mathbf{v}_b = (v_{b,1}, v_{b,2}, \dots, v_{b,m})^T$. (*n* = 2 in the figure.) Define $V_b = \text{diag}(\mathbf{v}_b + \epsilon)$

· Apply batch normalization function to each score vector:

$$\hat{\mathbf{s}}_i = V_b^{-\frac{1}{2}} (\mathbf{s}_i - \boldsymbol{\mu}_b)$$



- Want to compute
 ^{∂J}/_{∂si} for each s_i in the batch.
- The children of node s_i are {ŝ_i, v_b, μ_b} thus

 $\frac{\partial J}{\partial \mathbf{s}_i} = \frac{\partial J}{\partial \hat{\mathbf{s}}_i} \frac{\partial \hat{\mathbf{s}}_i}{\partial \mathbf{s}_i} + \frac{\partial J}{\partial \mathbf{v}_b} \frac{\partial \mathbf{v}_b}{\partial \mathbf{s}_i} + \frac{\partial J}{\partial \boldsymbol{\mu}_b} \frac{\partial \boldsymbol{\mu}_b}{\partial \mathbf{s}_i}$

· Let's look at the individual gradients and Jacobians.

Gradient Computations for a BN layer



- $\frac{\partial J}{\partial \mathbf{s}_i} = \frac{\partial J}{\partial \hat{\mathbf{s}}_i} \frac{\partial \hat{\mathbf{s}}_i}{\partial \mathbf{s}_i} + \frac{\partial J}{\partial \mathbf{v}_b} \frac{\partial \mathbf{v}_b}{\partial \mathbf{s}_i} + \frac{\partial J}{\partial \boldsymbol{\mu}_b} \frac{\partial \boldsymbol{\mu}_b}{\partial \mathbf{s}_i}$
- The equation relating ŝ_i to v_b (remember V_b = diag(v_b + c))

$$\hat{s}_{i} = V_{b}^{-\frac{1}{2}} (s_{i} - \mu_{b})$$

Therefore

$$\frac{\partial \hat{\mathbf{s}}_i}{\partial \mathbf{s}_i} = V_b^{-\frac{1}{2}}$$





Gradient Computations for a BN layer



- $\frac{\partial J}{\partial \mathbf{s}_i} = \frac{\partial J}{\partial \hat{\mathbf{s}}_i} \frac{\partial \hat{\mathbf{s}}_i}{\partial \mathbf{s}_i} + \frac{\partial J}{\partial \mathbf{v}_b} \frac{\partial \mathbf{v}_b}{\partial \mathbf{s}_i} + \frac{\partial J}{\partial \boldsymbol{\mu}_b} \frac{\partial \boldsymbol{\mu}_b}{\partial \mathbf{s}_i}$
- The children of node v_b are {ŝ₁,...,ŝ_n}
- Therefore

$$\frac{\partial J}{\partial \mathbf{v}_b} = \sum_{i=1}^n \frac{\partial J}{\partial \hat{\mathbf{s}}_i} \frac{\partial \hat{\mathbf{s}}}{\partial \mathbf{v}}$$



∂J	$\partial J \partial \hat{s}_i$	$\partial J \partial \mathbf{v}_b$	$\partial J \partial \mu_b$
∂s_i	$\partial \hat{\mathbf{s}}_i \partial \mathbf{s}_i$	$\partial \mathbf{v}_b \partial \mathbf{s}_i$	$\overline{\partial \mu_b} \overline{\partial \mathbf{s}_i}$

- The children of node v_b are {ŝ₁,...,ŝ_n}
- Therefore

$$\frac{\partial J}{\partial \mathbf{v}_b} = \sum_{i=1}^n \frac{\partial J}{\stackrel{\uparrow}{\underset{\uparrow}{\partial \mathbf{\hat{s}}_i}}} \frac{\partial \mathbf{\hat{s}}_i}{\partial \mathbf{v}_b}$$

Gradient Computations for a BN layer

The equation relating ŝ_i to v_b (remember V_b = diag(v_b + ε))

$$\hat{s}_i = V_b^{-\frac{1}{2}} (s_i - \mu_b)$$

The local Jacobian we want to compute

$$\frac{\partial \dot{\mathbf{x}}_i}{\partial \mathbf{v}_b} = \begin{pmatrix} \frac{\partial \dot{x}_{i,1}}{\partial v_{b,1}} & \cdots & \frac{\partial \dot{x}_{i,1}}{\partial v_{b,m}} \\ \vdots & \vdots & \vdots \\ \frac{\partial \dot{x}_{i,m}}{\partial v_{b,1}} & \cdots & \frac{\partial \dot{x}_{i,m}}{\partial v_{b,m}} \end{pmatrix}$$

· Computing the derivative for each individual element:

$$\frac{\partial \hat{s}_{i,j}}{\partial v_{b,k}} = \begin{cases} -\frac{1}{2}(v_{b,k} + \epsilon)^{-\frac{3}{2}}(s_{i,k} - \mu_{b,k}) & \text{if } j = k \\ 0 & \text{otherwise} \end{cases}$$

In matrix form

$$\frac{\partial \hat{\mathbf{s}}_i}{\partial \mathbf{v}_b} = -\frac{1}{2}V_b^{-\frac{3}{2}} \text{diag} (\mathbf{s}_i - \boldsymbol{\mu}_b)$$



- $\frac{\partial J}{\partial \mathbf{s}_{i}} = \frac{\partial J}{\partial \hat{\mathbf{s}}_{i}} \frac{\partial \hat{\mathbf{s}}_{i}}{\partial \mathbf{s}_{i}} + \frac{\partial J}{\partial \mathbf{v}_{b}} \frac{\partial \mathbf{v}_{b}}{\partial \mathbf{s}_{i}} + \frac{\partial J}{\partial \mu_{b}} \frac{\partial \mu_{b}}{\partial \mathbf{s}_{i}}$
- The children of node v_b are {ŝ₁,..., ŝ_n}
- Therefore

• As

and

 $\frac{\partial J}{\partial \mathbf{v}_b} = \sum_{i=1}^n \frac{\partial J}{\partial \hat{\mathbf{s}}_i} \quad \frac{\partial \hat{\mathbf{s}}_i}{\partial \mathbf{v}_b}$

Gradient Computations for a BN layer







- The children of node μ_b are {ŝ₁,..., ŝ_n, v_b}.
- Therefore

$$\frac{\partial J}{\partial \mu_b} = \sum_{i=1}^n \frac{\partial J}{\partial \hat{\mathbf{s}}_i} \frac{\partial \hat{\mathbf{s}}_i}{\partial \mu_b} + \frac{\partial J}{\partial \mathbf{v}_b} \frac{\partial \mathbf{v}_b}{\partial \mu_b}$$

$$\frac{\partial J}{\partial \boldsymbol{\mu}_b} = \sum_{i=1}^n \frac{\partial J}{\partial \hat{\mathbf{s}}_i} \frac{\partial \hat{\mathbf{s}}_i}{\partial \boldsymbol{\mu}_b} + \frac{\partial J}{\partial \mathbf{v}_b} \frac{\partial \mathbf{v}_b}{\partial \boldsymbol{\mu}_b}$$



The equation relating ŝ_i to μ_b (remember V_b = diag(v_b + ε))

$$\hat{\mathbf{s}}_i = V_b^{-\frac{1}{2}} (\mathbf{s}_i - \boldsymbol{\mu}_b)$$

· The local Jacobian we want to compute

 $\frac{\partial \hat{\mathbf{s}}_i}{\partial \mu_i} = -V_b^{-\frac{1}{2}}$

Gradient Computations for a BN layer

Gradient Computations for a BN layer

$$\frac{\partial J}{\partial \boldsymbol{\mu}_b} = \sum_{i=1}^n \frac{\partial J}{\partial \hat{\mathbf{s}}_i} \frac{\partial \hat{\mathbf{s}}_i}{\partial \boldsymbol{\mu}_b} + \frac{\partial J}{\partial \mathbf{v}_b} \frac{\partial \mathbf{v}_b}{\partial \boldsymbol{\mu}_b}$$



Next ^{∂v_b}/_{∂μ_b} = 0.
 As

$$v_{b,j} = \frac{1}{n} \sum_{i=1}^{n} (s_{i,j} - \mu_{b,j})^2$$

 $\frac{\partial v_{b,j}}{\partial \mu_{b,k}} = \begin{cases} -\frac{2}{n} \sum_{i=1}^{n} (s_{i,j} - \mu_{b,j}) = 0 & \text{if } j = k \\ 0 & \text{otherwise} \end{cases}$



aready calculated





∂J	$\partial J \partial \hat{s}_i$	$\partial J \partial \mathbf{v}_b$	$\partial J \partial \mu_b$
$\partial \mathbf{s}_i =$	$\partial \hat{\mathbf{s}}_i \partial \mathbf{s}_i^+$	$\frac{\partial \mathbf{v}_b}{\partial \mathbf{s}_i} +$	$\overline{\partial \mu_b} \overline{\partial \mathbf{s}_i}$

The equation relating µ_b to s_l's is

$$\boldsymbol{\mu}_{b} = \frac{1}{n} \sum_{l=1}^{n} \mathbf{s}_{l}$$

Therefore

$$\frac{\partial \mu_b}{\partial s_i} = \frac{1}{n}I_m$$

