Lecture 4 - k-layer Neural Networks

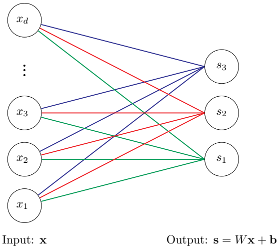
DD2424

April 8, 2017

A new class of scoring functions

Linear scoring function

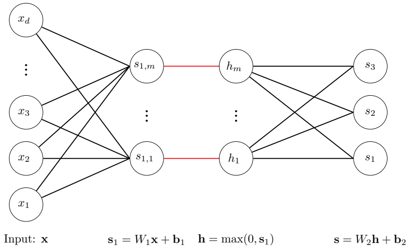
$$\mathbf{s} = W\mathbf{x} + \mathbf{b}$$



Before

2-layer Neural Network

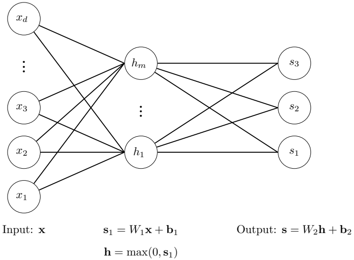
$$\mathbf{s}_1 = W_1\mathbf{x} + \mathbf{b}_1$$
$$\mathbf{h} = \max(0, \mathbf{s}_1)$$
$$\mathbf{s} = W_2\mathbf{h} + \mathbf{b}_2$$



Now

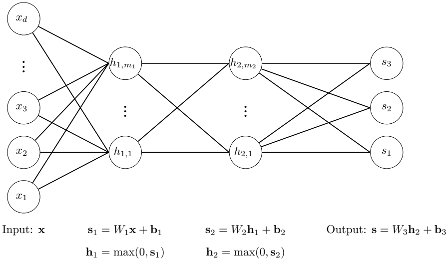
2-layer Neural Network

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



3-layer Neural Network

$$\mathbf{s}_1 = W_1\mathbf{x} + \mathbf{b}_1$$
$$\mathbf{h}_1 = \max(0, \mathbf{s}_1)$$
$$\mathbf{s}_2 = W_2\mathbf{h}_1 + \mathbf{b}_2$$
$$\mathbf{h}_2 = \max(0, \mathbf{s}_2)$$
$$\mathbf{s} = W_3\mathbf{h}_2 + \mathbf{b}_3$$



3-layer Neural Network

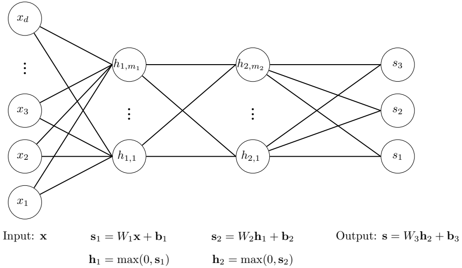
$\mathbf{s}_1 = W_1 \mathbf{x} + \mathbf{b}_1$ W_1 is $m_1 \times d$

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

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

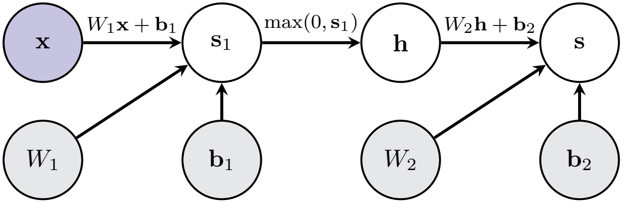
2nd hidden layer activations $\rightarrow$ $\mathbf{h}_2 = \max(0, \mathbf{s}_2)$ $\leftarrow$ apply non-linearity via **activation fn**

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

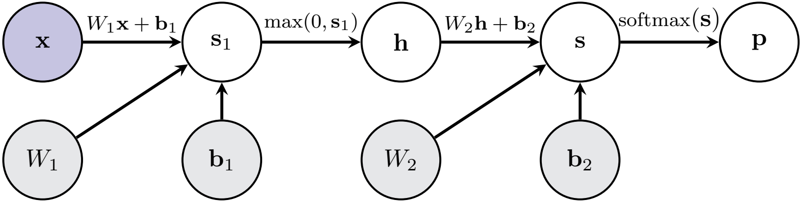


Sometimes referred to as a **2-hidden-layer neural network**.

Computational Graph of our 2-layer neural network

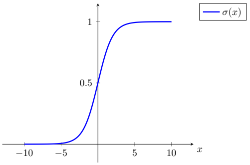


2-layer neural network with probabilistic outputs



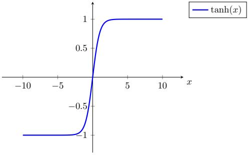
Options for activation functions

Sigmoid



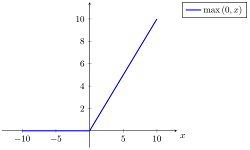
$$\sigma(x) = \frac{1}{1+\exp(-x)}$$

tanh



$$\mathsf{tanh}(x) = \frac{\exp(x)-\exp(-x)}{\exp(x)+\exp(-x)}$$

ReLu

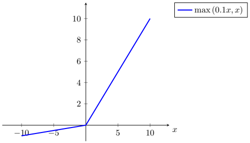


$$\mathsf{ReLu}(x) = \max(0, x)$$

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

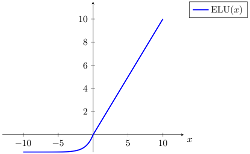
Options for activation Functions

Leaky ReLu



$\max(0.1x, x)$

ELU



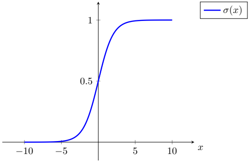
$$\mathsf{ELU}(x) = \begin{cases} x & \text{if } x > 0 \\ \alpha\left(\exp(x) - 1\right) & \text{otherwise} \end{cases}$$

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

Options for Activation Functions

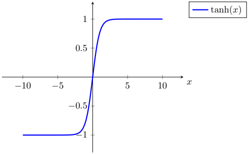
Sigmoid	**tanh**	**ReLu**

Sigmoid



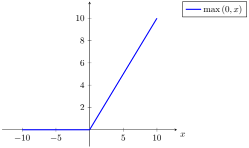
$\sigma(x) = \frac{1}{1+\exp(-x)}$

tanh



$\mathsf{tanh}(x) = \frac{\exp(x)-\exp(-x)}{\exp(x)+\exp(-x)}$

ReLu

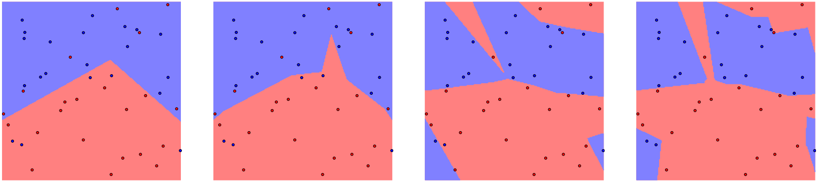


$\mathsf{ReLu}(x) = \max(0, x)$

✓

In modern networks ReLU is the most common activation function.

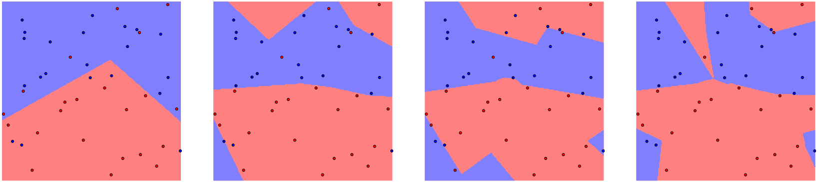
Effect of the number of hidden nodes in a 2 layer network



$m = 3$ $m = 20$ $m = 30$ $m = 100$

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

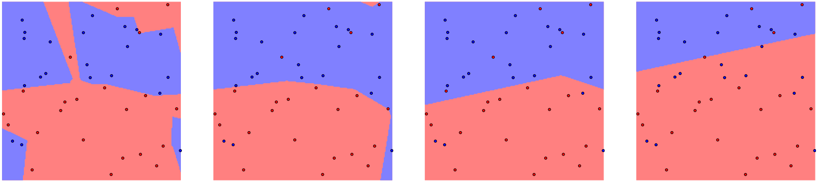
Result depends on parameter initialization



$m = 3$ $m = 20$ $m = 30$ $m = 100$

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

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



$\lambda = 0$ $\lambda = .001$ $\lambda = .01$ $\lambda = .1$

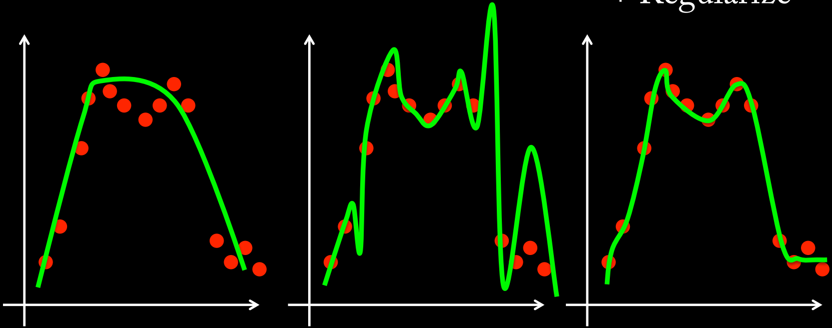
- $m = 100$ nodes in the hidden layer.
- L_2 regularization.

Do not use size of neural network as a regularizer.

Use stronger regularization.

Big Model + Regularize vs Small Model

Small model | Big model | Big model + Regularize



High-level overview of how to train network

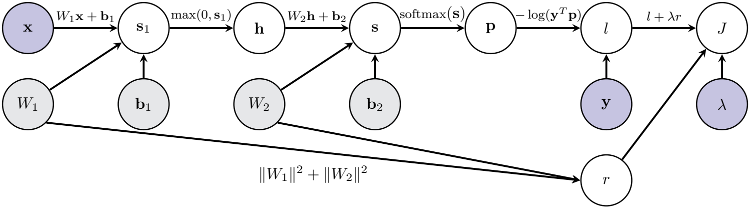
Mini-batch SGD (or variant)

Loop

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

Gradient Computations for a k-layer neural network

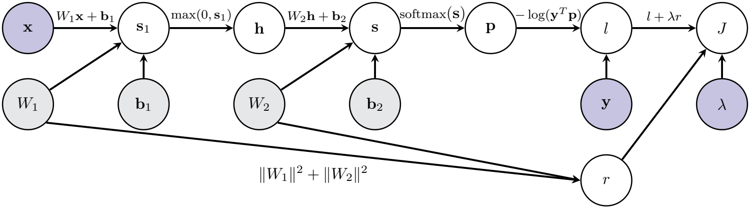
Back propagation for 2-layer neural network



For a single labelled training example:

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

Back propagation for 2-layer neural network



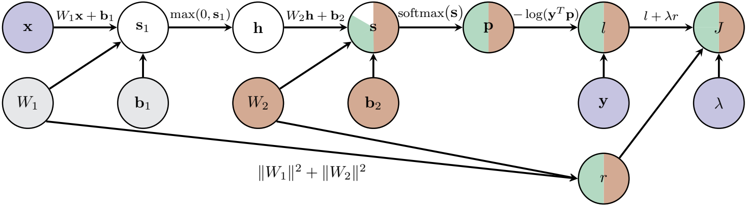
For a single labelled training example:

1. **Forward propagate** it through the graph and calculate loss.

   ↑ this is straightforward.

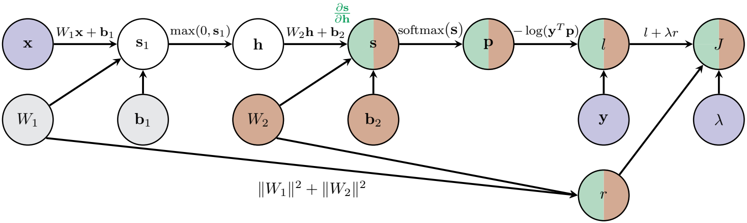
2. **Backward propagate** to calculate the gradients. ← Focus on this.

Starting point of our demonstration



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

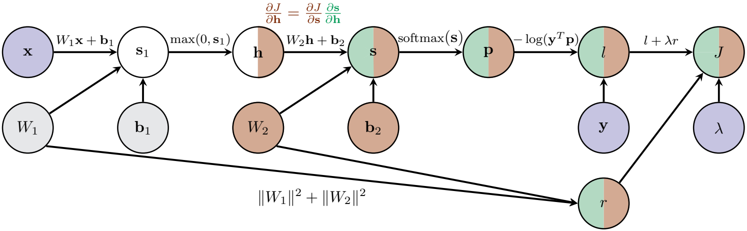
Compute local Jacobian of node $\mathbf{s}$ w.r.t. its child $\mathbf{h}$



$$\boxed{\mathbf{s} = W_2\mathbf{h} + \mathbf{b}_2}$$

- The Jacobian we need to compute: $\frac{\partial \mathbf{s}}{\partial \mathbf{h}} = \begin{pmatrix} \frac{\partial s_1}{\partial h_1} & \cdots & \frac{\partial s_1}{\partial h_m} \\ \vdots & \vdots & \vdots \\ \frac{\partial s_c}{\partial h_1} & \cdots & \frac{\partial s_c}{\partial h_m} \end{pmatrix}$
- The individual derivatives: $\frac{\partial s_i}{\partial h_j} = W_{2,ij}$
- In vector notation: $\frac{\partial \mathbf{s}}{\partial \mathbf{h}} = W_2$

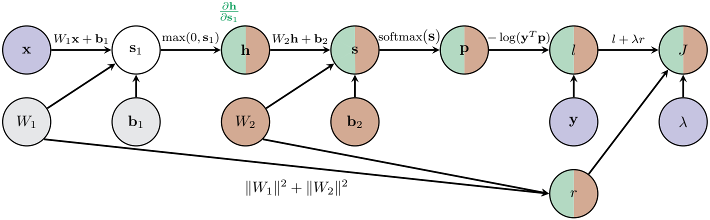
Compute gradient of J w.r.t. node $\mathbf{h}$



$$\boxed{\mathbf{s} = W_2\mathbf{h} + \mathbf{b}_2}$$

$$\frac{\partial J}{\partial \mathbf{h}} = \frac{\partial J}{\partial \mathbf{s}} \frac{\partial \mathbf{s}}{\partial \mathbf{h}}$$

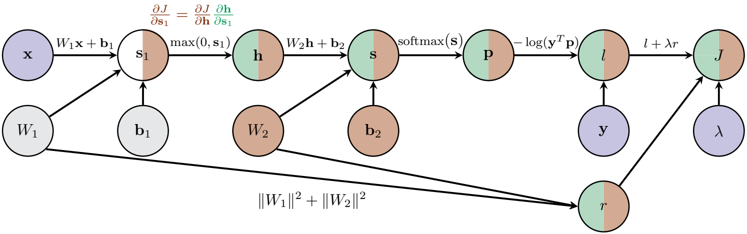
Compute local Jacobian of node $\mathbf{h}$ w.r.t. its child $\mathbf{s}_1$



$$\boxed{\mathbf{h} = \max(0, \mathbf{s}_1)}$$

- The Jacobian we need to compute: $\frac{\partial \mathbf{h}}{\partial \mathbf{s}_1} = \begin{pmatrix} \frac{\partial h_1}{\partial s_{1,1}} & \cdots & \frac{\partial h_1}{\partial s_{1,m}} \\ \vdots & \vdots & \vdots \\ \frac{\partial h_m}{\partial s_{1,1}} & \cdots & \frac{\partial h_c}{\partial s_{1,m}} \end{pmatrix}$
- The individual derivatives: $\frac{\partial h_i}{\partial s_{1,j}} = \begin{cases} \text{Ind}(s_{1,j} > 0) & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$
- In vector notation: $\frac{\partial \mathbf{h}}{\partial \mathbf{s}_1} = \text{diag}(\text{Ind}(\mathbf{s}_1 > 0))$

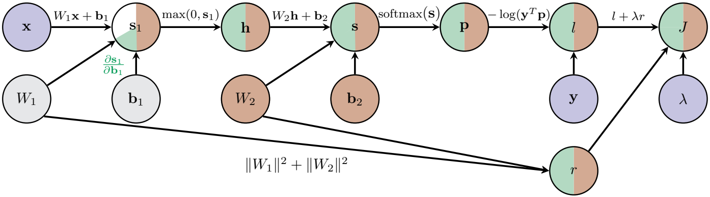
Compute gradient of J w.r.t. node $\mathbf{s}_1$



$$\mathbf{h} = \max(0, \mathbf{s}_1)$$

$$\frac{\partial J}{\partial \mathbf{s}_1} = \frac{\partial J}{\partial \mathbf{h}} \frac{\partial \mathbf{h}}{\partial \mathbf{s}_1}$$

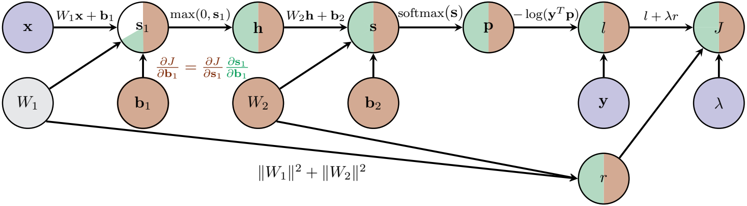
Compute local Jacobian of node $\mathbf{s}_1$ w.r.t. its child $\mathbf{b}_1$



$$\boxed{\mathbf{s}_1 = W_1\mathbf{x} + \mathbf{b}_1}$$

- The Jacobian we need to compute: $\frac{\partial \mathbf{s}_1}{\partial \mathbf{b}_1} = \begin{pmatrix} \frac{\partial s_{1,1}}{\partial b_{1,1}} & \cdots & \frac{\partial s_{1,1}}{\partial b_{1,m}} \\ \vdots & \vdots & \vdots \\ \frac{\partial s_{1,m}}{\partial b_{1,1}} & \cdots & \frac{\partial s_{1,m}}{\partial b_{1,m}} \end{pmatrix}$
- The individual derivatives: $\frac{\partial s_{1,i}}{\partial b_{1,j}} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$
- In vector notation: $\frac{\partial \mathbf{s}_1}{\partial \mathbf{b}_1} = I_m$

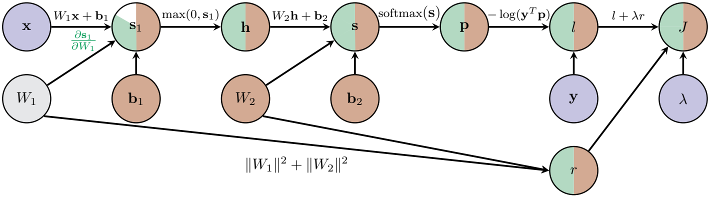
Compute gradient of J w.r.t. node $\mathbf{b}_1$



$$\boxed{\mathbf{s}_1 = W_1\mathbf{x} + \mathbf{b}_1}$$

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

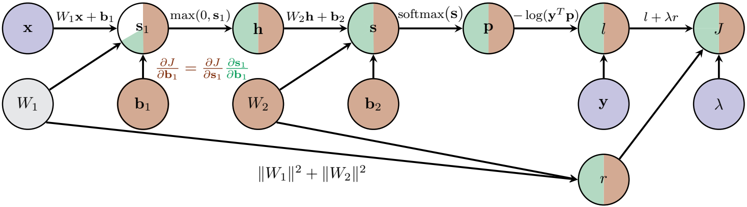
Compute local Jacobian of node s_1 w.r.t. its child W



$$\boxed{\mathbf{s}_1 = W_1\mathbf{x} + \mathbf{b}_1 = (I_m \otimes \mathbf{x})\,\mathrm{vec}(W_1)}$$

- Let $\mathbf{v} = \mathrm{vec}(W_1)$. Jacobian to compute: $\frac{\partial \mathbf{s}_1}{\partial \mathbf{v}} = \begin{pmatrix} \frac{\partial s_{1,1}}{\partial v_1} & \dots & \frac{\partial s_{1,1}}{\partial v_{dm}} \\ \vdots & \vdots & \vdots \\ \frac{\partial s_{1,m}}{\partial v_1} & \dots & \frac{\partial s_{1,m}}{\partial v_{dm}} \end{pmatrix}$
- The individual derivatives: $\frac{\partial s_{1,i}}{\partial v_j} = \begin{cases} x_{j-(i-1)d} & \text{if } (i-1)d+1 \le j \le id \\ 0 & \text{otherwise} \end{cases}$
- In vector notation: $\frac{\partial \mathbf{s}_1}{\partial \mathbf{v}} = I_m \otimes \mathbf{x}^T$

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



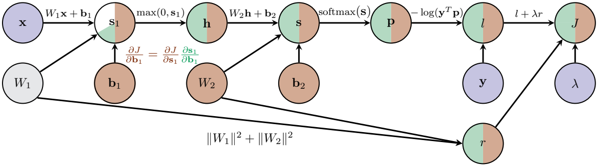
$$\mathbf{s}_1 = W_1\mathbf{x} + \mathbf{b}_1 = \left(I_m \otimes \mathbf{x}^T\right) \text{vec}(W_1) + \mathbf{b}_1$$

$$\frac{\partial J}{\partial \text{vec}(W_1)} = \frac{\partial J}{\partial \mathbf{s}_1} \frac{\partial \mathbf{s}_1}{\partial \text{vec}(W_1)} + \frac{\partial J}{\partial r} \frac{\partial r}{\partial \text{vec}(W_1)}$$

$$= \begin{pmatrix} g_1\mathbf{x}^T & g_2\mathbf{x}^T & \cdots & g_m\mathbf{x}^T \end{pmatrix} + \lambda\, \text{vec}(W_1)^T$$ ← gradient needed for learning

if we set $\mathbf{g} = \frac{\partial J}{\partial \mathbf{s}_1}$.

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



$$\boxed{\mathbf{s}_1 = W_1\mathbf{x} + \mathbf{b}_1 = \left(I_m \otimes \mathbf{x}^T\right)\text{vec}(W_1) + \mathbf{b}_1}$$

Can convert

$$\frac{\partial J}{\partial \text{vec}(W_1)} = \left(g_1\mathbf{x}^T \quad g_2\mathbf{x}^T \quad \cdots \quad g_m\mathbf{x}^T\right) + 2\lambda\,\text{vec}(W_1)^T$$

(where $\mathbf{g} = \frac{\partial J}{\partial \mathbf{s}_1}$) from a vector $(1 \times md)$ back to a 2D matrix $(m \times d)$:

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

Aggregated backward pass for a 2-layer neural network

1. Let
$$\mathbf{g} = -\frac{\mathbf{y}^T}{\mathbf{y}^T\mathbf{p}}\left(\text{diag}(\mathbf{p}) - \mathbf{p}\mathbf{p}^T\right)$$
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 $\mathbf{g}$ to the first layers
$$\mathbf{g} = \mathbf{g}W_2$$
$$\mathbf{g} = \mathbf{g}\,\text{diag}(\text{Ind}(\mathbf{s}_1 > 0)) \leftarrow \text{assuming ReLu activation}$$
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
$$\frac{\partial J}{\partial W_1} = \mathbf{g}^T\mathbf{x}^T + 2\lambda W_1$$

Gradient Computations for a mini-batch

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

- Compute gradients of l w.r.t. $W_1, W_2, \mathbf{b}_1, \mathbf{b}_2$ for each $(\mathbf{x}, y) \in \mathcal{D}^{(t)}$:
  - 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 $\mathbf{g} = -\frac{\mathbf{y}^T}{\mathbf{y}^T\mathbf{p}} \left(\text{diag}(\mathbf{p}) - \mathbf{p}\mathbf{p}^T\right)$
    2. Add gradient of l w.r.t. $\mathbf{b}_2$ computed at $(\mathbf{x}, y)$
    $$\frac{\partial L}{\partial \mathbf{b}_2} \mathrel{+}= \mathbf{g}, \quad \frac{\partial L}{\partial W_2} \mathrel{+}= \mathbf{g}^T\mathbf{h}^T$$
    3. Propagate the gradients
    $$\mathbf{g} = \mathbf{g}W_2$$
    $$\mathbf{g} = \mathbf{g}\ \text{diag}(\text{Ind}(\mathbf{s}_1 > 0))$$
    4. Add gradient of l w.r.t. first layer parameters computed at $(\mathbf{x}, y)$
    $$\frac{\partial L}{\partial \mathbf{b}_1} \mathrel{+}= \mathbf{g}, \quad \frac{\partial L}{\partial W_1} \mathrel{+}= \mathbf{g}^T\mathbf{x}^T$$
  - Divide by the number of entries in $\mathcal{D}^{(t)}$:
  $$\frac{\partial L}{\partial W_i} \mathrel{/}= |\mathcal{D}^{(t)}|, \quad \frac{\partial L}{\partial \mathbf{b}_i} \mathrel{/}= |\mathcal{D}^{(t)}| \quad \text{for } i = 1, 2$$
- Add the gradient for the regularization term
$$\frac{\partial J}{\partial W_i} = \frac{\partial L}{\partial W_i} + 2\lambda W_i, \quad \frac{\partial J}{\partial \mathbf{b}_i} = \frac{\partial L}{\partial \mathbf{b}_i} \quad \text{for } i = 1, 2$$

Forward pass for a k-layer neural network

- Let $\mathbf{x}^{(0)} = \mathbf{x}$ 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

$$\mathbf{s}^{(k)} = W_k \mathbf{x}^{(k-1)} + \mathbf{b}_k$$

- 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 $\mathbf{y}$

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

Assumed ReLu is the activation function at each intermediary layer.

Aggregated Backward pass for a k-layer neural network

The gradient computation for one training example $(\mathbf{x}, y)$:

- Let

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

- for $i = k, k-1, \ldots, 1$

  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 W_i

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

  3. Propagate the gradient vector $\mathbf{g}$ to the previous layer (if $i > 1$)

  $$\mathbf{g} = \mathbf{g} W_i$$
  $$\mathbf{g} = \mathbf{g} \, \text{diag}(\text{Ind}(\mathbf{s}^{(i)} > 0))$$

Training Neural Networks a little 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:

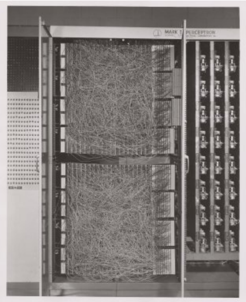
$$f(\mathbf{x}; \mathbf{w}) = \begin{cases} 1 & \text{if } \mathbf{w}^T\mathbf{x} + \mathbf{b} > 0 \\ 0 & \text{otherwise} \end{cases}$$

- For labelled training example $(\mathbf{x}, y)$ ($y \in \{-1, 1\}$) the Perceptron loss is

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

- **Update rule**: Use SGD to learn $\mathbf{w}$. If training example $(\mathbf{x}_i, y_i)$ is incorrectly classified then

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



A bit of history

- ADALINE (Adaptive Linear Element) developed by **Widrow** and **Hoff** at Stanford in 1960.
- Adaline a single layer neural network with one output

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

- **Loss function**: for labelled training example $(\mathbf{x}, y)$

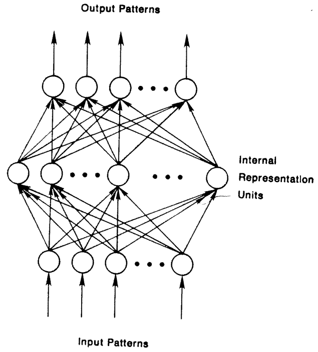
$$l(\mathbf{x}, y, \mathbf{w}) = (y - (\mathbf{w}^T\mathbf{x} + b))^2 = (y - \hat{y})^2$$

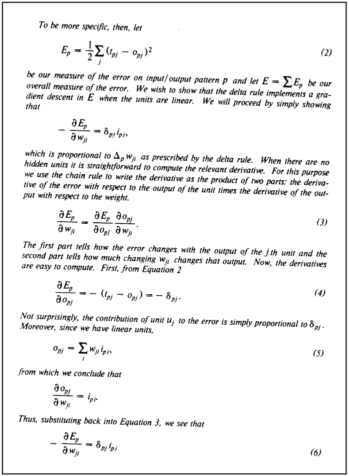
- **Update rule**: Use SGD with learning rate η to learn $\mathbf{w}$:

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

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

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





To be more specific, then, let

$$E_p = \frac{1}{2}\sum_j (t_{pj} - o_{pj})^2 \qquad (2)$$

be our measure of the error on input/output pattern p *and let* $E = \sum E_p$ *be our overall measure of the error. We wish to show that the delta rule implements a gradient descent in* E *when the units are linear. We will proceed by simply showing that*

$$-\frac{\partial E_p}{\partial w_{ji}} = \delta_{pj} i_{pi},$$

which is proportional to $\Delta_p w_{ji}$ *as prescribed by the delta rule. When there are no hidden units it is straightforward to compute the relevant derivative. For this purpose we use the chain rule to write the derivative as the product of two parts: the derivative of the error with respect to the output of the unit times the derivative of the output with respect to the weight.*

$$\frac{\partial E_p}{\partial w_{ji}} = \frac{\partial E_p}{\partial o_{pj}} \frac{\partial o_{pj}}{\partial w_{ji}}. \qquad (3)$$

The first part tells how the error changes with the output of the j*th unit and the second part tells how much changing* w_{ji} *changes that output. Now, the derivatives are easy to compute. First, from Equation 2*

$$\frac{\partial E_p}{\partial o_{pj}} = -(t_{pj} - o_{pj}) = -\delta_{pj}. \qquad (4)$$

Not surprisingly, the contribution of unit u_j *to the error is simply proportional to* δ_{pj}. *Moreover, since we have linear units,*

$$o_{pj} = \sum_i w_{ji} i_{pi}, \qquad (5)$$

from which we conclude that

$$\frac{\partial o_{pj}}{\partial w_{ji}} = i_{pi}.$$

Thus, substituting back into Equation 3, we see that

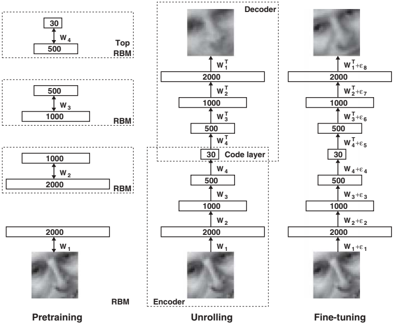
$$-\frac{\partial E_p}{\partial w_{ji}} = \delta_{pj} i_{pi} \qquad (6)$$

First time back-propagation became popular

A bit of history

New wave of research in Deep Learning.

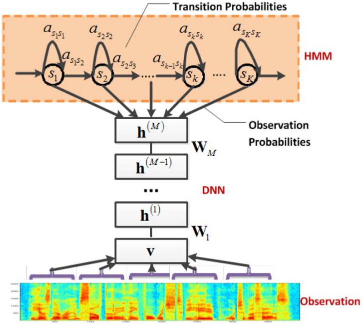
- Ability to train networks with many layers.
- Mixture of unsupervised and supervised training.
- **Unsupervised**: Encoding layers first learnt in stagewise manner using RBMs (restricted Boltzman machines).
- Decode layers using an auto-encoder.
- **Supervised**: Back-prop used to do final update of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



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

First Very Convincing Results

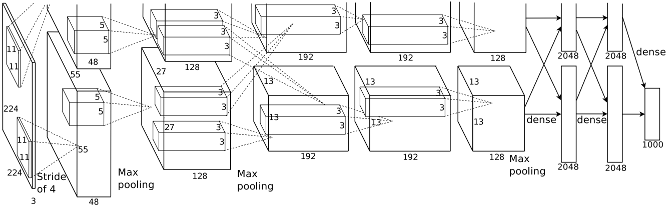
- **Context-Dependent Pre-trained Deep Neural Networks for Large Vocabulary Speech Recognition**, G. Dahl, D. Yu, L. Deng, A. Acero, 2010.



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

First Very Convincing Results

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



- Beat the stagnating established approaches of

  Handcrafted features + kernel SVM.

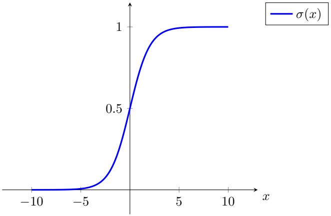
- Improved results on ImageNet by ∼11%.

Better understanding of gradient flows during BackProp helped with these breakthroughs

Understanding Effect of Activation Functions

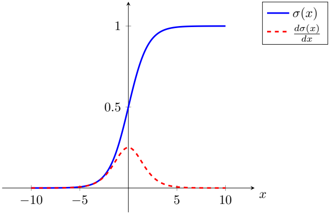
Sigmoid

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



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

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



Problems

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

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

   - Derivative of the sigmoid function is:

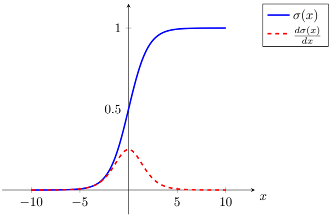
$$\frac{\partial h_i}{\partial s_j} = \begin{cases} \frac{\exp(-s_i)}{(1+\exp(-s_i))^2} \quad (= \sigma'(s_i)) & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$$

   - 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 $|s_i| > 5$?

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



Problems

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

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

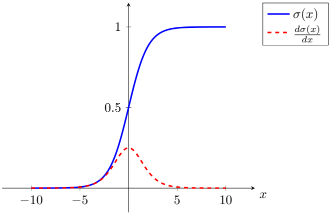
   - Then

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

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

Sigmoid

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



Problems

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

     $$\mathbf{s} = W\mathbf{x} + \mathbf{b}, \quad \mathbf{h} = \sigma(\mathbf{s})$$

   - Then

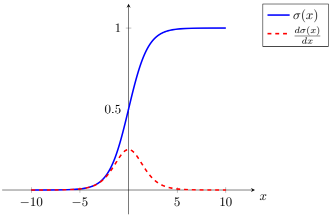
     $$\frac{\partial J}{\partial \mathbf{w}_i} = \frac{\partial J}{\partial h_i}\frac{\partial h_i}{\partial s_i}\frac{\partial s_i}{\partial \mathbf{w}_i} = \underbrace{\frac{\partial J}{\partial h_i}}_{\text{positive or negative}} \; \underbrace{\sigma'(s_i)}_{\text{positive}} \; \underbrace{\mathbf{x}^T}_{\text{all positive}}$$

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

$\Longrightarrow$ entries of $\frac{\partial J}{\partial \mathbf{w}_i}$ are either all positive or all negative.

Sigmoid

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



Problems

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

$$\mathbf{s} = W\mathbf{x} + \mathbf{b}, \quad \mathbf{h} = \sigma(\mathbf{s})$$

   - Then

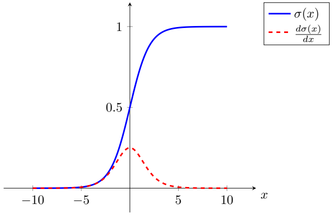
$$\frac{\partial J}{\partial \mathbf{w}_i} = \frac{\partial J}{\partial h_i}\frac{\partial h_i}{\partial s_i}\frac{\partial s_i}{\partial \mathbf{w}_i} = \frac{\partial J}{\partial \mathbf{w}_i} \quad = \frac{\partial J}{\partial h_i}\frac{\partial h_i}{\partial s_i}\frac{\partial s_i}{\partial \mathbf{w}_i}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

What is $\frac{\partial J}{\partial \mathbf{w}_i}$ when all entries in $\mathbf{x}$ are $+$tive? (occurs after applying sigmoid)

$\Longrightarrow$ entries of $\frac{\partial J}{\partial \mathbf{w}_i}$ are either all positive or all negative.

$\Longrightarrow$ inefficient zig-zag update paths to find optimal $\mathbf{w}_i$

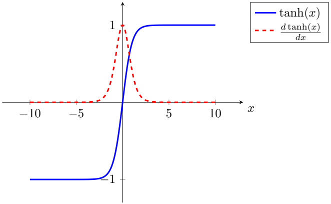
$$\sigma(x) = \frac{1}{1 + \exp(-x)}$$



Problems

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

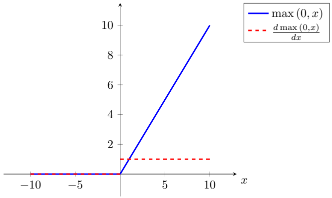
$$\tanh(x) = \frac{\exp(x) - \exp(-x)}{\exp(x) + \exp(-x)}$$



Properties

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

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

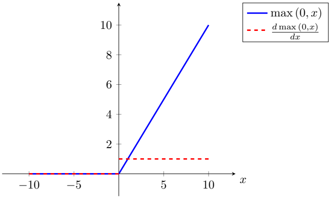


Pros

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.

Rectified Linear Unit (ReLu)

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



Problems

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

$$\mathbf{s} = W\mathbf{x} + \mathbf{b}$$
$$\mathbf{h} = \max(0, \mathbf{s})$$

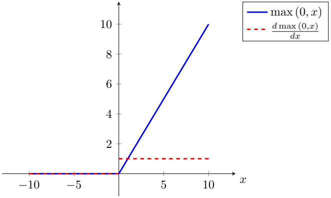
   - Derivative of the ReLu function is:

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

   - Then

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

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



Problems

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

   As

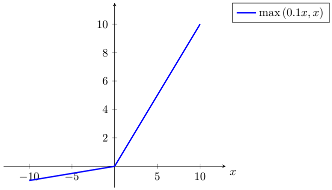
$$\mathbf{s} = W\mathbf{x} + \mathbf{b}, \quad \mathbf{h} = \max(0, \mathbf{s})$$

   then

$$\frac{\partial J}{\partial \mathbf{w}_i} = \frac{\partial J}{\partial h_i}\frac{\partial h_i}{\partial s_i}\frac{\partial s_i}{\partial \mathbf{w}_i} = \begin{cases} \frac{\partial J}{\partial h_i}\ \mathbf{x}^T & \text{if } s_i > 0 \\ \mathbf{0} & \text{otherwise} \end{cases}$$

$\Longrightarrow$ dead ReLU will never activate

$\Longrightarrow$ never update parameter weights.



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

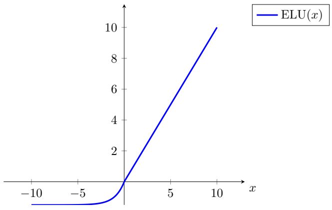
Pros

1. Does not saturate.
2. Computationally efficient.
3. 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]

Exponential Linear Units (ELU)

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



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]

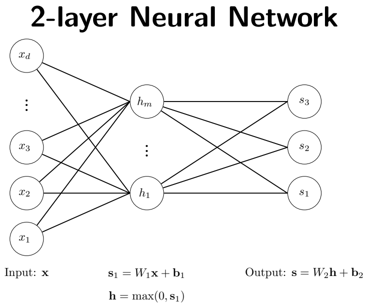
Which Activation Function?

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.

Effect of weight initialization & activation function on gradient flow

Pathological weight initialization



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

Initialize with small random numbers

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

What happens in this case?

Initialize with small random numbers

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

What happens in this case?

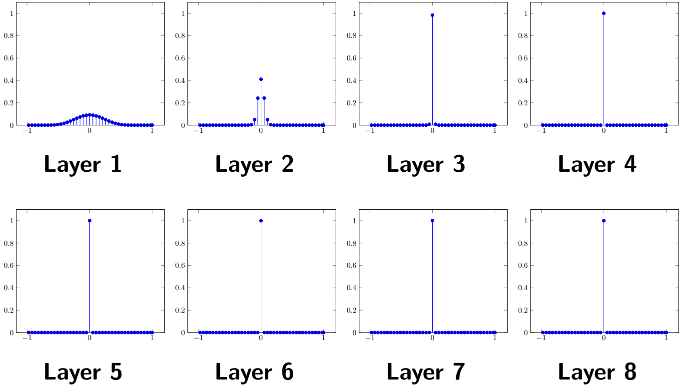
Works okay for small networks, but can lead to non-homogeneous distributions of activations across the layers of a deep network.

Some activation histograms

- 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 $(N(0, 1^2))$ with $d = 500$.

Some activation histograms

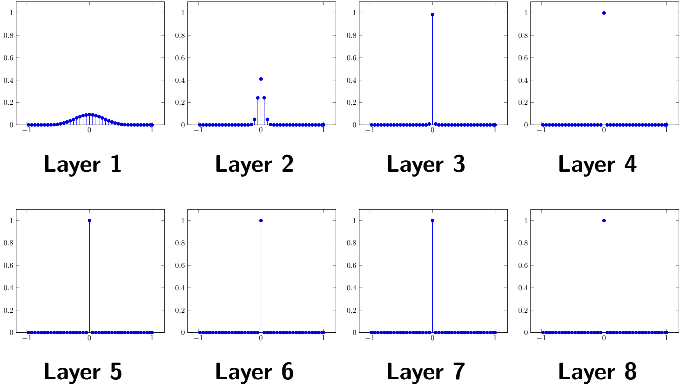
- Initialize a 10-layer network with 500 nodes at each layer.
- Use a `tanh` activation function at each layer.
- Initialize weights will small random numbers.
- Generate random input data $(N(0, 1^2))$ with $d = 500$.



Histograms of activations at each layer

Some activation histograms

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



Histograms of activations at each layer

Aggregated Backward pass for a k-layer neural network

The gradient computation for one training example $(\mathbf{x}, y)$:

- Let

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

- for $i = k, k-1, \ldots, 1$
  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 W_i

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

  3. Propagate the gradient vector $\mathbf{g}$ to the previous layer (if $i > 1$)

  $$\mathbf{g} = \mathbf{g}W_i$$

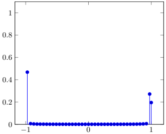
  $$\mathbf{g} = \mathbf{g}\ \text{diag}(\text{Ind}(\mathbf{s}^{(i)} > 0))$$

Change the initialization to bigger random numbers

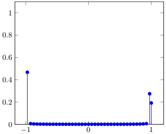
- Initialize a 10-layer network with 500 nodes at each layer.
- Use a `tanh` activation function at each layer.
- Initialize weights with bigger random numbers: $W_{i,lm} \sim N(w; 0, 1^2)$.
- Generate random input data $(N(0, 1^2))$ with $d = 500$.

Change the initialization to bigger random numbers

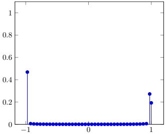
- Initialize a 10-layer network with 500 nodes at each layer.
- Use a `tanh` activation function at each layer.
- Initialize weights with bigger random numbers: $W_{i,lm} \sim N(w; 0, 1^2)$.
- Generate random input data ($N(0, 1^2)$) with $d = 500$.



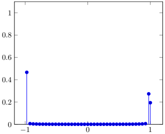
Layer 1



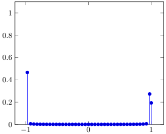
Layer 2



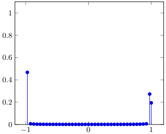
Layer 3



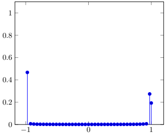
Layer 4



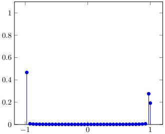
Layer 5



Layer 6



Layer 7

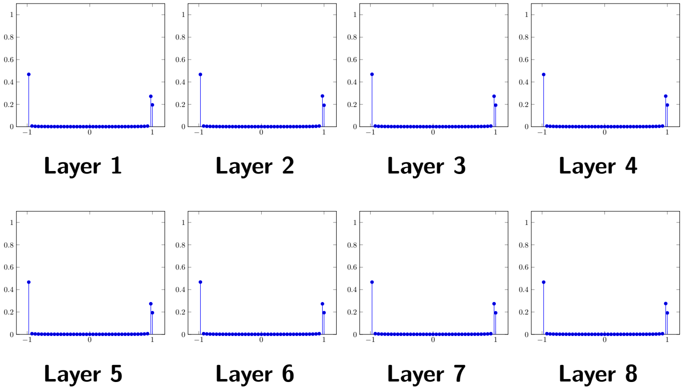


Layer 8

Histograms of activations at each layer

Change the initialization to bigger random numbers

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



Histograms of activations at each layer

Aggregated Backward pass for a k-layer neural network

The gradient computation for one training example $(\mathbf{x}, y)$:

- Let

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

- for $i = k, k-1, \ldots, 1$
  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 W_i

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

  3. Propagate the gradient vector $\mathbf{g}$ to the previous layer (if $i > 1$)

  $$\mathbf{g} = \mathbf{g} W_i$$

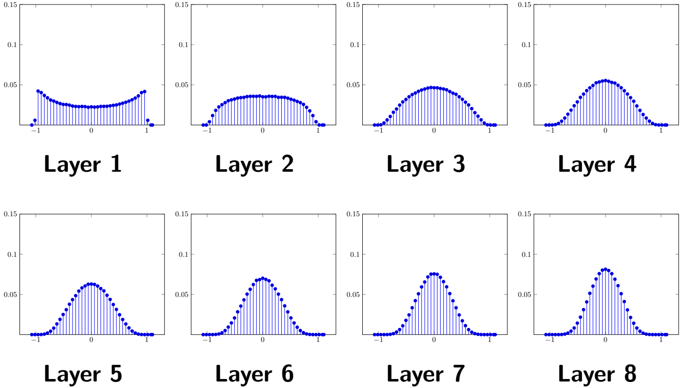
  $$\mathbf{g} = \mathbf{g}\ \text{diag}(\text{tanh}'(\mathbf{s}^{(i)}))$$

Change the initialization to Xavier initialization

- Initialize a 10-layer network with 500 nodes at each layer.
- Use a `tanh` activation function at each layer.
- Initialize weights with Xavier initialization: $W_{i,lm} \sim N(w; 0, 1/\sqrt{500})$.
- Generate random input data ($N(0, 1^2)$) with $d = 500$.

Change the initialization to Xavier initialization

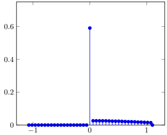
- Initialize a 10-layer network with 500 nodes at each layer.
- Use a `tanh` activation function at each layer.
- Initialize weights with Xavier initialization: $W_{i,lm} \sim N(w; 0, 1/\sqrt{500})$.
- Generate random input data $(N(0, 1^2))$ with $d = 500$.



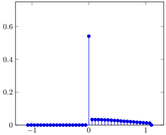
Histograms of activations at each layer

Xavier initialization doesn't work for ReLu activation

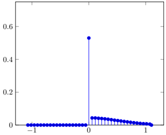
- Initialize a 10-layer network with 500 nodes at each layer.
- Use a `ReLu` activation function at each layer.
- Initialize weights with Xavier initialization: $W_{i,lm} \sim N(w; 0, 1/\sqrt{500})$.
- Generate random input data $(N(0, 1^2))$ with $d = 500$.



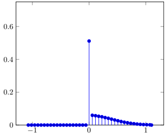
Layer 1



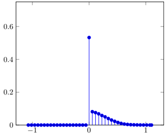
Layer 2



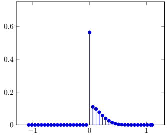
Layer 3



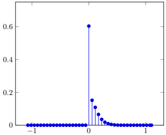
Layer 4



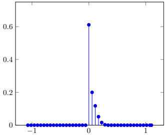
Layer 5



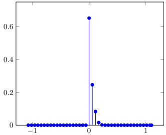
Layer 6



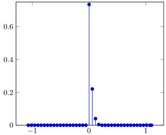
Layer 7



Layer 8



Layer 9



Layer 10

Histograms of activations at each layer

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

Lessening the effect of initialization: Batch normalization

- 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. Ioffe, C. Szegedy, arXiv 2015.

- Consider activations at some layer for a batch: $\mathbf{s}_1^{(j)}, \mathbf{s}_2^{(j)} \ldots, \mathbf{s}_n^{(j)}$

- To make each dimension unit gaussian, apply:

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

where

$$\boldsymbol{\mu} = \frac{1}{n}\sum_{i=1}^{n} \mathbf{s}_i^{(j)}, \quad \sigma_p^2 = \frac{1}{n}\sum_{i=1}^{n} (s_i^{(j)}, p - \mu_p)^2$$

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

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

    end
    Compute batch mean and variances of ith layer:

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

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

    $$\hat{\mathbf{s}}^{(i)} = \text{BatchNormalise}(\mathbf{s}^{(i)}, \boldsymbol{\mu}, \sigma_1, \ldots, \sigma_{m_i})$$
    $$\mathbf{x}^{(i)} = \max\left(0, \hat{\mathbf{s}}^{(i)}\right)$$

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

Batch Normalization: Scale & shift range

- 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 $\gamma^{(i)}$'s and $\beta^{(i)}$'s and add them as parameters of the network.

- To keep things simple this added complexity is often omitted.

Benefits of Batch Normalization

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

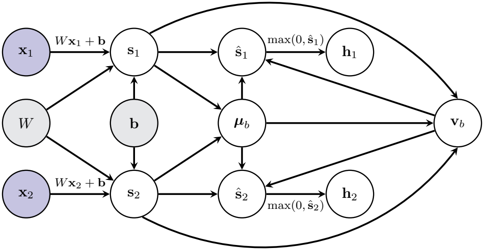
If training a deep network, you should use **Batch Normalization**.

Batch Normalization at Test Time

- 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).

Back-Prop for a Batch Normalization layer.

Computational Graph for a BN layer



- Compute the mean and variance for the *scores* in the batch:

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

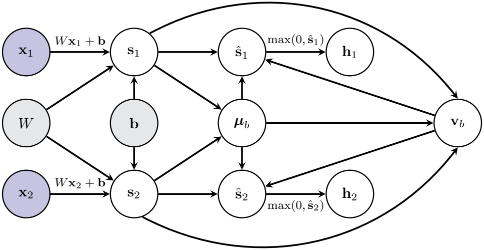
where $\mathbf{v}_b = (v_{b,1}, v_{b,2}, \ldots, v_{b,m})^T$. ($n = 2$ in the figure.) Define

$$V_b = \text{diag}(\mathbf{v}_b + \epsilon)$$

- Apply **batch normalization** function to each *score* vector:

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

Gradient Computations for a BN layer

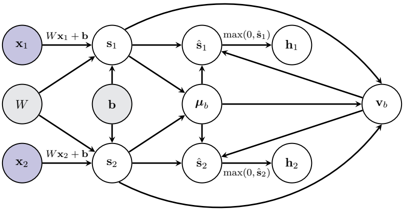


- Want to compute $\frac{\partial J}{\partial \mathbf{s}_i}$ for each $\mathbf{s}_i$ in the batch.
- The children of node $\mathbf{s}_i$ are $\{\hat{\mathbf{s}}_i, \mathbf{v}_b, \boldsymbol{\mu}_b\}$ thus

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

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

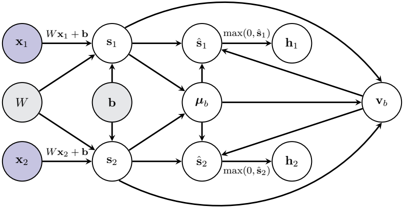
Gradient Computations for a BN layer



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

↑ assume already computed

Gradient Computations for a BN layer



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

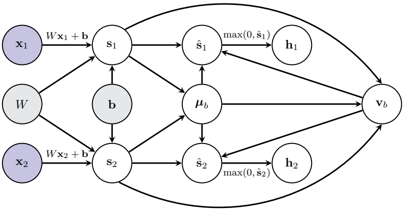
- The equation relating $\hat{\mathbf{s}}_i$ to $\mathbf{v}_b$ (remember $V_b = \text{diag}(\mathbf{v}_b + \epsilon)$)

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

- Therefore

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

Gradient Computations for a BN layer

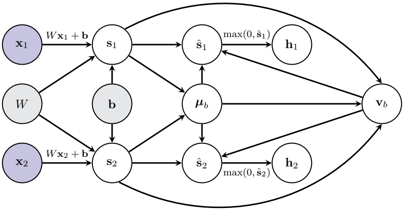


$$\frac{\partial J}{\partial \mathbf{s}_i} = \frac{\partial J}{\partial \hat{\mathbf{s}}_i}\frac{\partial \hat{\mathbf{s}}_i}{\partial \mathbf{s}_i} + \frac{\partial J}{\partial \mathbf{v}_b}\frac{\partial \mathbf{v}_b}{\partial \mathbf{s}_i} + \frac{\partial J}{\partial \boldsymbol{\mu}_b}\frac{\partial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

- The children of node $\mathbf{v}_b$ are $\{\hat{\mathbf{s}}_1, \ldots, \hat{\mathbf{s}}_n\}$
- Therefore

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

Gradient Computations for a BN layer

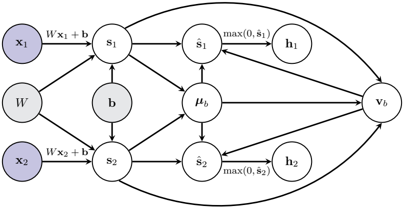


$$\frac{\partial J}{\partial \mathbf{s}_i} = \frac{\partial J}{\partial \hat{\mathbf{s}}_i}\frac{\partial \hat{\mathbf{s}}_i}{\partial \mathbf{s}_i} + \frac{\partial J}{\partial \mathbf{v}_b}\frac{\partial \mathbf{v}_b}{\partial \mathbf{s}_i} + \frac{\partial J}{\partial \boldsymbol{\mu}_b}\frac{\partial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

- The children of node $\mathbf{v}_b$ are $\{\hat{\mathbf{s}}_1, \ldots, \hat{\mathbf{s}}_n\}$
- Therefore

$$\frac{\partial J}{\partial \mathbf{v}_b} = \sum_{i=1}^{n} \underset{\substack{\uparrow \\ \text{assume known}}}{\frac{\partial J}{\partial \hat{\mathbf{s}}_i}} \quad \frac{\partial \hat{\mathbf{s}}_i}{\partial \mathbf{v}_b}$$

Gradient Computations for a BN layer



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

- The children of node $\mathbf{v}_b$ are $\{\hat{\mathbf{s}}_1, \ldots, \hat{\mathbf{s}}_n\}$
- Therefore

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

↑ compute now

Gradient Computations for a BN layer

- The equation relating $\hat{\mathbf{s}}_i$ to $\mathbf{v}_b$ (remember $V_b = \text{diag}(\mathbf{v}_b + \epsilon)$)

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

- The local Jacobian we want to compute

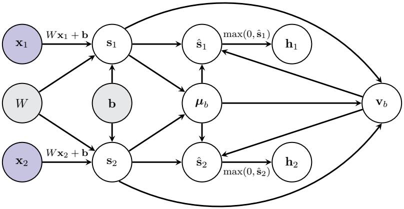
$$\frac{\partial \hat{\mathbf{s}}_i}{\partial \mathbf{v}_b} = \begin{pmatrix} \frac{\partial \hat{s}_{i,1}}{\partial v_{b,1}} & \cdots & \frac{\partial \hat{s}_{i,1}}{\partial v_{b,m}} \\ \vdots & \vdots & \vdots \\ \frac{\partial \hat{s}_{i,m}}{\partial v_{b,1}} & \cdots & \frac{\partial \hat{s}_{i,m}}{\partial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

- 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

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



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

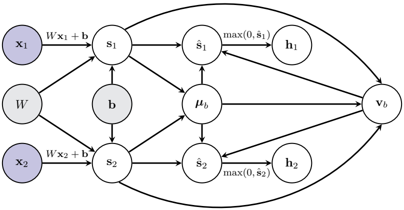
- Next $\frac{\partial \mathbf{v}_b}{\partial \mathbf{s}_i} = \frac{2}{n}\,\text{diag}\left(\mathbf{s}_i - \boldsymbol{\mu}_b\right)$.
- As

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

and

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

Gradient Computations for a BN layer



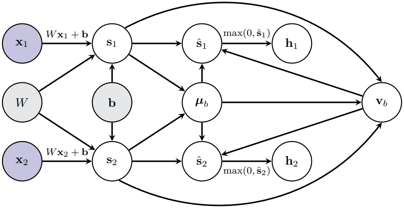
$$\frac{\partial J}{\partial \mathbf{s}_i} = \frac{\partial J}{\partial \hat{\mathbf{s}}_i}\frac{\partial \hat{\mathbf{s}}_i}{\partial \mathbf{s}_i} + \frac{\partial J}{\partial \mathbf{v}_b}\frac{\partial \mathbf{v}_b}{\partial \mathbf{s}_i} + \frac{\partial J}{\partial \boldsymbol{\mu}_b}\frac{\partial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

- The children of node $\boldsymbol{\mu}_b$ are $\{\hat{\mathbf{s}}_1, \ldots, \hat{\mathbf{s}}_n, \mathbf{v}_b\}$.
- Therefore

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

Gradient Computations for a BN layer

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



- The equation relating $\hat{\mathbf{s}}_i$ to $\boldsymbol{\mu}_b$ (remember $V_b = \text{diag}(\mathbf{v}_b + \epsilon)$)

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

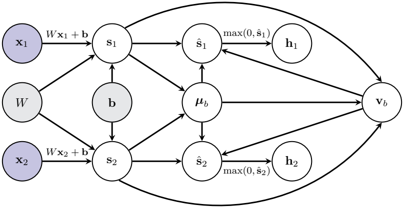
- The local Jacobian we want to compute

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

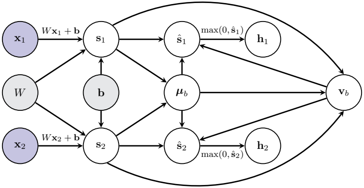
Gradient Computations for a BN layer

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

already calculated



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



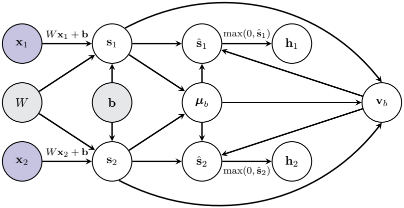
- Next $\frac{\partial \mathbf{v}_b}{\partial \boldsymbol{\mu}_b} = -\frac{2}{n} \operatorname{diag}\left(\sum_{i=1}^{n} (\mathbf{s}_i - \boldsymbol{\mu}_b)\right)$.
- As

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

and

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

Gradient Computations for a BN layer



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

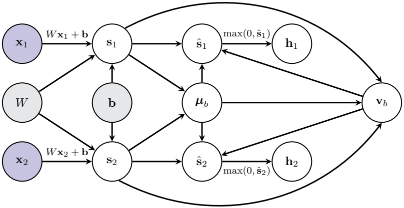
- The equation relating $\boldsymbol{\mu}_b$ to $\mathbf{s}_l$'s is

$$\boldsymbol{\mu}_b = \frac{1}{n}\sum_{l=1}^{n} \mathbf{s}_l$$

- Therefore

$$\frac{\partial \boldsymbol{\mu}_b}{\partial \mathbf{s}_i} = \frac{1}{n}$$

Putting everything together



$$\frac{\partial J}{\partial \mathbf{v}_b} = -\frac{1}{2} \sum_{i=1}^{n} \frac{\partial J}{\partial \hat{\mathbf{s}}_i} V_b^{-\frac{3}{2}} (\mathbf{s}_i - \boldsymbol{\mu}_b)$$

$$\frac{\partial J}{\partial \boldsymbol{\mu}_b} = -\sum_{i=1}^{n} \frac{\partial J}{\partial \hat{\mathbf{s}}_i} V_b^{-\frac{1}{2}} - \frac{2}{n} \frac{\partial J}{\partial \mathbf{v}_b} \,\mathsf{diag}\left(\sum_{i=1}^{n} (\mathbf{s}_i - \boldsymbol{\mu}_b) \right)$$

$$\frac{\partial J}{\partial \mathbf{s}_i} = \frac{\partial J}{\partial \hat{\mathbf{s}}_i} V_b^{-\frac{1}{2}} + \frac{2}{n} \frac{\partial J}{\partial \mathbf{v}_b} \mathsf{diag}\,(\mathbf{s}_i - \boldsymbol{\mu}_b) + \frac{\partial J}{\partial \boldsymbol{\mu}_b} \frac{1}{n}$$