Lecture 4 - k-layer Neural Networks

DD2424

April 8, 2017

Linear scoring function

$$e = W_{\mathbf{v}} \perp \mathbf{k}$$

2-layer Neural Network
$$\mathbf{s}_1 = W_1\mathbf{x} + \mathbf{b}_1$$

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

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

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



Before

Now

Some terminology

Not restricted to two layers

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

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

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



3-layer Neural Network

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

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

$$\mathbf{s}_2 = W_2 \mathbf{h}_1 + \mathbf{b}_2$$

$$\mathbf{h}_2 = \max(0, \mathbf{s}_2)$$

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

3-layer Neural Network

 $\mathbf{s}_1 = W_1\mathbf{x} + \mathbf{b}_1$ $W_1 = m_1 \times d$ 1st hidden layer activations o $h_1 = max(0, s_1) \leftarrow$ apply non-linearity via activation fn

 $s_2 = W_2 h_1 + b_2$ $W_2 is m_2 \times m_1$

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

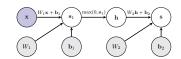
Sometimes referred to as a 2-hidden-layer neural network.

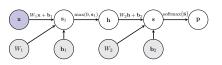
2-layer Neural Network

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



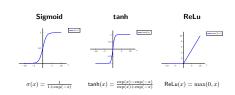
$$\mathbf{s} = W\mathbf{x} + \mathbf{b}$$



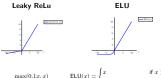


Options for activation functions

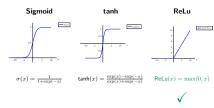
Options for activation Functions



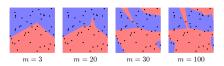
Activation function is applied independently to each element of the score vector.



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

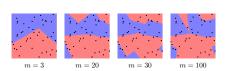


In modern networks ReLU is the most common activation function.



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

Result depends on parameter initialization



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

Effect of regularization

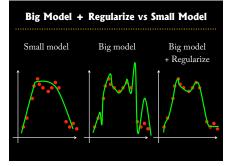
$$J(\mathcal{D},\lambda,\Theta) = \sum_{(\mathbf{x},y)\in\mathcal{D}} l(\mathbf{x},y,\Theta) + \lambda R(\Theta)$$

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

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

Do not use size of neural network as a regularizer.

Use stronger regularization.



Gradient Computations for a k-layer neural network

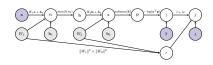
High-level overview of how to train network

Mini-batch SGD (or variant)

Loop

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

Back propagation for 2-layer neural network

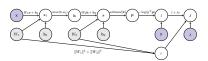


For a single labelled training example:

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

Back propagation for 2-layer neural network

Backward Pass: Gradient of current node



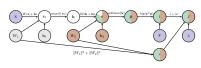
For a single labelled training example:

- 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

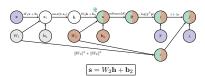


In Lecture 3 explicitly computed **filled in** *local Jacobians* and *gradients*.

Backward Pass

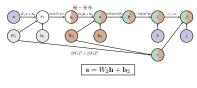
Backward Pass

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



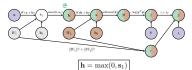
- The Jacobian we need to compute: $\frac{\partial x}{\partial h} = \begin{pmatrix} \frac{\partial x_1}{\partial h_1} & \cdots & \frac{\partial x_1}{\partial h_m} \\ \vdots & \vdots & \vdots \\ \frac{\partial x_n}{\partial h_n} & \cdots & \frac{\partial x_n}{\partial h_m} \end{pmatrix}$
- The individual derivatives: \$\frac{\partial s_i}{\partial h_i} = W_{2,ij}\$
- In vector notation: $\frac{\partial \mathbf{s}}{\partial \mathbf{b}} = W_2$

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



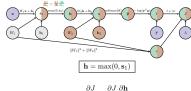
$$\frac{\partial J}{\partial \mathbf{h}} = \frac{\partial J}{\partial \mathbf{s}} \frac{\partial \mathbf{s}}{\partial \mathbf{h}}$$

Compute local Jacobian of node h w.r.t. its child si



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

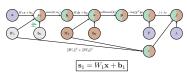
Compute gradient of J w.r.t. node s_1



Backward Pass

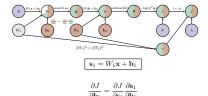
Backward Pass

Compute local Jacobian of node s1 w.r.t. its child b1

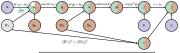


- The Jacobian we need to compute: $\frac{\partial s_1}{\partial b_1} = \begin{pmatrix} \frac{\partial s_1}{\partial b_1,1} & \cdots & \frac{\partial s_{1,1}}{\partial b_1,n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial s_1}{\partial b_1,1} & \cdots & \frac{\partial s_1}{\partial b_1,n} \end{pmatrix}$
- 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: ^{∂s₁}/_{∂b₁} = I_m

Compute gradient of J w.r.t. node b_1



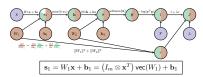
Compute local Jacobian of node \mathbf{s}_1 w.r.t. its child W



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

- Let $\mathbf{v} = \text{vec}(W_1)$. Jacobian to compute: $\frac{\partial s_1}{\partial \mathbf{v}} = \begin{pmatrix} \frac{\partial s_{1,1}}{\partial v_1} & \cdots & \frac{\partial s_{1,1}}{\partial v_1} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial s_{1,m}}{\partial v_1} & \cdots & \frac{\partial s_{1,m}}{\partial v_d} \end{pmatrix}$
- $\bullet \ \ \text{The individual derivatives:} \ \frac{\partial s_{1,i}}{\partial v_j} = \begin{cases} x_{j-(i-1)d} & \text{if } (i-1)d+1 \leq j \leq id \\ 0 & \text{otherwise} \end{cases}$
- In vector notation: ^{∂s₁}/_{∂v} = I_m ⊗ x^T

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

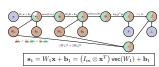


$$\begin{split} \frac{\partial J}{\partial \text{vec}(W_1)} &= \frac{\partial J}{\partial \mathbf{s}_1} \frac{\partial \mathbf{s}_1}{\partial \text{vec}(W_1)} + \frac{\partial J}{\partial r} \frac{\partial r}{\partial \text{vec}(W_1)} \\ &= \left(g_1 \mathbf{x}^T - g_2 \mathbf{x}^T - \cdots - g_m \mathbf{x}^T\right) + \lambda \text{vec}(W_1)^T & \leftarrow \text{gradient needed for learning} \end{split}$$

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

Backward Pass

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



Can convert

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

(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

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

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

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

Propagate the gradient vector g to the first layers

$$g = gW_2$$

$$\mathbf{g} = \mathbf{g} \operatorname{diag}(\operatorname{Ind}(\mathbf{s}_1 > 0)) \leftarrow \operatorname{assuming} \operatorname{ReLu} \operatorname{activation}$$

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

6. Gradient of
$$J$$
 w.r.t. the first weight matrix W_1 is the $m \times d$ matrix
$$\frac{\partial J}{\partial W_-} = \mathbf{g}^T \mathbf{x}^T + 2\lambda W_1$$

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

- Compute gradients of l w.r.t. $W_1, W_2, \mathbf{b}_1, \mathbf{b}_2$ for each $(\mathbf{x}, y) \in \mathcal{D}^{(t)}$:
 - Set all entries in \(\frac{\partial L}{\partial b_1}\), \(\frac{\partial L}{\partial b_2}\), \(\frac{\partial L}{\partial W_1}\) and \(\frac{\partial L}{\partial W_2}\) to zero.
 - for $(\mathbf{x}, y) \in \mathcal{D}^{(t)}$
 - 1. Let $g = -\frac{y^T}{T} \left(diag(p) pp^T \right)$
 - 2. Add gradient of l w.r.t. b2 computed at (x, y)

$$\frac{\partial L}{\partial \mathbf{h}_0}$$
 += \mathbf{g} , $\frac{\partial L}{\partial W_0}$ += $\mathbf{g}^T \mathbf{h}^T$

Propagate the gradients

$$g = gW_2$$

- $g = g \operatorname{diag}(\operatorname{Ind}(s_1 > 0))$ Add gradient of I w.r.t. first lawer parameter
- 4. Add gradient of l w.r.t. first layer parameters computed at (\mathbf{x}, y) $\frac{\partial L}{\partial x} + \mathbf{g} \mathbf{g}, \quad \frac{\partial L}{\partial x} + \mathbf{g} \mathbf{g}^T \mathbf{x}^T$
- Divide by the number of entries in $\mathcal{D}^{(t)}$:

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

Add the gradient for the regularization term

$$\frac{\partial J}{\partial W} = \frac{\partial L}{\partial W} + 2\lambda W_i, \quad \frac{\partial J}{\partial \mathbf{h}_i} = \frac{\partial L}{\partial \mathbf{h}_i} \quad \text{for } i = 1, 2$$

Aggregated Backward pass for a k-layer neural network

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

 $\mathbf{g} = -\frac{\mathbf{y}^T}{2}$ (diag

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

• for i = k, k - 1, ..., 1

Let

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)

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

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

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

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

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

- 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 \boldsymbol{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

- 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

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

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

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



- 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 (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:

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

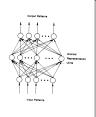
Extension Madaline: a three-layer, fully connected, feed-forward artificial neural network architecture for classification.

A bit of history

A bit of history

A bit of histo

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

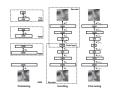




First time back-propagation became popular

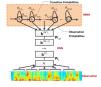
New wave of research in Deep Learning.

- 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.

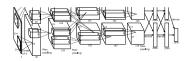


- Beat the widely established approach of GMM-HMM with a DNN-HMM.
- · Improved results on popular datasets by 5.8% and 9.2%.

Better understanding of gradient flows during BackProp helped with these breakthroughs

Understanding Effect of Activation Functions

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



- Beat the stagnating established approaches of Handcrafted features + kernel SVM.
- Improved results on ImageNet by ${\sim}11\%$.

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.

Sigmoid



Problems

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

$$s = Wx + b$$

 $h = \sigma(s)$

- Derivative of the sigmoid function is:

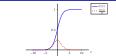
$$\frac{\partial h_i}{\partial s_j} = \begin{cases} \frac{\exp(-s_i)}{(1 + \exp(-s_i))^2} & (= \sigma'(s_i)) & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$$

- 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 $|s_i| > 5$?

Sigmoid



Problems

1. Saturated activations kill the gradients.

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

2. Sigmoid outputs are not zero-centered.

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

- Then

$$\frac{\partial J}{\partial \mathbf{w}_i} = \frac{\partial J}{\partial h_i} \frac{\partial h_i}{\partial s_i} \frac{\partial s_i}{\partial \mathbf{w}_i} = \underbrace{\frac{\partial J}{\partial h_i}}_{\text{positive or negative}} \overset{\mathbf{x}^T}{\underset{\text{positive or negative}}{\text{positive}}} \overset{\mathbf{x}^T}{\underset{\text{positive or negative}}{\text{positive}}}$$

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

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



Problems

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

$$s = Wx + b$$

 $h = \sigma(s)$

- Then

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

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

Sigmoid

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

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

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

What is $\frac{\partial J}{\partial w_i}$ when all entries in x are +tive? (occurs after applying sigmoid) \implies entries of $\frac{\partial J}{\partial \mathbf{w}_i}$ are either all positive or all negative.

⇒ inefficient zig-zag update paths to find optimal w_i

Sigmoid tanh

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



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

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

Rectified Linear Unit (ReLu)



Pros

- 1. Does not saturate for large positive \boldsymbol{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)





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 ReLu function is:

$$\frac{\mathbf{t}_i}{\mathbf{t}_j} = \begin{cases} 1 & \text{if } i = j & & s_j > 0 \\ 0 & \text{otherwise} \end{cases}$$

- Then

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





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.

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



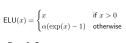
Pros

- 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)

Which Activation Function?





- 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]

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.

Pathological weight initialization



What happens when you initialize each weight matrix entry to

Effect of weight initialization & activation function on gradient flow

Initialize with small random numbers

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

What happens in this case?

Initialize with small random numbers

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

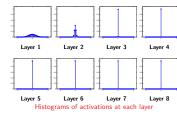
What happens in this case?

zero? (each $W_{i,lm} = 0$)

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

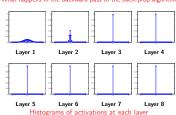
- Initialize a 10-layer network with 500 nodes at each layer.
- Use a tanh activation function at each laver.
- Initialize weights will small random numbers.
- Generate random input data ($N(0, 1^2)$) with d = 500.

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



Some activation histograms

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



Aggregated Backward pass for a k-layer neural network

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

Let

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

• for i = k, k - 1, ..., 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 g to the previous layer (if i > 1)

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

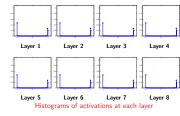
 $\mathbf{g} = \mathbf{g} \operatorname{diag}(\operatorname{Ind}(\mathbf{s}^{(i)} > 0))$

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} ~ N(w; 0, 1²).
- Generate random input data (N(0,1²)) with d = 500.

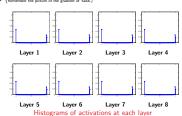
Change the initialization to bigger random numbers

- · Initialize a 10-layer network with 500 nodes at each layer.
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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

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

- for i = k, k 1, ..., 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

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

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

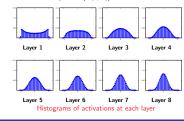
$$\begin{split} \mathbf{g} &= \mathbf{g} W_i \\ \mathbf{g} &= \mathbf{g} \; \mathsf{diag}(\mathsf{tanh}'(\mathbf{s}^{(i)})) \end{split}$$

Change the initialization to Xavier initialization

Change the initialization to Xavier initialization

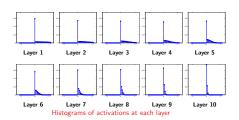
- Initialize a 10-layer network with 500 nodes at each layer.
- Use a tanh activation function at each laver.
- Initialize weights with Xavier initialization: W_{i Im} ~ N(w; 0, 1/√500).
- Generate random input data (N(0, 1²)) with d = 500.

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



Xavier initialization doesn't work for Rel u activation

- Initialize a 10-layer network with 500 nodes at each layer.
- Use a ReLu activation function at each laver.
- 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

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: $\mathbf{s}_1^{(j)}, \mathbf{s}_2^{(j)}, \dots, \mathbf{s}_n^{(j)}$
- 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

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

Batch Normalization

Batch Normalization: Scale & shift range

- Usually apply normalization after the fully connected layer before non-linearity.
- ullet Therefore for a k-layer network have

for
$$(\mathbf{x}^{(i-1)}, y) \in \mathcal{D} \leftarrow \mathsf{Apply}$$
 ith linear transformation to batch
$$\mathbf{s}^{(i)} = W_i \mathbf{x}^{(i-1)} + \mathbf{b}_i$$

Lessening the effect of initialization: Batch normalization

end

Compute batch mean and variances of ith layer:

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

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

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

end

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

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 $\gamma^{(i)}$'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

Batch Normalization at Test Time

- · 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.

Back-Prop for a Batch Normalization laver.

- 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



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

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

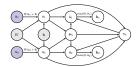
where $\mathbf{v}_b = (v_{b,1}, v_{b,2}, \dots, v_{b,m})^T$. (n=2 in the figure.) Define $V_b = \operatorname{diag}\left(\mathbf{v}_b + \epsilon\right)$

Apply batch normalization function to each score vector:

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

Gradient Computations for a BN layer

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 s_i are $\{\hat{s}_i, \mathbf{v}_b, \boldsymbol{\mu}_b\}$ thus

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

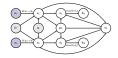
· Let's look at the individual gradients and Jacobians.

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

assume already computed

Gradient Computations for a BN layer

Gradient Computations for a BN layer



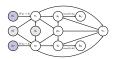
$$\frac{\partial J}{\partial \mathbf{s}_{i}} = \frac{\partial J}{\partial \hat{\mathbf{s}}_{i}} \frac{\partial \hat{\mathbf{s}}_{i}}{\partial \mathbf{s}_{i}} + \frac{\partial J}{\partial \mathbf{v}_{b}} \frac{\partial \mathbf{v}_{b}}{\partial \mathbf{s}_{i}} + \frac{\partial J}{\partial \boldsymbol{\mu}_{b}} \frac{\partial \boldsymbol{\mu}_{b}}{\partial \mathbf{s}_{i}}$$

• The equation relating \hat{s}_i to v_b (remember $V_b = \text{diag}(v_b + \epsilon)$)

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

Therefore

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



$$\frac{\partial J}{\partial \mathbf{s}_{i}} = \frac{\partial J}{\partial \hat{\mathbf{s}}_{i}} \frac{\partial \hat{\mathbf{s}}_{i}}{\partial \mathbf{s}_{i}} + \frac{\partial J}{\partial \mathbf{v}_{b}} \frac{\partial \mathbf{v}_{b}}{\partial \mathbf{s}_{i}} + \frac{\partial J}{\partial \boldsymbol{\mu}_{b}} \frac{\partial \boldsymbol{\mu}_{b}}{\partial \mathbf{s}_{i}}$$

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

Gradient Computations for a BN layer



$$\frac{\partial J}{\partial \mathbf{s}_{i}} = \frac{\partial J}{\partial \hat{\mathbf{s}}_{i}} \frac{\partial \hat{\mathbf{s}}_{i}}{\partial \mathbf{s}_{i}} + \frac{\partial J}{\partial \mathbf{v}_{b}} \frac{\partial \mathbf{v}_{b}}{\partial \mathbf{s}_{i}} + \frac{\partial J}{\partial \mathbf{\mu}_{b}} \frac{\partial \mathbf{\mu}_{b}}{\partial \mathbf{s}_{i}}$$

- The children of node v_b are {\$\hat{s}_1,...,\hat{s}_n\$}
- Therefore

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

$\frac{\partial J}{\partial \mathbf{s}_i} = \frac{\partial J}{\partial \hat{\mathbf{s}}_i} \frac{\partial \hat{\mathbf{s}}_i}{\partial \mathbf{s}_i} + \frac{\partial J}{\partial \mathbf{v}_b} \frac{\partial \mathbf{v}_b}{\partial \mathbf{s}_i} + \frac{\partial J}{\partial \mathbf{\mu}_b} \frac{\partial \mathbf{\mu}_b}{\partial \mathbf{s}_i}$ The children of node v_b are {\$\hat{s}_1, ..., \hat{s}_n\$}

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

Gradient Computations for a BN layer

Gradient Computations for a BN layer

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

$$\hat{\mathbf{s}}_{i} = V_{i}^{-\frac{1}{2}} (\mathbf{s}_{i} - \boldsymbol{\mu}_{i})$$

The local Jacobian we want to compute

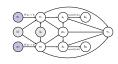
$$\frac{\partial \hat{\mathbf{s}}_i}{\partial \mathbf{v}_b} = \begin{pmatrix} \frac{\partial \hat{s}_{i,1}}{\partial v_{b,1}} & \cdots & \frac{\partial \hat{s}_{i,1}}{\partial v_{b,m}} \\ \vdots & \vdots & \vdots \\ \frac{\partial \hat{s}_{i,m}}{\partial s_{i,m}} & \cdots & \frac{\partial \hat{s}_{i,m}}{\partial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

· 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

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



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

- Next $\frac{\partial \mathbf{v}_b}{\partial \mathbf{s}_i} = \frac{2}{n} \operatorname{diag} (\mathbf{s}_i \boldsymbol{\mu}_b)$.

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

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 μ_b are {ŝ₁,...,ŝ_n, 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

$$\frac{\partial J}{\partial \pmb{\mu}_b} = \sum_{i=1}^n \frac{\partial J}{\partial \hat{\mathbf{s}}_i} \frac{\partial \hat{\mathbf{s}}_i}{\partial \pmb{\mu}_b} + \underbrace{\frac{\partial J}{\partial \pmb{\mathbf{v}}_b}}_{\text{already calculated}} \frac{\partial \mathbf{v}_b}{\partial \pmb{\mu}_b}$$



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



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

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

Gradient Computations for a BN layer

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



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

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

and

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



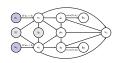
$$\frac{\partial J}{\partial \mathbf{s}_{i}} = \frac{\partial J}{\partial \hat{\mathbf{s}}_{i}} \frac{\partial \hat{\mathbf{s}}_{i}}{\partial \mathbf{s}_{i}} + \frac{\partial J}{\partial \mathbf{v}_{b}} \frac{\partial \mathbf{v}_{b}}{\partial \mathbf{s}_{i}} + \frac{\partial J}{\partial \boldsymbol{\mu}_{b}} \frac{\partial \boldsymbol{\mu}_{b}}{\partial \mathbf{s}_{i}}$$

• The equation relating μ_b to \mathbf{s}_l 's is

$$\mu_b = \frac{1}{n} \sum_{l=1}^{n} \mathbf{s}_l$$

Therefore

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



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

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

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