Machine Learning: Chenhao Tan

University of Colorado Boulder

LECTURE 15

Slides adapted from Jordan Boyd-Graber, Justin Johnson, Andrej Karpathy, Chris Ketelsen, Fei-Fei Li, Mike Mozer, Michael Nielson

Logistics

- Homework 3 is due next week
- Grading for homework 2 is done

Overview

Forward propagation recap

Back propagation

- Chain rule
- Back propagation
- Full algorithm

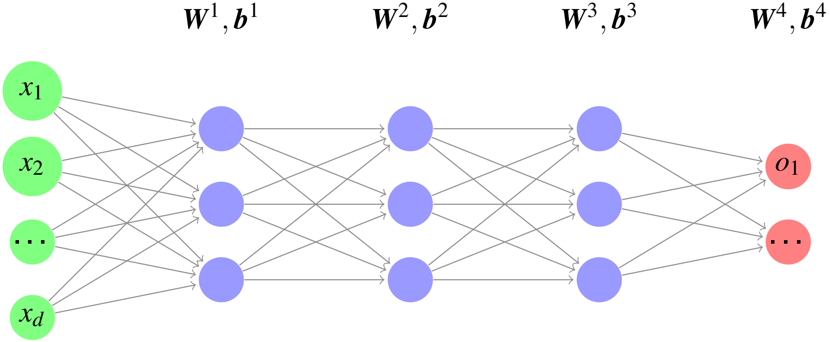
Practical issues of back propagation

- Unstable gradients
- Weight Initialization
- Alternative regularization
- Batch size

Outline

Forward propagation algorithm

How do we make predictions based on a multi-layer neural network?
Store the biases for layer l in $\boldsymbol{b}^l$, weight matrix in $\boldsymbol{W}^l$



Forward propagation algorithm

Suppose your network has L layers
Make prediction for an instance $\boldsymbol{x}$

1: Initialize $\boldsymbol{a}^0 = \boldsymbol{x}$
2: **for** $l = 1$ to L **do**
3: $\quad \boldsymbol{z}^l = \boldsymbol{W}^l \boldsymbol{a}^{l-1} + \boldsymbol{b}^l$
4: $\quad \boldsymbol{a}^l = g(\boldsymbol{z}^l)$ // g represents the nonlinear activation
5: **end for**
6: The prediction $\hat{y}$ is simply $\boldsymbol{a}^L$

Neural networks in a nutshell

- Training data $S_{\text{train}} = \{(\boldsymbol{x}, y)\}$
- Network architecture (model)

$$\hat{y} = f_w(\boldsymbol{x})$$

$$\boldsymbol{W}^l, \boldsymbol{b}^l, l = 1, \dots, L$$

- Loss function (objective function)

$$\mathscr{L}(y, \hat{y})$$

- How do we learn the parameters?

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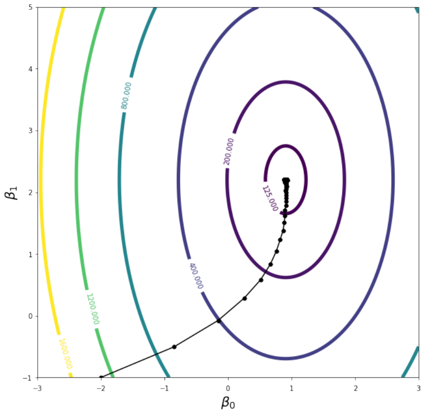
- How do we learn the parameters?
  Stochastic gradient descent,

$$\boldsymbol{W}^l \leftarrow \boldsymbol{W}^l - \eta \frac{\partial \mathscr{L}(y, \hat{y})}{\partial \boldsymbol{W}^l}$$

Reminder of gradient descent



Challenge

- **Challenge**: How do we compute derivatives of the loss function with respect to weights and biases?
- **Solution**: Back propagation

Outline

The Chain Rule

The chain rule allows us to take derivatives of nested functions.

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Univariate chain rule:

$$\frac{d}{dx} f(g(x)) = f'(g(x))\, g'(x) = \frac{df}{dg}\frac{dg}{dx}$$

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Example:

$$\frac{d}{dx} \frac{1}{1+\exp(-x)}$$

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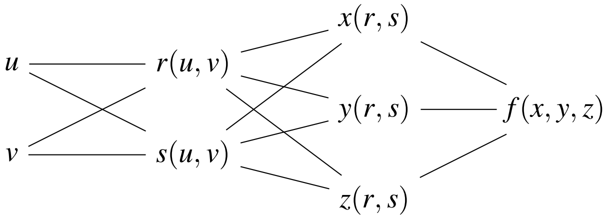
Example:

$$\frac{d}{dx}\, \frac{1}{1+\exp(-x)} = -\frac{1}{(1+\exp(-x))^2} \cdot \exp(-x) \cdot -1$$

$$\frac{d\sigma(x)}{dx} = \sigma(x)(1 - \sigma(x))$$

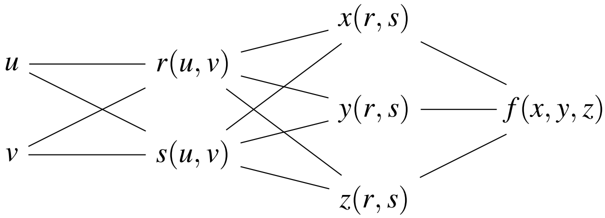
The Chain Rule

Multivariate chain rule:



The Chain Rule

Multivariate chain rule:



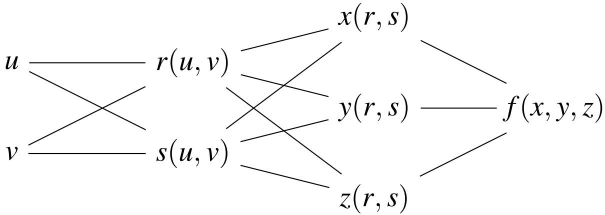
Derivative of $\mathscr{L}$ with respect to x:

$$\frac{\partial f}{\partial x}$$

Similarly, $\frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$

The Chain Rule

What is the derivative of f with respect to r?



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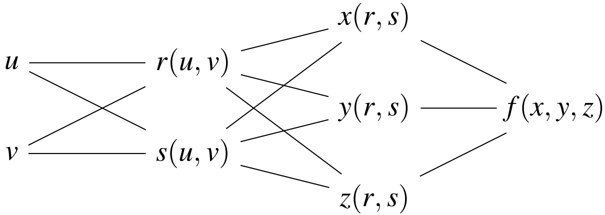

$$\frac{\partial f}{\partial r} = \frac{\partial f}{\partial x}\frac{\partial x}{\partial r} + \frac{\partial f}{\partial y}\frac{\partial y}{\partial r} + \frac{\partial f}{\partial z}\frac{\partial z}{\partial r}$$

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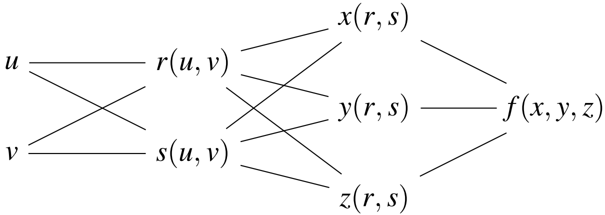
What is the derivative of f with respect to s?



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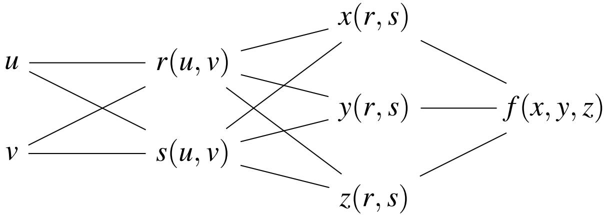

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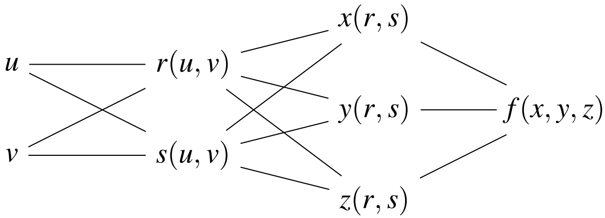

Example: Let $f = xyz$, $x = r$, $y = rs$, and $z = s$. Find $\partial f / \partial s$

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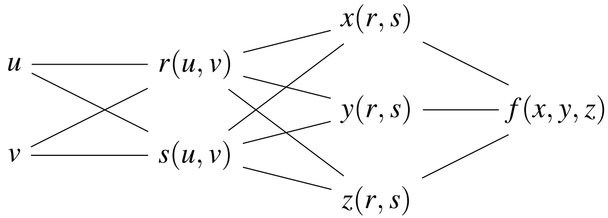

Example: Let $f = xyz$, $x = r$, $y = rs$, and $z = s$. Find $\partial f / \partial s$

$$\frac{\partial f}{\partial s} = yz \cdot 0 + xz \cdot r + xy \cdot 1$$

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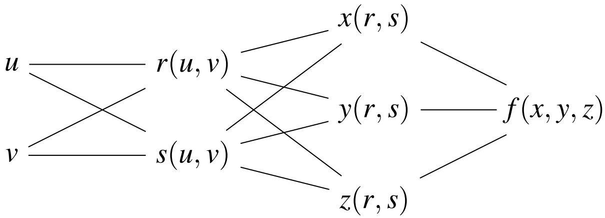
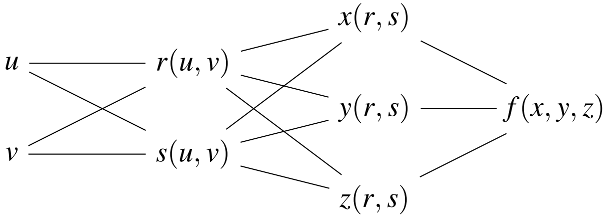


Example: Let $f = xyz$, $x = r$, $y = rs$, and $z = s$. Find $\partial f / \partial s$

$$\frac{\partial f}{\partial s} = rs^2 \cdot 0 + rs \cdot r + r^2 s \cdot 1$$

The Chain Rule

What is the derivative of f with respect to s?



Example: Let $f = xyz$, $x = r$, $y = rs$, and $z = s$. Find $\partial f / \partial s$

$$\frac{\partial f}{\partial s} = 2r^2 s$$

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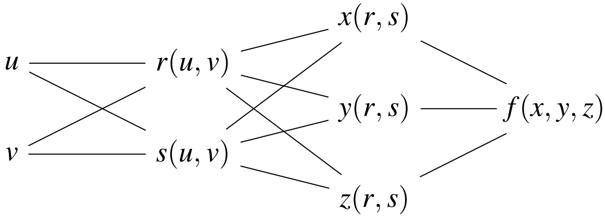
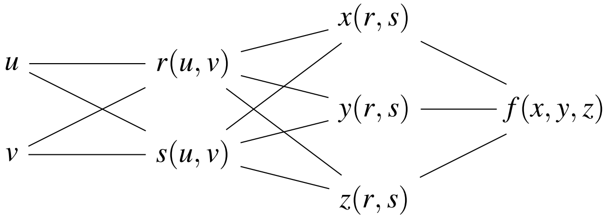


Example: Let $f = xyz$, $x = r$, $y = rs$, and $z = s$. Find $\partial f / \partial s$

$$f(r, s) = r \cdot rs \cdot s = r^2 s^2 \quad \Rightarrow \quad \frac{\partial f}{\partial s} = 2r^2 s \ \checkmark$$

The Chain Rule

What is the derivative of f with respect to u?



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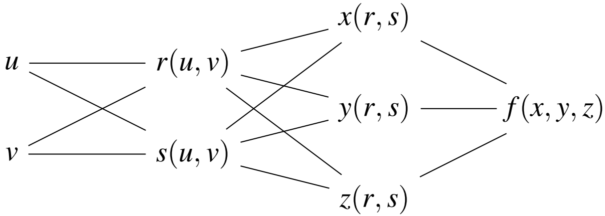

$$\frac{\partial f}{\partial u} = \frac{\partial f}{\partial r}\frac{\partial r}{\partial u} + \frac{\partial f}{\partial s}\frac{\partial s}{\partial u}$$

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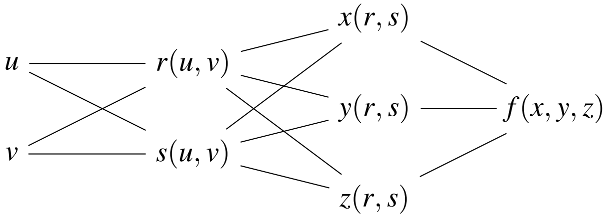

Crux: If you know the derivative of objective w.r.t. intermediate value in the chain, can eliminate everything in between.

The Chain Rule

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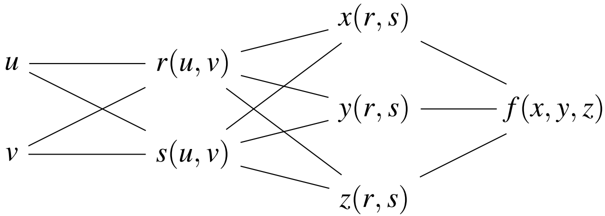
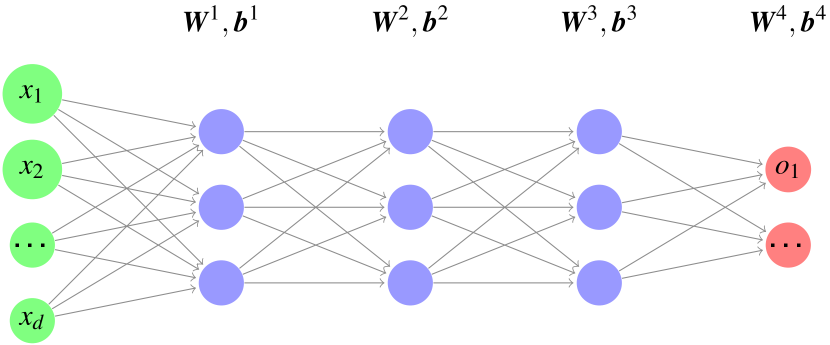


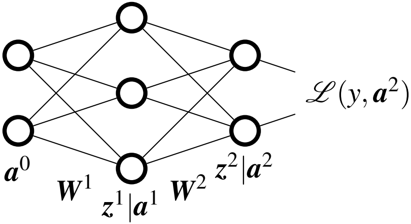
Crux: If you know the derivative of objective w.r.t. intermediate value in the chain, can eliminate everything in between.
This is the cornerstone of the *back propagation* algorithm.

Back Propagation



Back Propagation

For the derivation, we'll consider a simplified network



We want to use back propagation to compute partial derivative of $\mathscr{L}$ w.r.t. the weights and biases

$$\frac{\partial \mathscr{L}}{\partial w_{ij}^2}, \text{for } l = 1, 2$$

w_{ij}^l is the weight from node j in layer $l-1$ to node i in layer l.

Back Propagation

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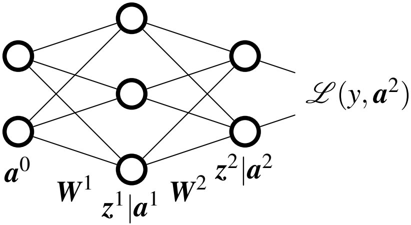

We need to choose an intermediate term that lives on the nodes, that we can easily compute derivative with respect to.
Could choose $\boldsymbol{a}$'s, but we'll choose $\boldsymbol{z}$'s because math is easier.

Back Propagation

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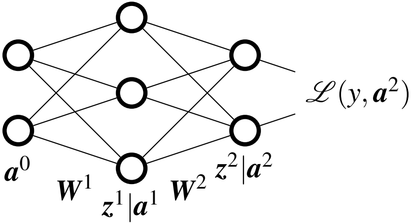

Define the derivative w.r.t. the z's by $\boldsymbol{\delta}$:

$$\delta_j^l = \frac{\partial \mathscr{L}}{\partial z_j^l}$$

Note that $\boldsymbol{\delta}^l$ has the same size as $\boldsymbol{z}^l$ and $\boldsymbol{a}^l$.

Back Propagation

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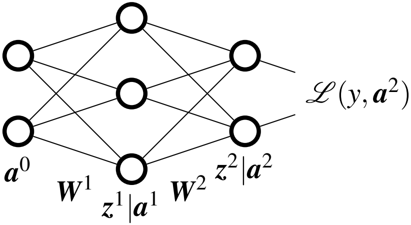

Let's compute δ^L for output layer L:

$$\delta_j^L = \frac{\partial \mathscr{L}}{\partial z_j^L} = \frac{\partial \mathscr{L}}{\partial a_j^L} \frac{da_j^L}{dz_j^L}$$

Back Propagation

$$\delta_j^L = \frac{\partial \mathscr{L}}{\partial z_j^L} = \frac{\partial \mathscr{L}}{\partial a_j^L} \frac{da_j^L}{dz_j^L}$$

We know that $a_j^L = g(z_j^L)$, so $\frac{da_j^L}{dz_j^L} = g'(z_j^L)$

$$\delta_j^L = \frac{\partial \mathscr{L}}{\partial a_j^L} g'(z_j^L)$$

Note: The first term is j^{th} entry of gradient of $\mathscr{L}$.

Back Propagation

$$\delta_j^L = \frac{\partial \mathscr{L}}{\partial a_j^L} g'(z_j^L)$$

We can combine all of these into a vector operation

$$\boldsymbol{\delta}^L = \frac{\partial \mathscr{L}}{\partial \boldsymbol{a}^L} \odot g'(\boldsymbol{z}^L)$$

Where $g'(\boldsymbol{z}^L)$ is the activation function applied elementwise to $\boldsymbol{z}^L$.
The symbol $\odot$ indicates element-wise multiplication of vectors.

Back Propagation

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The symbol $\odot$ indicates element-wise multiplication of vectors.
Notice that computing $\boldsymbol{\delta}^L$ requires knowing activations.
This means that before we can compute derivatives for SGD through back propagation, we first run forward propagation through the network.

Back Propagation

Example: Suppose we're in regression setting and choose a sigmoid activation function:

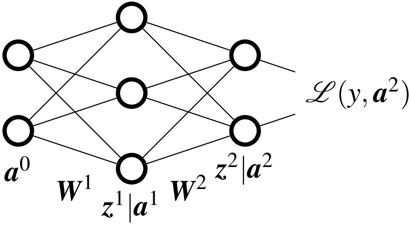
$$\mathscr{L} = \frac{1}{2}\sum_j (y_j - a_j^L)^2 \quad \text{and} \quad a_j^L = \sigma(z)$$

$$\frac{\partial \mathscr{L}}{\partial a_j^L} = (a_j^L - y_j), \quad \frac{da_j^L}{dz_j^L} = \sigma'(z_j^L) = \sigma(z_j^L)(1 - \sigma(z_j^L))$$

So $\boldsymbol{\delta}^L = (\boldsymbol{a}^L - y) \odot \sigma(\boldsymbol{z}^L) \odot (1 - \sigma(\boldsymbol{z}^L))$

Back Propagation

OK Great! Now we can easily-ish compute the δ's for the output layer.
But really we're after partials w.r.t. to weights and biases.



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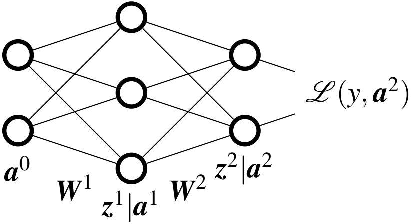
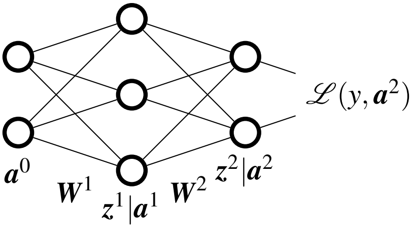


Question: What do you notice?

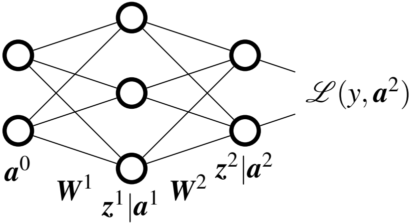
Back Propagation

We want to find derivative $\mathscr{L}$ w.r.t. to weights and biases



Every weight connected to a node in layer L depends on a single δ_j^L

Back Propagation

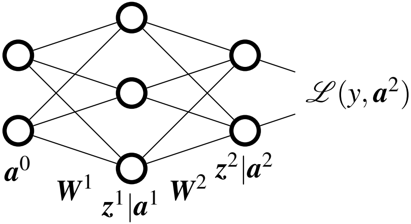


So we have $$\frac{\partial \mathscr{L}}{\partial w_{jk}^L} = \frac{\partial \mathscr{L}}{\partial z_j^L} \frac{\partial z_j^L}{\partial w_{jk}^L} = \delta_j^L \frac{\partial z_j^L}{\partial w_{jk}^L}$$

Need to compute $\frac{\partial z_j^L}{\partial w_{jk}^L}$. Recall $\mathbf{z}^L = W^L \mathbf{a}^{L-1} + \mathbf{b}^L$

$$j^{\text{th}} \text{ entry in vector} \Rightarrow \quad z_j^L = \sum_i w_{ji}^L a_i^{L-1} + b_j^L$$

Back Propagation



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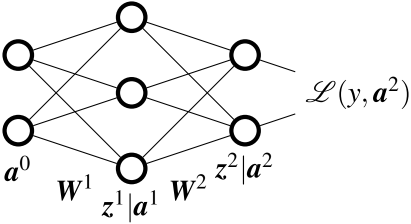
Taking derivative w.r.t. w_{jk}^L gives

$$\Rightarrow \quad \frac{\partial z_j^L}{\partial w_{jk}^L} = a_k^{L-1} \quad \Rightarrow \quad \frac{\partial \mathscr{L}}{\partial w_{jk}^L} = a_k^{L-1}\delta_j^L$$

Back Propagation



So we have $$\frac{\partial \mathcal{L}}{\partial w_{jk}^L} = a_k^{L-1} \delta_j^L$$

Easy expression for derivative w.r.t. every weight leading into layer L.

Back Propagation

Let's make the notation a little more practical.

$$\boldsymbol{W}^2 = \begin{bmatrix} w_{11}^2 & w_{12}^2 & w_{13}^2 \\ w_{21}^2 & w_{22}^2 & w_{23}^2 \end{bmatrix}$$

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Now we can write this as an outer-product of $\boldsymbol{\delta}^2$ and $\boldsymbol{a}^1$,

$$\frac{\partial \mathcal{L}}{\partial \boldsymbol{W}^2} = \boldsymbol{\delta}^2 (\boldsymbol{a}^1)^T$$

(Exercise for yourself, $\frac{\partial \mathcal{L}}{\partial \boldsymbol{b}^2}$)

Intermediate summary

For a giving training example $\boldsymbol{x}$, perform forward propagation to get $\boldsymbol{z}^l$ and $\boldsymbol{a}^l$ on each layer.
Then to get the partial derivatives for $\boldsymbol{W}^2$ or $\boldsymbol{W}^L$:

1. Compute $\boldsymbol{\delta}^L = \frac{\partial \mathcal{L}}{\partial a_j^L} \odot g'(\boldsymbol{z}^L)$
2. Compute $\frac{\partial \mathcal{L}}{\partial \boldsymbol{W}^L} = \boldsymbol{\delta}^L (\boldsymbol{a}^{L-1})^T$ and $\frac{\partial \mathcal{L}}{\partial \boldsymbol{b}^L} = \boldsymbol{\delta}^L$

OK, that wasn't so bad! We found very simple expressions for the derivatives with respect to the weights in the last hidden layer!

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OK, that wasn't so bad! We found very simple expressions for the derivatives with respect to the weights in the last hidden layer!
Problem: How do we do the other layers?
Since the formulas were so nice once we knew the adjacent $\boldsymbol{\delta}^l$, it sure would be nice if we could easily compute the $\boldsymbol{\delta}^l$'s on earlier layers.

Back Propagation

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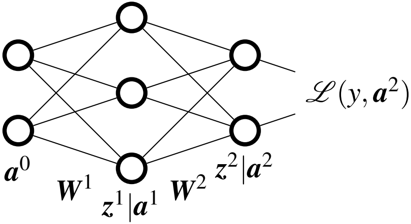
Notice that δ^1 depends on δ^2.



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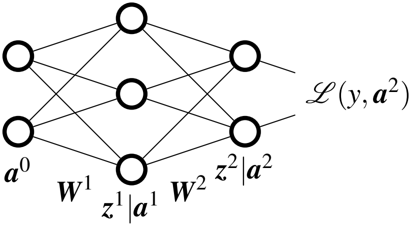

By multivariate chain rule,

$$\frac{\partial \mathscr{L}}{\partial z_k^{l-1}} = \sum_j \frac{\partial \mathscr{L}}{\partial z_j^l} \frac{\partial z_j^l}{\partial z_k^{l-1}}$$

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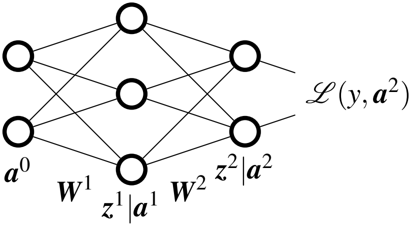
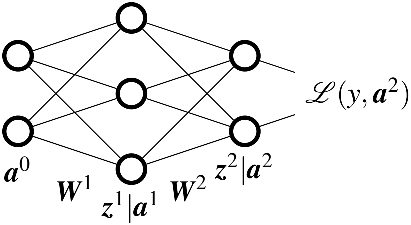


By multivariate chain rule,

$$\delta_k^{l-1} = \frac{\partial \mathcal{L}}{\partial z_k^{l-1}} = \sum_j \frac{\partial \mathcal{L}}{\partial z_j^l} \frac{\partial z_j^l}{\partial z_k^{l-1}} = \sum_j \delta_j^l \frac{\partial z_j^l}{\partial z_k^{l-1}}$$

Back Propagation

Notice that δ^1 depends on δ^2.



By multivariate chain rule,

$$\delta_2^1 = \frac{\partial \mathscr{L}}{\partial z_2^1} = \delta_1^2 \frac{\partial z_1^2}{\partial z_2^1} + \delta_2^2 \frac{\partial z_2^2}{\partial z_2^1}$$

Back Propagation

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Recall that $\boldsymbol{z}^2 = \boldsymbol{W}^2 a^1 + \boldsymbol{b}^2$, it follows that

$$z_i^2 = w_{i1}^2 a_1^1 + w_{i2}^2 a_2^1 + w_{i3}^2 a_3^1 + b_i^2$$

Taking the derivative $\frac{\partial z_i^2}{\partial z_2^1} = w_{i2}^2 g'(z_2^1)$, and plugging in gives

$$\delta_2^1 = \frac{\partial \mathcal{L}}{\partial z_2^1} = \delta_1^2 w_{12}^2 g'(z_2^1) + \delta_2^2 w_{22}^2 g'(z_2^1)$$

Back Propagation

If we do this for each of the 3 δ_i^1's, something nice happens:
(Exercise for yourself: work out δ_1^1 and δ_3^1 for yourself)

$$\begin{aligned}
\delta_1^1 &= \delta_1^2 w_{11}^2 g'(z_1^1) + \delta_2^2 w_{21}^2 g'(z_1^1) \\
\delta_2^1 &= \delta_1^2 w_{12}^2 g'(z_2^1) + \delta_2^2 w_{22}^2 g'(z_2^1) \\
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\end{aligned}
$$

Notice that each row of the system gets multiplied by $g'(z_i^1)$, so let's factor those out.

Back Propagation

If we do this for each of the 3 δ_i^2's, something nice happens:

$$
\begin{aligned}
\delta_1^1 &= (\delta_1^2 w_{11}^2 + \delta_2^2 w_{21}^2) \cdot g'(z_1^1) \\
\delta_2^1 &= (\delta_1^2 w_{12}^2 + \delta_2^2 w_{22}^2) \cdot g'(z_2^1) \\
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\end{aligned}
$$

Remember $\boldsymbol{\delta}^2 = \begin{bmatrix} \delta_1^2 \\ \delta_2^2 \end{bmatrix}$, $\boldsymbol{W}^2 = \begin{bmatrix} w_{11}^2 & w_{12}^2 & w_{13}^2 \\ w_{21}^2 & w_{22}^2 & w_{23}^2 \end{bmatrix}$

Do you see $\boldsymbol{\delta}^2$ and $\boldsymbol{W}^2$ lurking anywhere in the above system?

Back Propagation

If we do this for each of the 3 δ_i^2's, something nice happens:

$$\begin{aligned}
\delta_1^1 &= (\delta_1^2 w_{11}^2 + \delta_2^2 w_{21}^2) \cdot g'(z_1^1) \\
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\delta_3^2 &= (\delta_1^2 w_{13}^2 + \delta_2^2 w_{23}^2) \cdot g'(z_3^1)
\end{aligned}$$

Does this help?

$$(\boldsymbol{W}^2)^T = \begin{bmatrix} w_{11}^2 & w_{21}^2 \\ w_{12}^2 & w_{22}^2 \\ w_{13}^2 & w_{23}^2 \end{bmatrix}, \boldsymbol{\delta}^2 = \begin{bmatrix} \delta_1^2 \\ \delta_2^2 \end{bmatrix}.$$

Back Propagation

If we do this for each of the 3 δ_i^2's, something nice happens:

$$
\begin{aligned}
\delta_1^1 &= (\delta_1^2 w_{11}^2 + \delta_2^2 w_{21}^2) \cdot g'(z_1^1) \\
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\end{aligned}
$$

$$
\boldsymbol{\delta}^1 = (\boldsymbol{W}^2)^T \boldsymbol{\delta}^2 \odot g'(\boldsymbol{z}^1)
$$

Back Propagation

OK Great!
We can easily compute $\boldsymbol{\delta}^1$ from $\boldsymbol{\delta}^2$
Then we can compute derivatives of $\mathscr{L}$ w.r.t. weights $\boldsymbol{W}^1$ and biases $\boldsymbol{b}^1$ exactly the way we did for $\boldsymbol{W}^2$ and biases $\boldsymbol{b}^2$

1. Compute $\boldsymbol{\delta}^1 = (\boldsymbol{W}^2)^T \boldsymbol{\delta}^2 \odot g'(\boldsymbol{z}^1)$
2. Compute $\frac{\partial \mathscr{L}}{\partial \boldsymbol{W}^1} = \boldsymbol{\delta}^1 (\boldsymbol{a}^0)^T$ and $\frac{\partial \mathscr{L}}{\partial \boldsymbol{b}^1} = \boldsymbol{\delta}^1$

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We've worked this out for a simple network with one hidden layer.

Nothing we've done assumed anything about the number of layers, so we can apply the same procedure recursively with any number of layers.

Back Propagation

$\delta^L = \frac{\partial \mathscr{L}}{\partial a_j^L} \odot g'(\mathbf{z}^L)$ # Compute δ's on output layer

For $\ell = L, \ldots, 1$

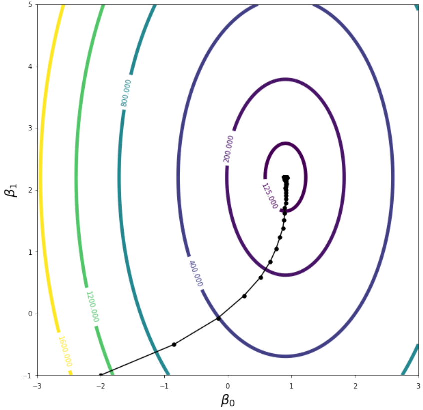
$\frac{\partial \mathscr{L}}{\partial \boldsymbol{W}^\ell} = \boldsymbol{\delta}^\ell (\boldsymbol{a}^{l-1})^T$ # Compute weight derivatives

$$\frac{\partial \mathscr{L}}{\partial \boldsymbol{b}^\ell} = \boldsymbol{\delta}^\ell$$ # Compute bias derivatives

$\boldsymbol{\delta}^{\ell-1} = \left(W^\ell\right)^T \boldsymbol{\delta}^\ell \odot g'(\mathbf{z}^{\ell-1})$ # Back prop $\boldsymbol{\delta}$'s to previous layer

(After this, ready to do a SGD update on weights/biases)

Reminder of gradient descent



Training a Feed-Forward Neural Network

Given initial guess for weights and biases.
Loop over each training example in random order:

1. Forward propagate to get activations on each layer
2. Back propagate to get derivatives
3. Update weights and biases via stochastic gradient descent
4. Repeat

Outline

Forward propagation recap

Back propagation
- Chain rule
- Back propagation
- Full algorithm

Practical issues of back propagation
- Unstable gradients
- Weight Initialization
- Alternative regularization
- Batch size

Back Propagation

In practice, many remaining questions may arise.

$\delta^L = \frac{\partial \mathscr{L}}{\partial a_j^L} \odot g'(\mathbf{z}^L)$ # Compute δ's on output layer

For $\ell = L, \dots, 1$

$\frac{\partial \mathscr{L}}{\partial \boldsymbol{W}^\ell} = \boldsymbol{\delta}^\ell (\boldsymbol{a}^{l-1})^T$ # Compute weight derivatives

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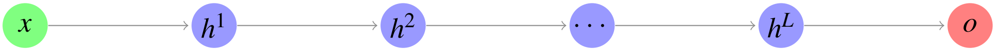
Unstable gradients

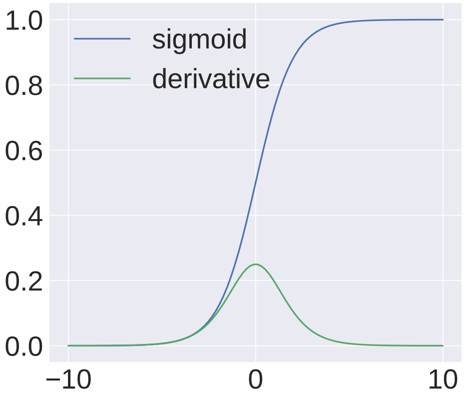


Unstable gradients

$$x \longrightarrow h^1 \longrightarrow h^2 \longrightarrow \cdots \longrightarrow h^L \longrightarrow o$$

$$\frac{\partial \mathcal{L}}{\partial b^1} = g'(z^1) \times w^2 \times g'(z^2) \times w^3 \ldots g'(z^L) \frac{\partial \mathcal{L}}{\partial a^L}$$

Unstable gradients



Vanishing gradients

If we use Gaussian initialization for weights, $w^j \sim \mathcal{N}(0, 1)$,

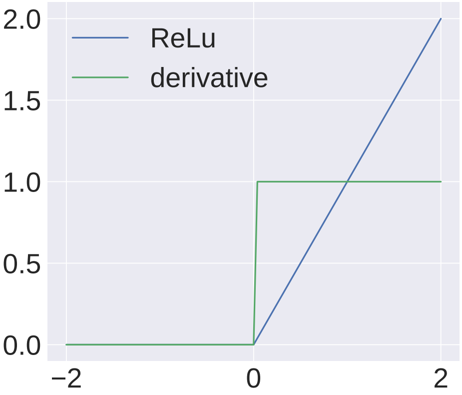
$$|w^j| < 1$$

$$|w^j \sigma'(z_j)| < \frac{1}{4}$$

$$\frac{\partial \mathcal{L}}{\partial b^1} \text{ decay to zero exponentially}$$

Vanishing gradients

ReLu



Exploding gradients

If $w^j = 100$,

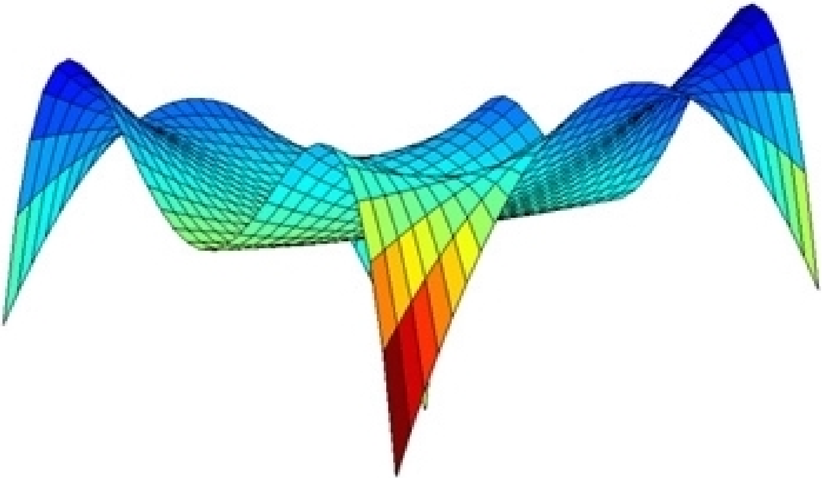
$$|w^j \sigma'(z_j)| \approx k > 1$$

Training a Feed-Forward Neural Network

In practice, many remaining questions may arise, more examples:

1. How do we initialize weights and biases?
2. How do we regularize?
3. Can I batch this?

Non-convexity



Weight initialization

Old idea: $W = 0$, what happens?

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$\delta^L = \nabla_{\boldsymbol{a}^L} \mathscr{L} \odot g'(\mathbf{z}^L)$ # Compute δ's on output layer

For $\ell = L, \ldots, 1$

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$\frac{\partial \mathscr{L}}{\partial \boldsymbol{b}^\ell} = \boldsymbol{\delta}^\ell$ # Compute bias derivatives

$\boldsymbol{\delta}^{\ell-1} = \left(W^\ell\right)^T \boldsymbol{\delta}^\ell \odot g'(\mathbf{z}^{\ell-1})$ # Back prop $\boldsymbol{\delta}$'s to previous layer

Weight initialization

First idea: small random numbers, $W \sim \mathcal{N}(0, 0.01)$

Weight initialization

$$
\begin{aligned}
Var(z) &= Var(\sum_i w_i x_i) \\
&= nVar(w_i)Var(x_i)
\end{aligned}
$$

Weight initialization

Xavier initialization [Glorot and Bengio, 2010]

$$W \sim \mathcal{N}(0, \frac{2}{n_{in} + n_{out}})$$

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He initialization [He et al., 2015]

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$$W \sim \mathcal{N}(0, \frac{2}{n_{in} + n_{out}})$$

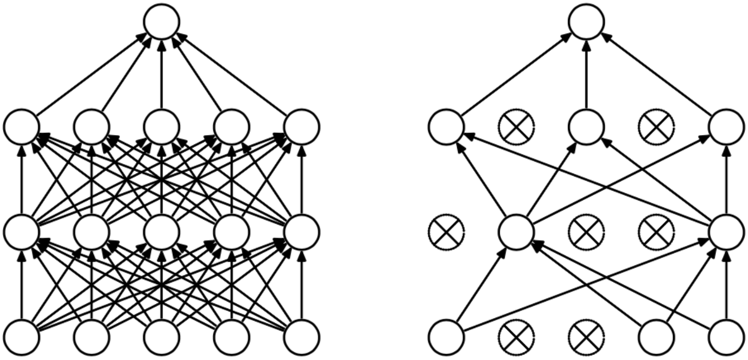
He initialization [He et al., 2015]

$$W \sim \mathcal{N}(0, \frac{2}{n_{in}})$$

This is an actively research area and next great idea may come from you!

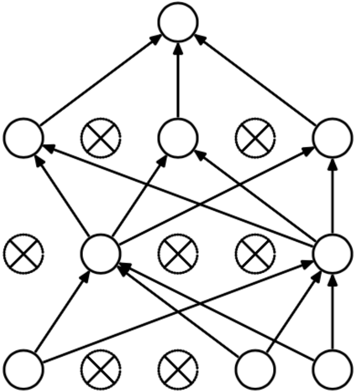
Dropout layer

"randomly set some neurons to zero in the forward pass" [Srivastava et al., 2014]



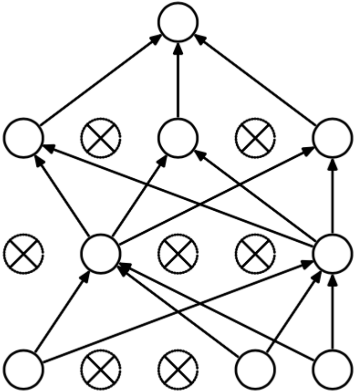
(a) Standard Neural Net   (b) After applying dropout.

Dropout layer



Forces the network to have a redundant representation.

Dropout layer



Another interpretation: Dropout is training a large ensemble of models.

Batch size

We have so far learned gradient descent which uses all training data to compute gradients.

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Alternatively, we use a single instance to compute gradients in stochastic gradient descent.

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Alternatively, we use a single instance to compute gradients in stochastic gradient descent.

In general, we can use a parameter batch size to compute the gradients from a few instances.

- N (the entire training data)
- 1 (a single instance)
- More common values: 16, 32, 64, 128

Wrap up

Back propagation allows for computing the gradients of the parameters and watch out for unstable gradients!

$\delta^L = \frac{\partial \mathscr{L}}{\partial a_j^L} \odot g'(\mathbf{z}^L)$ # Compute δ's on output layer

For $\ell = L, \ldots, 1$

$\frac{\partial \mathscr{L}}{\partial \boldsymbol{W}^\ell} = \boldsymbol{\delta}^\ell (\boldsymbol{a}^{l-1})^T$ # Compute weight derivatives

$\frac{\partial \mathscr{L}}{\partial \boldsymbol{b}^\ell} = \boldsymbol{\delta}^\ell$ # Compute bias derivatives

$\boldsymbol{\delta}^{\ell-1} = \left(W^\ell\right)^T \boldsymbol{\delta}^\ell \odot g'(\mathbf{z}^{\ell-1})$ # Back prop $\boldsymbol{\delta}$'s to previous layer

References

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