ECE595 / STAT598: Machine Learning I
Lecture 18 Multi-Layer Perceptron

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Outline

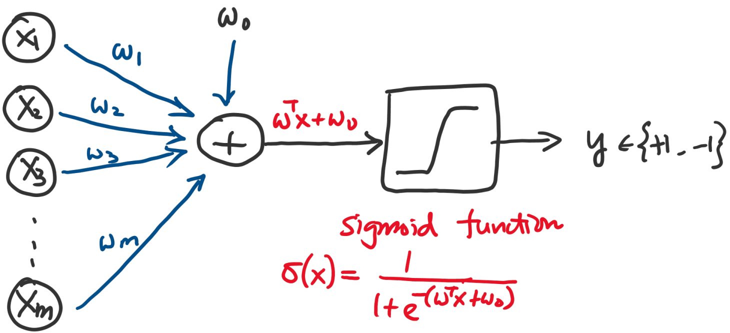
Discriminative Approaches

- Lecture 16 Perceptron 1: Definition and Basic Concepts
- Lecture 17 Perceptron 2: Algorithm and Property
- Lecture 18 Multi-Layer Perceptron: Back Propagation

This lecture: Multi-Layer Perceptron: Back Propagation

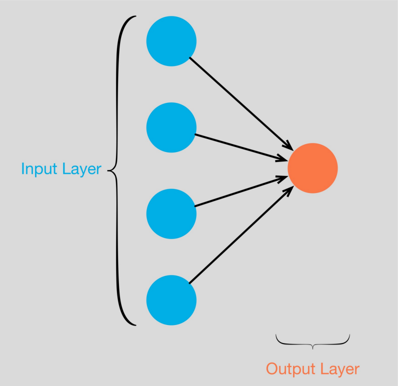
- Multi-Layer Perceptron
  - Hidden Layer
  - Matrix Representation
- Back Propagation
  - Chain Rule
  - 4 Fundamental Equations
  - Algorithm
  - Interpretation

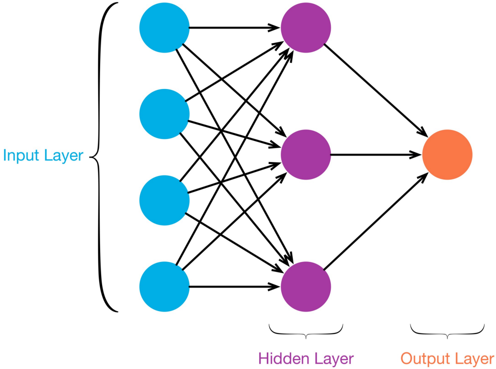
Single-Layer Perceptron



- Input neurons $\boldsymbol{x}$
- Weights $\boldsymbol{w}$
- Predicted label $= \sigma(\boldsymbol{w}^T\boldsymbol{x} + w_0)$.

Multi-Layer Network

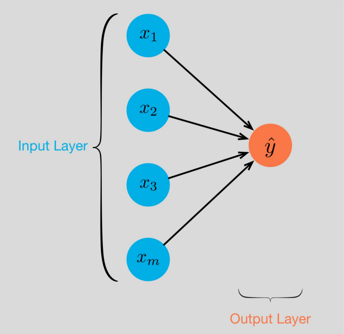


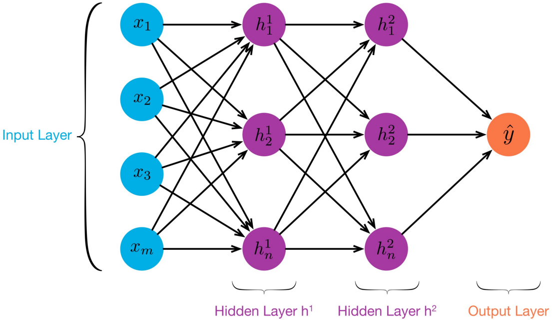


https://towardsdatascience.com/multi-layer-neural-networks-with-sigmoid-function-deep-learning-for-rookies-2-bf464f09eb7f

- Introduce a layer of **hidden** neurons
- So now you have two sets of weights: from input to hidden, and from hidden to output

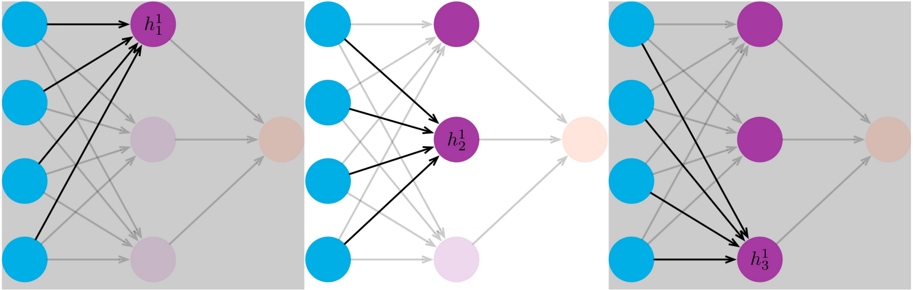
Many Hidden Layers





- You can introduce as many hidden layers as you want.
- Every time you add a hidden layer, you add a set of weights.

Understanding the Weights



- Each hidden neuron is an **output** of a perceptron
- So you will have

$$\begin{bmatrix} h_1^1 \\ h_2^1 \\ \dots \\ h_n^1 \end{bmatrix} = \begin{bmatrix} w_{11}^1 & w_{12}^1 & \dots & w_{1n}^1 \\ w_{21}^1 & w_{22}^1 & \dots & w_{2n}^1 \\ \vdots & \vdots & \ddots & \vdots \\ w_{m1}^1 & w_{m2}^1 & \dots & w_{mn}^1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_m \end{bmatrix}$$

Progression to DEEP (Linear) Neural Networks

- Single-layer:

$$h = \boldsymbol{w}^T \boldsymbol{x}$$

- Hidden-layer:

$$\boldsymbol{h} = \boldsymbol{W}^T \boldsymbol{x}$$

- Two Hidden Layers:

$$\boldsymbol{h} = \boldsymbol{W}_2^T \boldsymbol{W}_1^T \boldsymbol{x}$$

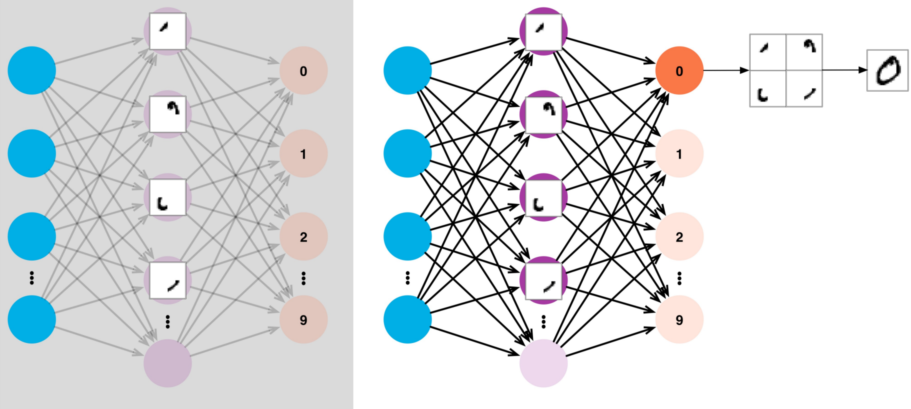
- Three Hidden Layers:

$$\boldsymbol{h} = \boldsymbol{W}_3^T \boldsymbol{W}_2^T \boldsymbol{W}_1^T \boldsymbol{x}$$

- A LOT of Hidden Layers:

$$\boldsymbol{h} = \boldsymbol{W}_N^T \dots \boldsymbol{W}_2^T \boldsymbol{W}_1^T \boldsymbol{x}$$

Interpreting the Hidden Layer

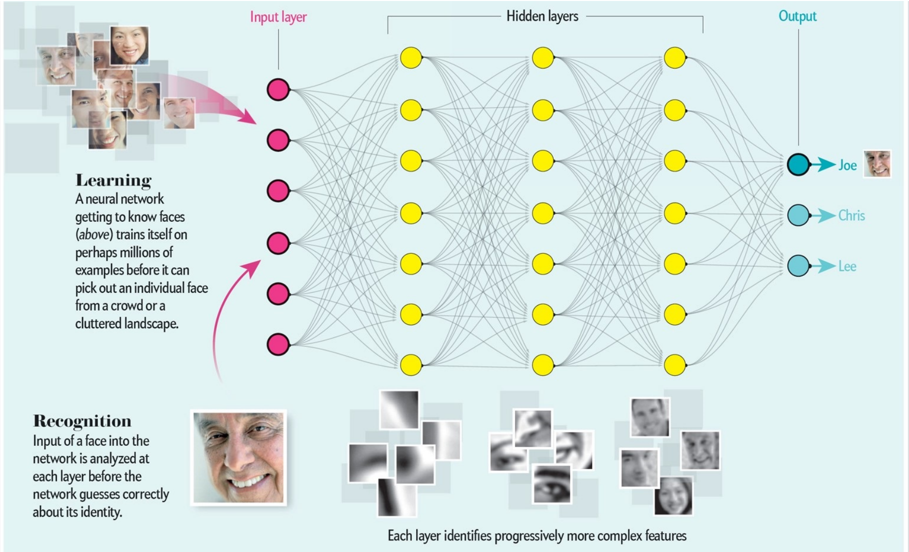


A Trained Neural Network in which each hidden neuron classifies certain pattern

Feeding a handwritten digit of 0 should trigger the 4 hidden layer neurons, and then the first output neuron

- Each hidden neuron is responsible for certain features.
- Given an object, the network identifies the most likely features.

Interpreting the Hidden Layer



https://www.scientificamerican.com/article/springtime-for-ai-the-rise-of-deep-learning/

Two Questions about Multi-Layer Network

- How do we **efficiently** learn the weights?
  - Ultimately we need to minimize the loss

$$J(\boldsymbol{W}_1, \ldots, \boldsymbol{W}_L) = \sum_{i=1}^{N} \|\boldsymbol{W}_L^T \ldots \boldsymbol{W}_2^T \boldsymbol{W}_1^T \boldsymbol{x}_i - \boldsymbol{y}_i\|^2$$

  - One layer: Gradient descent. Multi-layer: Also gradient descent, also known as Back propagation (BP) by Rumelhart, Hinton and Williams (1986)
  - Back propagation = Very careful book-keeping and chain rule
- What is the optimization **landscape**?
  - Convex? Global minimum? Saddle point?
  - Two-layer case is proved by Baldi and Hornik (1989)
  - All local minima are global.
  - A critical point is either a saddle point or global minimum.
  - L-layer case is proved by Kawaguchi (2016). Also proved L-layer nonlinear network (with sigmoid between adjacent layers.)

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Back Propagation: A 20-Minute Tour

- You will be able to find **A LOT OF** blogs on the internet discussing how back propagation is being implemented.
- Some are **mystifying** back propagation
- Some literally just teach you the procedure of back propagation without telling you the intuition
- I find the following online book by Mike Nielsen fairly well-written
- http://neuralnetworksanddeeplearning.com/
- The following slides are written based on Nielsen's book
- We will not go into great details
- The purpose to get you exposed to the idea, and de-mystify back propagation
- As stated before, back propagation is chain rule + very careful book keeping

Back Propagation

- Here is the loss function you want to minimize:

$$J(\boldsymbol{W}_1, \ldots, \boldsymbol{W}_L) = \sum_{i=1}^{N} \|\sigma(\boldsymbol{W}_L^T \ldots \sigma(\boldsymbol{W}_2^T \sigma(\boldsymbol{W}_1^T \boldsymbol{x}_i))) - \boldsymbol{y}_i\|^2$$

- You have a set of nonlinear activation functions, usually the sigmoid.
- To optimize, you need gradient descent. For example, for $\boldsymbol{W}_1$

$$\boldsymbol{W}_1^{t+1} = \boldsymbol{W}_1^t - \alpha \nabla J(\boldsymbol{W}_1^t)$$

- But you need to do this for all $\boldsymbol{W}_1, \ldots, \boldsymbol{W}_L$.
- And there are lots of sigmoid functions.
- Let us do the brute force.
- And this is back-propagation. (Really? Yes...)

Let us See an Example

- Let us look at two layers

$$J(\boldsymbol{W}_1, \boldsymbol{W}_2) = \|\underbrace{\sigma(\boldsymbol{W}_2^T \sigma(\boldsymbol{W}_1^T \boldsymbol{x}))}_{\boldsymbol{a}_2} - \boldsymbol{y}\|^2$$

- Let us go **backward**:

$$\frac{\partial J}{\partial \boldsymbol{W}_2} = \frac{\partial J}{\partial \boldsymbol{a}_2} \cdot \frac{\partial \boldsymbol{a}_2}{\partial \boldsymbol{W}_2}$$

- Now, what is $\boldsymbol{a}_2$?

$$\boldsymbol{a}_2 = \sigma(\underbrace{\boldsymbol{W}_2^T \sigma(\boldsymbol{W}_1^T \boldsymbol{x}))}_{\boldsymbol{z}_2}$$

So let us compute:

$$\frac{\partial \boldsymbol{a}_2}{\partial \boldsymbol{W}_2} = \frac{\partial \boldsymbol{a}_2}{\partial \boldsymbol{z}_2} \cdot \frac{\partial \boldsymbol{z}_2}{\partial \boldsymbol{W}_2}.$$

Let us See an Example

$$J(\boldsymbol{W}_1, \boldsymbol{W}_2) = \|\sigma(\boldsymbol{W}_2^T \underbrace{\sigma(\boldsymbol{W}_1^T \boldsymbol{x})}_{\boldsymbol{a}_1}) - \boldsymbol{y}\|^2$$

- How about $\boldsymbol{W}_1$? Again, let us go **backward**:

$$\frac{\partial J}{\partial \boldsymbol{W}_1} = \frac{\partial J}{\partial \boldsymbol{a}_2} \cdot \frac{\partial \boldsymbol{a}_2}{\partial \boldsymbol{W}_1}$$

- But you can now repeat the calculation as follows (Let $\boldsymbol{z}_1 = \boldsymbol{W}_1^T \boldsymbol{x}$)

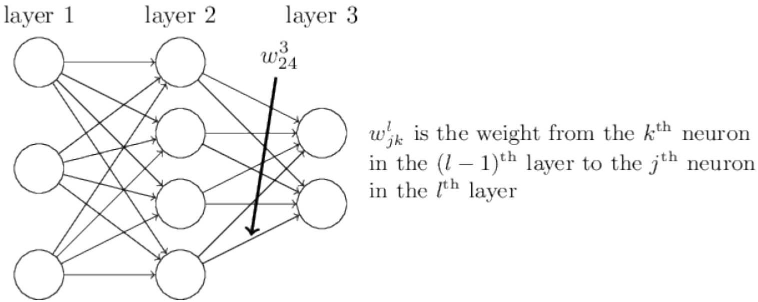
$$\begin{aligned} \frac{\partial \boldsymbol{a}_2}{\partial \boldsymbol{W}_1} &= \frac{\partial \boldsymbol{a}_2}{\partial \boldsymbol{a}_1} \frac{\partial \boldsymbol{a}_1}{\partial \boldsymbol{W}_1} \\ &= \frac{\partial \boldsymbol{a}_2}{\partial \boldsymbol{a}_1} \frac{\partial \boldsymbol{a}_1}{\partial \boldsymbol{z}_1} \frac{\partial \boldsymbol{z}_1}{\boldsymbol{W}_1} \end{aligned}$$

- So it is just a very long sequence of chain rule.

Notations for Back Propagation

- The following notations are based on Nielsen's online book.
- The purpose of doing these is to write down a concise algorithm.

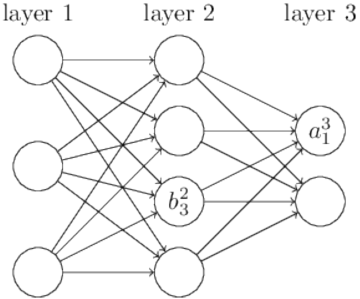
Weights:



- w^{3}_{24}: The 3rd layer
- w^3_{24}: From 4-th neuron to 2-nd neuron

Notations for Back Propagation

Activation and Bias:



- a_1^3: 3rd layer, 1st activation
- b_3^2: 2nd layer, 3rd bias
- Here is the relationship. Think of $\sigma(\boldsymbol{w}^T\boldsymbol{x} + w_0)$:

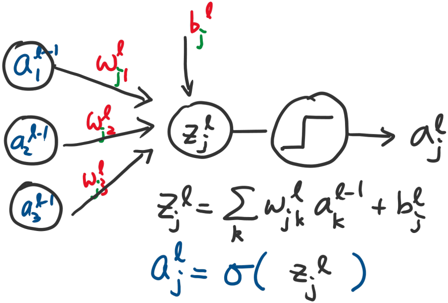
$$a_j^\ell = \sigma\left(\sum_k w_{jk}^\ell a_k^{\ell-1} + b_j^\ell\right).$$

Understanding Back Propagation

- This is the main equation

$$a_j^\ell = \sigma\underbrace{\left(\sum_k w_{jk}^\ell a_k^{\ell-1} + b_j^\ell\right)}_{z_j^\ell}, \quad \text{or} \quad a_j^\ell = \sigma(z_j^\ell).$$

- a_j^ℓ: activation, z_j^ℓ: intermediate.

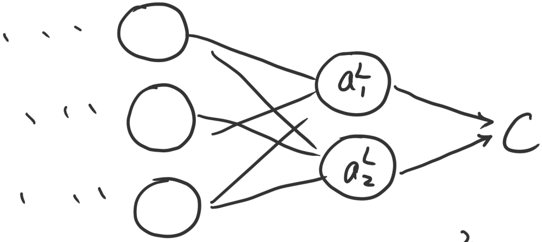


Loss

- The loss takes the form of

$$C = \sum_j (a_j^L - y_j)^2$$

- Think of two-class cross-entropy where each $\boldsymbol{a}^L$ is a 2-by-1 vector

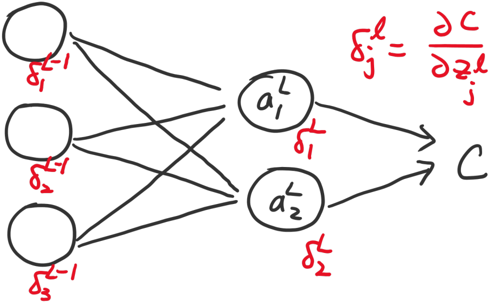


$$C = (a_1^L - y_1)^2 + (a_2^L - y_2)^2$$

Error Term

- The error is defined as

$$\delta_j^\ell = \frac{\partial C}{\partial z_j^\ell}$$



- You can show that at the output,

$$\delta_j^L = \frac{\partial C}{\partial a_j^L}\frac{\partial a_j^L}{\partial z_j^L} = \frac{\partial C}{\partial a_j^L}\sigma'(z_j^L).$$

4 Fundamental Equations for Back Propagation

BP Equation 1: For the error in the output layer:

$$\delta_j^L = \frac{\partial C}{\partial a_j^L} \sigma'(z_j^L). \qquad \text{(BP-1)}$$

- First term: $\frac{\partial C}{\partial a_j^L}$ is rate of change w.r.t. a_j^L
- Second term: $\sigma'(z_j^L) =$ rate of change w.r.t. z_j^L.
- So it is just **chain rule**.
- Example: If $C = \frac{1}{2}\sum_j (y_j - a_j^L)^2$, then

$$\frac{\partial C}{\partial a_j^L} = (a_j^L - y_j)$$

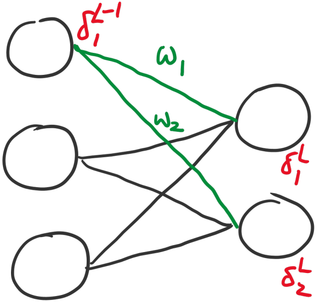
- Matrix-vector form: $\boldsymbol{\delta}^L = \nabla_a C \odot \sigma'(\boldsymbol{z}^L)$

4 Fundamental Equations for Back Propagation

BP Equation 2: An equation for the error δ^ℓ in terms of the error in the next layer, $\delta^{\ell+1}$

$$\boldsymbol{\delta}^\ell = ((\boldsymbol{w}^{\ell+1})^T \boldsymbol{\delta}^{\ell+1}) \odot \sigma'(\boldsymbol{z}^\ell). \quad \text{(BP-2)}$$

- You start with $\boldsymbol{\delta}^{\ell+1}$. Take weighted average $\boldsymbol{w}^{\ell+1}$.



- (BP-1) and (BP-2) can help you determine error at any layer.

4 Fundamental Equations for Back Propagation

Equation 3: An equation for the rate of change of the cost with respect to any bias in the network.

$$\frac{\partial C}{\partial b_j^\ell} = \delta_j^\ell. \qquad \text{(BP-3)}$$

- Good news: We have already known δ_j^ℓ from Equation 1na dn 2.
- So computing $\frac{\partial C}{\partial b_j^\ell}$ is easy.

Equation 4: An equation for the rate of change of the cost with respect to any weight in the network.

$$\frac{\partial C}{\partial w_{jk}^\ell} = a_k^{\ell-1}\delta_j^\ell \qquad \text{(BP-4)}$$

- Again, everything on the right is known. So it is easy to compute.

Back Propagation Algorithm

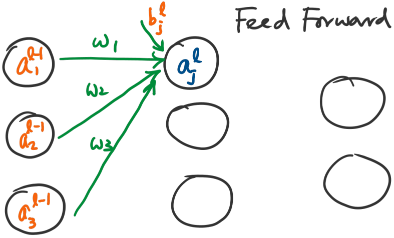
- Below is a very concise summary of the BP algorithm

1. **Input x:** Set the corresponding activation a^1 for the input layer.
2. **Feedforward:** For each $l = 2, 3, \ldots, L$ compute $z^l = w^l a^{l-1} + b^l$ and $a^l = \sigma(z^l)$.
3. **Output error δ^L:** Compute the vector $\delta^L = \nabla_a C \odot \sigma'(z^L)$.
4. **Backpropagate the error:** For each $l = L-1, L-2, \ldots, 2$ compute $\delta^l = ((w^{l+1})^T \delta^{l+1}) \odot \sigma'(z^l)$.
5. **Output:** The gradient of the cost function is given by $\frac{\partial C}{\partial w^l_{jk}} = a^{l-1}_k \delta^l_j$ and $\frac{\partial C}{\partial b^l_j} = \delta^l_j$.

Step 2: Feed Forward Step

- Let us take a closer look at Step 2
- The feed forward step computes the intermediate variables and the activations

$$
\begin{aligned}
\boldsymbol{z}^{\ell} &= (\boldsymbol{w}^{\ell})^T \boldsymbol{a}^{\ell-1} + b^{\ell} \\
\boldsymbol{a}^{\ell} &= \sigma(\boldsymbol{z}^{\ell}).
\end{aligned}
$$

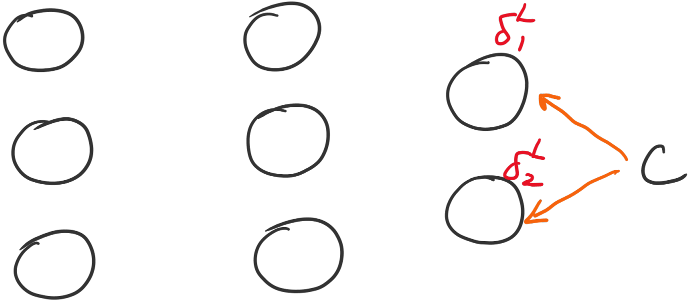


$$a_j^\ell = \sigma(z_j^\ell) = \sigma\left((w^\ell)^T a^{\ell-1} + b_j^\ell\right)$$

Step 3: Output Error

- Let us take a closer look at Step 3
- The output error is given by (BP-1)

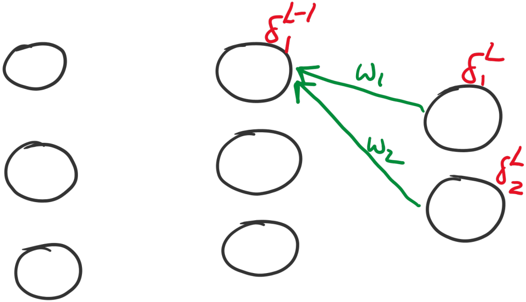
$$\boldsymbol{\delta}^L = \nabla_a C \odot \sigma'(\boldsymbol{z}^L)$$



Step 4: Output Error

- Let us take a closer look at Step 4
- The error back propagation is given by (BP-2)

$$\boldsymbol{\delta}^{\ell} = ((\boldsymbol{w}^{\ell+1})^T \boldsymbol{\delta}^{\ell+1}) \odot \sigma'(\boldsymbol{z}^{\ell}).$$



Summary of Back Propagation

- There is no dark magic behind back propagation
- It is literally just **chain rule**
- You need to do this chain rule very systematically and **carefully**
- Then you can derive the back propagation steps
- Nielsen wrote in his book that

> ... How backpropagation could have been discovered in the first place? In fact, if you follow the approach I just sketched you will discover a proof of backpropagation...You make those simplifications, get a shorter proof, and write that out....The result after a few iterations is the one we saw earlier, short but somewhat obscure...

- Most deep learning libraries have built-in back propagation steps.
- You don't have to implement it yourself, but you need to know what's behind it.

Reading List

- Michael Nielsen, Neural Networks and Deep Learning, http://neuralnetworksanddeeplearning.com/chap2.html
  - Very well written. Easy to follow.
- Duda, Hart, Stork, Pattern Classification, Chapter 5
  - Classical treatment. Comprehensive. Readable.
- Bishop, Pattern Recognition and Machine Learning, Chapter 5
  - Somewhat Bayesian. Good for those who like statistics
- Stanford CS 231N, http://cs231n.stanford.edu/slides/2017/cs231n_2017_lecture4.pdf
  - Good numerical example.
- CMU https://www.cs.cmu.edu/~mgormley/courses/10601-s17/slides/lecture20-backprop.pdf
- Cornell https://www.cs.cornell.edu/courses/cs5740/2016sp/resources/backprop.pdf