Tools & Models for Data Science

Deep Neural Networks (2): Learning

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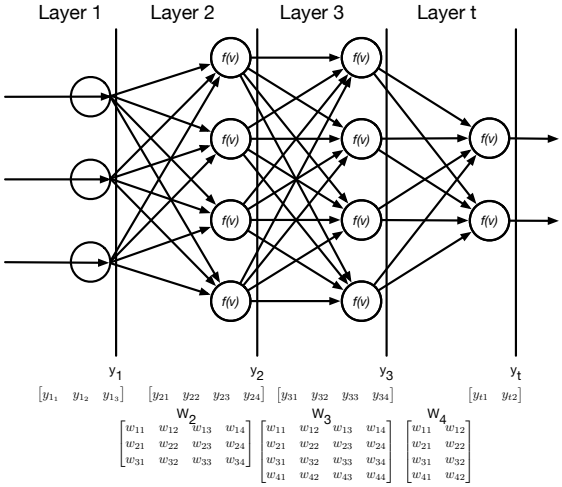
Learning Is Accomplished Via GD

- GD in the context of a NN gives rise to the “back-propagation” algorithm
  - First described in 1975
  - Recall params to deep network are all of the weight matrices: $W = W_1, W_2, ...$
  - “Learning” involves tweaking values of those matrices
  - … to minimize a loss function

NN Variables



- $w_{i,j,k}$:
- $i =$ layer
- $j =$ input neuron
- $k =$ output neuron

GD for Deep NNs

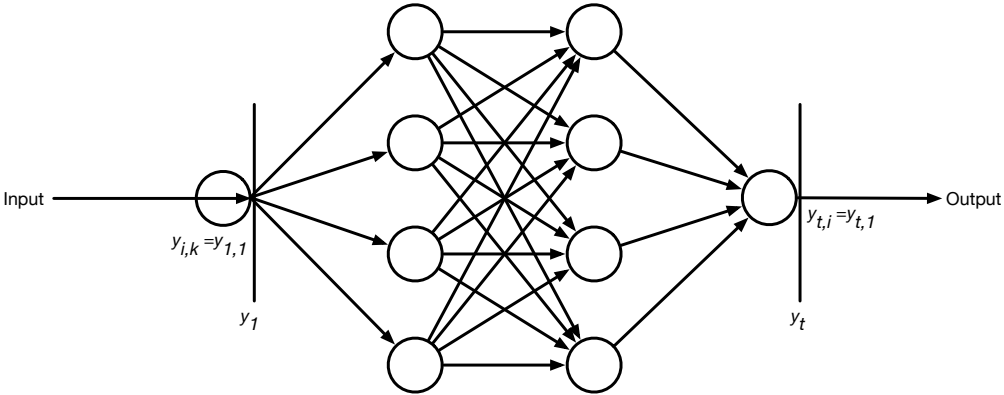
- Just like all GD algorithms, it is iterative
  - Assume loss function $L(W)$
  - with learning rate, λ
  - and where W is a tensor of 2D weight matrices
  - Then we have

Make a non-stupid guess for each W_i;
repeat {
  $W \leftarrow W - \lambda \nabla L(W)$;
} **while** (change in loss $> \varepsilon$)

Choosing a Loss Function

- There are many possible loss functions
- Let's assume one output neuron, one input data point;
  - Use $y_{i,k}$ to denote output from layer i, neuron k
  - So in layer t ("top") just have $y_{t,1}$
  - Hoped-for value is y^*
  - Let's use squared loss: $L(W) = (y_{t,1} - y^*)^2$
- Extension to many data points, many outputs straightforward.

Our 1 I/O NN

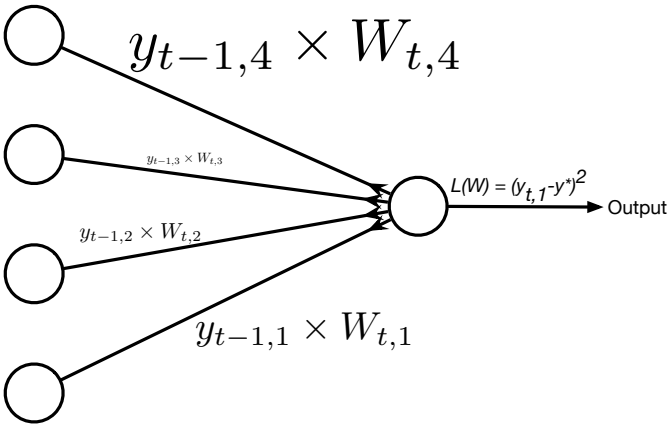


Big Picture

1. Make a non-stupid guess for the weights
2. Compute the value of the Loss function
3. Redistribute the error from the Loss function among the weights

- Weights that cause the error to increase will have larger activation values (y)
- And these will have larger values for $\frac{\partial L}{\partial W}$

Push Back Loss



From Inputs to Outputs to Weights

- Each input data point contributes to the cost and to the gradient
- Each “pulls” gradient descent in a certain direction
- Sum together the contribution to determine the overall direction of the gradient
- Move the weights that way

Computing the Gradient

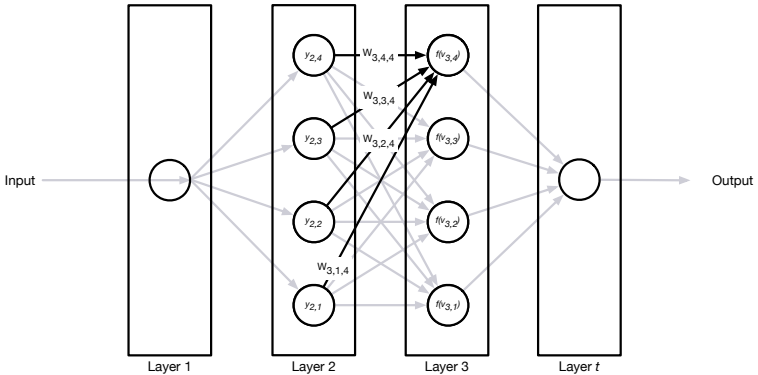
- Need to be able to differentiate L wrt each weight
- Done by applying the chain rule:

$$\frac{\partial L}{\partial w_{i,j,k}} = \frac{\partial L}{\partial y_{i,k}} \frac{\partial y_{i,k}}{\partial v_{i,k}} \frac{\partial v_{i,k}}{\partial w_{i,j,k}}$$

- $v_{i,k}$ is the weighted sum of activations sent into layer i, neuron k
- $v_{i,k} = \sum_{j'} w_{i,j',k} y_{i-1,j'}$

Computing the Neuron Input

$$v_{3,4} = \sum_{j'} w_{3,j',4} y_{2,j'}$$



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$$= \frac{\text{Loss}}{\text{Neuron Output}} \frac{\text{Neuron Output}}{\text{Neuron input}} \frac{\text{Neuron Input}}{\text{Weights}}$$

- Application of chain rule comes from chain of dependencies:
  - neuron output $y_{i,k}$ used to compute the loss
  - neuron input $v_{i,k}$ used to compute neuron output $y_{i,k}$
  - weight $w_{i,j,k}$ used to compute neuron input $v_{i,k}$
- Note: No one actually does the math!

Now We Look At the Different Parts

- Explain

$$\frac{\partial L}{\partial w_{i,j,k}} = \frac{\partial L}{\partial y_{i,k}} \frac{\partial y_{i,k}}{\partial v_{i,k}} \frac{\partial v_{i,k}}{\partial w_{i,j,k}}$$

$$\frac{\partial L}{\partial w_{i,j,k}} = 3 \times 1 \times 2$$

1. Start with differentiating neuron output
2. Then differentiating the neuron input
3. And finally differentiating the loss

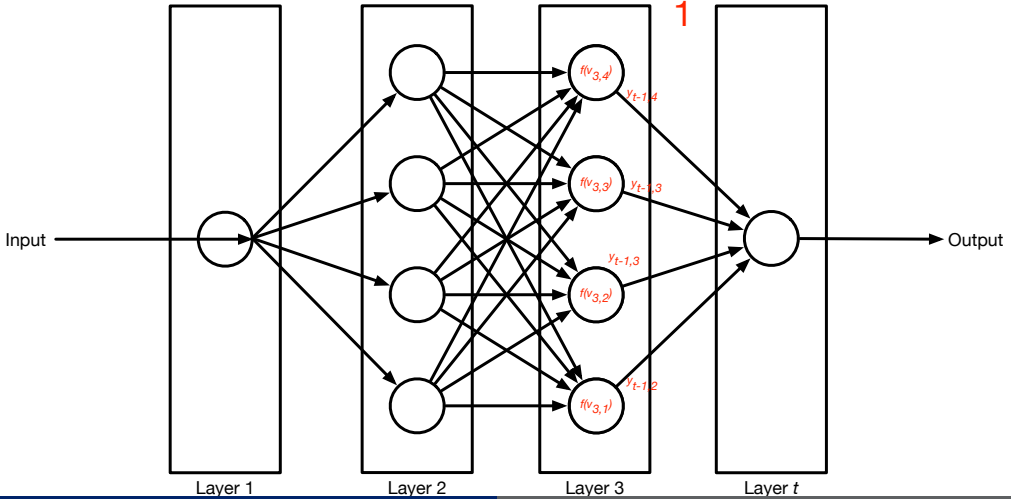
Differentiating Neuron Output

- We start with neuron output
- That is,

$$\frac{\partial y_{i,j}}{\partial v_{i,j}}$$

Computing the Gradient - Neuron Output

$$\frac{\partial y_{i,j}}{\partial v_{i,j}}$$



Differentiating Neuron Output

- Assume activation function is the logistic function

$$f(v_{i,j}) = \frac{1}{1+e^{-v_{i,j}}}$$

- Popular because result is magically simple
- Will skip algebra, but differentiating the logistic function gives us:

$$\frac{df}{dv_{i,j}} = f(v_{i,j})(1-f(v_{i,j}))$$

- So, since $y_{i,j} = f(v_{i,j})$,

$$\frac{\partial y_{i,j}}{\partial v_{i,j}} = \frac{df}{dv_{i,j}} = f(v_{i,j})(1-f(v_{i,j}))$$

- Which is surprisingly nice for Logistic Regression

Differentiating Neuron Input

- Now time to deal with

$$\frac{\partial v_{i,k}}{\partial w_{i,j,k}}$$

- Note that $v_{i,k}$ computes a dot product, so:x

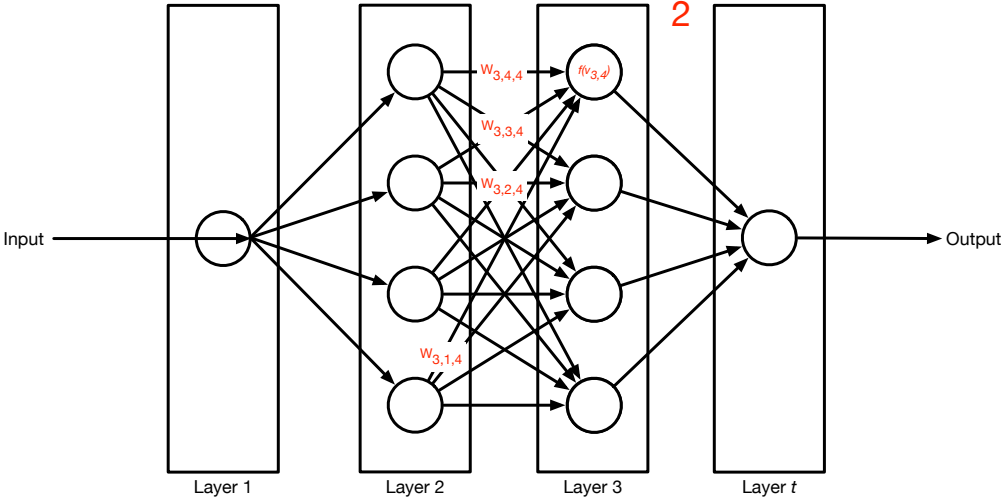
$$\frac{\partial v_{i,k}}{\partial w_{i,j,k}} = \frac{\partial}{\partial w_{i,j,k}} \sum_{j'} w_{i,j',k} y_{i-1,j'}$$

- This is just $y_{i-1,j}$, since all the j's drop out, except for the case where $j' = j$
- We are summing over the prior layer's neurons
- Multiplying those outputs by the weights leading to the current layer
- For each neuron input, we only care about weights that go INTO this neuron
- Can ignore all the other weights in this layer

Computing the Gradient - Neuron Input

$$\frac{\partial v_{i,k}}{\partial w_{i,j,k}}$$

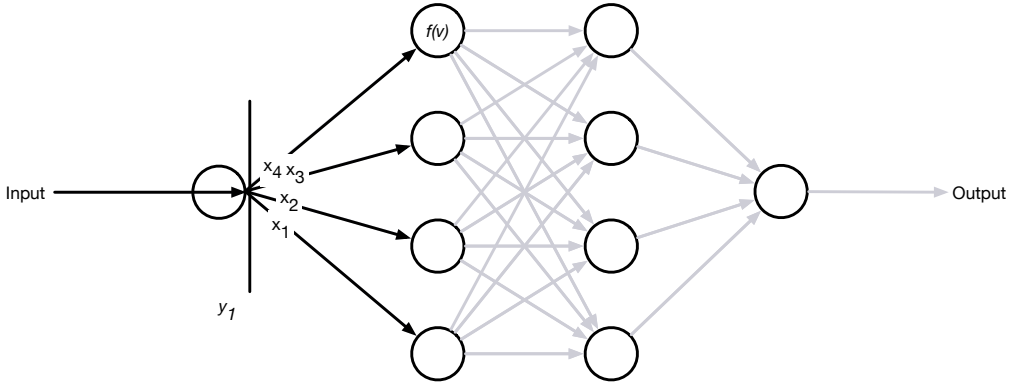
2



Differentiating Neuron Input from the Input Layer

- Note that if $i-1$ is the input layer, then $y_{i-1,j} = x_j$
  - Where x_j is the jth entry in the input vector

Computing the Gradient - Neuron Input



Differentiating the Loss

- Next, need to be able to deal with differentiating the loss

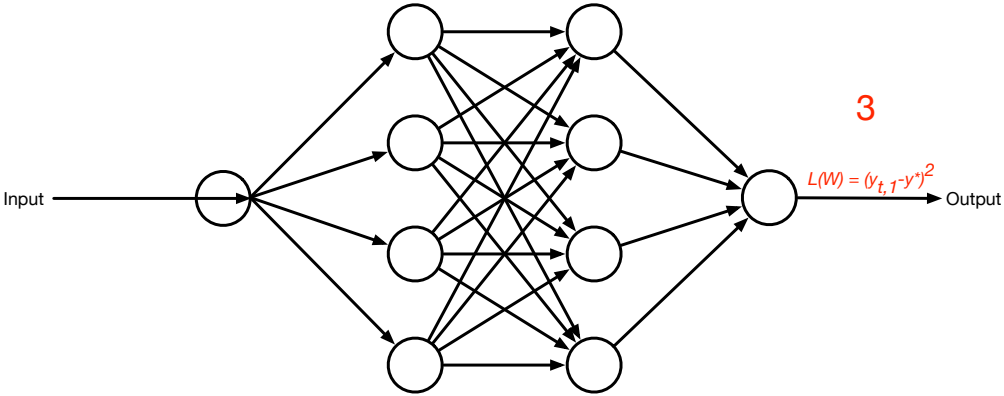
$$\frac{\partial L}{\partial y_{i,j}}$$

- If this is the output layer, it is easy:

$$\frac{\partial L}{\partial y_{t,1}} = 2(y_{t,1} - y^*) \approx (y_{t,1} - y^*)$$

- Recall: y^* is the hoped for output
- Can drop the 2 since will be swallowed into the learning rate

Computing the Gradient - Loss for Output Layer



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? But what about the other layers?

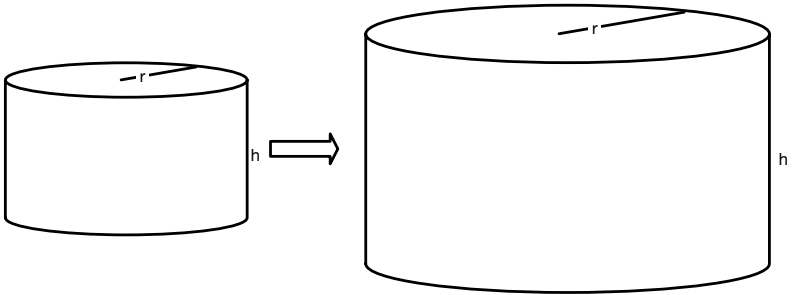
Sidebar: the Total Derivative

- Quick detour: idea of a "total derivative" (consequence of chain rule)
  - Say we have a function f of several variables $x_1, x_2, ...$
  - Each of which is a function of variable t; we want $\frac{df}{dt}$
  - Is computed via the "total derivative":

$$\frac{df}{dt} = \frac{\partial f}{\partial x_1}\frac{\partial x_1}{\partial t} + \frac{\partial f}{\partial x_2}\frac{\partial x_2}{\partial t} + ...$$

Total Derivative Example

- A cylinder has radius and height of 2 units
  - Recall $V = \pi r^2 h$
  - It's getting bigger...
  - Radius increases at 2 units/sec, height at 1 unit/sec



Total Derivative Example

- A cylinder has radius, height of 2 units
  - Recall $V = \pi r^2 h$
  - It's getting bigger...
  - Radius increases at 2 units/sec, height at 1 unit/sec
  - What is the instantaneous rate of increase in volume?

$$\begin{aligned}\frac{dV}{dt} &= \frac{\partial V}{\partial r}\frac{\partial r}{\partial t} + \frac{\partial V}{\partial h}\frac{\partial h}{\partial t} \\ &= \pi 2rh \times \left(\frac{\partial r}{\partial t}\right) + \pi r^2 \times \left(\frac{\partial h}{\partial t}\right) \\ &= \pi \times 2 \times 2 \times 2 \times (2) + \pi \times 2^2 \times (1) = 20\pi \text{ units}^3/\text{sec}\end{aligned}$$

  - Note: could substitute $r = 2 + 2t, h = 2 + t$ in $V = \pi r^2 h$
  - Would get same answer using "classic" derivative over this new expression

Total Derivative vs. Partial Derivative

- Partial derivative: Other variables are treated as constants
- Total derivative: Other variables are NOT constant

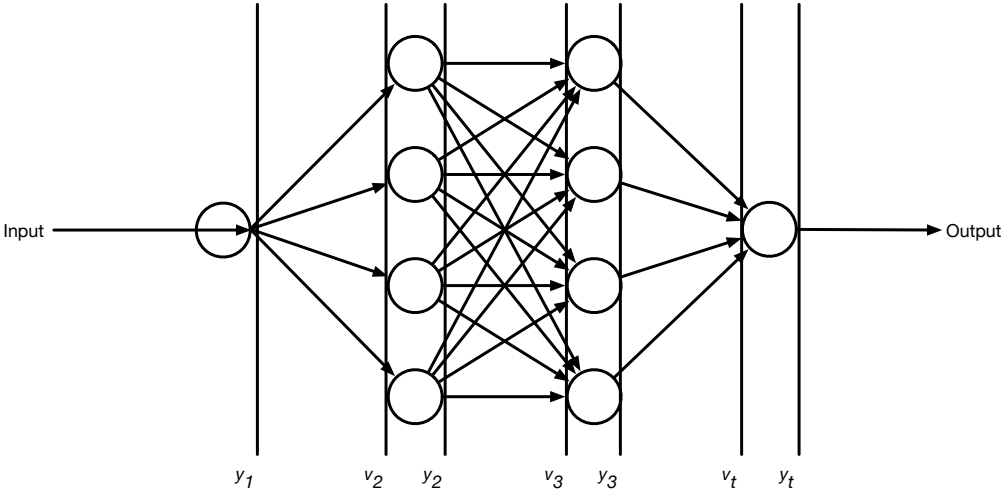
Differentiating Loss for Hidden Layers

- Why is total derivative relevant?
  - Note that Loss is a function of all the neuron inputs
  - All v's at layer $i+1$: $v_{i+1,1}, v_{i+1,2}, v_{i+1,3}, \ldots$
  - Where $v_{i+1,k}$ is itself a function of $y_{i,j}$
  - (Plus a lot of other things we'll treat as constants)
  - This is exactly the case where $\frac{\partial L}{\partial y_{i,j}}$ must be computed using total derivative
  - So take the total derivative wrt $y_{i,j}$:

$$\frac{\partial L}{\partial y_{i,j}} = \sum_k \frac{\partial L}{\partial v_{i+1,k}} \frac{\partial v_{i+1,k}}{\partial y_{i,j}}$$

  - Partial of L wrt the jth neuron in layer i
  - Recall that $y_{i,j}$ depends on all of the input weights

Computing the Gradient - Loss for Hidden Layers



Differentiating the Loss for Hidden Layers

- And since $\frac{\partial v_{i+1,k}}{\partial y_{i,j}} = w_{i+1,j,k}$
- We have:

$$\frac{\partial L}{\partial y_{i,j}} = \sum_k \frac{\partial L}{\partial v_{i+1,k}} w_{i+1,j,k}$$

  - Further, note that, by chain rule:

$$\frac{\partial L}{\partial v_{i+1,k}} = \frac{\partial L}{\partial y_{i+1,k}} \frac{\partial y_{i+1,k}}{\partial v_{i+1,k}}$$

- Refer to $\frac{\partial L}{\partial v_{i+1,k}}$ as $\delta_{i+1,k}$.
  - So

$$\frac{\partial L}{\partial y_{i,j}} = \sum_k \delta_{i+1,k} w_{i+1,j,k}$$

Recursion!!

- Recall,

$$\frac{\partial L}{\partial w_{i,j,k}} = \frac{\partial L}{\partial y_{i,k}} \frac{\partial y_{i,k}}{\partial v_{i,k}} \frac{\partial v_{i,k}}{\partial w_{i,j,k}}$$

  - And we can write this as:

$$\begin{aligned}\frac{\partial L}{\partial w_{i,j,k}} &= \left(\sum_{k'} \delta_{i+1,k'} w_{i+1,k,k'} \right) \left(f(v_{i,k})(1 - f(v_{i,k})) \right) \left(y_{i-1,j} \right) \\ &= \delta_{i,k} \left(y_{i-1,j} \right)\end{aligned}$$

Breaking down the Transition

$$\frac{\partial L}{\partial w_{i,j,k}} = \frac{\partial L}{\partial y_{i,k}} \frac{\partial y_{i,k}}{\partial v_{i,k}} \frac{\partial v_{i,k}}{\partial w_{i,j,k}}$$

$$\frac{\partial L}{\partial w_{i,j,k}} = \left(\sum_{k'} \delta_{i+1,k'} w_{i+1,k,k'} \right) \left(f(v_{i,k})(1 - f(v_{i,k})) \right) \left(y_{i-1,j} \right)$$

$$\frac{\partial L}{\partial v_{i+1,k}} = \delta_{i+1,k}$$

$$= \delta_{i,k} \left(y_{i-1,j} \right)$$

Recursion!!

- Remember our goal
- To be able to differentiate L wrt each weight

$$\begin{aligned}\frac{\partial L}{\partial w_{i,j,k}} &= \left(\sum_{k'} \delta_{i+1,k'} w_{i+1,k,k'}\right)\left(f(v_{i,k})(1-f(v_{i,k}))\right)(y_{i-1,j}) \\ &= \delta_{i,k}\,(y_{i-1,j})\end{aligned}$$

- This suggests a dynamic programming algorithm!
  - Start at top, recurse back
  - At layer i, to compute each $\frac{\partial L}{\partial w_{i,j,k}}$ you use each $\delta_{i+1,k'}$ from previous layer
  - As a side-effect of computing each $\frac{\partial L}{\partial w_{i,j,k}}$, you compute $\delta_{i,k}$
  - Can record this and use when computing layer $i-1$

Dynamic Programming Algorithm

- First, make a forward pass thru the network
  - Compute each $y_{i,k}$, $v_{i,k}$, $w_{i,j,k}$
  - For each possible i, j, k
- Then, make a backward pass thru the network, starting at the top layer
  - Top layer is base case; compute

$$\delta_{t,1} = \frac{\partial L}{\partial y_{t,1}} \frac{\partial y_{t,1}}{\partial v_{t,1}} = f(v_{t,1})(1 - f(v_{t,1}))(y_{t,1} - y^*)$$

  - And then

$$\frac{\partial L}{\partial w_{t,j,1}} = \delta_{t,1} y_{t-1,j}$$

DP for Back-propagation: Other Layers

- Then at every other layer, want $\frac{\partial L}{\partial w_{i,j,k}}$, for each j, k pair
- To do this:
  - At layer i, for a given j, k pair
  - First compute $\delta_{i,k} = \left(\sum_{k'} \delta_{i+1,k'} w_{i+1,k,k'}\right) \left(f(v_{i,k})(1 - f(v_{i,k}))\right)$; save this value
  - Next compute $\frac{\partial L}{\partial w_{i,j,k}} = \delta_{i,k} y_{i-1,j}$
- Keep recursing until you have each $\frac{\partial L}{\partial w_{2,j,k}}$
- All of the $\frac{\partial L}{\partial w_{i,j,k}}$ values together then constitute $\nabla L(W)$
- Use in an iteration of GD

How To Implement Learning?

- This math has been known for many years
- Once you understand it, is quite simple
- So would be easy to implement learning directly in Python
- But applies to particular narrow case:
  - Fully-connected network
  - Logistic activation
  - Feed-forward
  - L2 loss
  - One output neuron
  - One data item

What If Your Network Is Different?

- Some changes are easy:
  - Different loss: only changes $\frac{\partial L}{\partial y_{t,1}}$
  - Multiple data points in a batch: compute $\frac{\partial L}{\partial w_{i,j,k}}$ wrt each, and then add them up (can be made efficient with vector/matrix ops)
  - Different activation: only changes $\frac{\partial y_{i,j}}{\partial v_{i,j}}$
- But some are hard...
- What about adding convolutional layers?
- Pooling layers?
- Suddenly a lot of error-prone math and code needs to be written

So In Practice...

- ...automatic differentiation tools are used
- This is a large part of TensorFlow
- Idea:
  - You describe your network in a high level language
  - Maybe just fit together layers
  - And the system generates the learning algorithm for you
  - Automatically figuring out necessary partial derivatives

Auto Differentiation

- Long history in CS (compilers in particular)
- Actually quite simple
  - Idea: don't generate code to actually execute math ops
  - Rather, they generate code to differentiate wrt that math operation
  - Example: user writes code $f(x,y,z) = exp_1 \times exp_2$
  - Wants partial derivative of f wrt x
  - Compiler won't generate code for $exp_1 \times exp_2$
  - Rather, compiler will generate code $exp_1 \frac{\partial exp_2}{\partial x} + exp_2 \frac{\partial exp_1}{\partial x}$
  - Using the chain rule

Auto Differentiation Example

- I write code to multiply two values
- The program overloads the multiplication operation
- And generates code that computes the partial derivative of the operation

Good/Bad of this Approach

- Good
  - Good: much less error prone
  - Good: very high programmer/data scientist productivity
  - Good: automatically generate algorithms that use hardware well
  - There care be an optimization step
  - Which provides an abstract representation of the partial derivative
- Bad
  - Bad: challenging to debug, since algorithm generated by compiler may look nothing like original code
  - Bad: algorithm will not be as efficient as one written by hard-core expert

Huh?

- You could spend some time and implement back propagation
- Then you could debug it, since it's your code
- Instead, you have to debug generated code
- You build (e.g. in TensorFlow) a computation graph
- And ask the system to differentiate it for you
- You get a new compute graph
- If it doesn't work
- it's much harder to debug the automatically generated code

Questions?