Lecture 4
Backpropagation
CMSC 35246: Deep Learning

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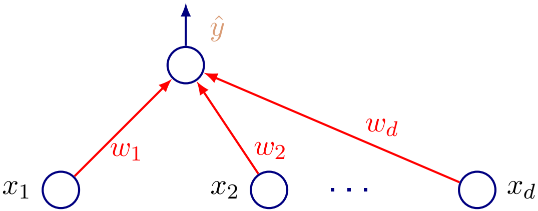
- Things we will look at today
  - More Backpropagation
  - Still more backpropagation
  - Quiz at 4:05 PM

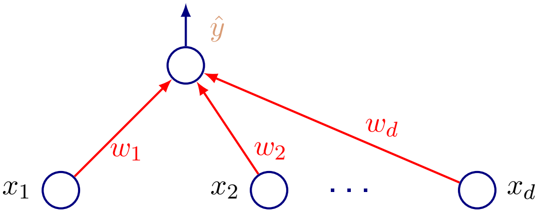
To understand, let us just calculate!

One Neuron Again



- Consider example $\mathbf{x}$; Output for $\mathbf{x}$ is $\hat{y}$; Correct Answer is y
- Loss $L = (y - \hat{y})^2$
- $\hat{y} = \mathbf{x}^T \mathbf{w} = x_1 w_1 + x_2 w_2 + \dots x_d w_d$

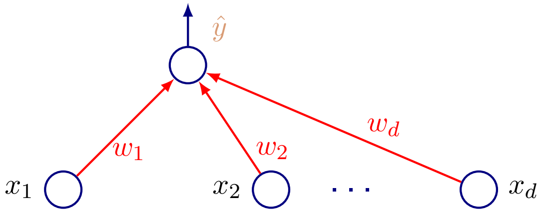
One Neuron Again



- Want to update w_i (forget closed form solution for a bit!)
- Update rule: $w_i := w_i - \eta \frac{\partial L}{\partial w_i}$
- Now

$$\frac{\partial L}{\partial w_i} = \frac{\partial (\hat{y} - y)^2}{\partial w_i} = 2(\hat{y} - y) \frac{\partial (x_1 w_1 + x_2 w_2 + \ldots x_d w_d)}{\partial w_i}$$

One Neuron Again

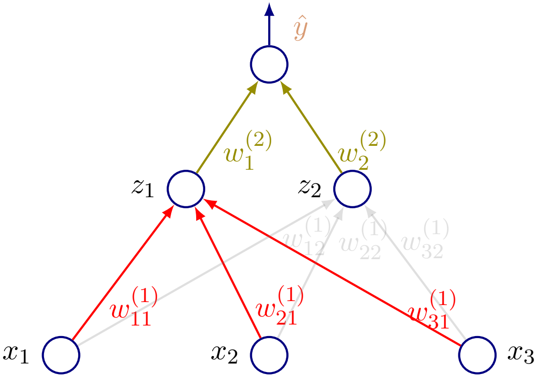


- We have: $\dfrac{\partial L}{\partial w_i} = 2(\hat{y} - y)x_i$
- Update Rule:

$$w_i := w_i - \eta(\hat{y} - y)x_i = w_i - \eta\delta x_i \text{ where } \delta = (\hat{y} - y)$$

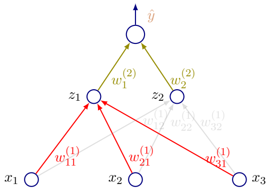
- In vector form: $\mathbf{w} := \mathbf{w} - \eta\delta\mathbf{x}$
- Simple enough! Now let's graduate ...

Simple Feedforward Network



- $\hat{y} = w_1^{(2)} z_1 + w_2^{(2)} z_2$
- $z_1 = \tanh(a_1)$ where $a_1 = w_{11}^{(1)} x_1 + w_{21}^{(1)} x_2 + w_{31}^{(1)} x_3$ likewise for z_2

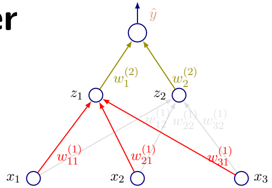
Simple Feedforward Network



- $z_1 = \tanh(a_1)$ where $a_1 = w_{11}^{(1)} x_1 + w_{21}^{(1)} x_2 + w_{31}^{(1)} x_3$
- $z_2 = \tanh(a_2)$ where $a_2 = w_{12}^{(1)} x_1 + w_{22}^{(1)} x_2 + w_{32}^{(1)} x_3$

- Output $\hat{y} = w_1^{(2)} z_1 + w_2^{(2)} z_2$; Loss $L = (\hat{y} - y)^2$
- Want to assign credit for the loss L to each weight

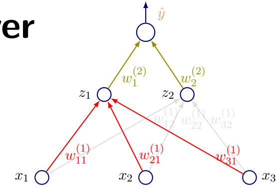
Top Layer



- Want to find: $\frac{\partial L}{\partial w_1^{(2)}}$ and $\frac{\partial L}{\partial w_2^{(2)}}$
- Consider $w_1^{(2)}$ first

- $\frac{\partial L}{\partial w_1^{(2)}} = \frac{\partial (\hat{y}-y)^2}{\partial w_1^{(2)}} = 2(\hat{y}-y)\frac{\partial (w_1^{(2)}z_1 + w_2^{(2)}z_2)}{\partial w_1^{(2)}} = 2(\hat{y}-y)z_1$
- Familiar from earlier! Update for $w_1^{(2)}$ would be $w_1^{(2)} := w_1^{(2)} - \eta \frac{\partial L}{\partial w_1^{(2)}} = w_1^{(2)} - \eta \delta z_1$ with $\delta = (\hat{y}-y)$
- Likewise, for $w_2^{(2)}$ update would be $w_2^{(2)} := w_2^{(2)} - \eta \delta z_2$

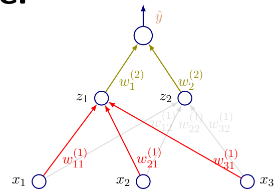
Next Layer



- There are six weights to assign credit for the loss incurred
- Consider $w_{11}^{(1)}$ for an illustration
- Rest are similar

- $\frac{\partial L}{\partial w_{11}^{(1)}} = \frac{\partial (\hat{y}-y)^2}{\partial w_{11}^{(1)}} = 2(\hat{y}-y)\frac{\partial (w_1^{(2)} z_1 + w_2^{(2)} z_2)}{\partial w_{11}^{(21)}}$
- Now: $\frac{\partial (w_1^{(2)} z_1 + w_2^{(2)} z_2)}{\partial w_{11}^{(1)}} = w_1^{(2)} \frac{\partial (\tanh(w_{11}^{(1)} x_1 + w_{21}^{(1)} x_2 + w_{31}^{(1)} x_3))}{\partial w_{11}^{(1)}} + 0$
- Which is: $w_1^{(2)}(1-\tanh^2(a_1))x_1$ recall $a_1 =?$
- So we have: $\frac{\partial L}{\partial w_{11}^{(1)}} = 2(\hat{y}-y) w_1^{(2)} (1-\tanh^2(a_1))x_1$

Next Layer



- $\frac{\partial L}{\partial w_{11}^{(1)}} =$
  $2(\hat{y} - y)w_1^{(2)}(1 - \tanh^2(a_1))x_1$
- Weight update:
  $w_{11}^{(1)} := w_{11}^{(1)} - \eta \frac{\partial L}{\partial w_{11}^{(1)}}$

- Likewise, if we were considering $w_{22}^{(1)}$, we'd have:
- $\frac{\partial L}{\partial w_{22}^{(1)}} = 2(\hat{y} - y)w_2^{(2)}(1 - \tanh^2(a_2))x_2$
- Weight update: $w_{22}^{(1)} := w_{22}^{(1)} - \eta \frac{\partial L}{\partial w_{22}^{(1)}}$

Let's clean this up...

- Recall, for top layer: $\frac{\partial L}{\partial w_i^{(2)}} = (\hat{y} - y)z_i = \delta z_i$ (ignoring 2)
- One can think of this as: $\frac{\partial L}{\partial w_i^{(2)}} = \underbrace{\delta}_{\text{local error}} \underbrace{z_i}_{\text{local input}}$
- For next layer we had: $\frac{\partial L}{\partial w_{ij}^{(1)}} = (\hat{y} - y)w_j^{(2)}(1 - \tanh^2(a_j))x_i$
- Let $\delta_j = (\hat{y} - y)w_j^{(2)}(1 - \tanh^2(a_j)) = \delta w_j^{(2)}(1 - \tanh^2(a_j))$ (Notice that δ_j contains the δ term (which is the error!))
- Then: $\frac{\partial L}{\partial w_{ij}^{(1)}} = \underbrace{\delta_j}_{\text{local error}} \underbrace{x_i}_{\text{local input}}$
- Neat!

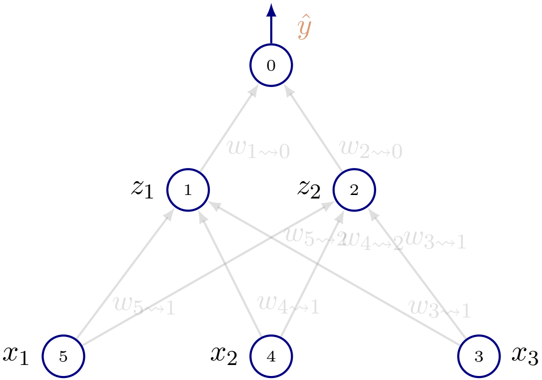
Let's clean this up...

- Let's get a cleaner notation to summarize this
- Let $w_{i \rightsquigarrow j}$ be the weight for the connection FROM node i to node j
- Then

$$\frac{\partial L}{\partial w_{i \rightsquigarrow j}} = \delta_j z_i$$

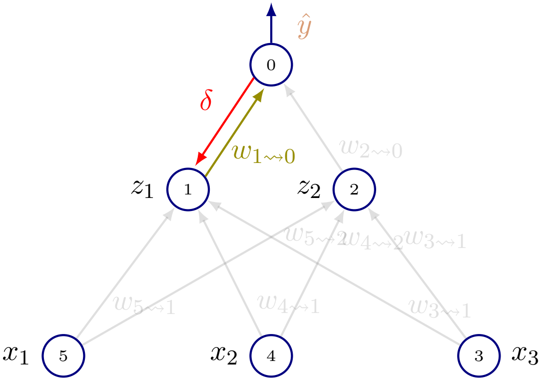
- δ_j is the local error (going from j backwards) and z_i is the local input coming from i

Credit Assignment: A Graphical Revision



- Let's redraw our toy network with new notation and label nodes

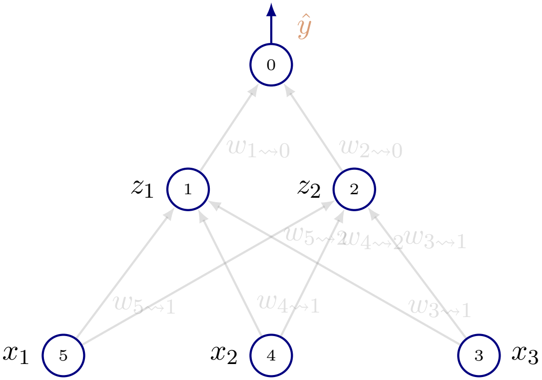
Credit Assignment: Top Layer



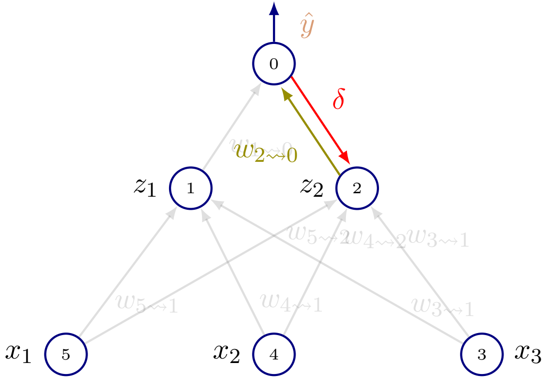
- Local error from 0: $\delta = (\hat{y} - y)$, local input from 1: z_1

$$\therefore \frac{\partial L}{\partial w_{1\rightsquigarrow 0}} = \delta z_1; \text{ and update } w_{1\rightsquigarrow 0} := w_{1\rightsquigarrow 0} - \eta \delta z_1$$

Credit Assignment: Top Layer



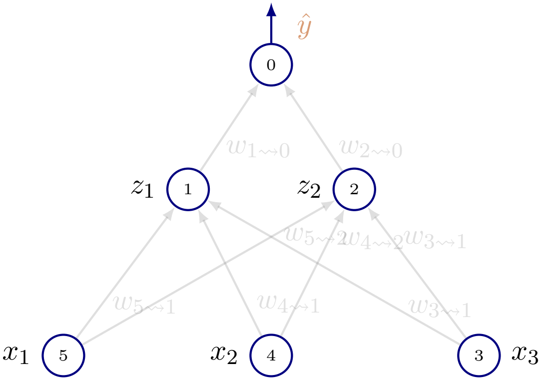
Credit Assignment: Top Layer



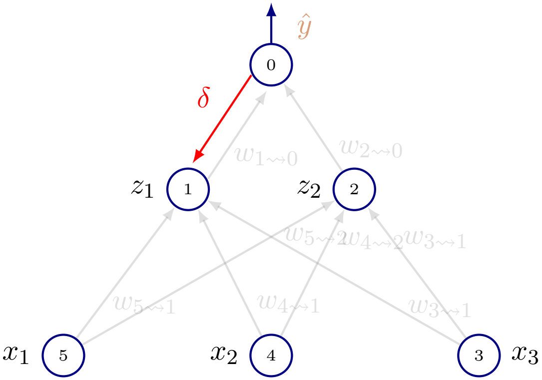
- Local error from 0: $\delta = (\hat{y} - y)$, local input from 2: z_2

$$\therefore \frac{\partial L}{\partial w_{2\rightsquigarrow 0}} = \delta z_2 \text{ and update } w_{2\rightsquigarrow 0} := w_{2\rightsquigarrow 0} - \eta \delta z_2$$

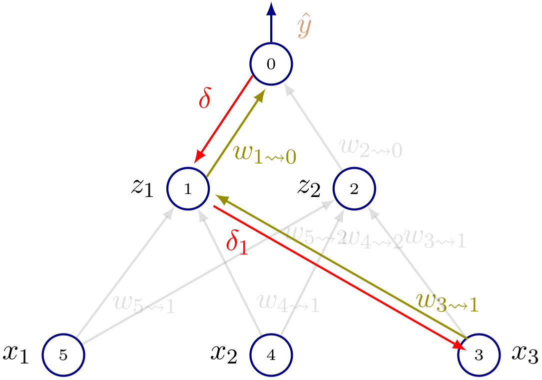
Credit Assignment: Next Layer



Credit Assignment: Next Layer



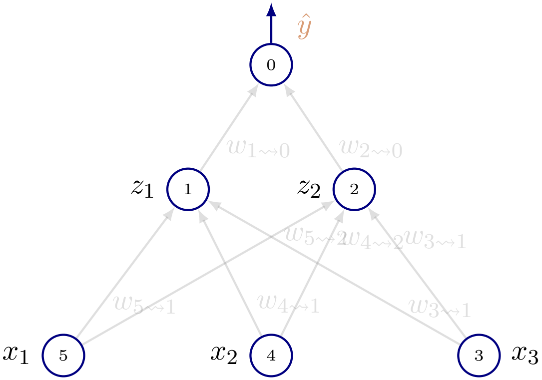
Credit Assignment: Next Layer



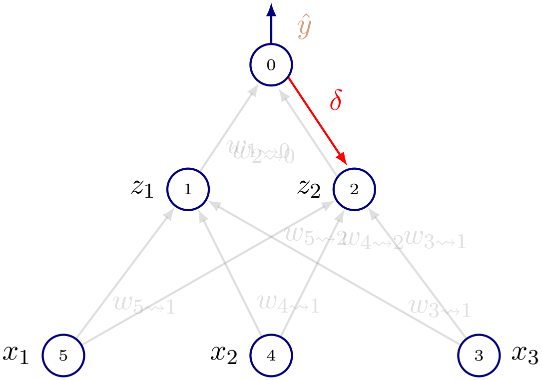
- Local error from 1: $\delta_1 = (\delta)(w_{1\rightsquigarrow 0})(1 - \tanh^2(a_1))$, local input from 3: x_3

$$\therefore \frac{\partial L}{\partial w_{3\rightsquigarrow 1}} = \delta_1 x_3 \text{ and update } w_{3\rightsquigarrow 1} := w_{3\rightsquigarrow 1} - \eta \delta_1 x_3$$

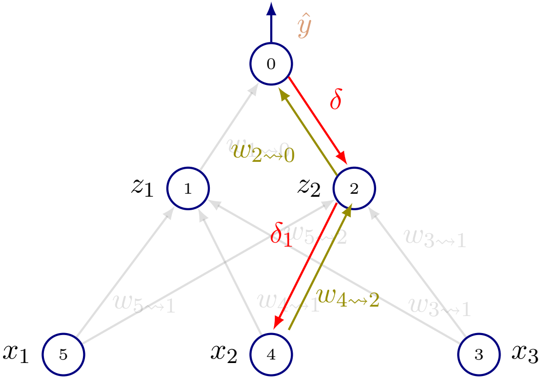
Credit Assignment: Next Layer



Credit Assignment: Next Layer



Credit Assignment: Next Layer



- Local error from 2: $\delta_2 = (\delta)(w_{2\rightsquigarrow 0})(1 - \tanh^2(a_2))$, local input from 4: x_2

$$\therefore \frac{\partial L}{\partial w_{4\rightsquigarrow 2}} = \delta_2 x_2 \text{ and update } w_{4\rightsquigarrow 2} := w_{4\rightsquigarrow 2} - \eta \delta_2 x_2$$

Let's Vectorize

- Let $W^{(2)} = \begin{bmatrix} w_{1 \rightsquigarrow 0} \\ w_{2 \rightsquigarrow 0} \end{bmatrix}$ (ignore that $W^{(2)}$ is a vector and hence more appropriate to use $\mathbf{w}^{(2)}$)
- Let
$$W^{(1)} = \begin{bmatrix} w_{5 \rightsquigarrow 1} & w_{5 \rightsquigarrow 2} \\ w_{4 \rightsquigarrow 1} & w_{4 \rightsquigarrow 2} \\ w_{3 \rightsquigarrow 1} & w_{3 \rightsquigarrow 2} \end{bmatrix}$$
- Let
$$Z^{(1)} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \text{ and } Z^{(2)} = \begin{bmatrix} z_1 \\ z_2 \end{bmatrix}$$

Feedforward Computation

1. Compute $A^{(1)} = {Z^{(1)}}^T W^{(1)}$
2. Applying element-wise non-linearity $Z^{(2)} = \tanh A^{(1)}$
3. Compute Output $\hat{y} = {Z^{(2)}}^T W^{(2)}$
4. Compute Loss on example $(\hat{y} - y)^2$

Flowing Backward

1. Top: Compute δ
2. Gradient w.r.t $W^{(2)} = \delta Z^{(2)}$
3. Compute $\delta_1 = (W^{(2)^T}\delta) \odot (1 - \tanh(A^{(1)})^2)$
   Notes: (a): $\odot$ is Hadamard product. (b) have written $W^{(2)^T}\delta$ as δ can be a vector when there are multiple outputs
4. Gradient w.r.t $W^{(1)} = \delta_1 Z^{(1)}$
5. Update $W^{(2)} := W^{(2)} - \eta\delta Z^{(2)}$
6. Update $W^{(1)} := W^{(1)} - \eta\delta_1 Z^{(1)}$
7. All the dimensionalities nicely check out!

So Far

- Backpropagation in the context of neural networks is all about assigning credit (or blame!) for error incurred to the weights
  - We follow the path from the output (where we have an error signal) to the edge we want to consider
  - We find the δs from the top to the edge concerned by using the chain rule
  - Once we have the partial derivative, we can write the update rule for that weight

What did we miss?

- Exercise: What if there are multiple outputs? (look at slide from last class)
- Another exercise: Add bias neurons. What changes?
- As we go down the network, notice that we need previous δs
- If we recompute them each time, it can blow up!
- Need to book-keep derivatives as we go down the network and reuse them

A General View of Backpropagation

Some redundancy in upcoming slides, but redundancy can be good!

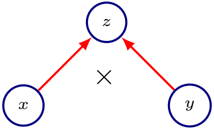
An Aside

- Backpropagation only refers to the method for computing the gradient
- This is used with another algorithm such as SGD for learning using the gradient
- Next: Computing gradient $\nabla_x f(x, y)$ for arbitrary f
- x is the set of variables whose derivatives are desired
- Often we require the gradient of the cost $J(\theta)$ with respect to parameters θ i.e $\nabla_\theta J(\theta)$
- Note: We restrict to case where f has a single output
- First: Move to more precise computational graph language!

Computational Graphs

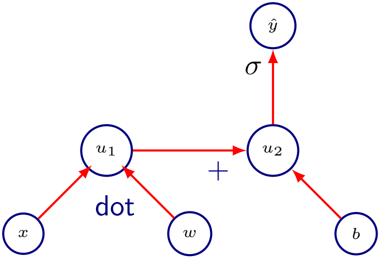
- Formalize computation as graphs
- **Nodes** indicate variables (scalar, vector, tensor or another variable)
- **Operations** are simple functions of one or more variables
- Our graph language comes with a set of **allowable** operations
- Examples:

$$z = xy$$



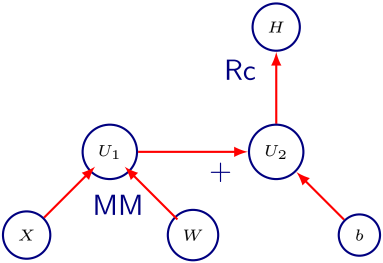
- Graph uses $\times$ operation for the computation

Logistic Regression



- Computes $\hat{y} = \sigma(\mathbf{x}^T \mathbf{w} + b)$

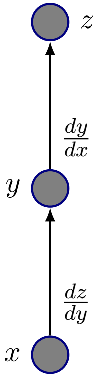
$$H = \max\{0, XW + b\}$$



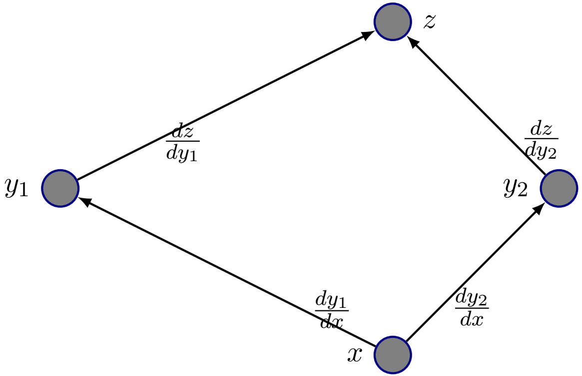
MM is matrix multiplication and Rc is ReLU activation

Back to backprop: Chain Rule

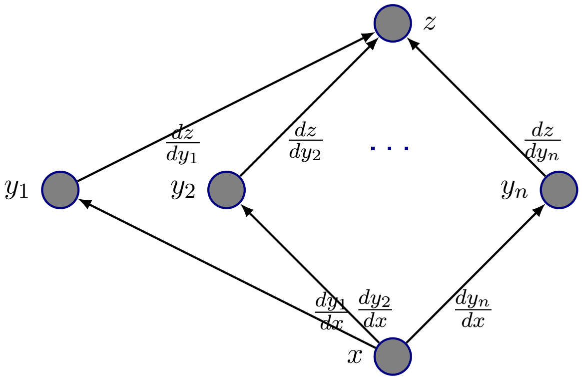
- Backpropagation computes the chain rule, in a manner that is highly efficient
- Let $f, g : \mathbb{R} \to \mathbb{R}$
- Suppose $y = g(x)$ and $z = f(y) = f(g(x))$
- Chain rule:
$$\frac{dz}{dx} = \frac{dz}{dy}\frac{dy}{dx}$$



Chain rule: $\frac{dz}{dx} = \frac{dz}{dy}\frac{dy}{dx}$



Multiple Paths: $\frac{dz}{dx} = \frac{dz}{dy_1}\frac{dy_1}{dx} + \frac{dz}{dy_2}\frac{dy_2}{dx}$



Multiple Paths: $$\frac{dz}{dx} = \sum_j \frac{dz}{dy_j} \frac{dy_j}{dx}$$

Chain Rule

- Consider $\mathbf{x} \in \mathbb{R}^m, \mathbf{y} \in \mathbb{R}^n$
- Let $g : \mathbb{R}^m \to \mathbb{R}^n$ and $f : \mathbb{R}^n \to \mathbb{R}$
- Suppose $\mathbf{y} = g(\mathbf{x})$ and $z = f(\mathbf{y})$, then

$$\frac{\partial z}{\partial x_i} = \sum_j \frac{\partial z}{\partial y_j} \frac{\partial y_j}{\partial x_i}$$

- In vector notation:

$$\begin{pmatrix} \frac{\partial z}{\partial x_1} \\ \vdots \\ \frac{\partial z}{\partial x_m} \end{pmatrix} = \begin{pmatrix} \sum_j \frac{\partial z}{\partial y_j} \frac{\partial y_j}{\partial x_1} \\ \vdots \\ \sum_j \frac{\partial z}{\partial y_j} \frac{\partial y_j}{\partial x_m} \end{pmatrix} = \nabla_{\mathbf{x}} z = \left(\frac{\partial \mathbf{y}}{\partial \mathbf{x}} \right)^T \nabla_{\mathbf{y}} z$$

Chain Rule

$$\nabla_{\mathbf{x}} z = \left(\frac{\partial \mathbf{y}}{\partial \mathbf{x}}\right)^T \nabla_{\mathbf{y}} z$$

- $\left(\frac{\partial \mathbf{y}}{\partial \mathbf{x}}\right)$ is the $n \times m$ Jacobian matrix of g
- **Gradient** of $\mathbf{x}$ is a multiplication of a Jacobian matrix $\left(\frac{\partial \mathbf{y}}{\partial \mathbf{x}}\right)$ with a vector i.e. the gradient $\nabla_{\mathbf{y}} z$
- Backpropagation consists of applying such Jacobian-gradient products to each operation in the computational graph
- In general this need not only apply to vectors, but can apply to tensors w.l.o.g

Chain Rule

- We can ofcourse also write this in terms of tensors
- Let the gradient of z with respect to a tensor $\mathbf{X}$ be $\nabla_{\mathbf{X}} z$
- If $\mathbf{Y} = g(\mathbf{X})$ and $z = f(\mathbf{Y})$, then:

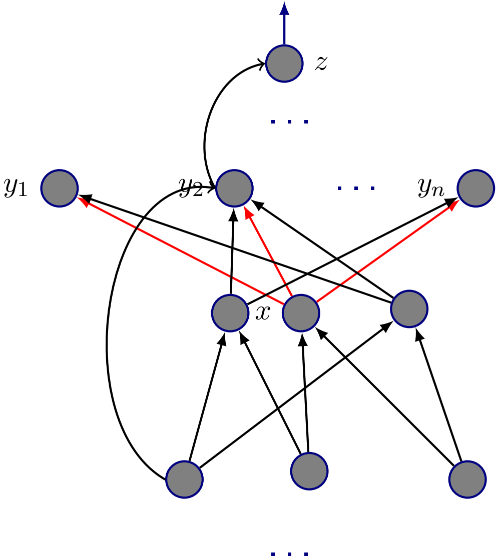
$$\nabla_{\mathbf{X}} z = \sum_j (\nabla_{\mathbf{X}} Y_j) \frac{\partial z}{\partial Y_j}$$

Recursive Application in a Computational Graph

- Writing an algebraic expression for the gradient of a scalar with respect to *any* node in the computational graph that *produced* that scalar is straightforward using the chain-rule
- Let for some node x the successors be: $\{y_1, y_2, \ldots y_n\}$
- Node: Computation result
- Edge: Computation dependency

$$\frac{dz}{dx} = \sum_{i=1}^{n} \frac{dz}{dy_i} \frac{dy_i}{dx}$$

Flow Graph (for previous slide)



Recursive Application in a Computational Graph

- Fpropagation: Visit nodes in the order after a topological sort
- Compute the value of each node given its ancestors
- Bpropagation: Output gradient $= 1$
- Now visit nods in reverse order
- Compute gradient with respect to each node using gradient with respect to successors
- Successors of x in previous slide $\{y_1, y_2, \dots y_n\}$:

$$\frac{dz}{dx} = \sum_{i=1}^{n} \frac{dz}{dy_i} \frac{dy_i}{dx}$$

Automatic Differentiation

- Computation of the gradient can be automatically inferred from the symbolic expression of fprop
- Every node type needs to know:
  - How to compute its output
  - How to compute its gradients with respect to its inputs *given* the gradient w.r.t its outputs
- Makes for rapid prototyping

Computational Graph for a MLP

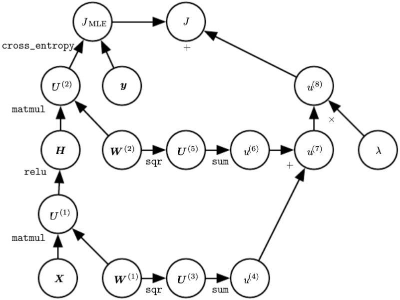


Figure: Goodfellow *et al.*

- To train we want to compute $\nabla_{W^{(1)}} J$ and $\nabla_{W^{(2)}} J$
- Two paths lead backwards from J to weights: Through cross entropy and through regularization cost

Computational Graph for a MLP

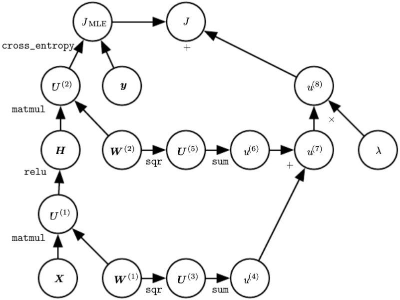


Figure: Goodfellow *et al.*

- Weight decay cost is relatively simple: Will always contribute $2\lambda W^{(i)}$ to gradient on $W^{(i)}$
- Two paths lead backwards from J to weights: Through cross entropy and through regularization cost

Symbol to Symbol

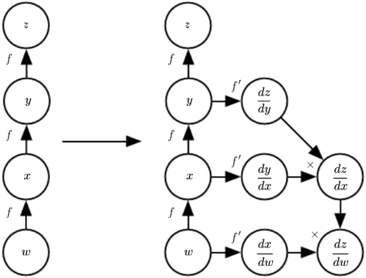


Figure: Goodfellow *et al.*

- In this approach backpropagation never accesses any numerical values
- Instead it just adds nodes to the graph that describe how to compute derivatives
- A graph evaluation engine will then do the actual computation
- Approach taken by Theano and TensorFlow

Next time

- Regularization Methods for Deep Neural Networks