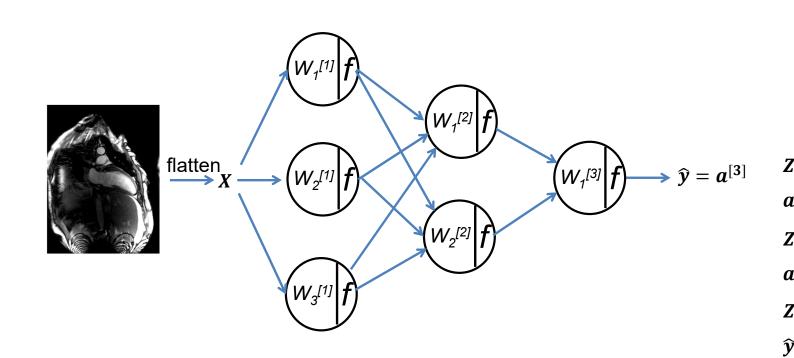
Deep Learning Crash Course



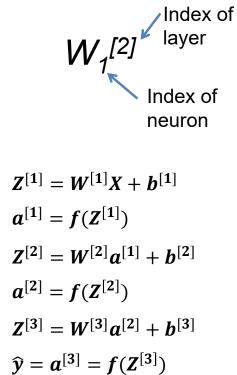
Hui Xue

Fall 2021

Recap: MLP



The i-th sample $(X^{(i)}, y^{(i)})$



Recap: Cross-Entropy Loss

Multi-class classification:

Given two probability distribution p and q, cross-entropy:

$$H(p,q) = -\sum_{\text{for all possible } x} p(x) \log[q(x)]$$

$$L_{CE_loss}(y, \hat{y}) = -\sum_{k=0}^{4} y[k] \log(\hat{y}[k])$$
$$L_{CE_loss}(y, \hat{y}) = -\log(\hat{y}[y_k])$$

Binary classification:

$$L_{BCE_loss}(y, \widehat{y}) = -[y \cdot log(\widehat{y}) + (1 - y) \cdot log(1 - \widehat{y})]$$

Recap: Mini-batch Gradient Descent

Initialize weights and bias

Random shuffle dataset

BatchSize = 32

for epoch in range(E):

select #BatchSize samples

Evaluate loss function (forward pass) at this batch

$$L = \frac{1}{B} \sum_{i=0}^{B-1} L(\boldsymbol{y}^{(i)}, \widehat{\boldsymbol{y}}^{(i)}(\boldsymbol{W}, \boldsymbol{b}))$$

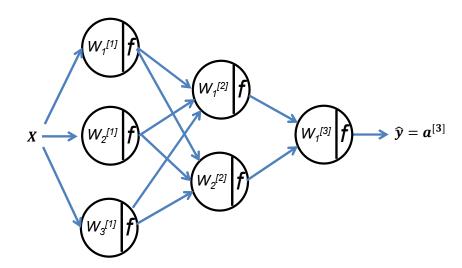
Compute gradient $\frac{\partial L}{\partial \boldsymbol{W}^{[l]}}, \frac{\partial L}{\partial \boldsymbol{b}^{[l]}}$

Update parameter $\mathbf{W}^{[l]} = \mathbf{W}^{[l]} - \alpha \frac{\partial L}{\partial \mathbf{W}^{[l]}}$, $\mathbf{b}^{[l]} = \mathbf{b}^{[l]} - \alpha \frac{\partial L}{\partial \mathbf{b}^{[l]}}$

Lecture 3

Backprop

To find the good model parameter



Evaluate loss function (forward pass) at this batch

$$L = \frac{1}{B} \sum_{i=0}^{B-1} L(\boldsymbol{y}^{(i)}, \widehat{\boldsymbol{y}}^{(i)}(\boldsymbol{W}, \boldsymbol{b}))$$

Compute gradient $\frac{\partial L}{\partial \boldsymbol{w}^{[l]}}$, $\frac{\partial L}{\partial \boldsymbol{b}^{[l]}}$

Update parameter $\mathbf{W}^{[l]} = \mathbf{W}^{[l]} - \alpha \frac{\partial L}{\partial \mathbf{W}^{[l]}}$, $\mathbf{b}^{[l]} = \mathbf{b}^{[l]} - \alpha \frac{\partial L}{\partial \mathbf{b}^{[l]}}$

Evaluate loss function: A forward pass

Evaluate loss function (forward pass) at this batch

$$L = \frac{1}{B} \sum_{i=0}^{B-1} L(\boldsymbol{y}^{(i)}, \widehat{\boldsymbol{y}}^{(i)}(\boldsymbol{W}, \boldsymbol{b}))$$

Let's look at one sample and write $y^{(i)}$ as y:

$$L(y, \hat{y}(\boldsymbol{W}, \boldsymbol{b})) = -[y \boldsymbol{log}(\hat{y}) + (1 - y) \boldsymbol{log}(1 - \hat{y})]$$

For every sample, we input (X, y) and model outputs \hat{y}

$$Z^{[1]} = W^{[1]}X + b^{[1]}$$
 $a^{[1]} = f(Z^{[1]})$
 $Z^{[2]} = W^{[2]}a^{[1]} + b^{[2]}$
 $a^{[2]} = f(Z^{[2]})$
 $Z^{[3]} = W^{[3]}a^{[2]} + b^{[3]}$
 $\hat{y} = a^{[3]} = f(Z^{[3]})$

Compute gradient: Is it easy to do?

Compute gradient
$$\frac{\partial L}{\partial \boldsymbol{w}^{[1]}}$$
, $\frac{\partial L}{\partial \boldsymbol{b}^{[1]}}$, $\frac{\partial L}{\partial \boldsymbol{w}^{[2]}}$, $\frac{\partial L}{\partial \boldsymbol{b}^{[2]}}$, $\frac{\partial L}{\partial \boldsymbol{w}^{[3]}}$, $\frac{\partial L}{\partial \boldsymbol{b}^{[3]}}$

First idea, compute analytical derivative

$$\hat{y} = a^{[3]} = f(Z^{[3]})$$

$$= f(W^{[3]}a^{[2]} + b^{[3]})$$

$$= f(W^{[3]}f(Z^{[2]}) + b^{[3]})$$

$$= f(W^{[3]}f(W^{[2]}a^{[1]} + b^{[2]}) + b^{[3]})$$

$$= f(W^{[3]}f(W^{[2]}f(Z^{[1]}) + b^{[2]}) + b^{[3]})$$

$$= f(W^{[3]}f(W^{[2]}f(W^{[1]}X + b^{[1]}) + b^{[2]}) + b^{[3]})$$

$$a^{[1]} = f(Z^{[1]})$$
 $Z^{[2]} = W^{[2]}a^{[1]} + b^{[2]}$
 $a^{[2]} = f(Z^{[2]})$
 $Z^{[3]} = W^{[3]}a^{[2]} + b^{[3]}$
 $\hat{y} = a^{[3]} = f(Z^{[3]})$

 $Z^{[1]} = W^{[1]}X + b^{[1]}$

Compute analytical gradient: hard to do

Compute gradient
$$\frac{\partial L}{\partial \boldsymbol{w}^{[1]}}$$
, $\frac{\partial L}{\partial \boldsymbol{b}^{[1]}}$, $\frac{\partial L}{\partial \boldsymbol{w}^{[2]}}$, $\frac{\partial L}{\partial \boldsymbol{b}^{[2]}}$, $\frac{\partial L}{\partial \boldsymbol{w}^{[3]}}$, $\frac{\partial L}{\partial \boldsymbol{b}^{[3]}}$

So, let's compute:

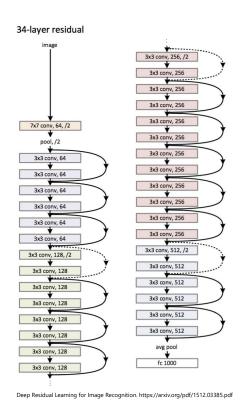
$$\frac{\partial L}{\partial W^{[1]}} = -\frac{\partial \{ [ylog(\widehat{y}) + (1-y)\log(1-\widehat{y})] \}}{\partial W^{[1]}}$$

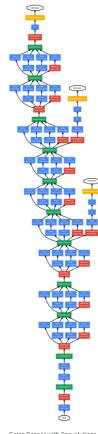
$$= -\frac{\partial \left\{ \left[ylog(f(W^{[3]}f(W^{[2]}f(W^{[1]}X + b^{[1]}) + b^{[2]}) + b^{[3]}) \right] \right\} - \frac{\partial \left\{ \left[ylog(\widehat{y}) + (1-y)\log(f(W^{[3]}f(W^{[2]}f(W^{[1]}X + b^{[1]}) + b^{[2]}) + b^{[3]}) \right] \right\}}{\partial W^{[1]}}$$

Compute derivative gradient is hard ... for this small MLP

$$Z^{[1]} = W^{[1]}X + b^{[1]}$$
 $a^{[1]} = f(Z^{[1]})$
 $Z^{[2]} = W^{[2]}a^{[1]} + b^{[2]}$
 $a^{[2]} = f(Z^{[2]})$
 $Z^{[3]} = W^{[3]}a^{[2]} + b^{[3]}$
 $\hat{y} = a^{[3]} = f(Z^{[3]})$

Compute derivative gradient : cannot be done





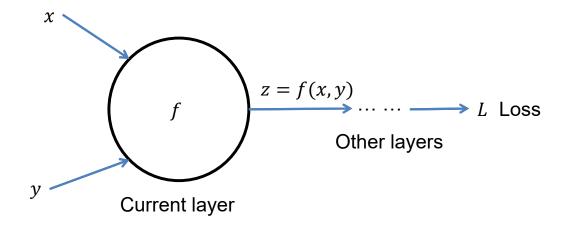
Compute analytical gradient becomes impossible for deep neural networks!

Don't try it!

Compute derivative gradient becomes impossible for deep neural networks. We need back prop.

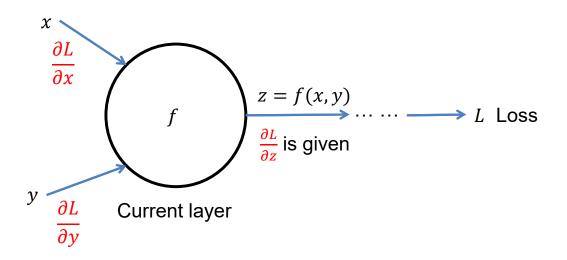
Three ideas behind BackProp:

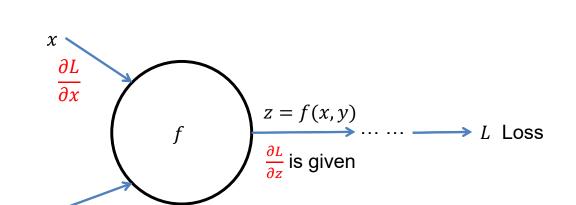
- Divide and conquer
- · Chain-rule
- · Let computer do the job AutoDiff



For this current layer, what we want to do:

- Given the gradient from the loss to output parameter z
- Compute gradient from the loss to input x and y





Current layer

· Chain rule

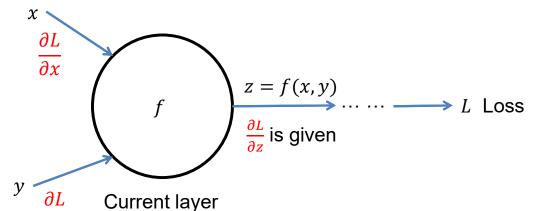
$$\frac{\partial L}{\partial x} = \frac{\partial L}{\partial z} \frac{\partial z}{\partial x}$$

$$\frac{\partial L}{\partial y} = \frac{\partial L}{\partial z} \frac{\partial z}{\partial y}$$

Divide and conquer

We only need to know:

- 1) the current layer to produce z from x and y
- 2) the upstream gradient



Chain rule

$$\frac{\partial L}{\partial x} = \frac{\partial L}{\partial z} \frac{\partial z}{\partial x} = \frac{\partial L}{\partial z} \frac{\partial f(x, y)}{\partial x}$$

$$\frac{\partial L}{\partial y} = \frac{\partial L}{\partial z} \frac{\partial z}{\partial y} = \frac{\partial L}{\partial z} \frac{\partial f(x,y)}{\partial y}$$

Divide and conquer

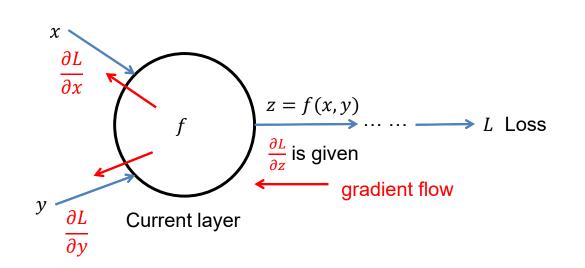
We know the current **function** to compute z from x and y

We know the gradient of loss to output z

Enough information to compute derivative of loss to input x and y

$$\frac{\partial z}{\partial x} = \frac{\partial f(x,y)}{\partial x} \qquad \frac{\partial z}{\partial y} = \frac{\partial f(x,y)}{\partial y}$$

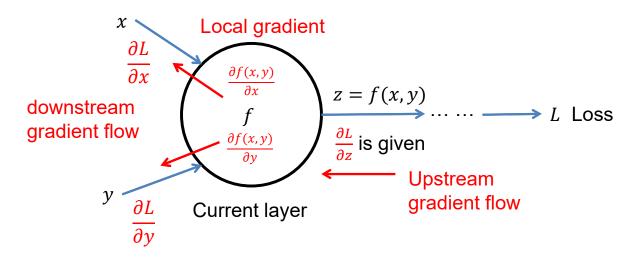
To compute current gradient, only need upstream gradient and local function



$$\frac{\partial L}{\partial y} = \frac{\partial L}{\partial z} \frac{\partial z}{\partial y} = \frac{\partial L}{\partial z} \frac{\partial f(x,y)}{\partial y}$$

$$\frac{\partial L}{\partial x} = \frac{\partial L}{\partial z} \frac{\partial z}{\partial x} = \begin{bmatrix} \frac{\partial L}{\partial z} & \frac{\partial f(x,y)}{\partial x} \\ \frac{\partial f(x,y)}{\partial x} & \frac{\partial f(x,y)}{\partial x} \end{bmatrix}$$

To compute current gradient, only need upstream gradient and local gradient



- 1) Inputs flow through the model to compute loss
- 2) Gradient of loss flows back to compute gradient to inputs (and all others ...)
- 3) Upstream gradient is combined with local gradient to compute downstream gradient

$$L = x^{2} + 2xy x = 1, y = 4$$

$$\frac{\partial L}{\partial x} = 2x + 2y = 2 + 8 = 10$$

$$\frac{\partial L}{\partial y} = 2x = 2$$

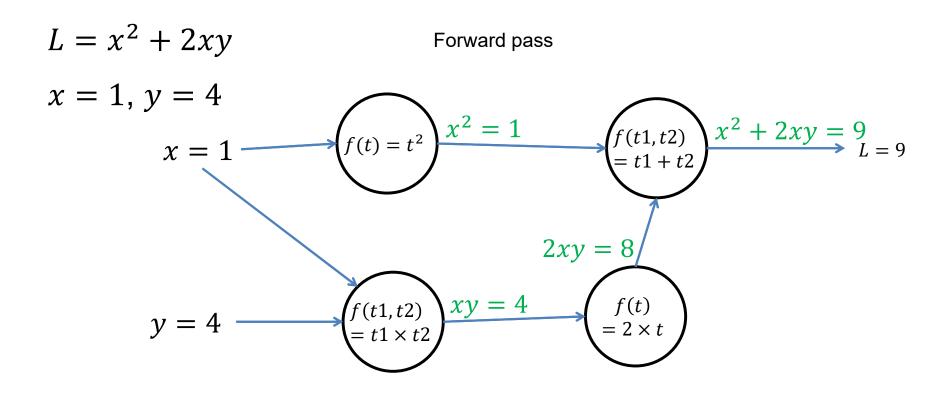
$$L = x^{2} + 2xy$$

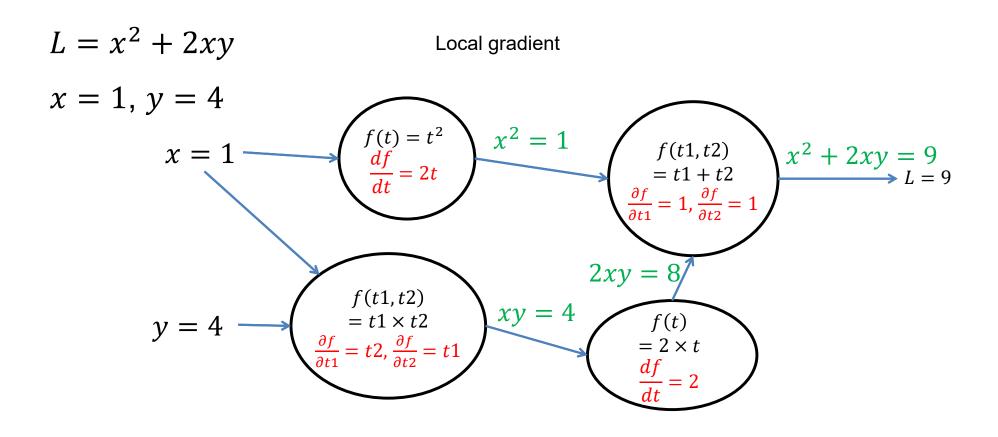
$$x = 1, y = 4$$

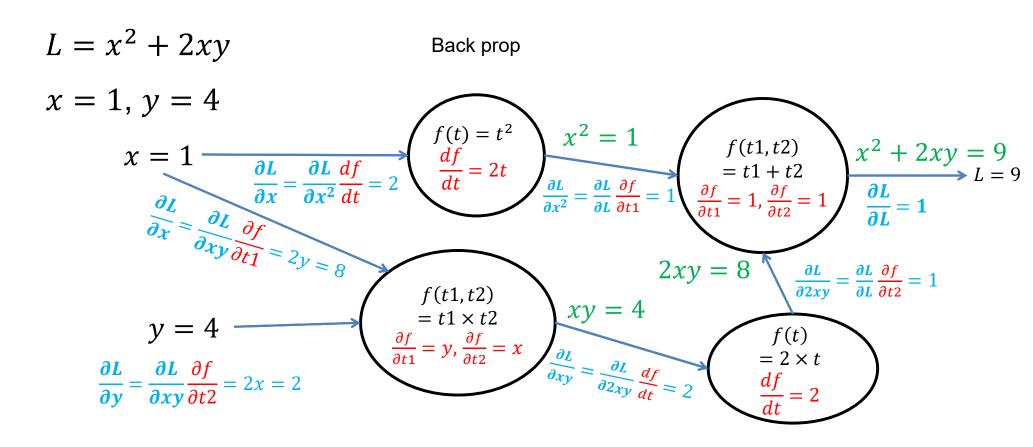
$$x = x^{2} + 2xy$$

$$x = x^{2} + 2xy$$

$$y = x^{2} + 2xy$$







$$L = x^{2} + 2xy$$

$$x = 1, y = 4$$

$$\frac{\partial L}{\partial x} = 2x + 2y = 2 + 8 = 10$$

$$\frac{\partial L}{\partial y} = 2x = 2$$

$$y = 4$$

$$\frac{\partial L}{\partial y} = \frac{\partial L}{\partial x} \frac{\partial f}{\partial t} = 2x$$

$$\frac{\partial L}{\partial y} = \frac{\partial L}{\partial x} \frac{\partial f}{\partial t} = 2x$$

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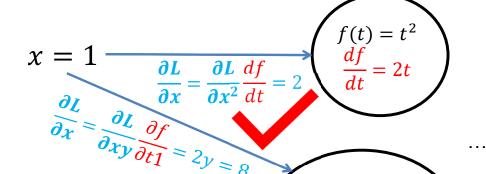
$$\frac{\partial L}{\partial y} = \frac{\partial L}{\partial x} \frac{\partial f}{\partial t} = 2x$$

$$L = x^2 + 2xy$$

$$x = 1, y = 4$$

$$\frac{\partial L}{\partial x} = 2x + 2y = 2 + 8 = 10$$

Back prop



Two paths contribute to one variable:

Sum contributions from all paths

$$f(t1, t2)$$

$$= t1 \times t2$$

$$\frac{\partial f}{\partial t1} = t2, \frac{\partial f}{\partial t2} = t1$$

Derivative of Scalar to Vector and Matrix

Loss is a scalar $L \in \mathbb{R}$

If x is a scalar, then

 $\frac{\partial L}{\partial x}$ is a scalar

Derivative of a scalar function to a scalar variable is a scalar.

If x is a vector, $x \in \mathbb{R}^{N \times 1}$

 $\frac{\partial L}{\partial x}$ is a vector in the same shape as x

$$\boldsymbol{x} = \begin{bmatrix} x_0 & x_1 & \dots & x_{N-2} & x_{N-1} \end{bmatrix}^T$$

$$\frac{\partial L}{\partial x} = \begin{bmatrix} \frac{\partial L}{\partial x_0} & \frac{\partial L}{\partial x_1} & \dots & \frac{\partial L}{\partial x_{N-2}} & \frac{\partial L}{\partial x_{N-1}} \end{bmatrix}^T$$

If x is a matrix, $x \in \mathbb{R}^{N \times M}$

 $\frac{\partial L}{\partial x}$ still has in the same shape as x

$$x = \begin{bmatrix} x_{00} & x_{01} & \dots & x_{0,M-1} \\ x_{10} & x_{11} & \dots & x_{1,M-1} \\ \dots & \dots & \dots & \dots \end{bmatrix}$$

$$x_{N-1,0} & x_{N-1,M-1} & \dots & x_{N-1,M-1}$$

$$\frac{\partial L}{\partial x} = \begin{bmatrix} \frac{\partial L}{\partial x_{ij}} \end{bmatrix}_{i=0:N-1,j=0:M-1}$$

Vector to Vector: Jacobian matrix

$$f \in \mathbb{R}^N \to \mathbb{R}^M$$
 $\mathbf{y} = f(\mathbf{x})$ $\mathbf{x} \in \mathbb{R}^N$ $\mathbf{y} \in \mathbb{R}^M$

$$\mathbf{y} = f(\mathbf{x})$$

$$x \in \mathbb{R}^N$$

$$y \in \mathbb{R}^M$$

$$\boldsymbol{x}$$
 is a vector of length $\boldsymbol{\mathsf{N}}$ $\boldsymbol{x} = [x_0 \ x_1 \ \dots \ x_{N-2} \ x_{N-1}]^T$

$$y$$
 is a vector of length M $y = [y_0 \ y_1 \ \dots \ y_{M-2} \ x_{M-1}]^T$

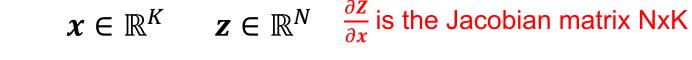
$$\frac{\partial \boldsymbol{y}}{\partial \boldsymbol{x}} = \begin{bmatrix} \frac{\partial y_i}{\partial x_j} \end{bmatrix}_{i=0:M-1,j=0:N-1} \begin{bmatrix} \frac{\partial y_0}{\partial x_0} & \dots & \frac{\partial y_0}{\partial x_{N-1}} \\ \vdots & \ddots & \vdots \\ \frac{\partial y_{M-1}}{\partial x_0} & \dots & \frac{\partial y_{M-1}}{\partial x_{N-1}} \end{bmatrix}$$
 Jacobian matrix: MxN output length x input length

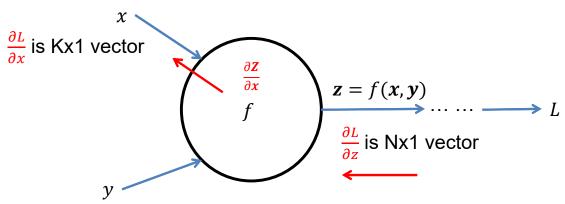
$$\begin{bmatrix} \frac{\partial y_0}{\partial x_0} & \cdots & \frac{\partial y_0}{\partial x_{N-1}} \\ \vdots & \ddots & \vdots \\ \frac{\partial y_{M-1}}{\partial x_0} & \cdots & \frac{\partial y_{M-1}}{\partial x_{N-1}} \end{bmatrix}$$

Derivative of every element of y to every element of x

Backprop for Vector

Apply Jacobian matrix as local gradient





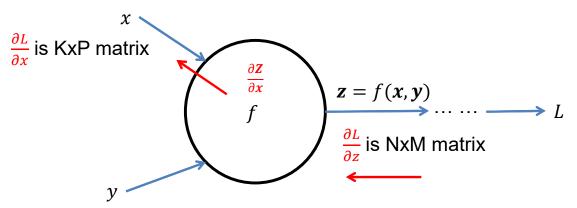
$$\frac{\partial L}{\partial x} = \begin{bmatrix} \frac{\partial \mathbf{Z}}{\partial \mathbf{x}} \end{bmatrix}^T \cdot \frac{\partial L}{\partial \mathbf{z}} \qquad \frac{\partial L}{\partial y} = \begin{bmatrix} \frac{\partial \mathbf{Z}}{\partial \mathbf{y}} \end{bmatrix}^T \cdot \frac{\partial L}{\partial \mathbf{z}}$$

- Unlike the scalar case, backprop for vectors requires matrix multiplication
- Only one way to put together equation

Backprop for Matrix and Tensors

$$\mathbf{x} \in \mathbb{R}^{K \times P} \ \mathbf{z} \in \mathbb{R}^{N \times M}$$

 $\boldsymbol{x} \in \mathbb{R}^{K \times P}$ $\boldsymbol{z} \in \mathbb{R}^{N \times M}$ $\frac{\partial \boldsymbol{z}}{\partial \boldsymbol{x}}$ is the Jacobian Tensor (NxM) x (KxP)



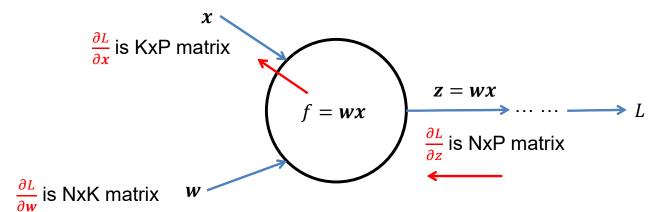
- Often use backprop to computer Jacobian Tensor
- · Still only one way to put together equation

$$\frac{\partial L}{\partial \boldsymbol{x}} = \begin{bmatrix} \partial \boldsymbol{z} \\ \partial \boldsymbol{x} \end{bmatrix}^T \cdot \frac{\partial L}{\partial \boldsymbol{z}} \qquad \frac{\partial L}{\partial \boldsymbol{y}} = \begin{bmatrix} \partial \boldsymbol{z} \\ \partial \boldsymbol{y} \end{bmatrix}^T \cdot \frac{\partial L}{\partial \boldsymbol{z}}$$

$$\frac{\partial L}{\partial \boldsymbol{y}} = \left[\frac{\partial \boldsymbol{z}}{\partial \boldsymbol{y}}\right]^T \cdot \frac{\partial L}{\partial \boldsymbol{z}}$$

Backprop for Matrix multiplication

$$\boldsymbol{x} \in \mathbb{R}^{K \times P} \quad \boldsymbol{w} \in \mathbb{R}^{N \times K} \quad \boldsymbol{z} \in \mathbb{R}^{N \times P}$$



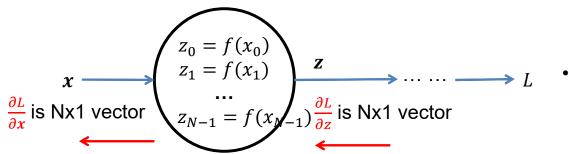
- Matrix multiplication formula is useful
- Only one way to put together them

$$\frac{\partial L}{\partial \mathbf{x}} = \mathbf{w}^T \cdot \frac{\partial L}{\partial \mathbf{z}}$$

$$\frac{\partial L}{\partial \mathbf{w}} = \frac{\partial L}{\partial \mathbf{z}} \cdot \mathbf{x}^T$$

Backprop for Element-wise operation

$$x \in \mathbb{R}^{N \times 1}$$
 $z \in \mathbb{R}^{N \times 1}$

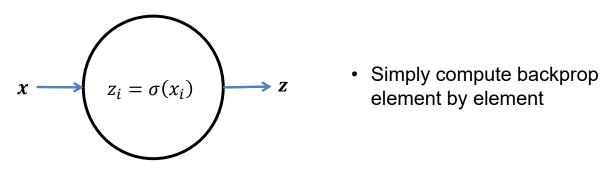


 Simply compute backprop element by element

$$\frac{\partial L}{\partial x_i} = \frac{df(x_i)}{dx_i} \frac{\partial L}{\partial z_i} \qquad i = 0: N - 1$$

Backprop for Sigmoid

$$\mathbf{x} \in \mathbb{R}^{N \times 1}$$
 $\mathbf{z} \in \mathbb{R}^{N \times 1}$ $\frac{\partial L}{\partial x_i} = \frac{df(x_i)}{dx_i} \frac{\partial L}{\partial z_i}$ $i = 0: N - 1$

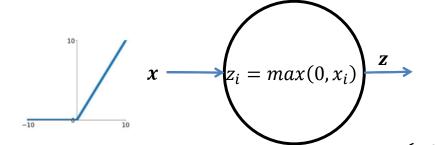


$$\frac{d\sigma(t)}{dt} = \sigma(t)[1 - \sigma(t)] \qquad \frac{\partial L}{\partial x_i} = \sigma(x_i)[1 - \sigma(x_i)] \frac{\partial L}{\partial z_i}$$

Backprop for ReLU activation function

$$\mathbf{x} \in \mathbb{R}^{N \times 1}$$
 $\mathbf{z} \in \mathbb{R}^{N \times 1}$ $\frac{\partial L}{\partial x_i} = \frac{df(x_i)}{dx_i} \frac{\partial L}{\partial z_i}$ $i = 0: N - 1$

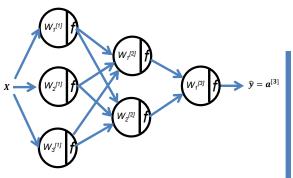
 $\begin{array}{l} \textbf{ReLU} \\ \max(0,x) \end{array}$



 compute backprop element by element

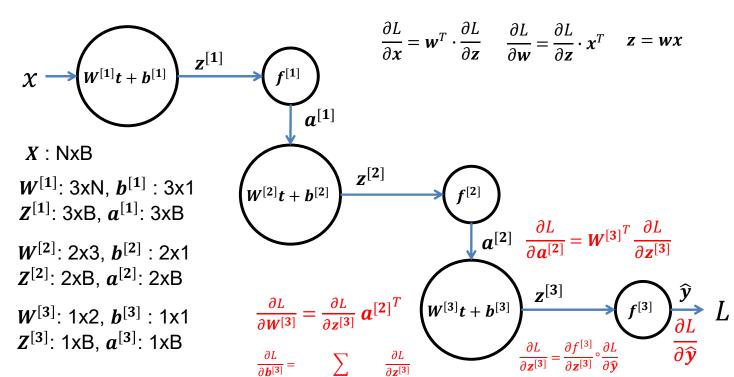
$$\frac{dmax(0,t)}{dt} = \begin{cases} 1, t > 0 \\ 0.5, t = 0 \\ 0, otherwise \end{cases} \frac{\partial L}{\partial x_i} = \begin{cases} \frac{\partial L}{\partial z_i}, x_i > 0 \\ \frac{\partial L}{\partial z_i}, x_i = 0 \\ 0, x_i < 0 \end{cases}$$

Computational Graph for MLP

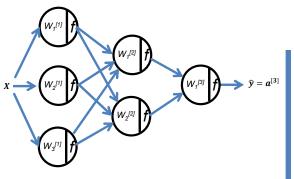


$$Z^{[1]} = W^{[1]}X + b^{[1]}$$
 $a^{[1]} = f(Z^{[1]})$
 $Z^{[2]} = W^{[2]}a^{[1]} + b^{[2]}$
 $a^{[2]} = f(Z^{[2]})$
 $Z^{[3]} = W^{[3]}a^{[2]} + b^{[3]}$
 $\widehat{y} = a^{[3]} = f(Z^{[3]})$

Compute gradient $\frac{\partial L}{\partial \boldsymbol{w}^{[1]}}$, $\frac{\partial L}{\partial \boldsymbol{b}^{[1]}}$, $\frac{\partial L}{\partial \boldsymbol{w}^{[2]}}$, $\frac{\partial L}{\partial \boldsymbol{b}^{[2]}}$, $\frac{\partial L}{\partial \boldsymbol{w}^{[3]}}$, $\frac{\partial L}{\partial \boldsymbol{b}^{[3]}}$

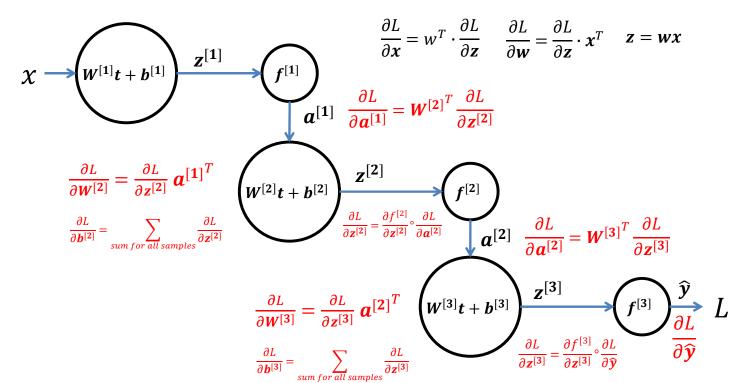


Computational Graph for MLP



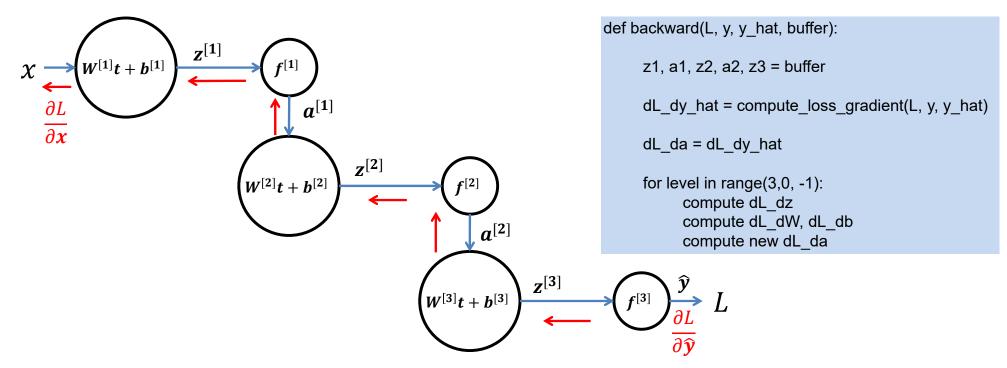
$$Z^{[1]} = W^{[1]}X + b^{[1]}$$
 $a^{[1]} = f(Z^{[1]})$
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 $a^{[2]} = f(Z^{[2]})$
 $Z^{[3]} = W^{[3]}a^{[2]} + b^{[3]}$
 $\widehat{y} = a^{[3]} = f(Z^{[3]})$

Compute gradient $\frac{\partial L}{\partial \boldsymbol{W}^{[1]}}$, $\frac{\partial L}{\partial \boldsymbol{b}^{[1]}}$, $\frac{\partial L}{\partial \boldsymbol{W}^{[2]}}$, $\frac{\partial L}{\partial \boldsymbol{b}^{[2]}}$, $\frac{\partial L}{\partial \boldsymbol{W}^{[3]}}$, $\frac{\partial L}{\partial \boldsymbol{b}^{[3]}}$



Backprop for MLP

Compute gradient
$$\frac{\partial L}{\partial \boldsymbol{w}^{[1]}}$$
, $\frac{\partial L}{\partial \boldsymbol{b}^{[1]}}$, $\frac{\partial L}{\partial \boldsymbol{w}^{[2]}}$, $\frac{\partial L}{\partial \boldsymbol{b}^{[2]}}$, $\frac{\partial L}{\partial \boldsymbol{w}^{[3]}}$, $\frac{\partial L}{\partial \boldsymbol{b}^{[3]}}$



Start the backprop

Given a batch (x, y), the mini-batch loss is:

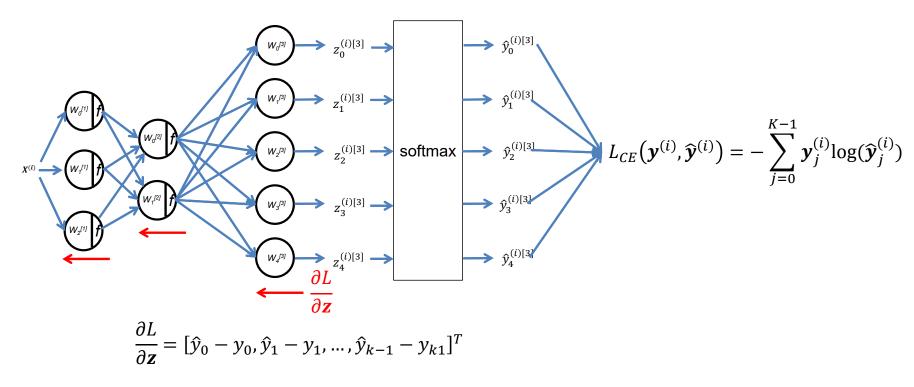
$$L = \frac{1}{B} \sum_{i=0}^{B-1} L^{(i)} (y^{(i)}, \hat{y}^{(i)})$$

$$L^{(i)}(y^{(i)}, \hat{y}^{(i)}) = -[y^{(i)} log(\hat{y}^{(i)}) + (1 - y^{(i)}) log(1 - \hat{y}^{(i)})]$$

$$\frac{\partial L}{\partial \hat{\mathbf{y}}} = \left[\frac{\partial L}{\partial \hat{\mathbf{y}}^{(i)}} \right]_{i=0:B-1} \qquad \frac{\partial L}{\partial \hat{\mathbf{y}}^{(i)}} = \frac{1}{B} \frac{\partial L^{(i)} \left(\mathbf{y}^{(i)}, \hat{\mathbf{y}}^{(i)} \right)}{\partial \hat{\mathbf{y}}^{(i)}} = \frac{1}{B} \left[\frac{\mathbf{y}^{(i)}}{\hat{\mathbf{y}}^{(i)}} - \frac{1-\mathbf{y}^{(i)}}{1-\hat{\mathbf{y}}^{(i)}} \right]$$

Start the backprop

K=5, 5 class classification



We have all ingredients for MB-SGD

Initialize weights and bias Forward pass Run data through model to compute output Random shuffle dataset BatchSize = 32 Backward pass or backprop for epoch in range(E): Starting from loss, compute gradient to all parameters select #BatchSize samples 1. Evaluate loss function (forward pass) at this batch $L = \frac{1}{B} \sum_{i=0}^{B-1} L(y^{(i)}, \widehat{y}^{(i)}(W, b))$ **Update** Use gradient information to update 2. Compute gradient $\frac{\partial L}{\partial w^{[l]}}, \frac{\partial L}{\partial \mathbf{p}^{[l]}}$ parameters 3. Update parameter $\boldsymbol{W}^{[l]} = \boldsymbol{W}^{[l]} - \alpha \frac{\partial L}{\partial \boldsymbol{W}^{[l]}}, \ \boldsymbol{b}^{[l]} = \boldsymbol{b}^{[l]} - \alpha \frac{\partial L}{\partial \boldsymbol{b}^{[l]}}$

