CS 4803 / 7643: Deep Learning

Topics:

- Optimization
- Computing Gradients

Dhruv Batra Georgia Tech

Administrativia

- HW0 Reminder
 - Due: 09/05, 11:55pm
- A note on expectations
 - Act like a responsible adult
- Thursday 09/06
 - Guest Lecture by Peter Anderson
- No class next week
 - 09/11, 09/13
- HW1 out next week (09/11)

Recap from last time

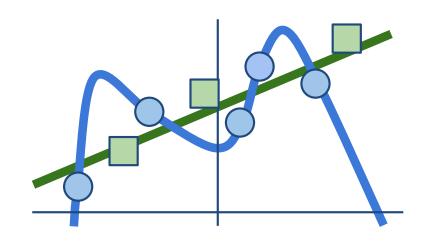
Regularization

 $\lambda_{.}$ = regularization strength (hyperparameter)

$$L(W) = \frac{1}{N} \sum_{i=1}^{N} L_i(f(x_i, W), y_i) + \lambda R(W)$$

Data loss: Model predictions should match training data

Regularization: Prevent the model from doing *too* well on training data



Occam's Razor:

"Among competing hypotheses, the simplest is the best" William of Ockham, 1285 - 1347

Regularization

 $\lambda_{.}$ = regularization strength (hyperparameter)

$$L(W) = \frac{1}{N} \sum_{i=1}^{N} L_i(f(x_i, W), y_i) + \lambda R(W)$$

Data loss: Model predictions should match training data

Regularization: Prevent the model from doing *too* well on training data

Simple examples

<u>L2 regularization:</u> $R(W) = \sum_{k} \sum_{l} W_{k,l}^2$ L1 regularization: $R(W) = \sum_{k} \sum_{l} |W_{k,l}|$ Elastic net (L1 + L2): $R(W) = \sum_{k} \sum_{l} \beta W_{k,l}^2 + |W_{k,l}|$

More complex:DropoutBatch normalizationVk,lStochastic depth, fractional pooling, etc

(Before) Linear score function:

$$f = Wx$$

(**Before**) Linear score function: (**Now**) 2-layer Neural Network

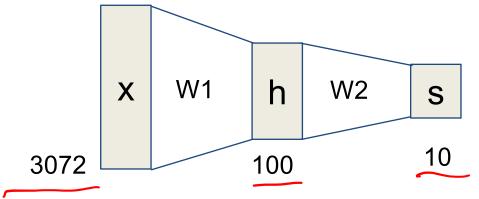
$$egin{aligned} f &= Wx \ f &= W_2 \max(0, W_1 x) \end{aligned}$$

(**Before**) Linear score function:

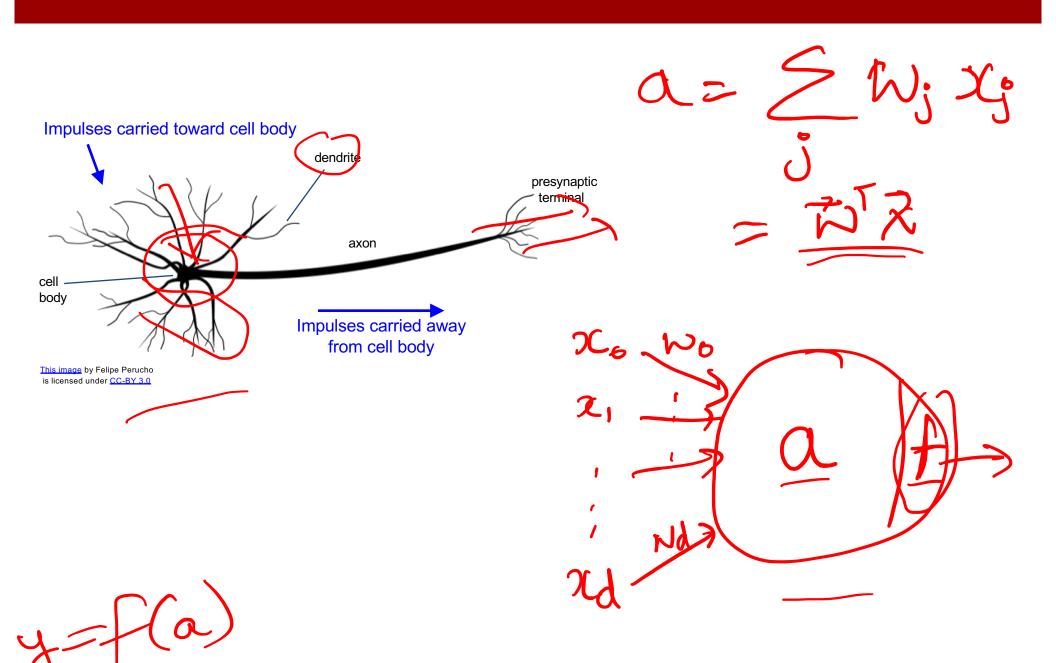
(Now) 2-layer Neural Network

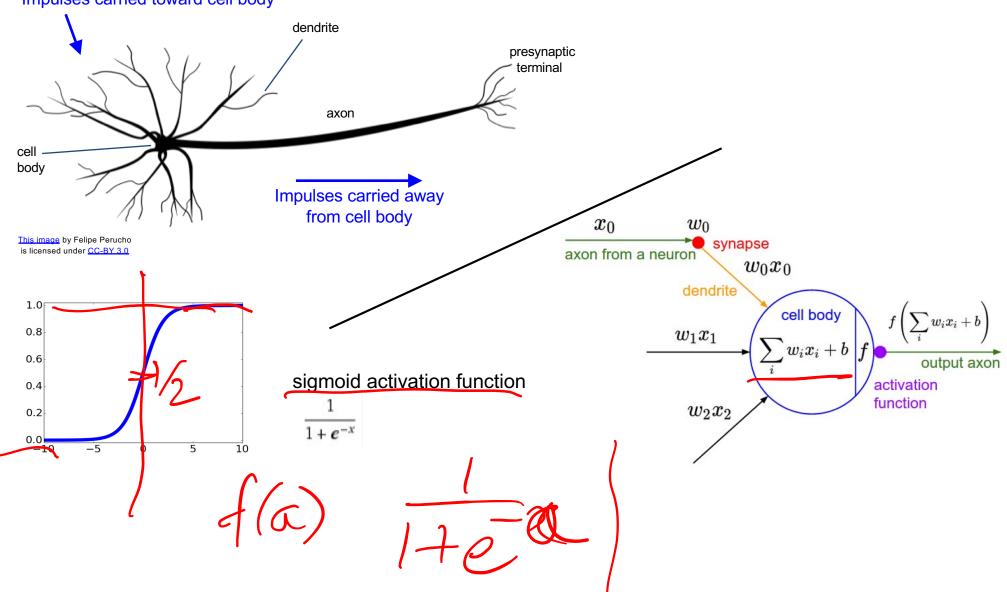
$$f = Wx$$

$$f=W_2\max(0,W_1x)$$



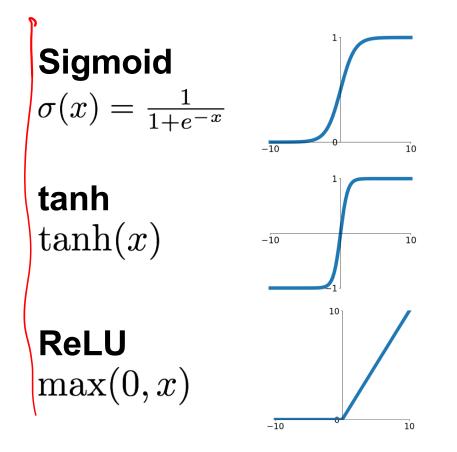
(Before) Linear score function: f = Wx(Now) 2-layer Neural Network $f = W_2 \max(0, W_1x)$ or 3-layer Neural Network $f = W_3 \max(0, W_2 \max(0, W_1x))$

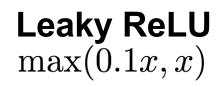


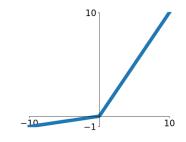


Impulses carried toward cell body

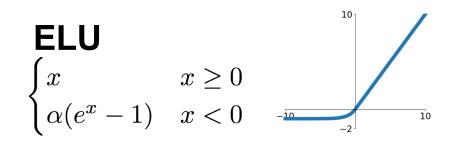
Activation functions

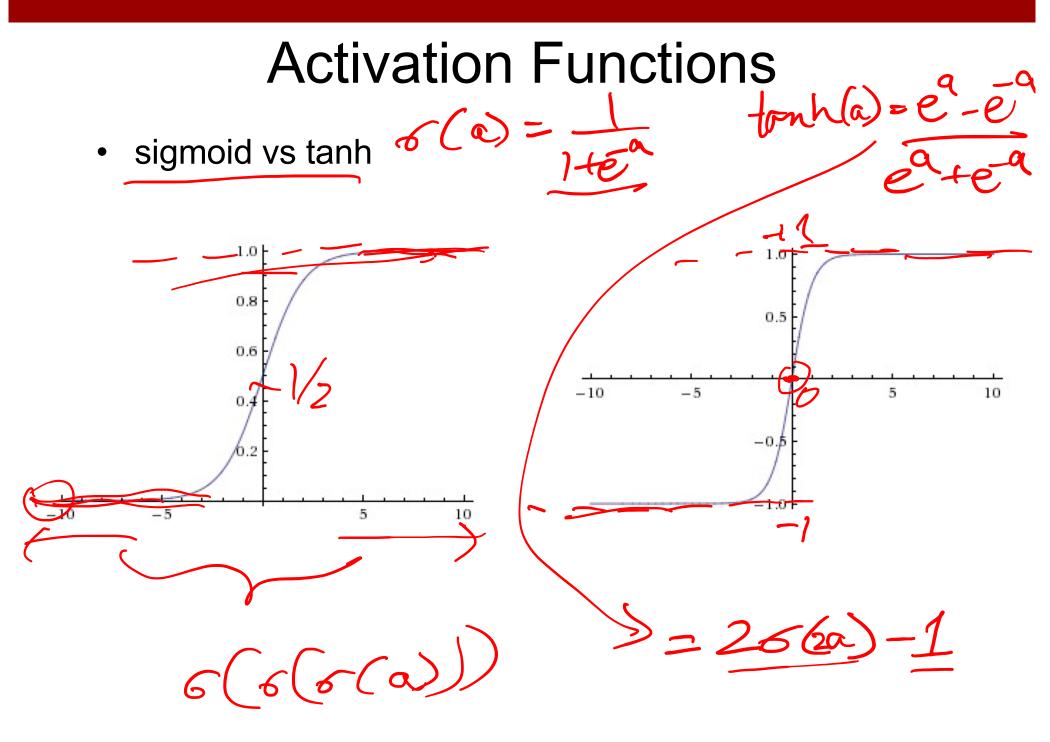






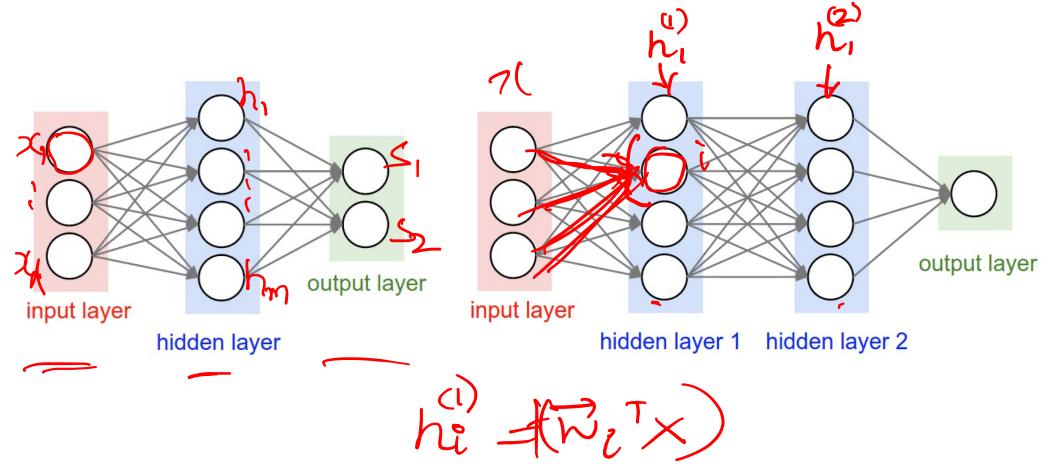
 $\begin{array}{l} \textbf{Maxout} \\ \max(w_1^T x + b_1, w_2^T x + b_2) \end{array}$





Multilayer Networks

- Cascade Neurons together
- The output from one layer is the input to the next
- Each Layer has its own sets of weights



Plan for Today

- (Finish) Optimization
- Computing Gradients

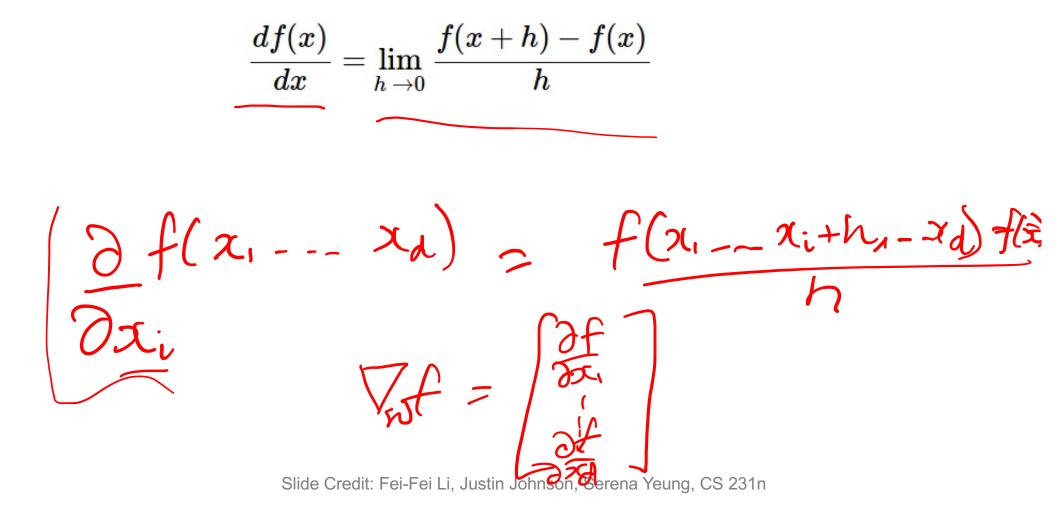
Optimization





Strategy: Follow the slope

In 1-dimension, the derivative of a function:



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In 1-dimension, the derivative of a function:

$$rac{df(x)}{dx} = \lim_{h o 0} rac{f(x+h) - f(x)}{h}$$

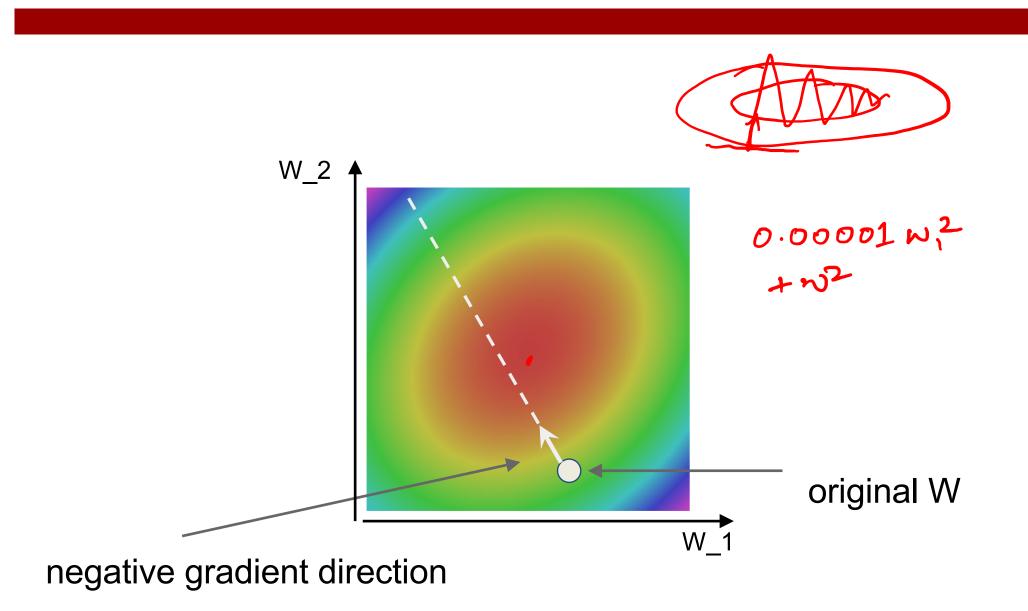
In multiple dimensions, the **gradient** is the vector of (partial derivatives) along each dimension

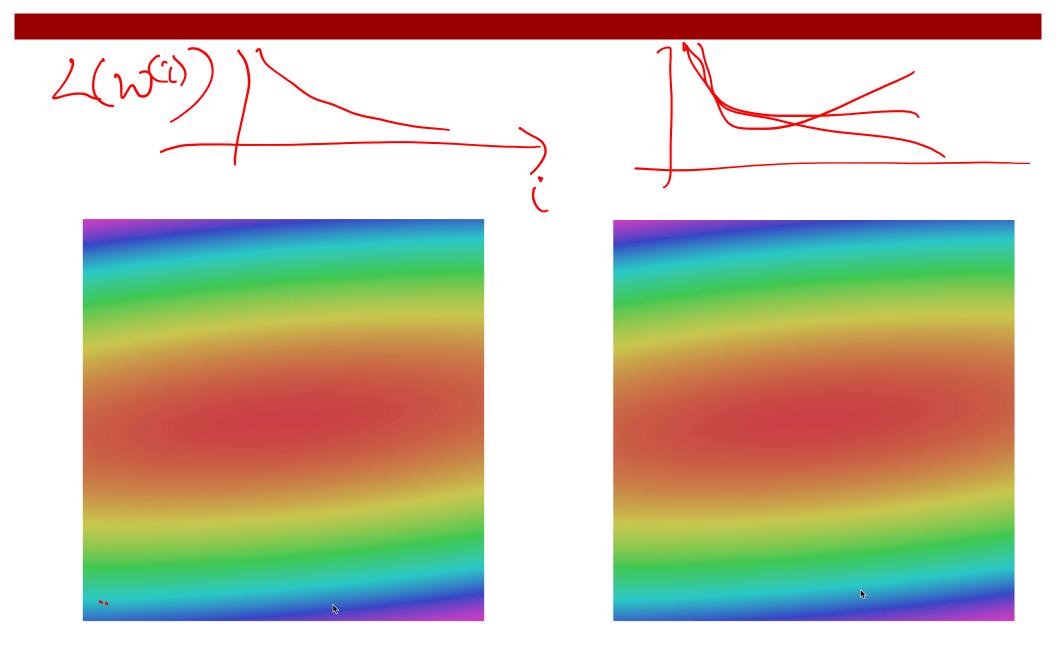
The slope in any direction is the **dot product** of the direction with the gradient The direction of steepest descent is the **negative gradient**



2 backt # Vanilla Gradient Descent while True: weights_grad = evaluate_gradient(loss_fun, data, weights) weights += - step size * weights grad # perform parameter update

 $1^{(0)} = init$ for t=1--- tired D(EH) = DE - N





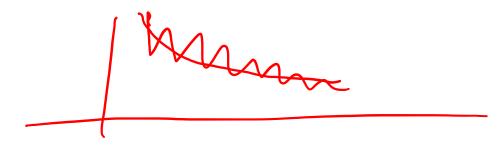
Stochastic Gradient Descent (SGD)

$$L(W) = \frac{1}{N} \sum_{i=1}^{N} L_i(x_i, y_i, W) + \lambda R(W)$$
$$\nabla_W L(W) = \frac{1}{N} \sum_{i=1}^{N} \nabla_W L_i(x_i, y_i, W) + \lambda \nabla_W R(W)$$

Full sum expensive when N is large!

Approximate sum using a **minibatch** of examples 32 / 64 / 128 common

```
# Vanilla Minibatch Gradient Descent
while True:
    data_batch = sample_training data(data, 256) # sample 256 examples
    weights_grad = evaluate gradient(loss_fun, data_batch, weights)
    weights += - step_size * weights_grad # perform parameter update
```



Stochastic Gradient Descent (SGD)

$$L(W) = \frac{1}{N} \sum_{i=1}^{N} L_i(x_i, y_i, W)$$

$$\nabla_W L(W) = \frac{1}{N} \sum_{i=1}^{N} \nabla_W L_i(x_i, y_i, W) = \sum_{i} \left(\frac{1}{N} \right) \nabla_U L_i$$

$$I = i \in (1, --, N)$$

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$$I = V \cup (1, N)$$

Stochastic Gradient Descent (SGD) $\int_{z} \sum V_{w} L(a,y,w) p^{*}(x,y) dx$ $= E \left[V_{\omega} L \right] \approx \frac{1}{m} \sum_{k=1}^{\infty} \sum_{k=1}^{\infty}$

Stochastic Gradient Descent (SGD)

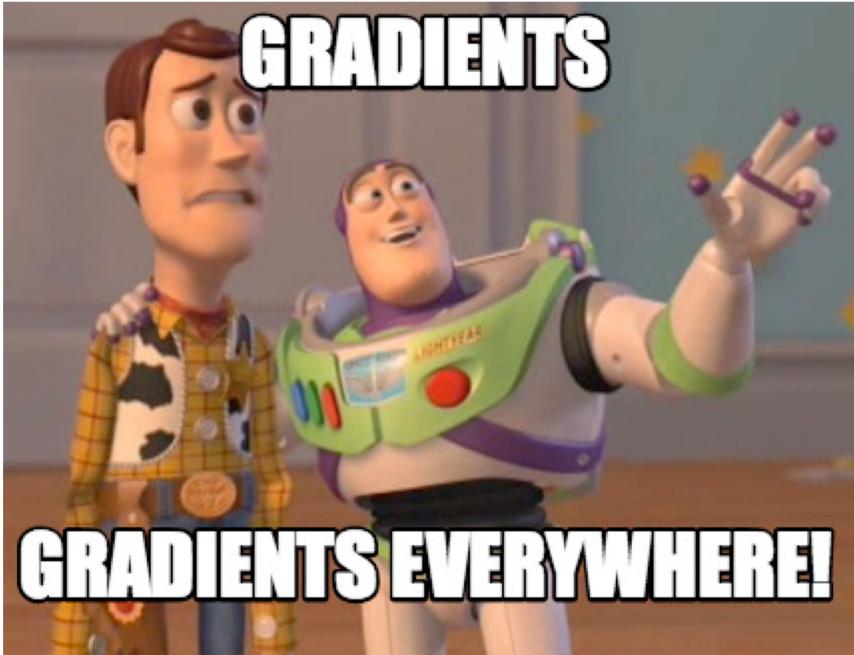
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Vanilla Minibatch Gradient Descent

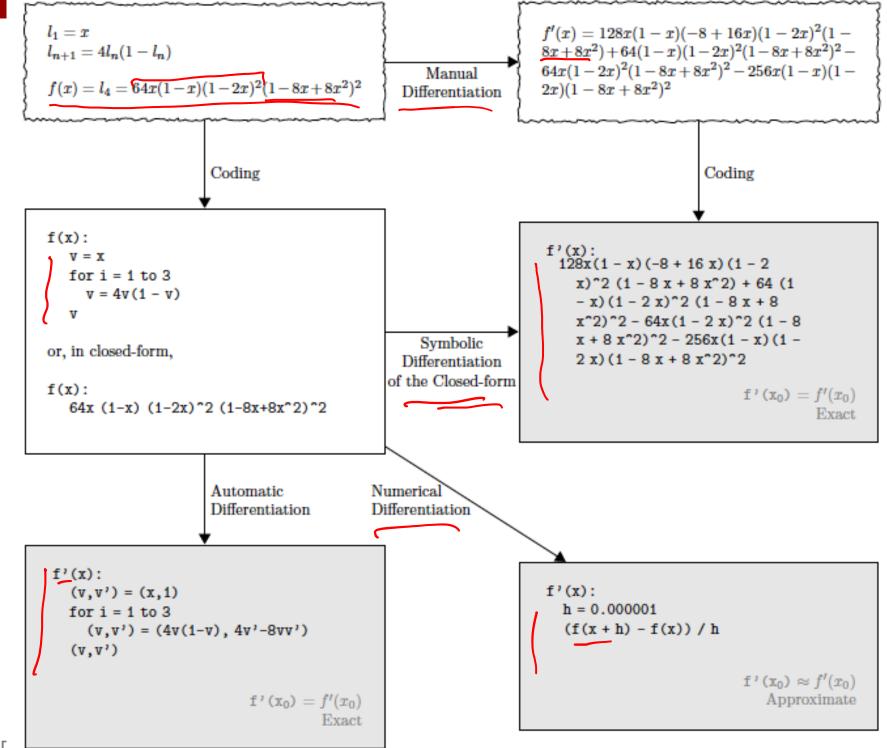
while True: data_batch = sample_training_data(data, 256) # sample 256 examples weights_grad = evaluate_gradient(loss_fun, data_batch, weights) weights += - step_size * weights_grad # perform parameter update



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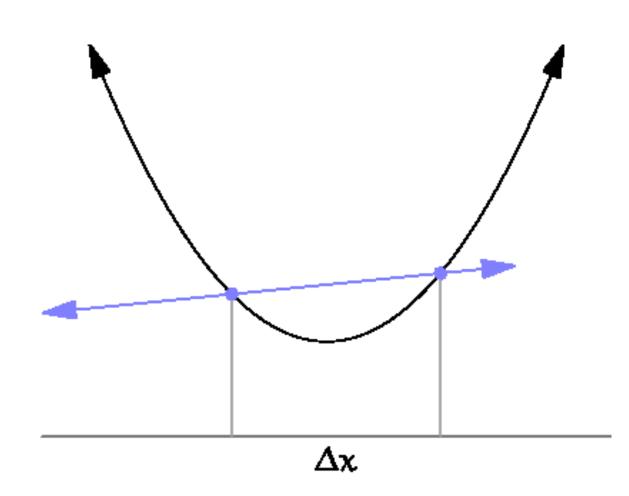
How do we compute gradients?

- Analytic or "Manual" Differentiation
- Symbolic Differentiation
- Numerical Differentiation
- Automatic Differentiation
 - Forward mode AD
 - Reverse mode AD
 - aka "backprop"



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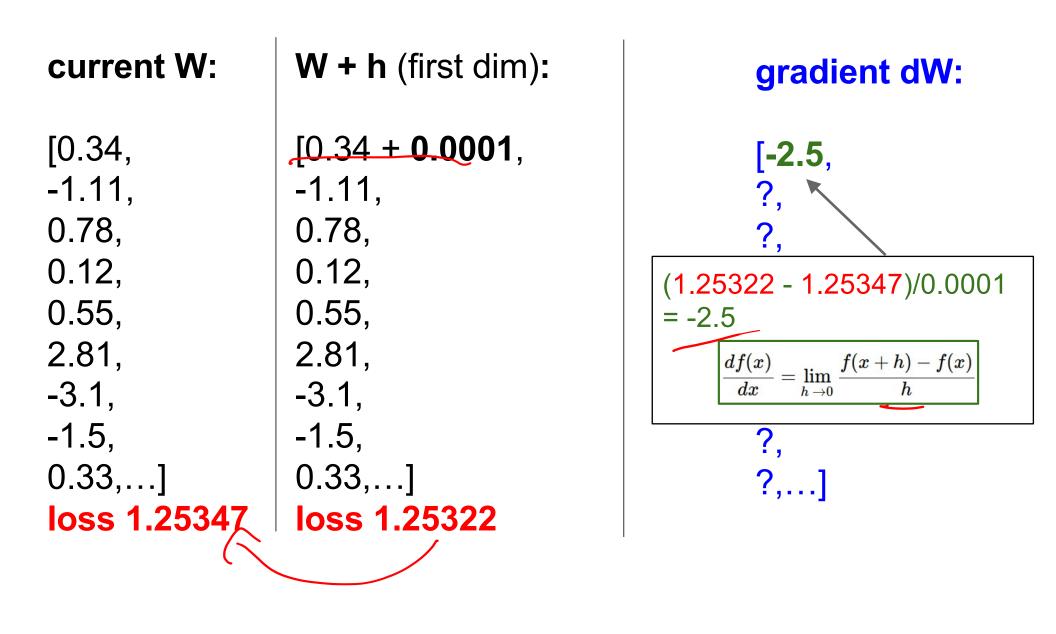
current W: 3 [0.34, -1.11, 0.78, 0.12, 0.55, 2.81, -3.1, -1.5, 0.33,...] loss 1.25347

[?, ?, ?, ?, ?, ?, ?, ?,

?,...]

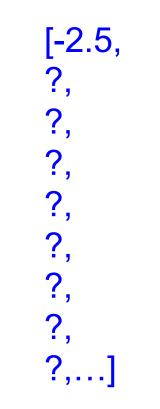
gradient dW:

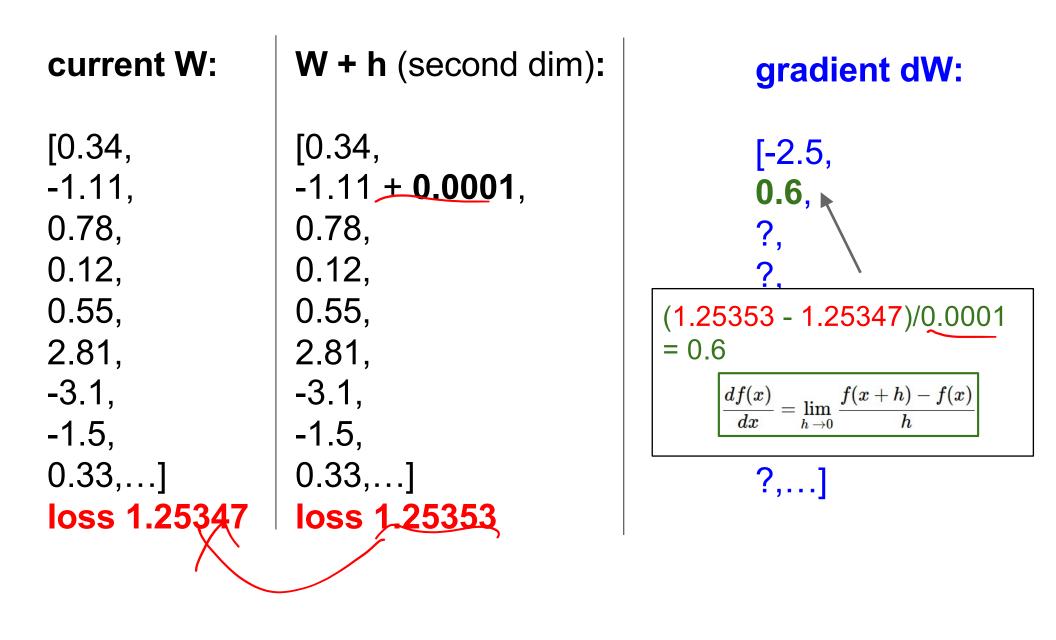
current W:	W + h (first dim):	gradient dW:
[0.34, -1.11, 0.78, 0.12, 0.55, 2.81, -3.1,	[0.34 + 0.0001, -1.11, 0.78, 0.12, 0.55, 2.81, -3.1,	[?, ?, ?, ?, ?, ?, ?, ?, ?,
-1.5, 0.33,…] loss 1.25347	-1.5, 0.33,] loss 1.25322	?, ?,]



current W:	W + h (second dim):
[0.34,	[0.34,
-1.11,	-1.11 + 0.0001 ,
0.78,	0.78,
0.12,	0.12,
0.55,	0.55,
2.81,	2.81,
-3.1,	-3.1,
-1.5,	-1.5,
0.33,]	0.33,]
loss 1.25347	loss 1.25353

gradient dW:





current W:	W + h (third dim):	gradient dW:
[0.34,	[0.34,	[-2.5,
-1.11, 0.78,	-1.11, 0.78 + 0.0001 ,	0.6, ?,
0.12,	0.12,	?,
0.55, 2.81,	0.55, 2.81,	?,
-3.1,	-3.1,	?, ?,
-1.5,	-1.5,	?,
0.33,…] loss 1.25347	0.33,…] loss 1.25347	?,]

current W:	W + h (third dim):	gradient dW:
[0.34, -1.11, 0.78, 0.12, 0.55, 2.81, -3.1, -1.5, 0.33,] Ioss 1.25347	[0.34, -1.11, 0.78 + 0.0001 , 0.12, 0.55, 2.81, -3.1, -1.5, 0.33,] Ioss 1.25347	$[-2.5, 0.6, 0.6, 0.6]$ $(1.25347 - 1.25347)/0.0001 = 0$ $\frac{df(x)}{dx} = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$ $f(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$

Numerical vs Analytic Gradients

$$rac{df(x)}{dx} = \lim_{h o 0} rac{f(x+h) - f(x)}{h}$$

Numerical gradient: slow :(, approximate :(, easy to write :) Analytic gradient: fast :), exact :), error-prone :(

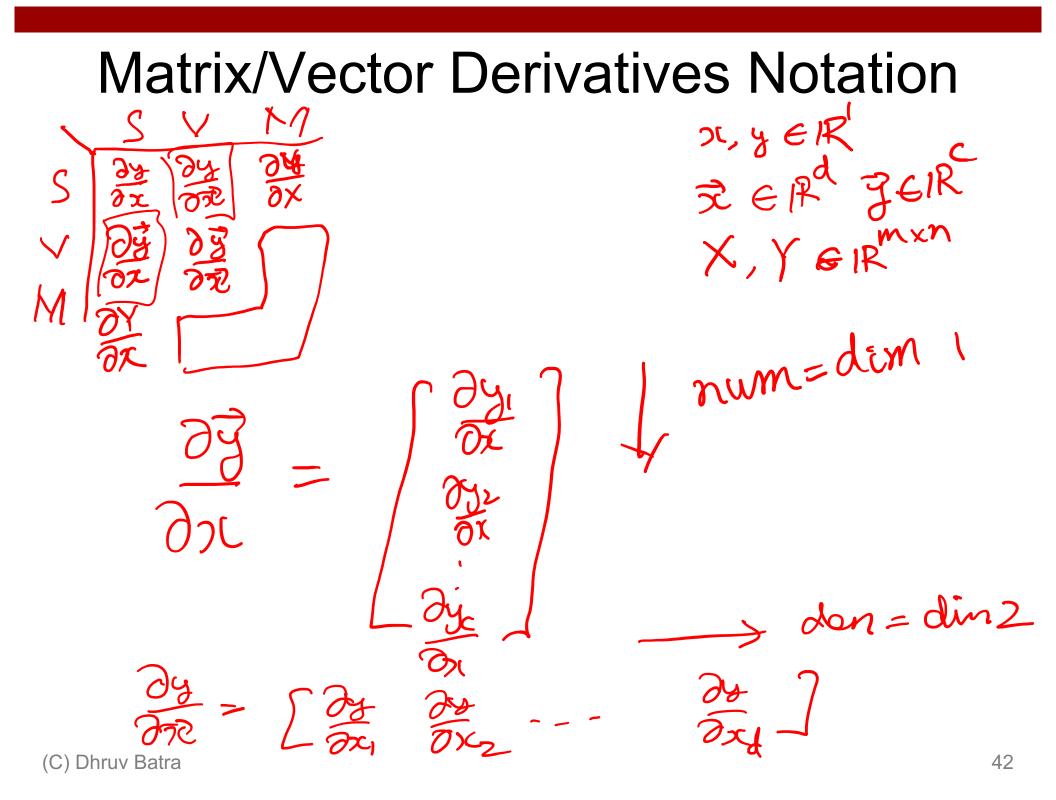
In practice: Derive analytic gradient, check your implementation with numerical gradient. This is called a **gradient check.**

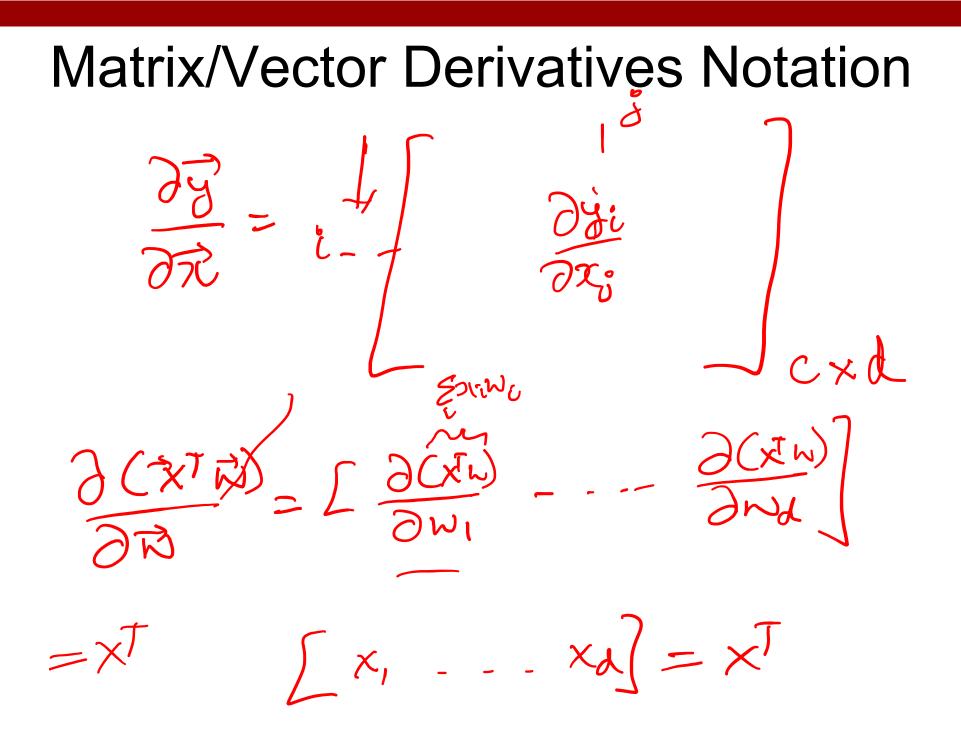
How do we compute gradients?

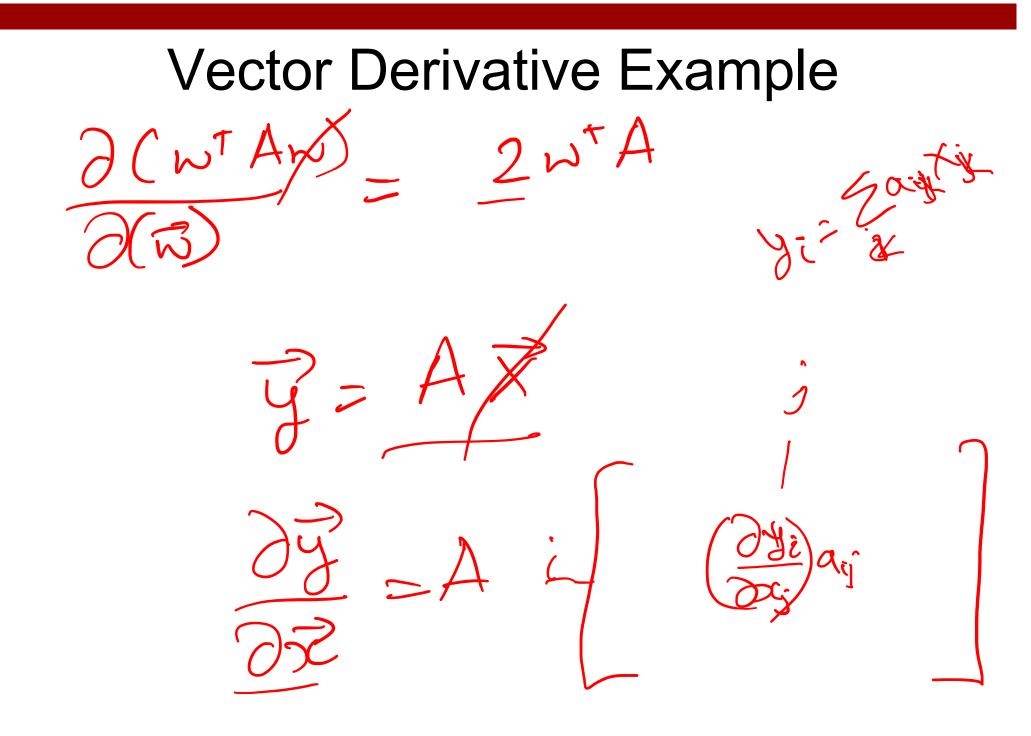
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- Symbolic Differentiation

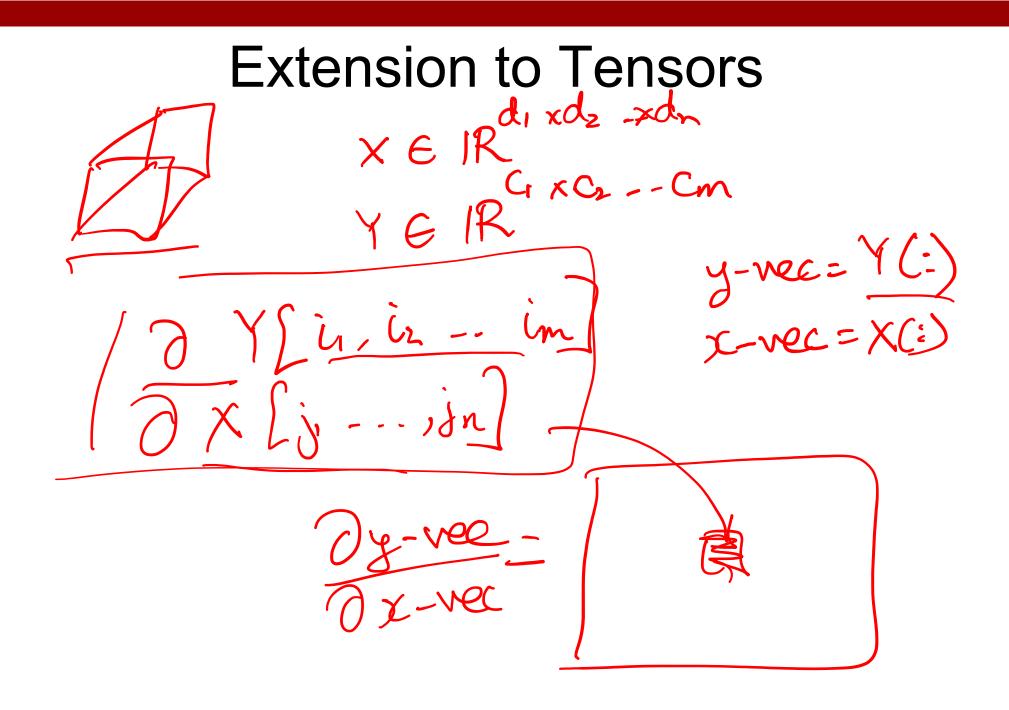
Numerical Differentiation

- Automatic Differentiation
 - Forward mode AD
 - Reverse mode AD
 - aka "backprop"



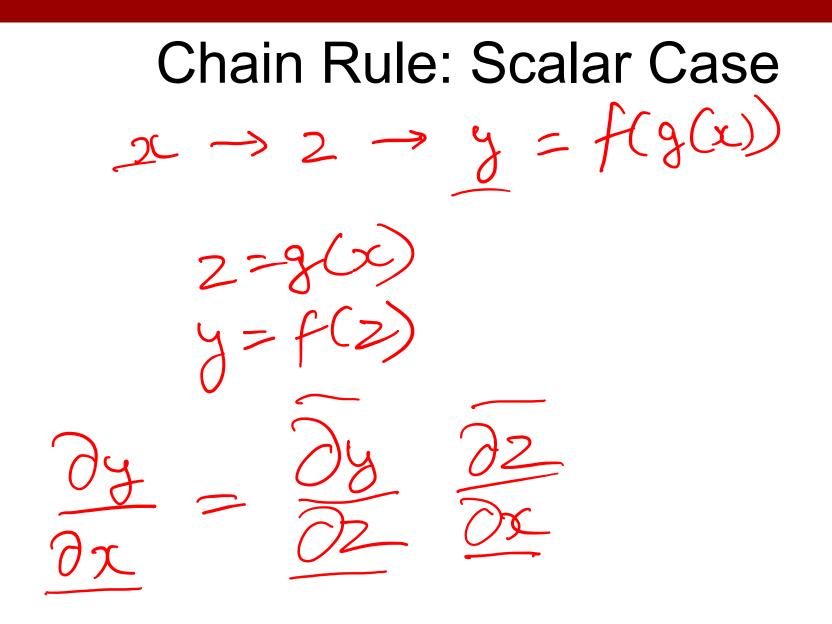




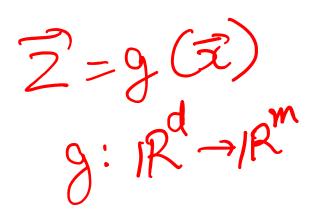


Chain Rule: Composite Functions $\mathcal{L}(x) = f(g(x)) = (f \circ g)(x)$



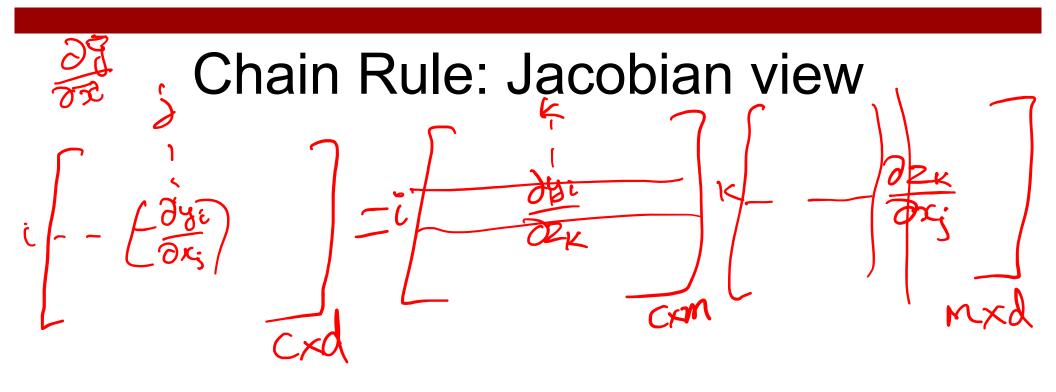




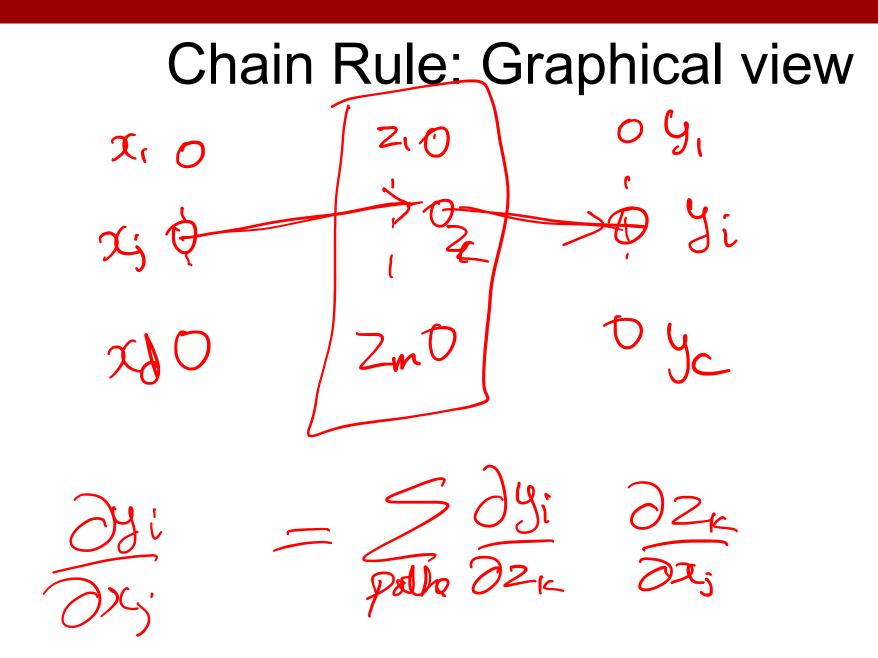


 $\vec{y} = f(\vec{z})$ $f: R^m \rightarrow R^c$

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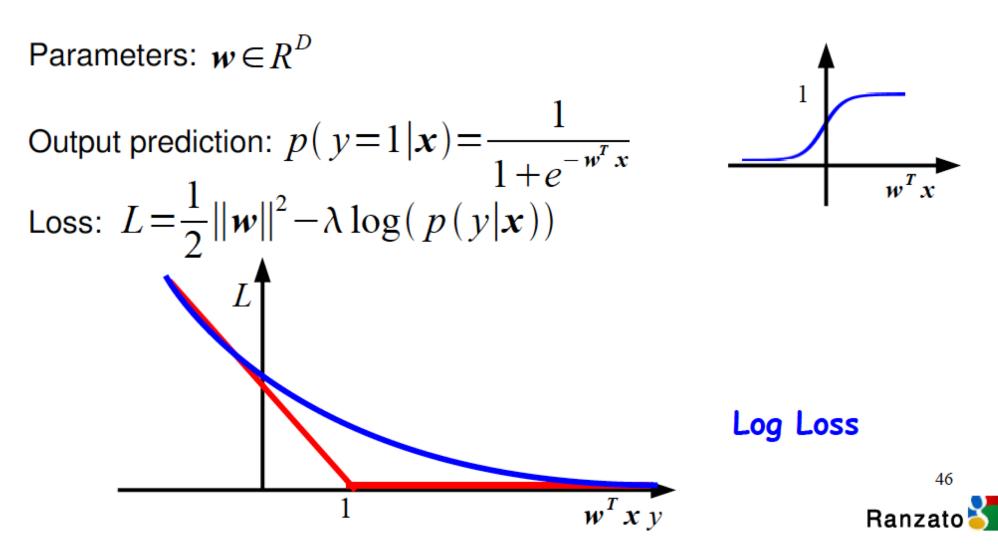
 $\frac{\partial y_i}{\partial x_g} = \sum_{\substack{K_i \\ K_i}} \frac{\partial y_i}{\partial x_k} \frac{\partial z_k}{\partial x_j}$



Linear Classifier: Logistic Regression

Input: $x \in R^{D}$

Binary label: $y \in \{-1, +1\}$



Logistic Regression Derivatives

Logistic Regression Derivatives

Convolutional network (AlexNet)

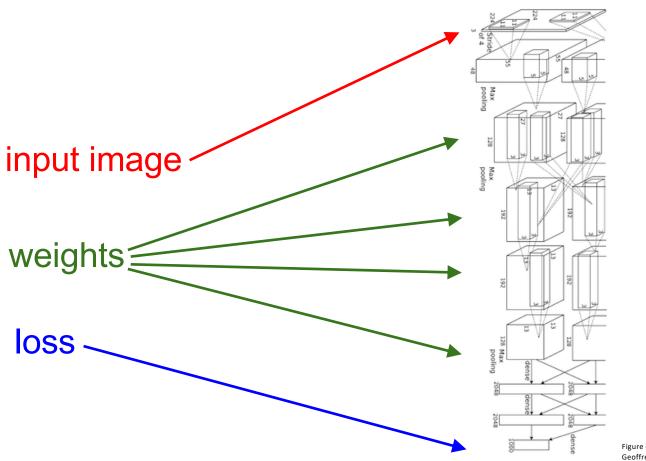


Figure copyright Alex Krizhevsky, Ilya Sutskever, and Geoffrey Hinton, 2012. Reproduced with permission.

Neural Turing Machine

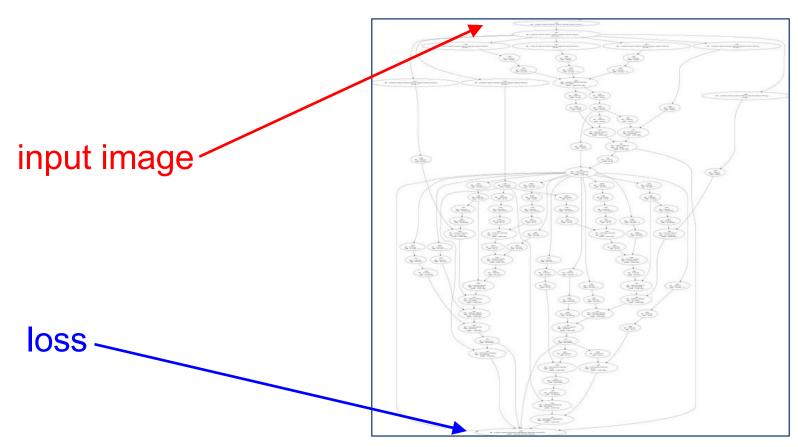
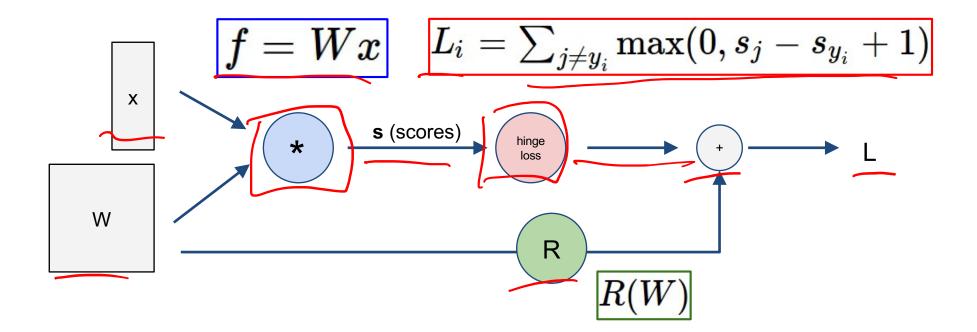


Figure reproduced with permission from a Twitter post by Andrej Karpathy.

How do we compute gradients?

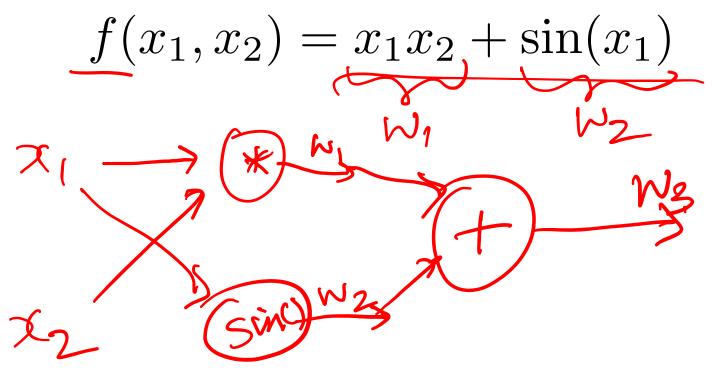
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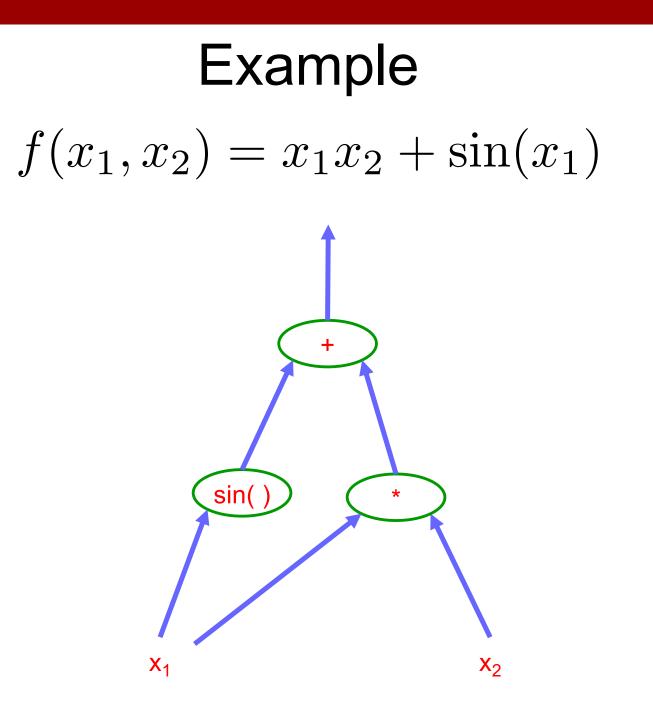
Computational Graph

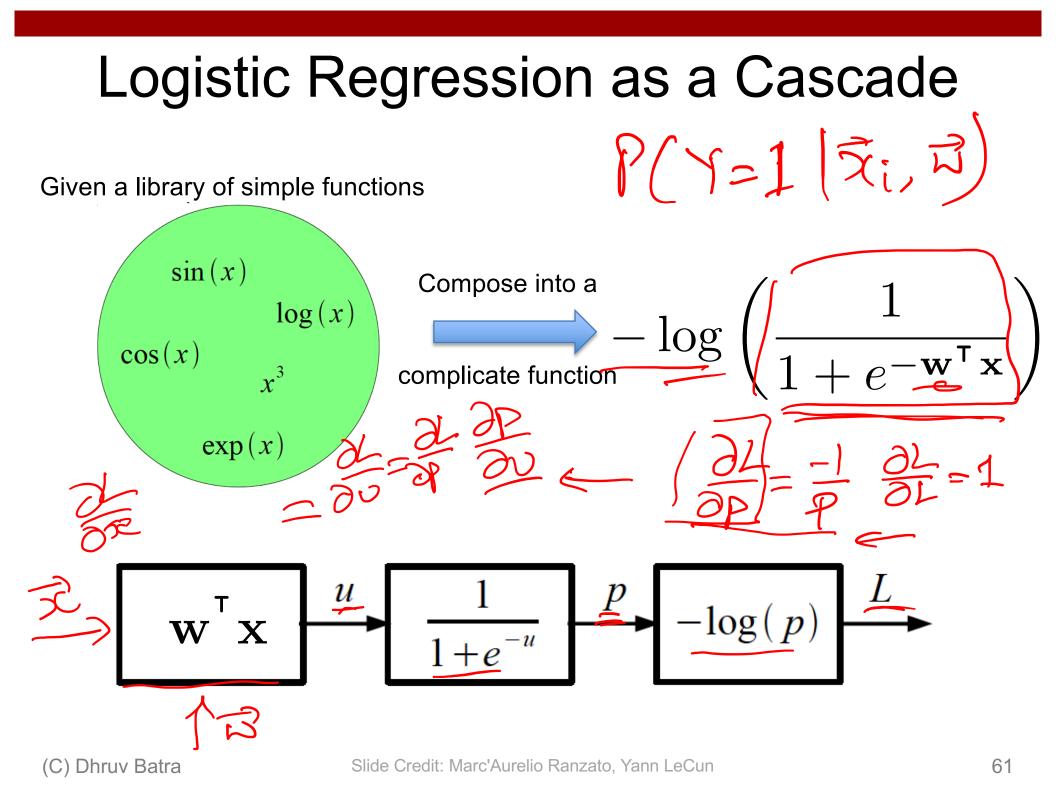


Computational Graphs

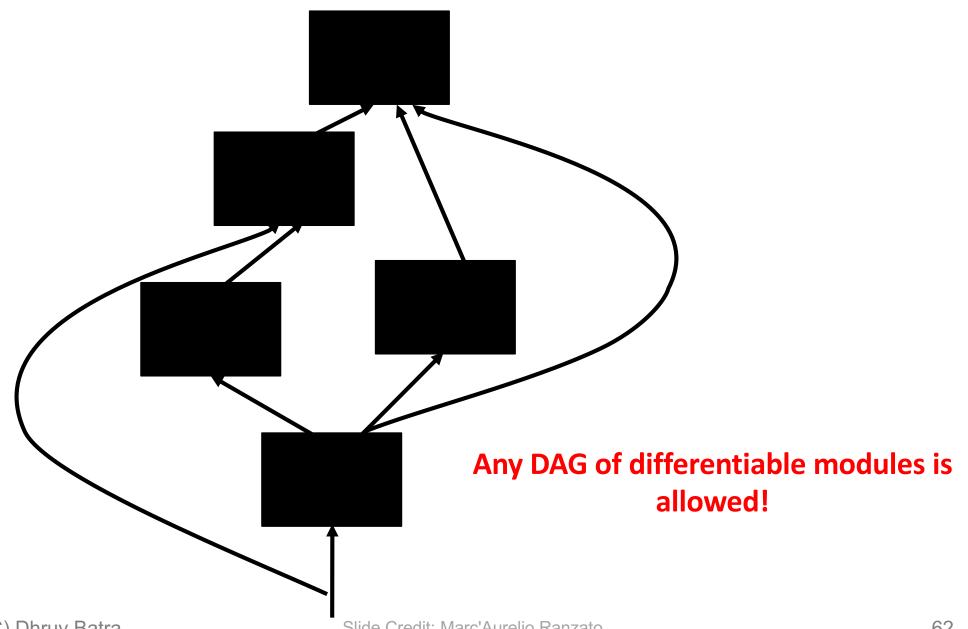
Notation



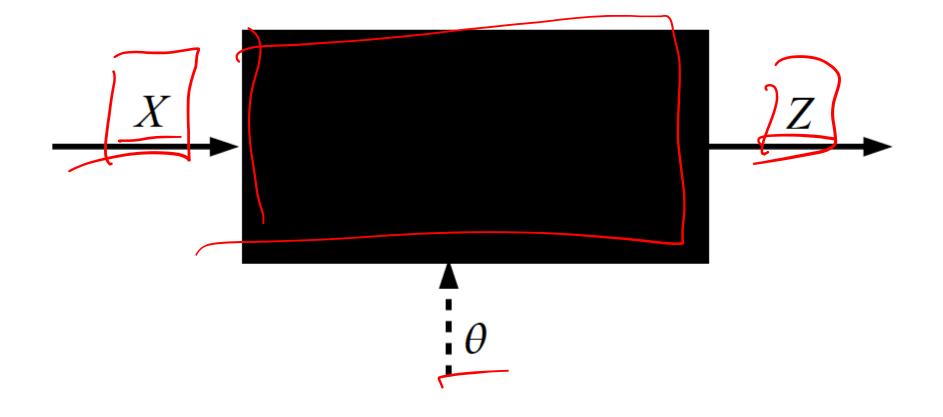




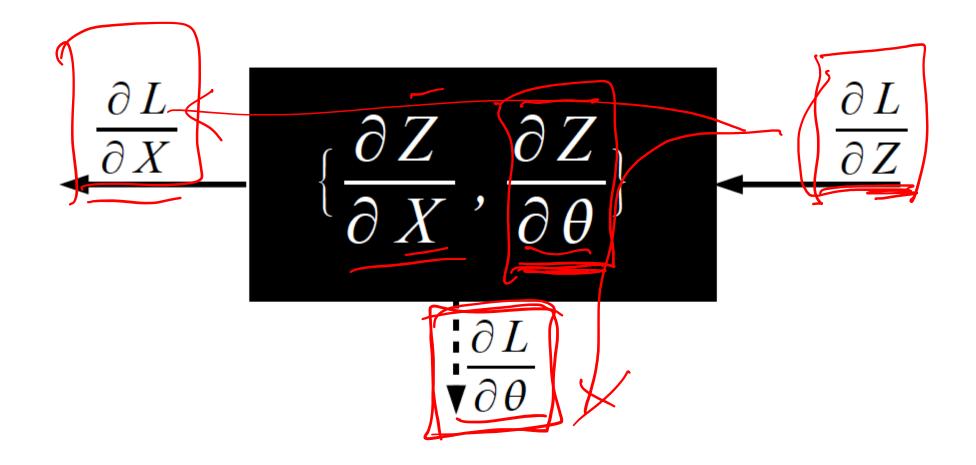
Computational Graph



Key Computation: Forward-Prop



Key Computation: Back-Prop

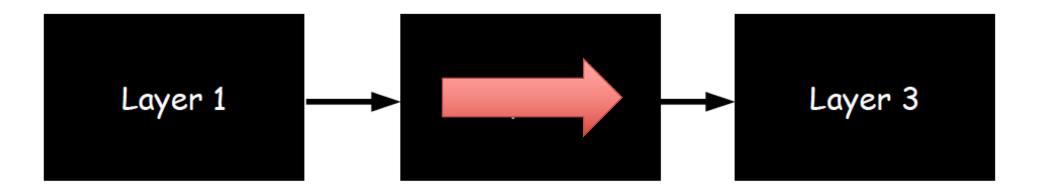


Step 1: Compute Loss on mini-batch



[F-Pass]

Step 1: Compute Loss on mini-batch
 [F-Pass]



Step 1: Compute Loss on mini-batch
 [F-Pass]

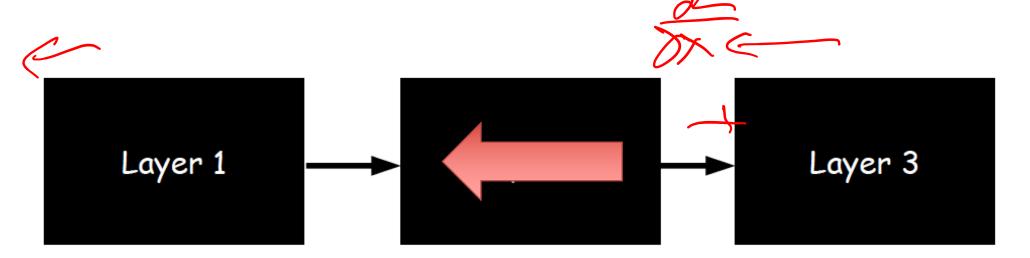


- Step 1: Compute Loss on mini-batch
- Step 2: Compute gradients wrt parameters [B-Pass]



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- Step 1: Compute Loss on mini-batch
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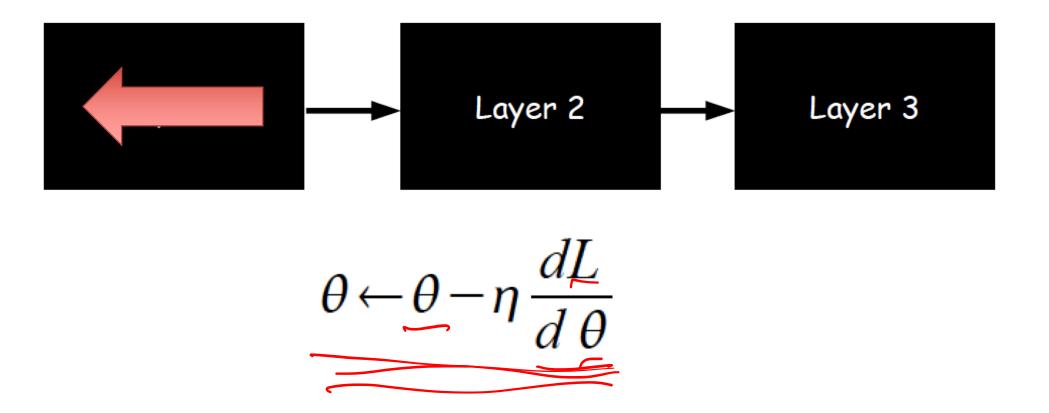


[F-Pass]

- Step 1: Compute Loss on mini-batch
 [F-Pass]
- Step 2: Compute gradients wrt parameters [B-Pass]



- Step 1: Compute Loss on mini-batch
- Step 2: Compute gradients wrt parameters [E
- [F-Pass] [B-Pass]
- Step 3: Use gradient to update parameters

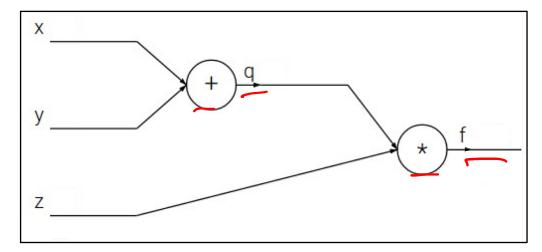


Backpropagation: a simple example

f(x,y,z) = (x+y)z

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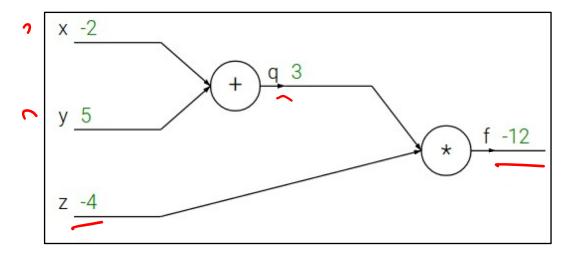
$$f(x,y,z) = \underbrace{(x+y)z}$$



Backpropagation: a simple example

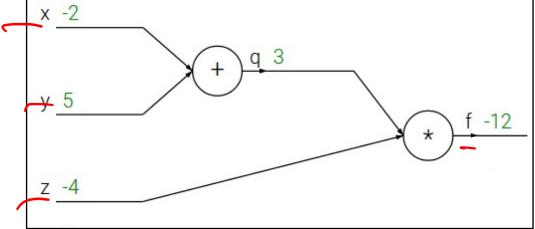
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e.g. x = -2, y = 5, z = -4



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Want:
$$\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$$

$$f(x, y, z) = (x + y)z$$

e.g. x = -2, y = 5, z = -4
$$q = x + y \quad \frac{\partial q}{\partial x} = 1, \frac{\partial q}{\partial y} = 1$$

Want:
$$\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$$

x -2

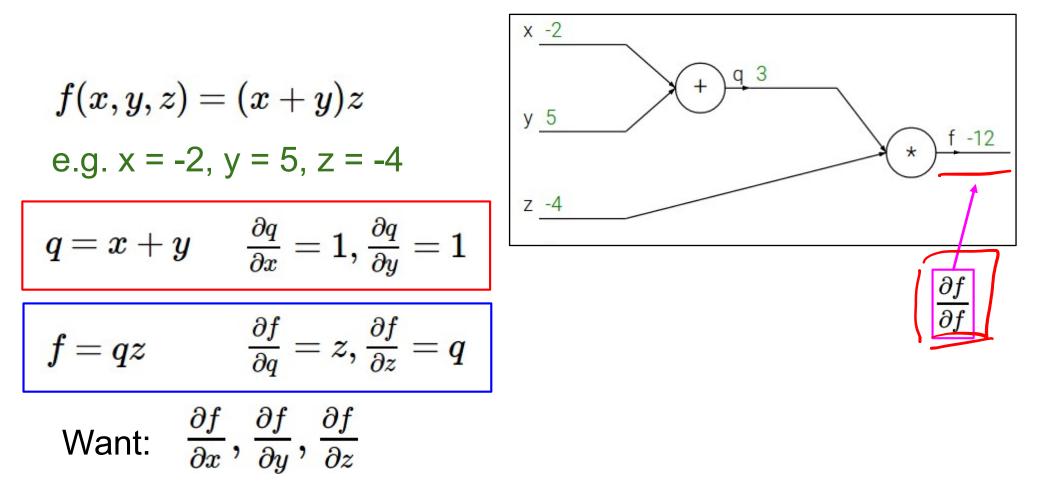
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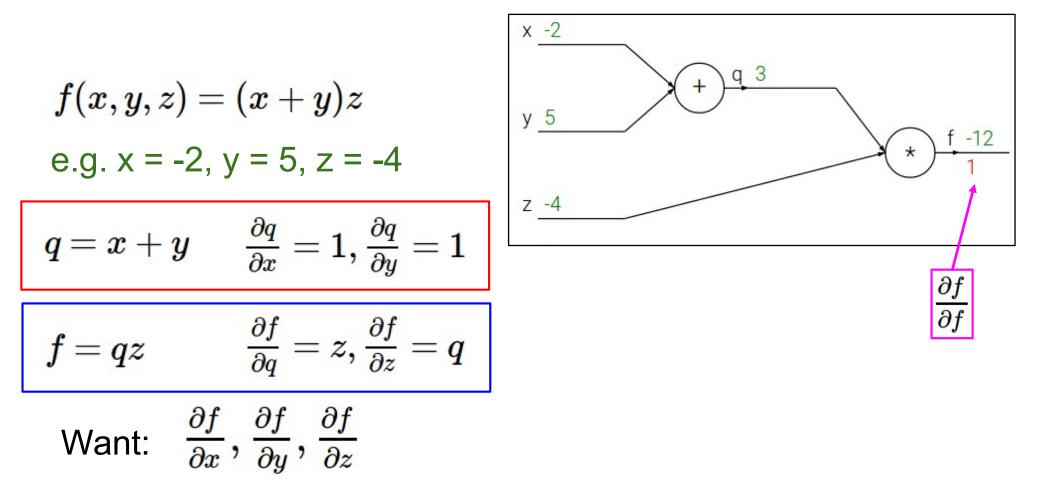
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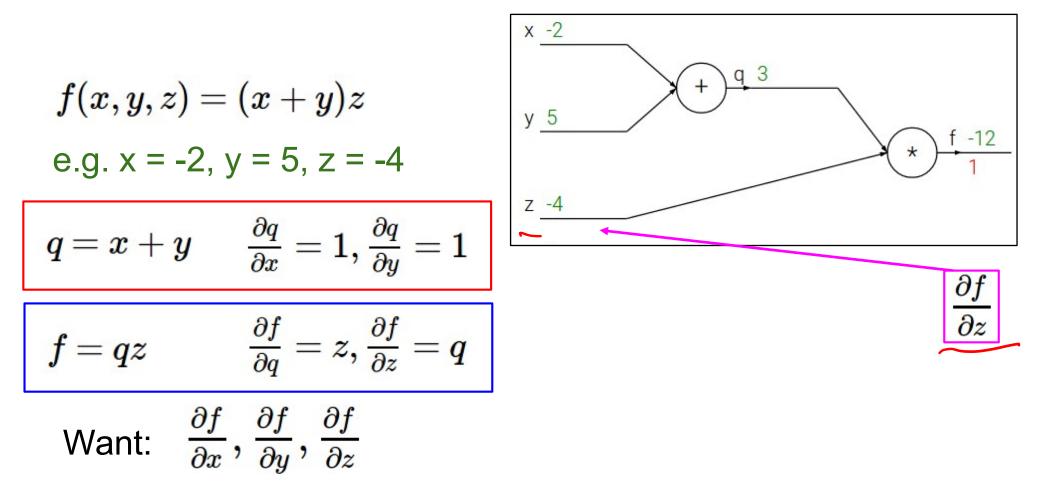
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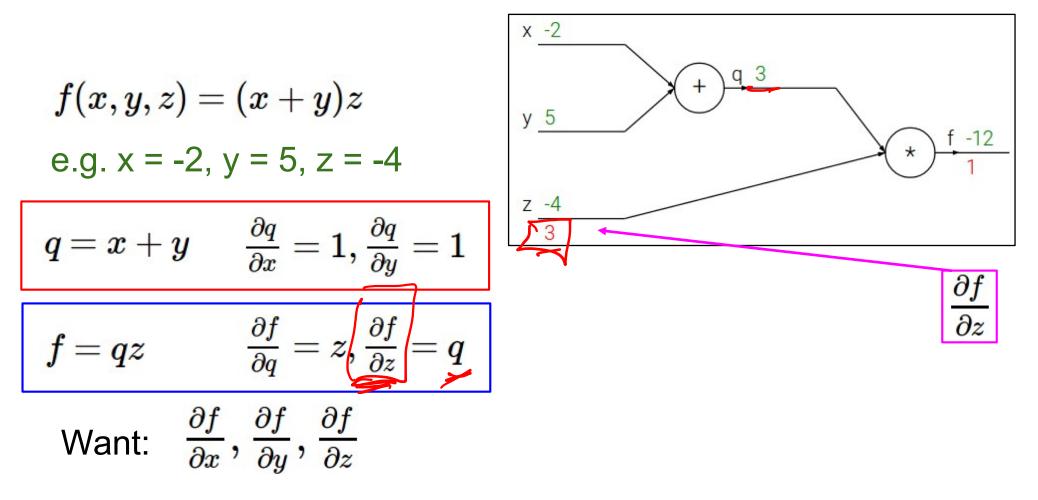
$$f = qz \qquad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q$$

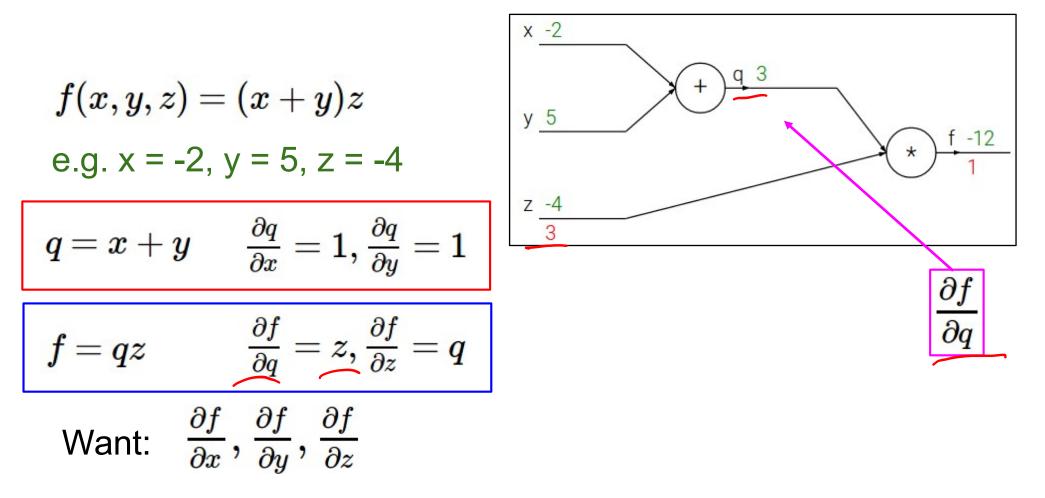
Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$











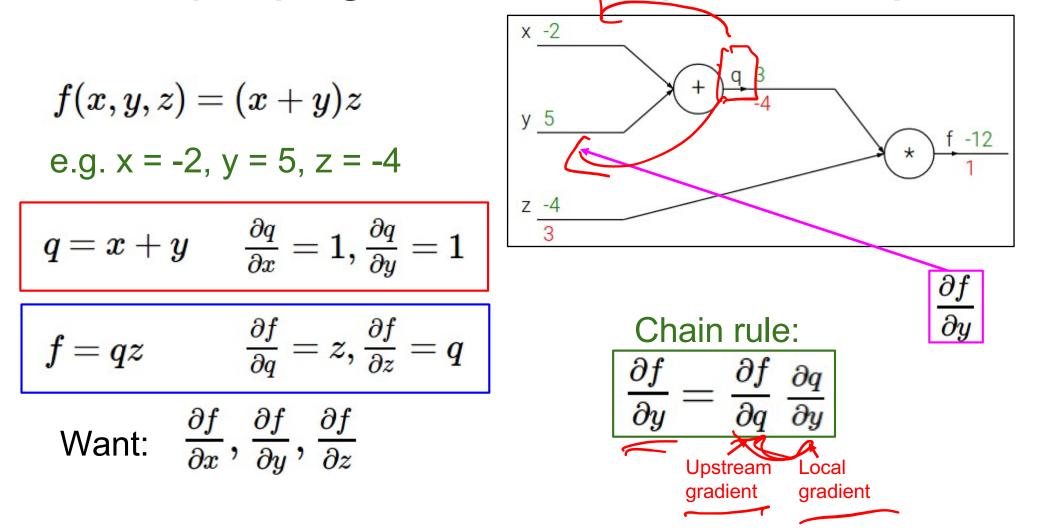
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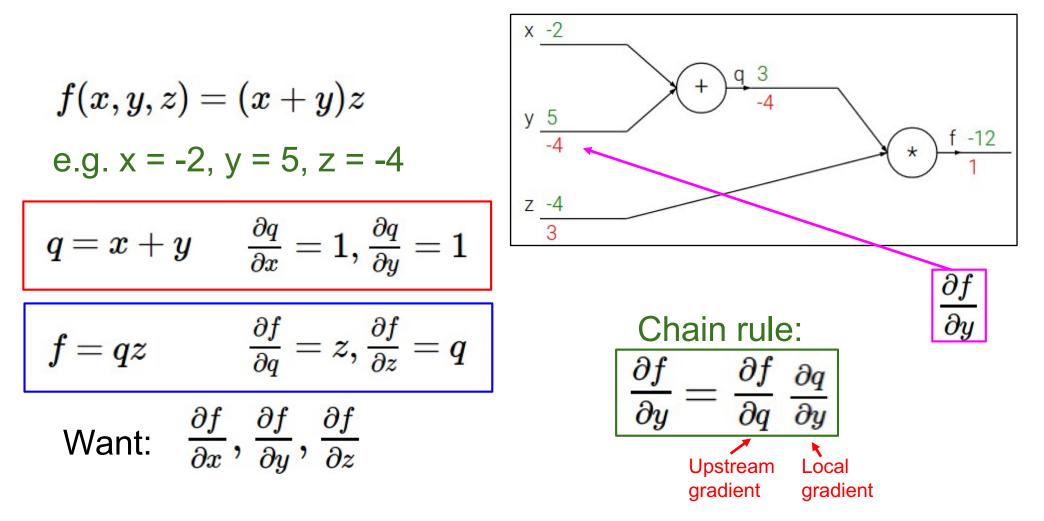
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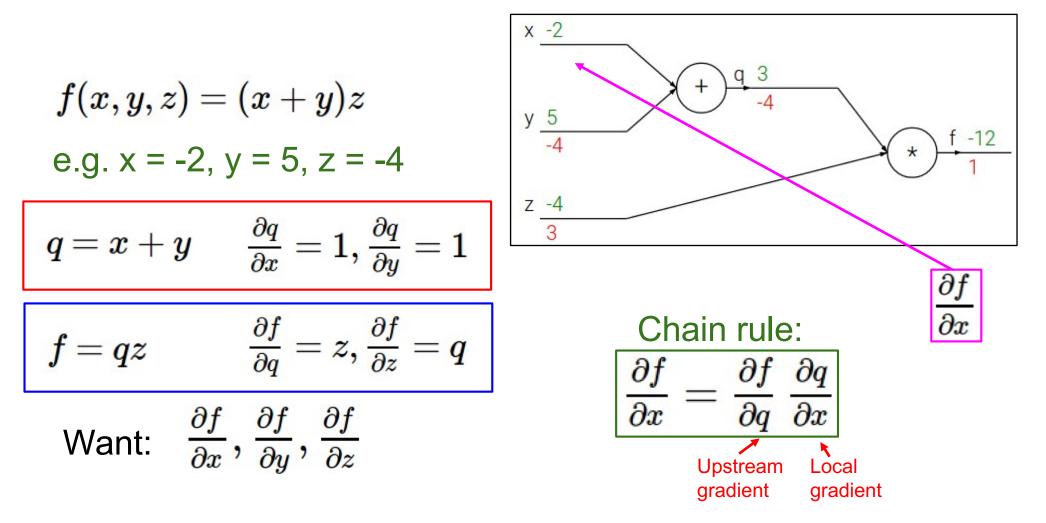
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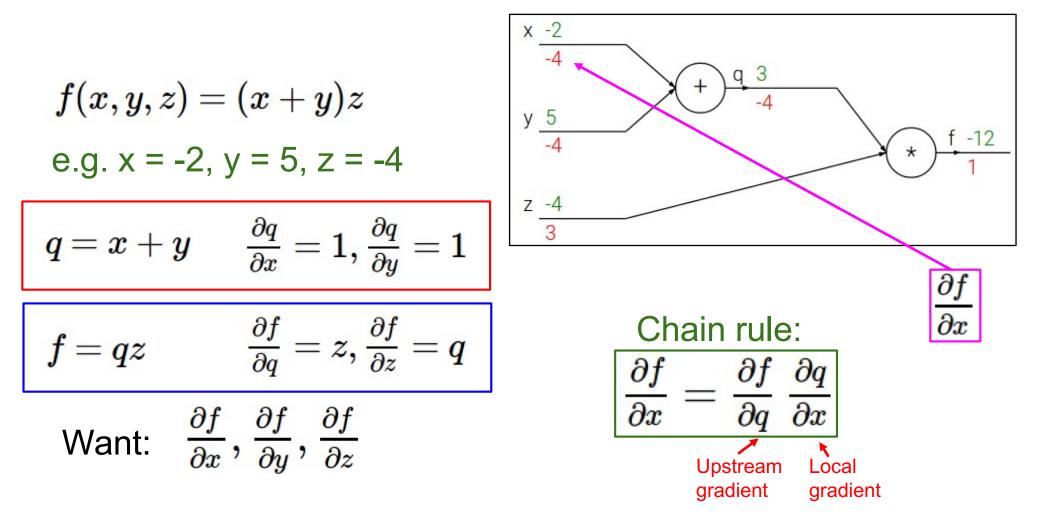
$$f = qz \qquad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q$$

Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



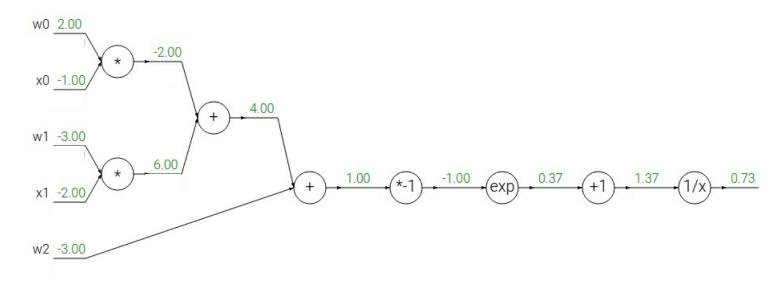




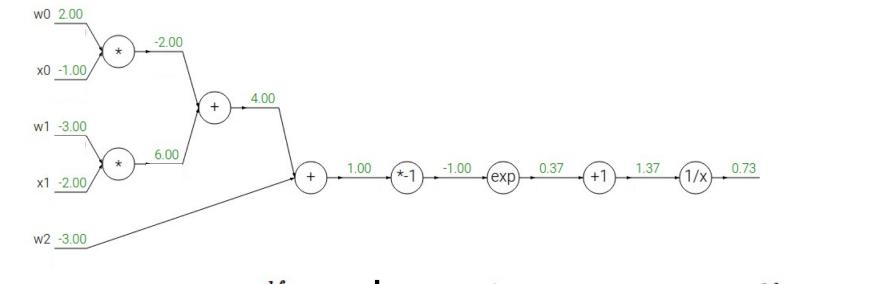


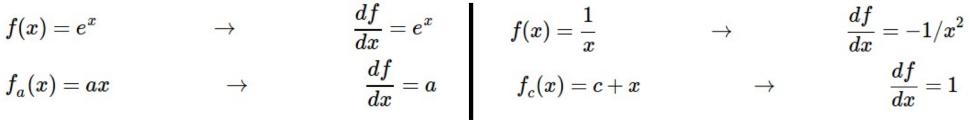
Another example: $f(w,x) = \frac{1}{1 + e^{-(w_0x_0 + w_1x_1 + w_2)}}$

$$f(w,x)=rac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$

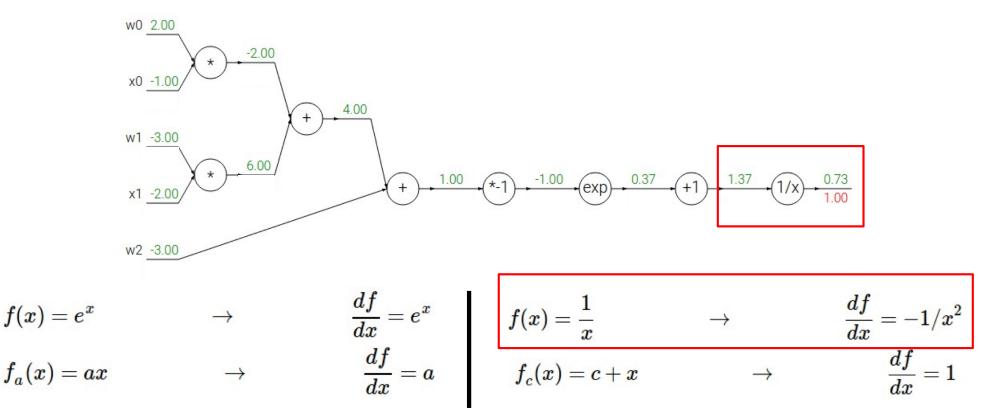


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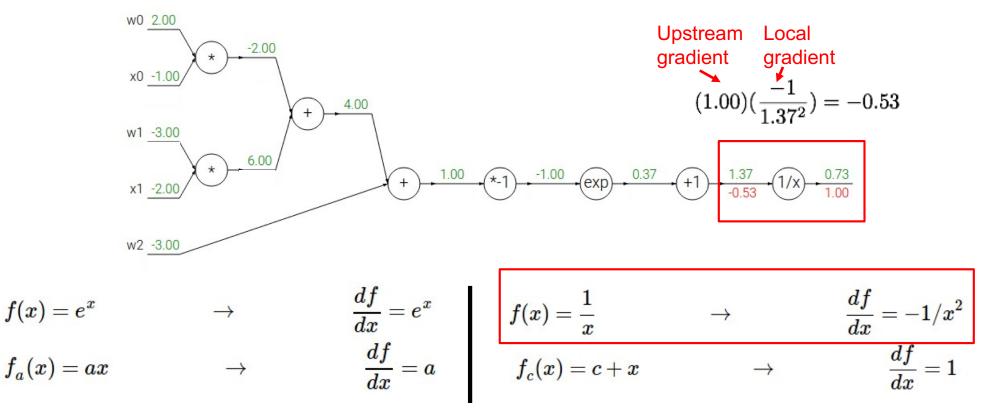




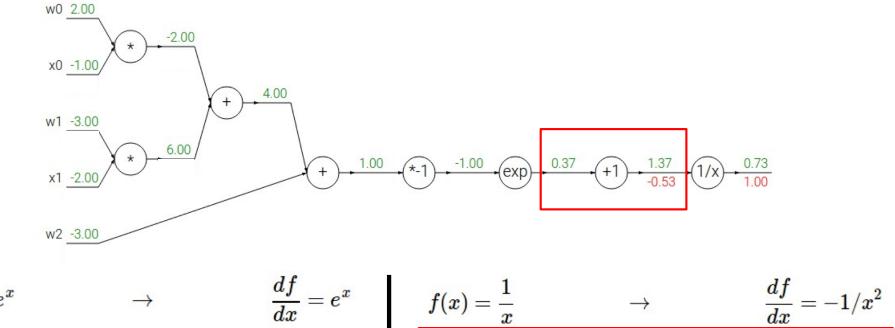
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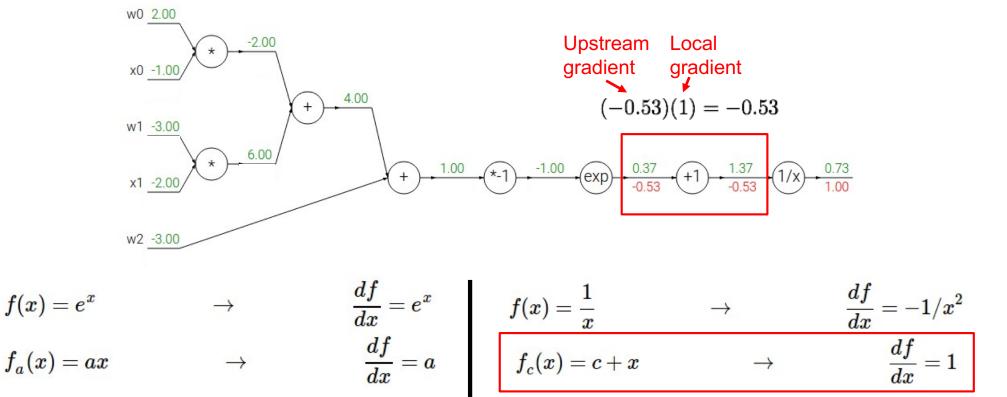


$$f(w,x)=rac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$



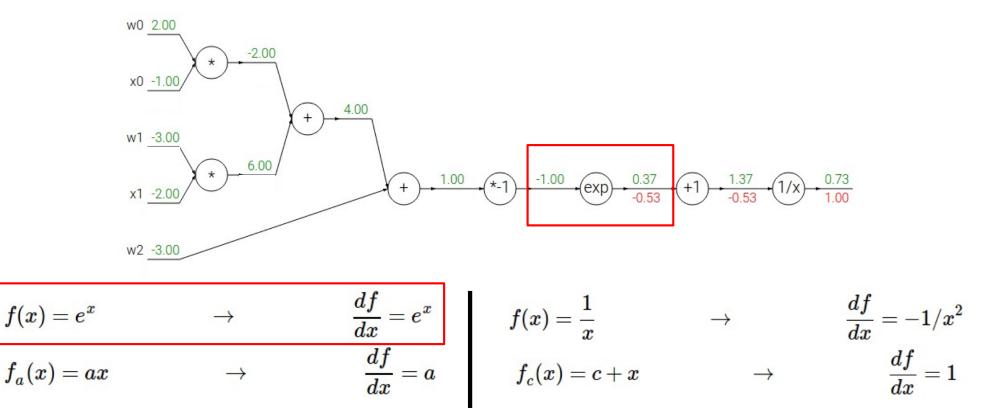
 $egin{array}{lll} f(x)=e^x &
ightarrow & \displaystyle rac{df}{dx}=e^x & f(x)=\displaystyle rac{1}{x} &
ightarrow & \displaystyle rac{df}{dx}=-1/x^2 & \ f_a(x)=ax &
ightarrow & \displaystyle rac{df}{dx}=a & \ f_c(x)=c+x &
ightarrow & \displaystyle rac{df}{dx}=1 & \ \end{array}$

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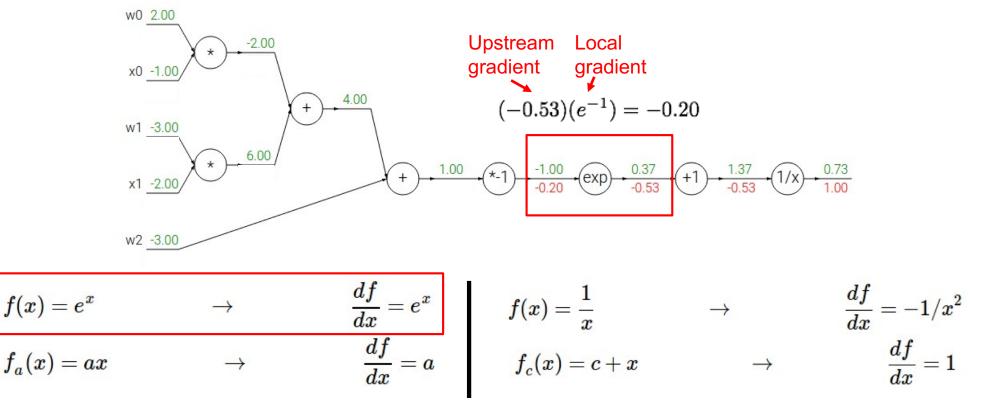


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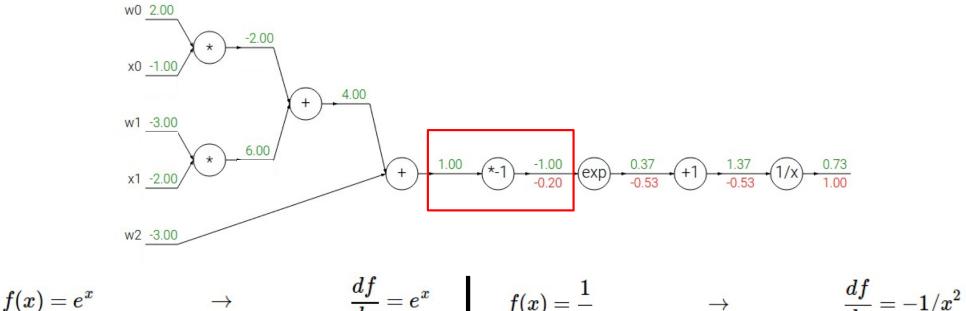
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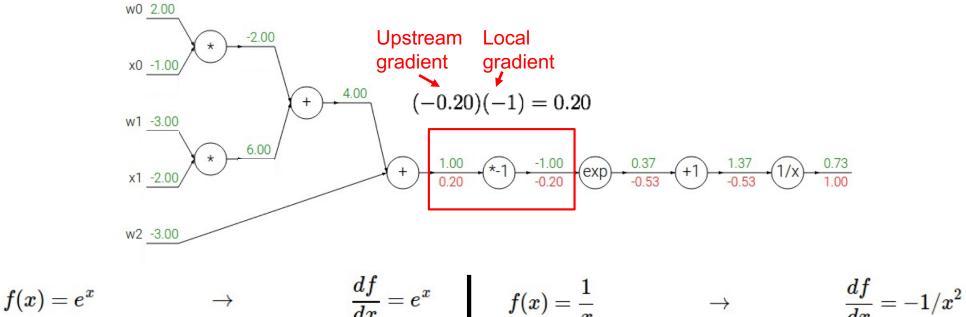


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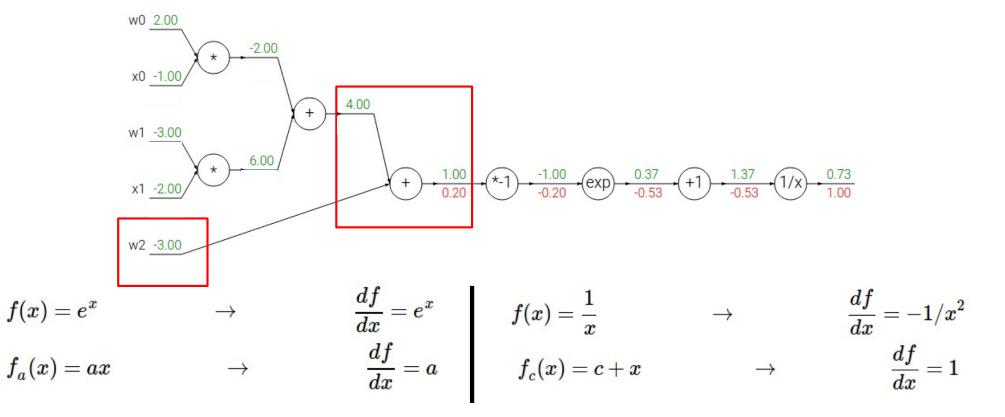


J(w) = c	,	dx	$J(x) = \frac{1}{x}$	~	$\frac{dx}{dx} = -1/x$
$f_a(x)=ax$	\rightarrow	$rac{df}{dx}=a$	$f_c(x)=c+x$	\rightarrow	$rac{df}{dx}=1$

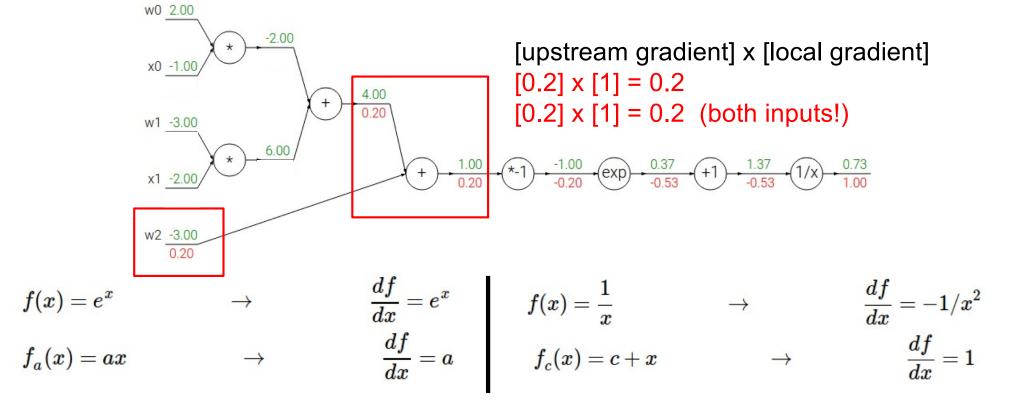
$$f(w,x)=rac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$

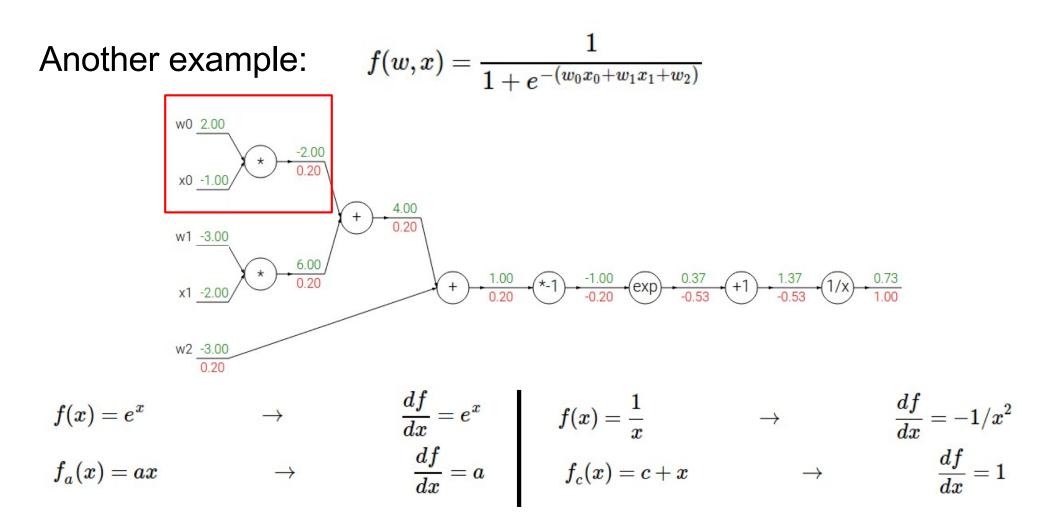


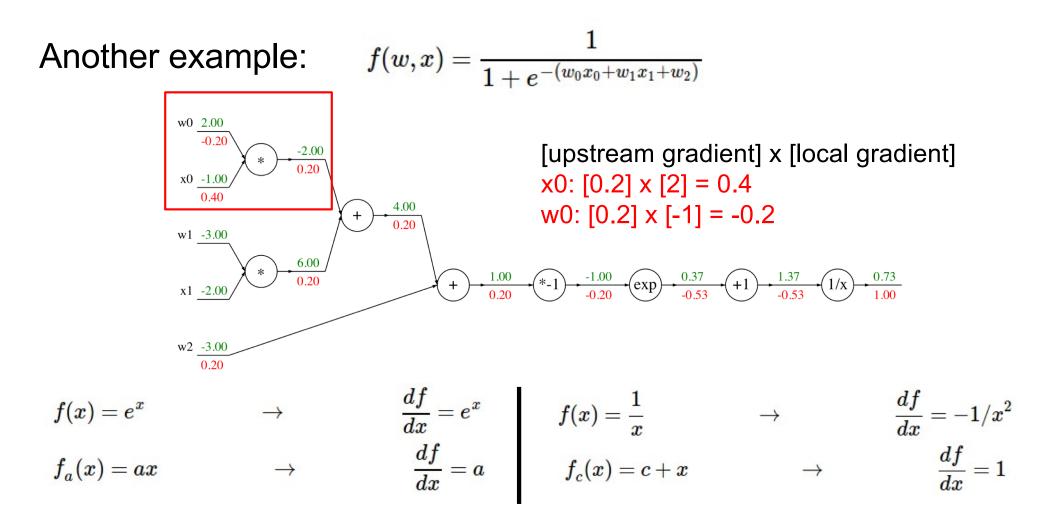
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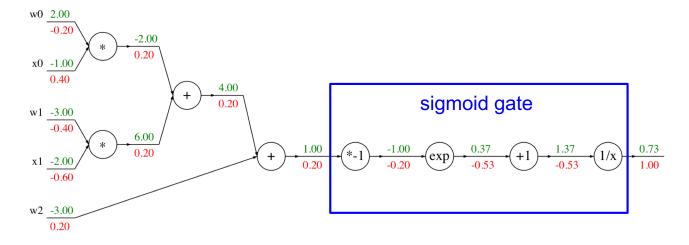


$$f(w,x)=rac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$

 $\sigma(x)$

Computational graph representation may not be unique. Choose one where local gradients at each node can be easily expressed!

$$\frac{\sigma(x) = \frac{1}{1 + e^{-x}}}{\text{sigmoid function}} \quad \frac{d\sigma(x)}{dx} = \frac{e^{-x}}{(1 + e^{-x})^2} = \left(\frac{1 + e^{-x} - 1}{1 + e^{-x}}\right) \left(\frac{1}{1 + e^{-x}}\right) = (1 - \sigma(x))\sigma(x)$$



$$f(w,x)=rac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$

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Computational graph representation may not be unique. Choose one where local gradients at each node can be easily expressed!

$$\sigma(x) = \frac{1}{1+e^{-x}} \qquad \frac{d\sigma(x)}{dx} = \frac{e^{-x}}{(1+e^{-x})^2} = \left(\frac{1+e^{-x}-1}{1+e^{-x}}\right) \left(\frac{1}{1+e^{-x}}\right) = (1-\sigma(x))\sigma(x)$$
sigmoid function

