Lecture 11: Backpropagation

Machine Learning and Imaging

BME 548L
Roarke Horstmeyer

This lecture uses material from:

- A. Baydin et al., Automatic Differentiation in Machine Learning: a Survey
- Stanford CS231n
- *Deep Learning* by I. Goodfellow

Important components of a CNN

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CNN Architecture

Architecture choices

- CONV size, stride, pad, depth
- ReLU & other nonlinearities
- POOL methods
- # of layers, dimensions per layer
- Fully connected layers

Loss function & optimization

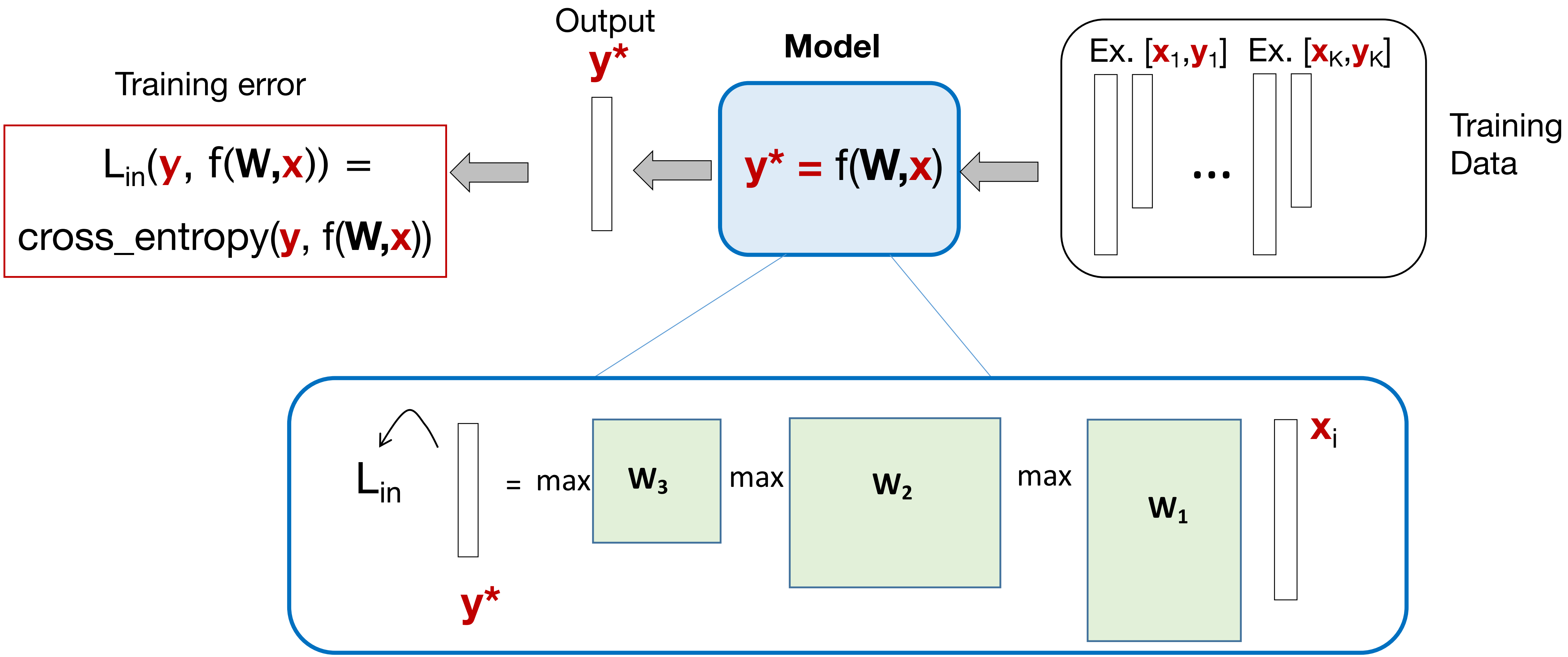
- Type of loss function
- Regularization
- Gradient descent method
- SGD batch and step size

Optimization choices

How does the optimizer actually work???

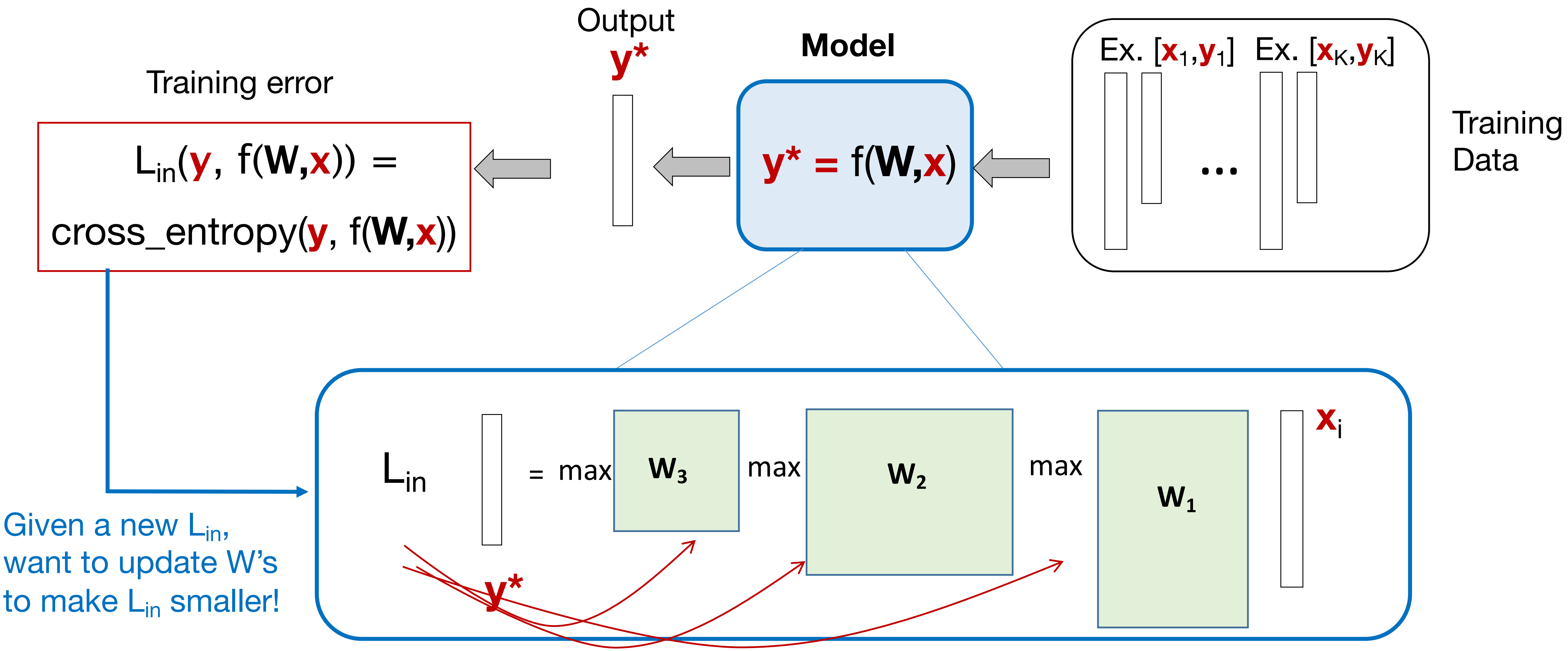
Other specifics: Pre-processing**,** initialization**,** dropout, batch normalization, augmentation

Our very basic convolutional neural network



Forward pass: from $\mathbf{x}_i$ and current **W**’s, find L_{in}

Our very basic convolutional neural network



Backwards pass: from new $L_{in,}$ need to update **W**'s! How?

Review: how can we determine the optimal W?

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- Here, let's assume we'll use the steepest descent algorithm to "go down the hill":

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Input: labeled training examples [$\mathbf{x}_i$,$\mathbf{y}_i$] for i=1 to N, initial guess of **W**'s

while loss function is still decreasing:
    Compute loss function L(**W**,$\mathbf{x}_i$,$\mathbf{y}_i$)
    Update **W** to make L smaller:
        dL/d**W** = evaluate_gradient(**W**,$\mathbf{x}_i$,$\mathbf{y}_i$,L)
        W = **W** – step_size * dL/d**W**

```
while previous_step_size > precision and iters < max_iters
    prev_W = cur_W
    cur_W -= gamma * differential_dL(CNN_model, prev_W)
    previous_step_size = abs(cur_W - prev_W)
    iters+=1
```

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Review: how can we determine the optimal W?

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W = **W** – step_size * dL/d**W**

Options to evaluate dL/d**W**:
1. Numerical gradient
2. Analytic gradient
3. Automatic differentiation

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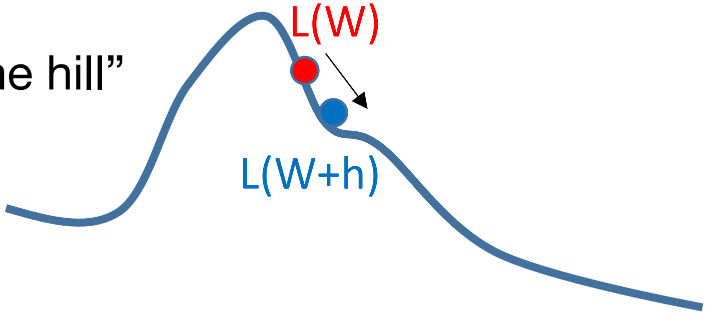
*Note: Other gradient descent methods require the same fundamental calculation. So how gradient *is computed* is a different problem then how it is *used*

1. Numerical gradient, a simple example



"Go down the hill"

With a matrix, compute this for each entry:

$$\frac{dL(W_i)}{dW_i} = \lim_{h \to 0} \frac{L(W_i + h) - L(W_i)}{h}$$

<u>Example:</u>

W = [1,2;3,4]
L(W, x, y) = 12.79

W_1+h = [1.001,2;3,4]
L(W_1+h, x, y) = 12.8

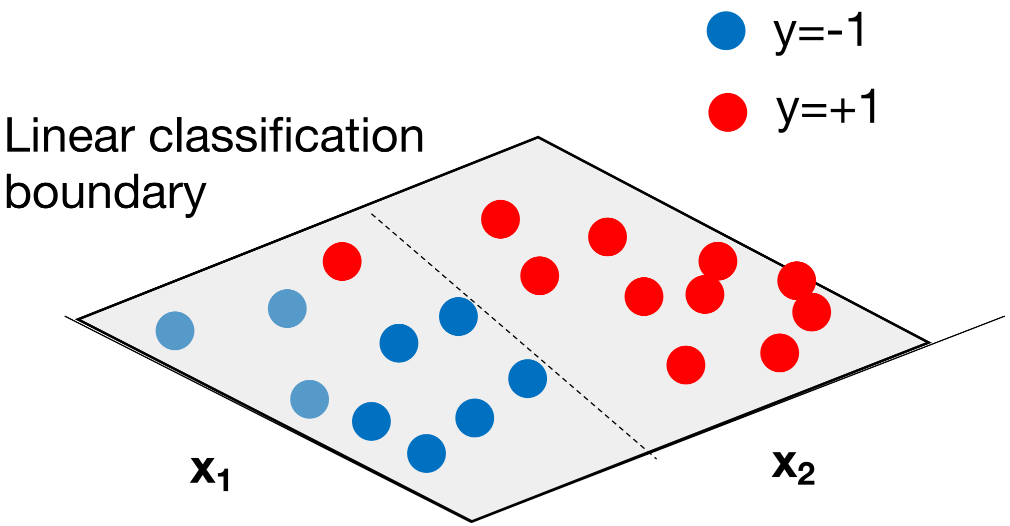
d$L(W_1)$/dW_1 = 12.8-12.79/.001

d$L(W_1)$/dW_1 = 10

Pros: Simple! Easy to code up!

Cons: Slow…really slow. And approximate

2. Analytic gradient, a simple example



$$L = \frac{1}{N}\sum_{i=1}^{N}(w^T x_i - y_i)^2$$

Analytically compute new function

$$\nabla L(w) = \frac{2}{N} X^T (Xw - y)$$

Evaluate this function and use to iterative update weights **W**

Pros: Fast and exact

Cons: Error prone, especially with deep networks…

3. Automatic differentiation – what we'll use without knowing it

Resources:

- Stanford CS231n, Lecture 4 notes and resources
    - http://cs231n.stanford.edu/syllabus

- I. Goodfellow et al., Deep Learning Chapter 6 Section 5
    - https://www.deeplearningbook.org/contents/mlp.html

- A. Baydin et al., "Automatic differentiation in machine learning: a survey"
    - https://arxiv.org/pdf/1502.05767.pdf

3. Automatic differentiation – what is it?

- Not solely numerical or analytic
- Use insights into formation of final function
- Split into elementary operations
- Perform analytic (symbolic) differentiation at elementary operation level
- Keep intermediate numeric results
- *Repeat process in lock-step with evaluation of final function*

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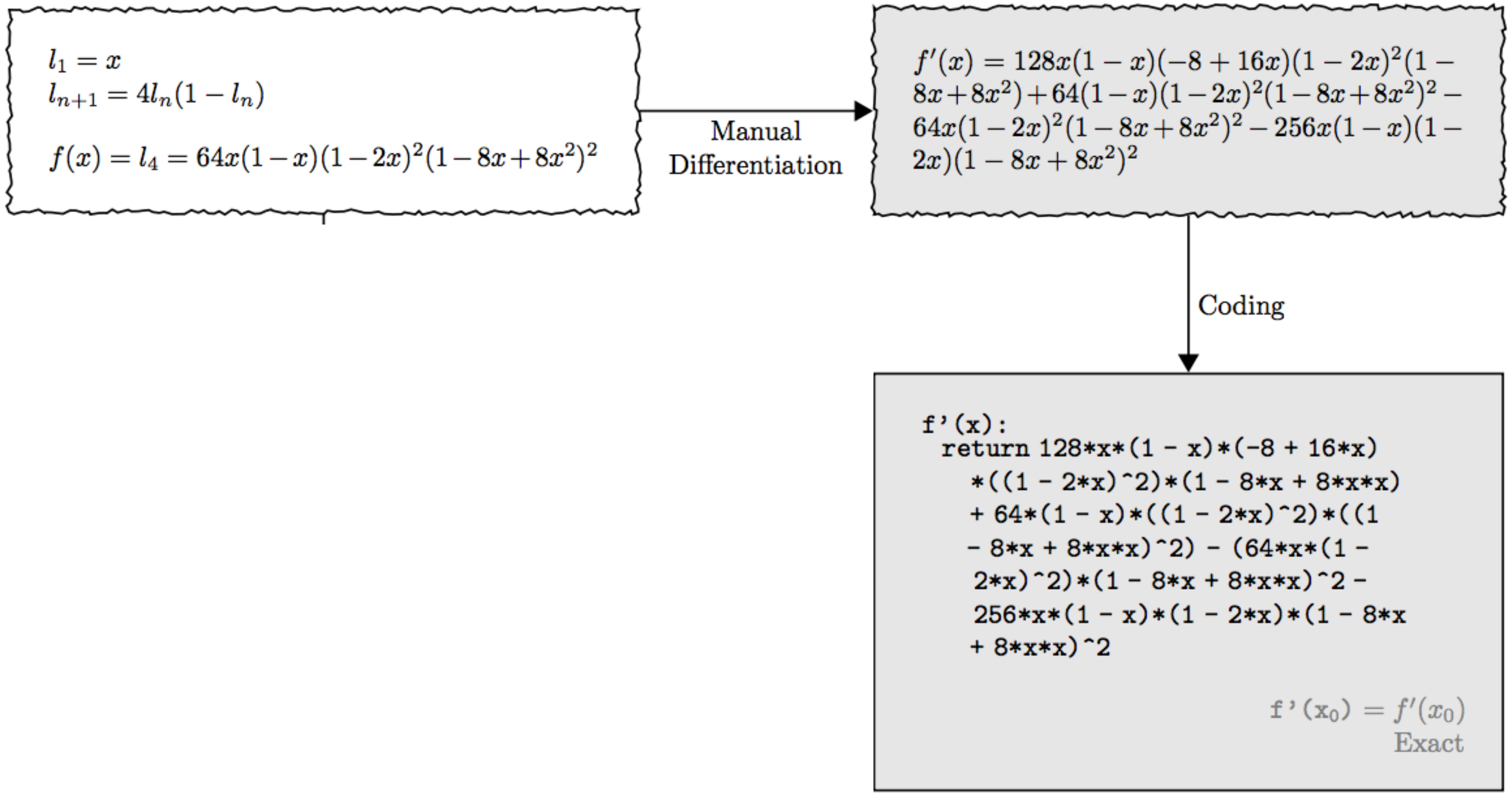

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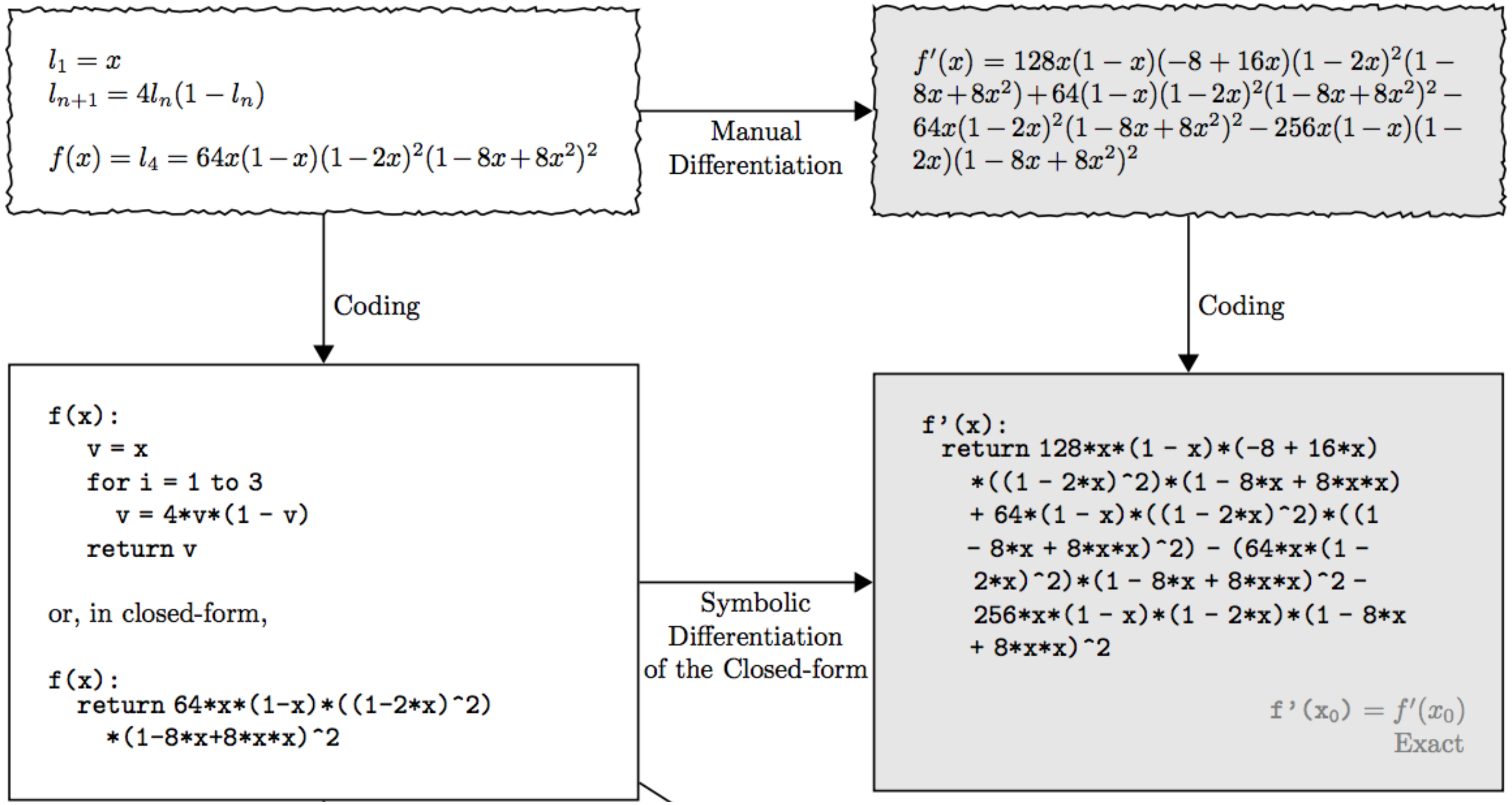

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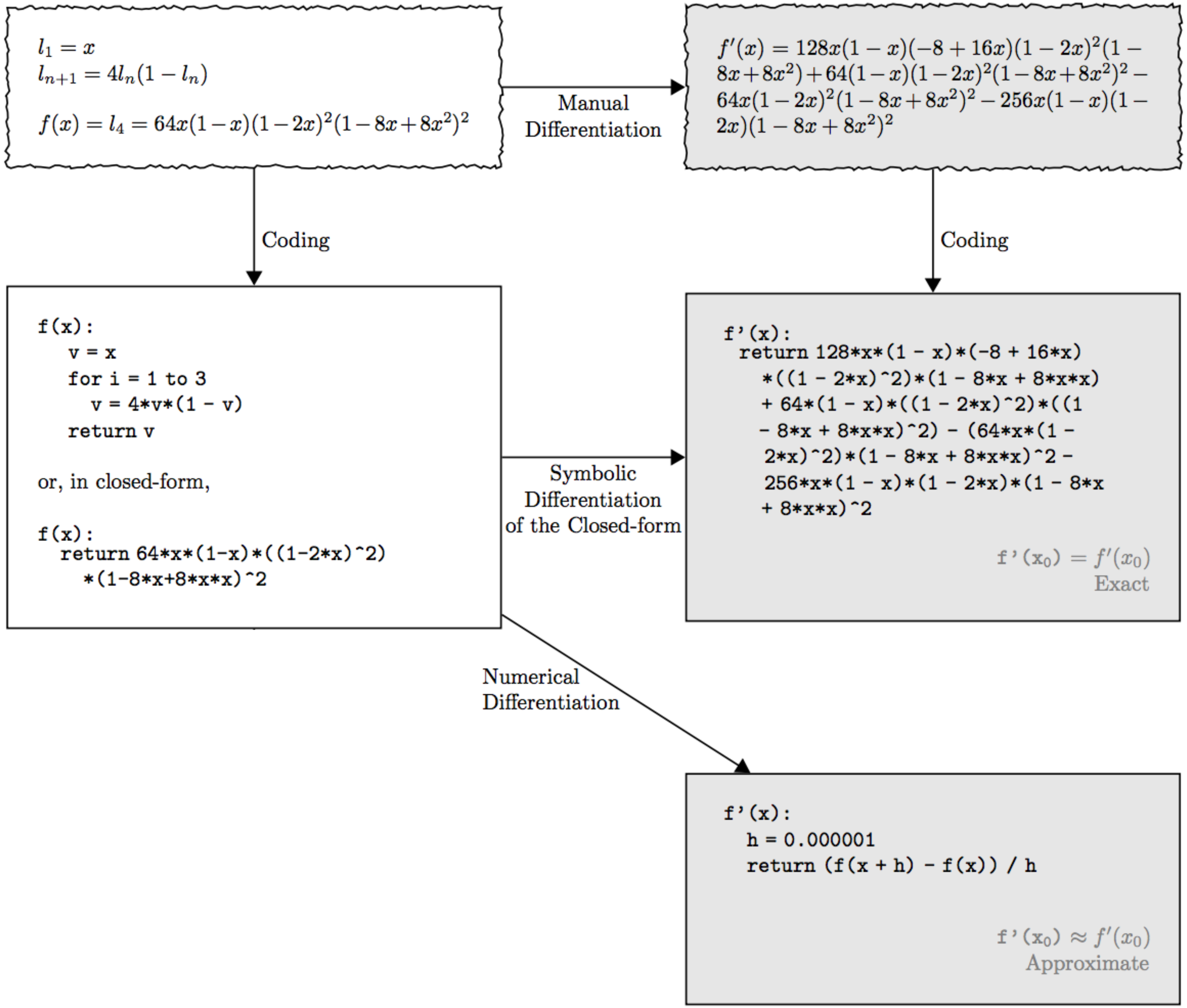

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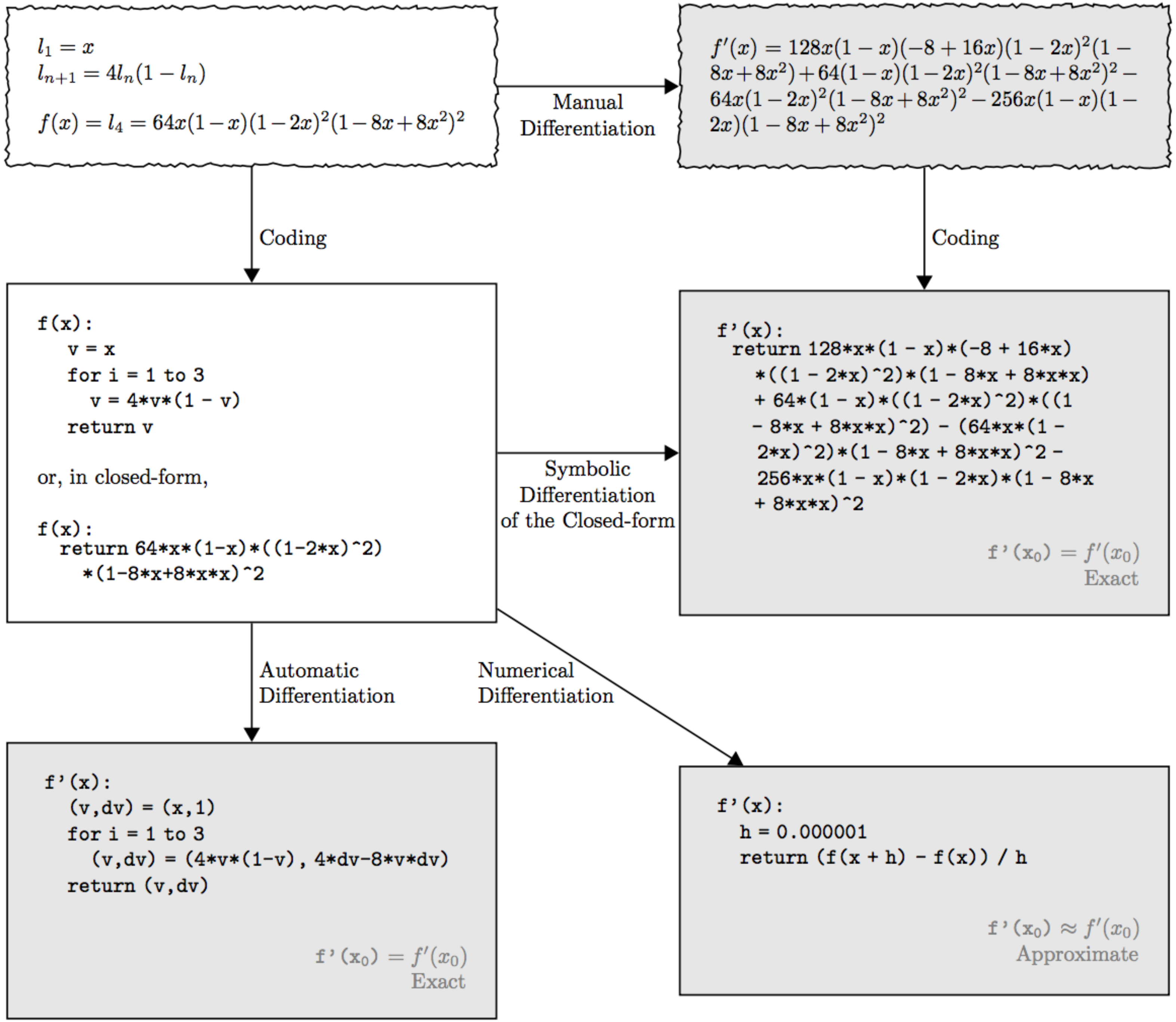

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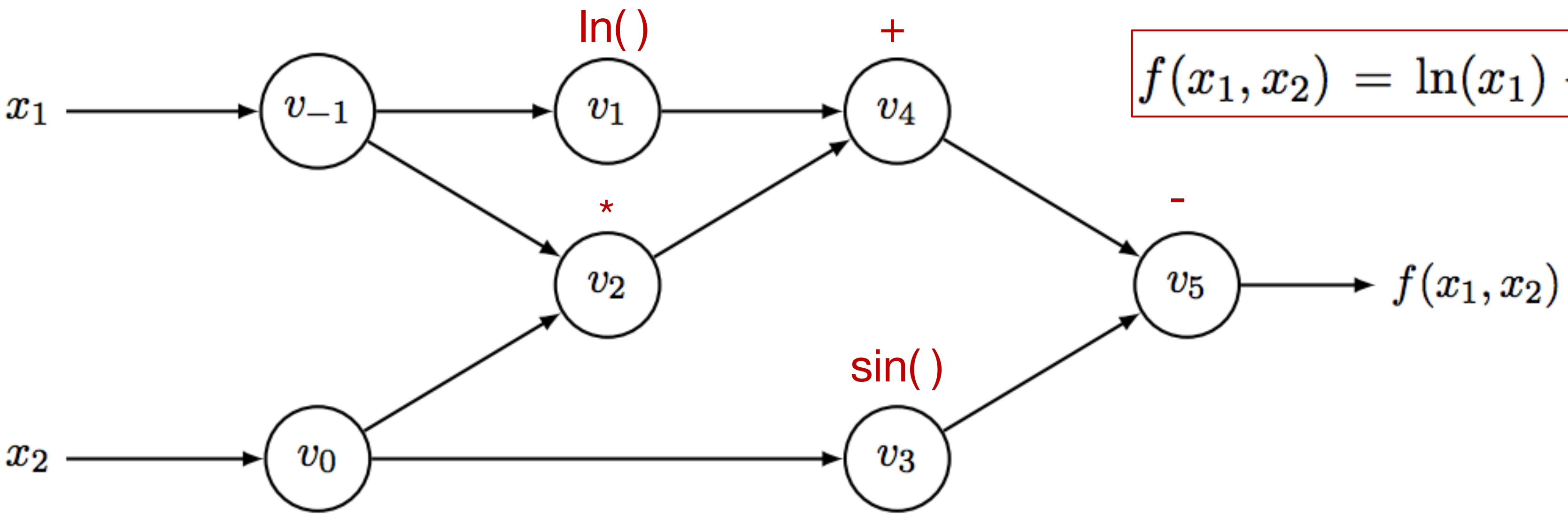
Automatic differentiation on computational graphs

$$\boxed{f(x_1, x_2) = \ln(x_1) + x_1 x_2 - \sin(x_2)}$$



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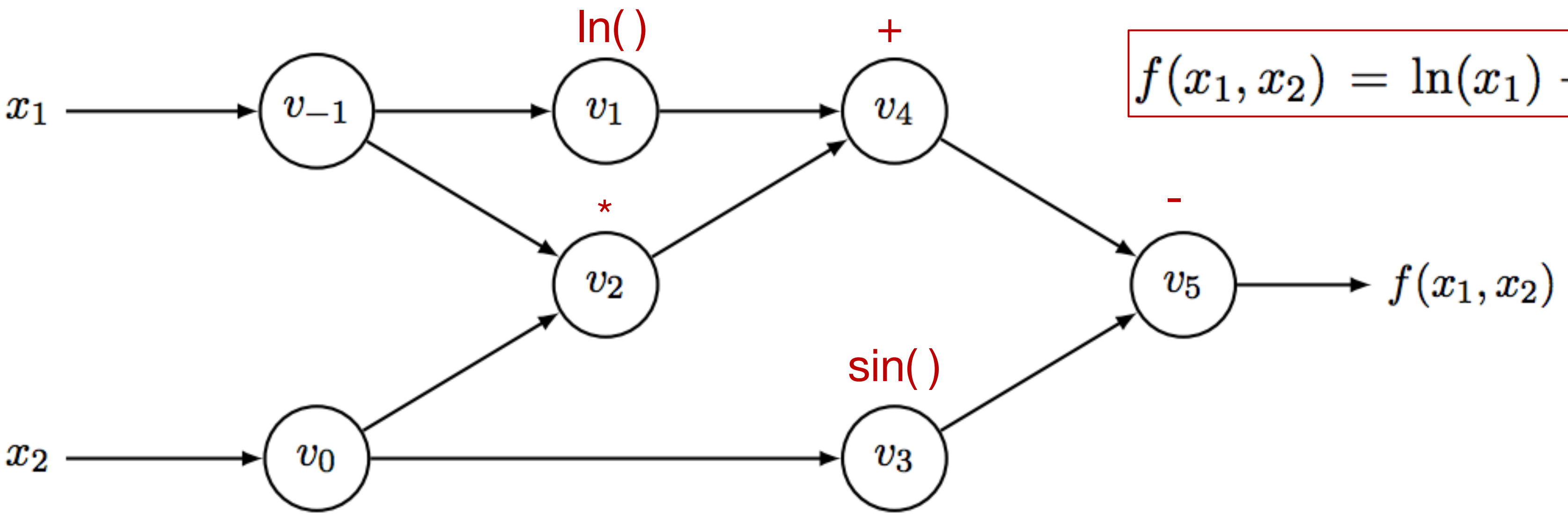

$$\boxed{f(x_1, x_2) = \ln(x_1) + x_1 x_2 - \sin(x_2)}$$

To both determine f and find df/dx_i :

- Create graph of local operations
- Compute analytic (symbolic) gradient at each node (unit) in graph
- Use inter-relationships to establish final desired gradient, df/dx_1
  - Forward differentiation
  - Backwards differentiation = Backpropagation

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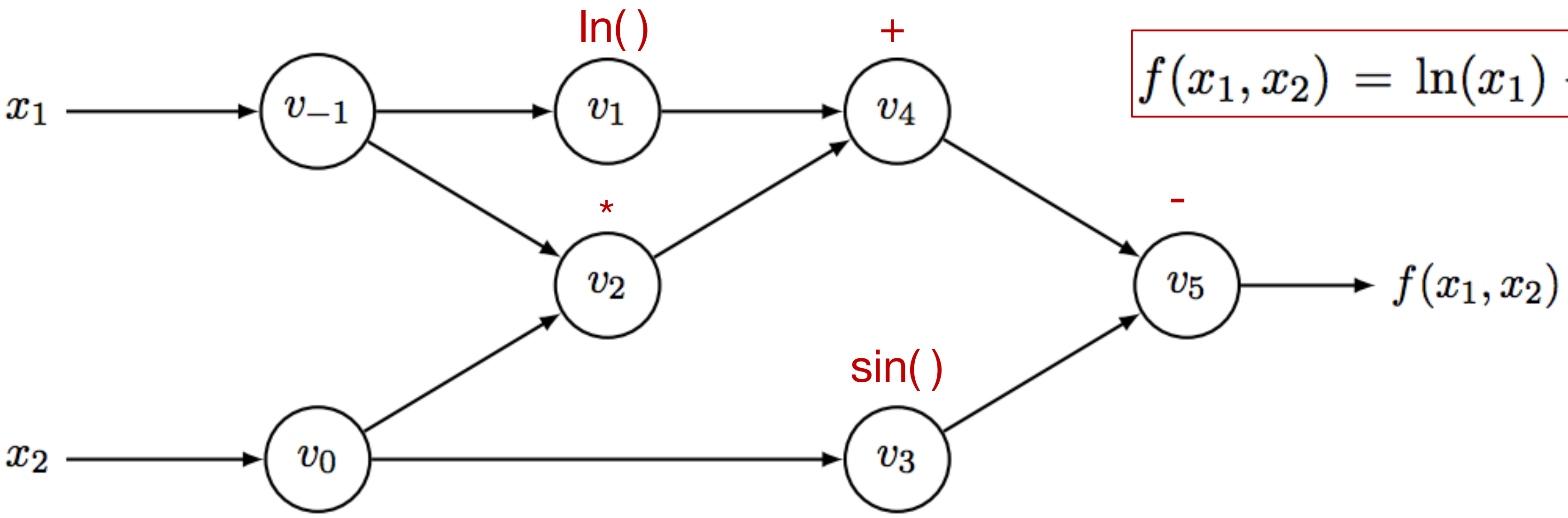

Forward Primal Trace

v_{-1}	$= x_1$	$= 2$
v_0	$= x_2$	$= 5$
v_1	$= \ln v_{-1}$	$= \ln 2$
v_2	$= v_{-1} \times v_0$	$= 2 \times 5$
v_3	$= \sin v_0$	$= \sin 5$
v_4	$= v_1 + v_2$	$= 0.693 + 10$
v_5	$= v_4 - v_3$	$= 10.693 + 0.959$
y	$= v_5$	$= 11.652$

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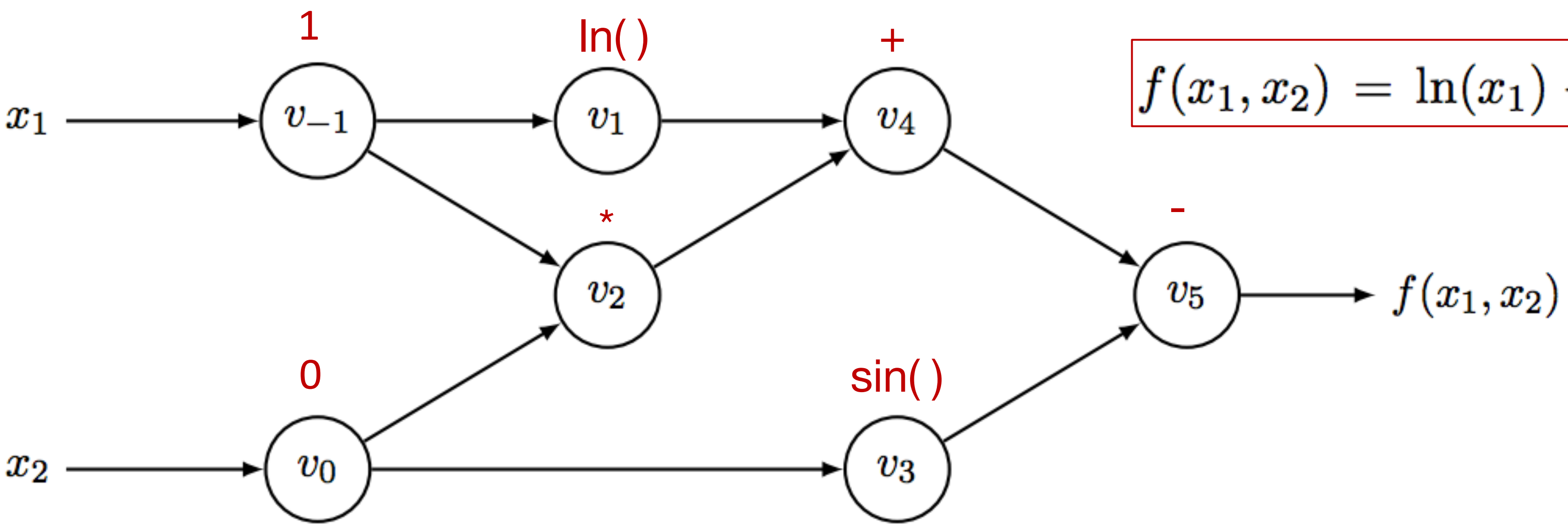

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Forward Tangent (Derivative) Trace		
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$\dot{v}_2$	$= \dot{v}_{-1} \times v_0 + \dot{v}_0 \times v_{-1}$	$= 1 \times 5 + 0 \times 2$
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$\dot{\boldsymbol{y}}$	$= \dot{\boldsymbol{v}}_5$	$= \mathbf{5.5}$

Set to 1 because we want df/dx_1

Forward automatic differentiation

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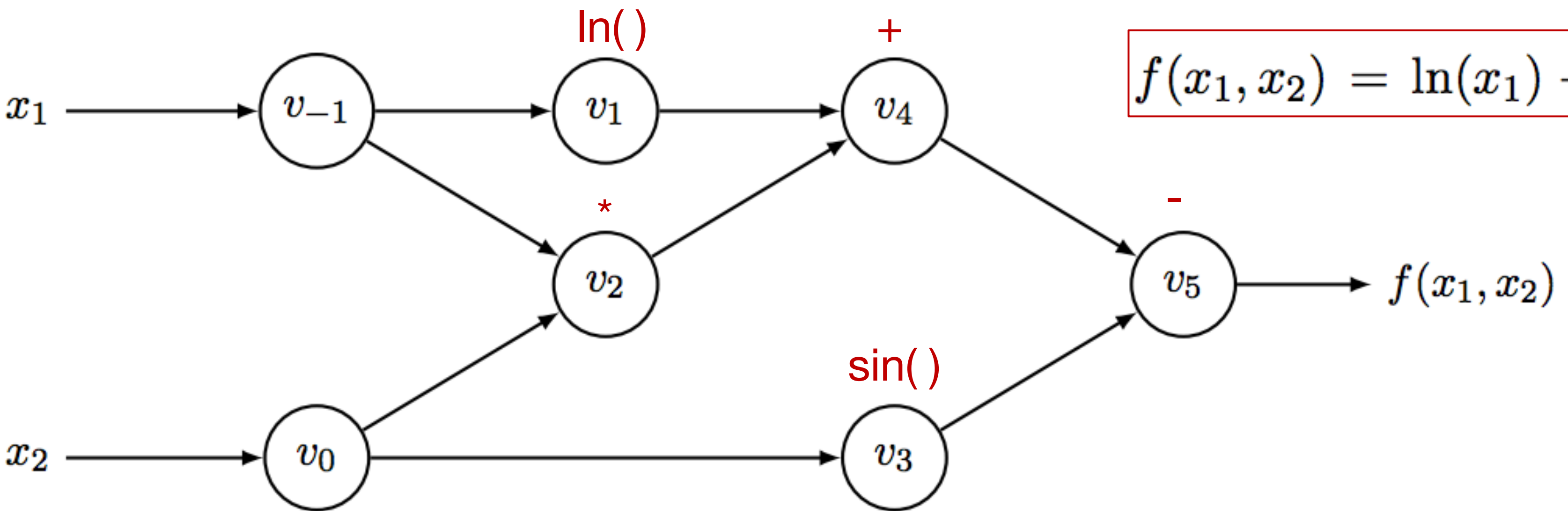

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Compute local derivative for *all inputs and accumulate* with chain rule

Forward automatic differentiation

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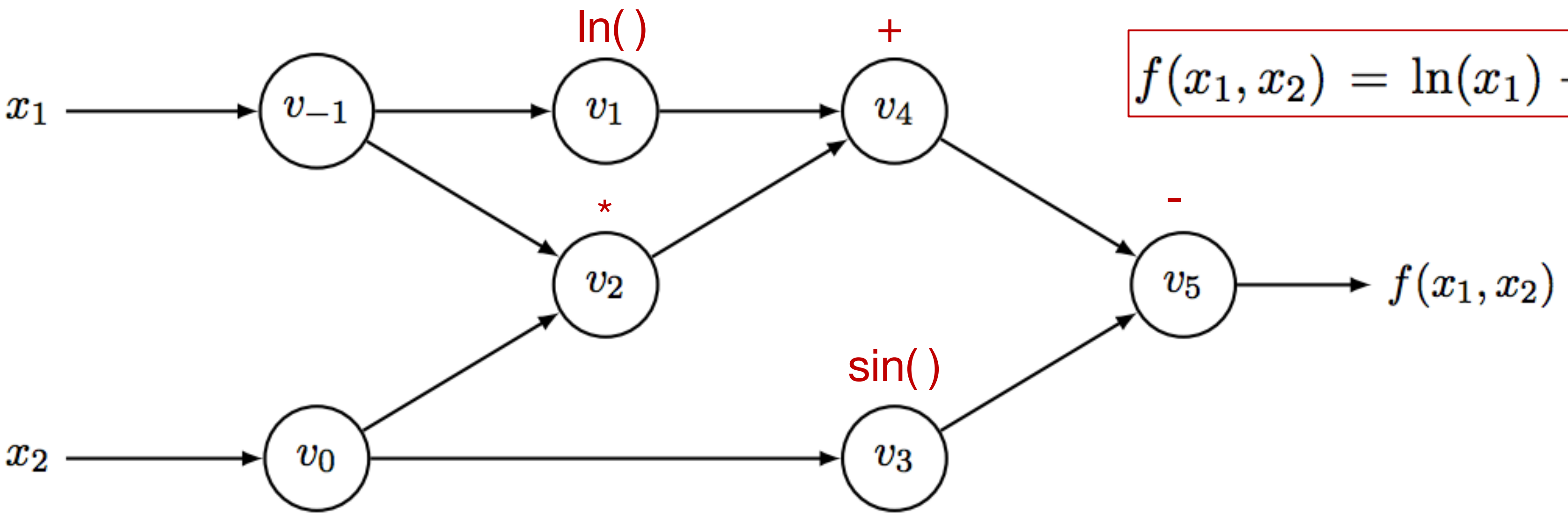

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Leads to final desired df/dx_1

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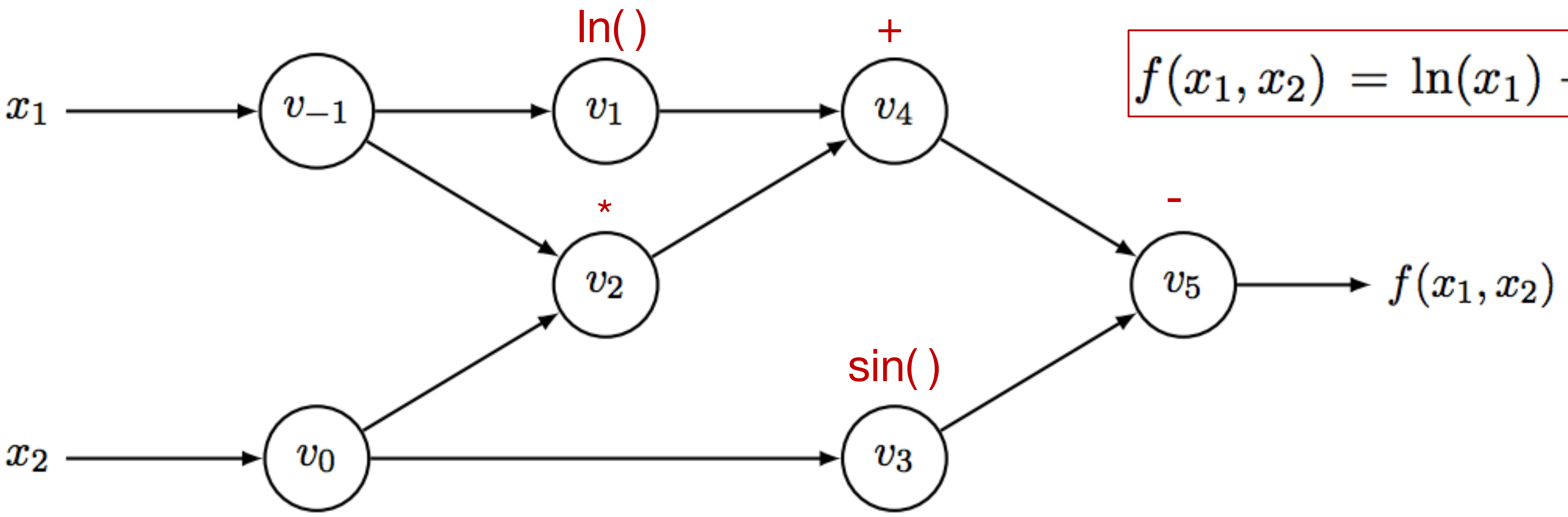

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Problem:

- For N inputs, need to compute this N times, setting x_i to 1 each time…

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Forward automatic differentiation

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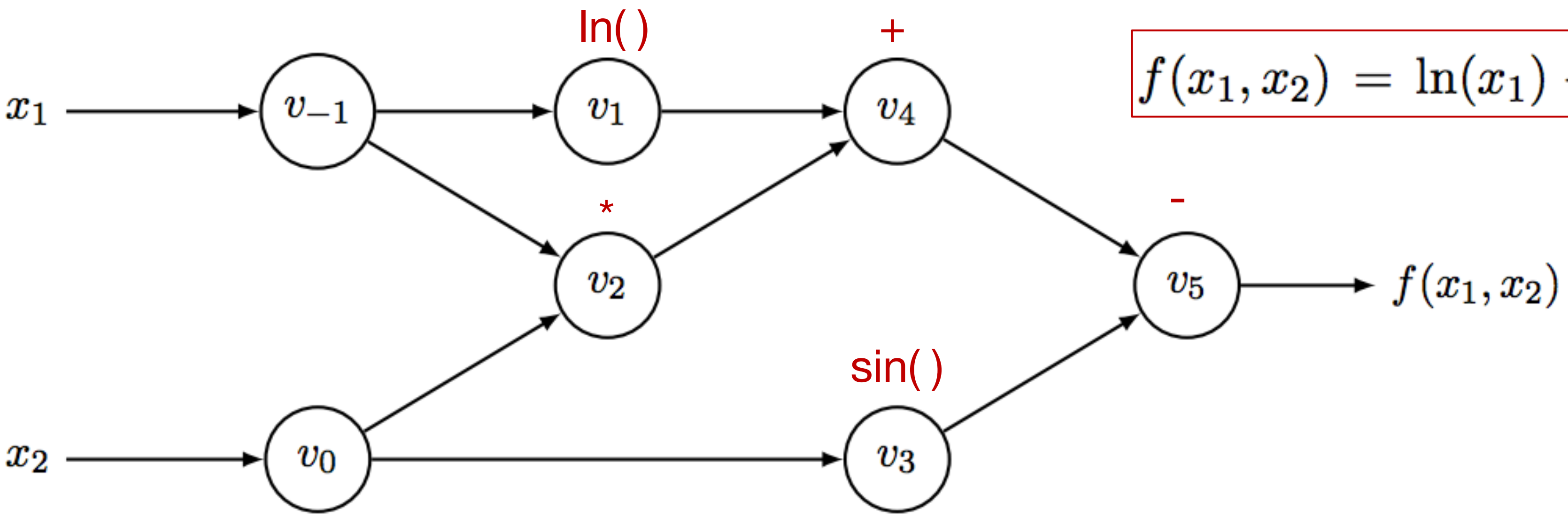

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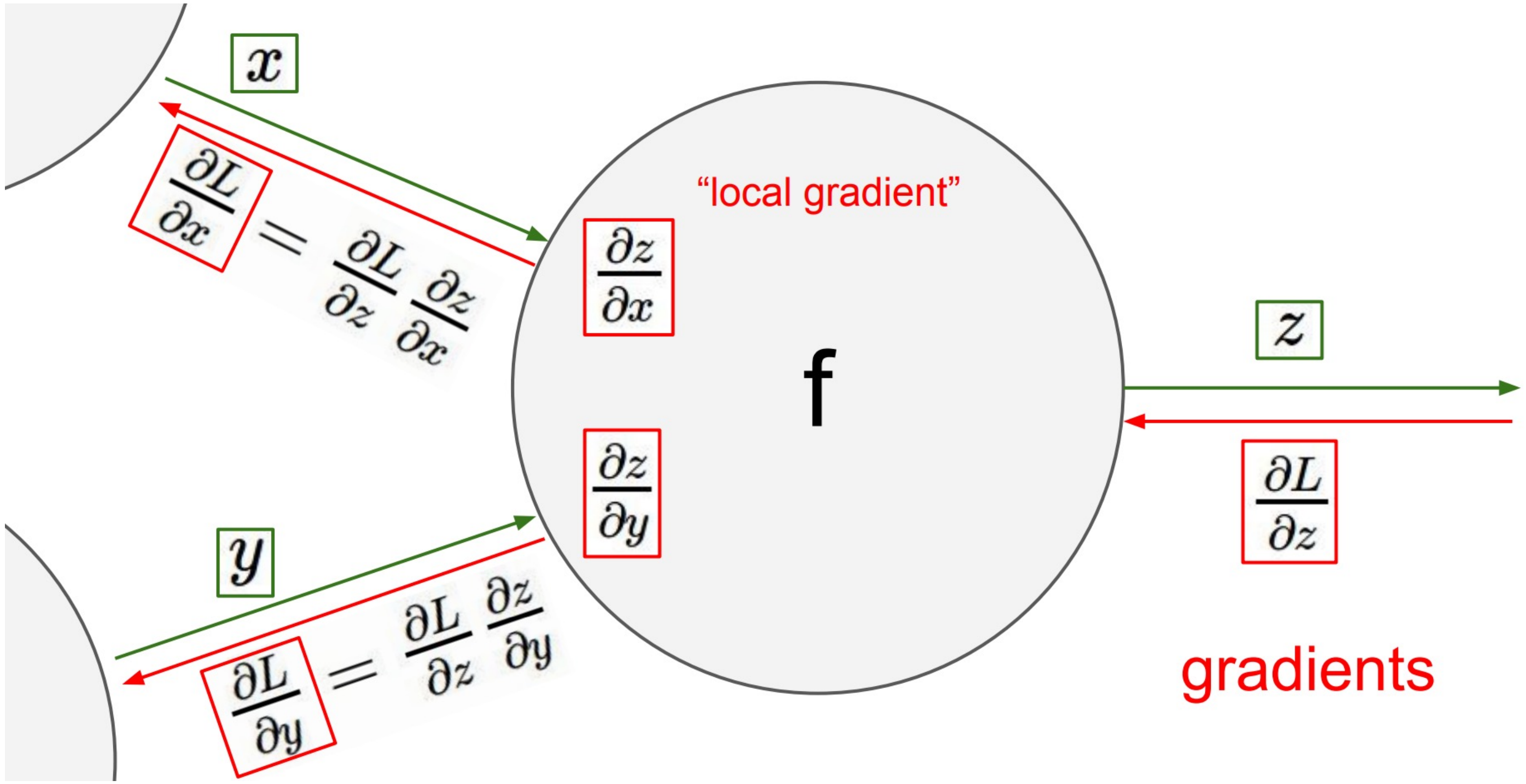
Solution:
Work backwards from end to start with back-propagation

Backpropagation explanation from Stanford CS231N Slides

Treat intermediate nodes like a dummy variable z, for $L(w_1)$

Key Idea: $dL/dw_1 = (dL/dz)(dz/dw_1)$



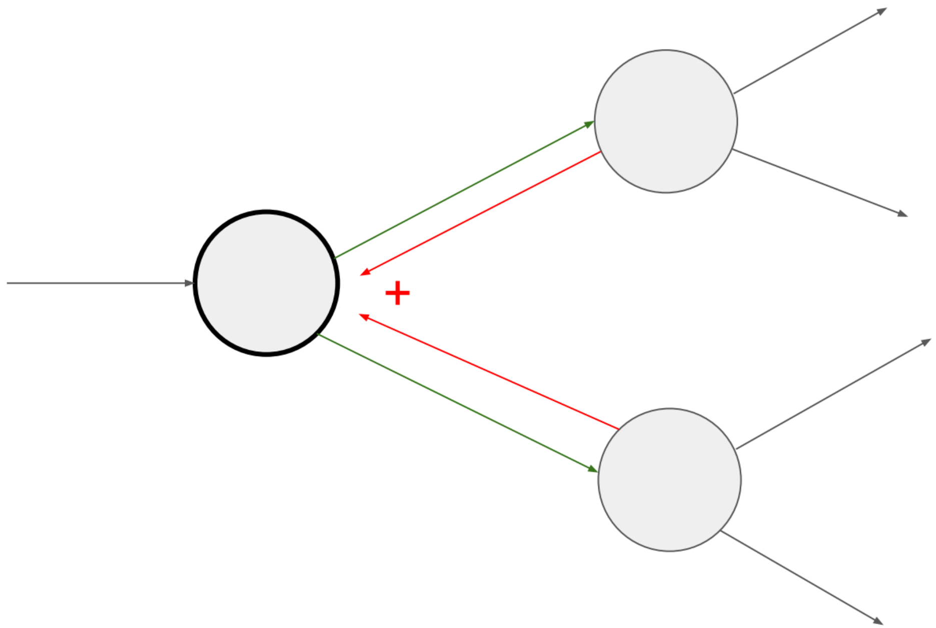
Backpropagation explanation from Stanford CS231N Slides

Go over slides 12-44 here: http://cs231n.stanford.edu/slides/2017/cs231n_2017_lecture4.pdf

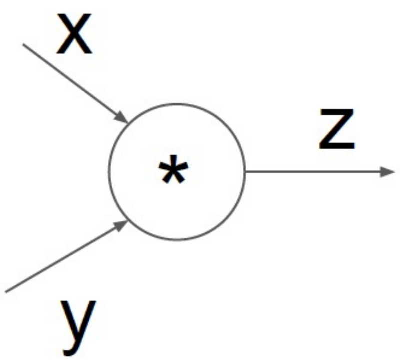
Other useful info here: http://cs231n.github.io/optimization-2/

What happens during backpropagation when multiple gradients come into an operation?

Answer: Gradients add at branches



Modularized implementation: forward / backward API



(x,y,z are scalars)

```
class MultiplyGate(object):
    def forward(x,y):
        z = x*y
        self.x = x # must keep these around!
        self.y = y
        return z
    def backward(dz):
        dx = self.y * dz # [dz/dx * dL/dz]
        dy = self.x * dz # [dz/dy * dL/dz]
        return [dx, dy]
```

Local gradient Upstream gradient variable

How exactly does Tensorflow create a graph structure for back-prop?

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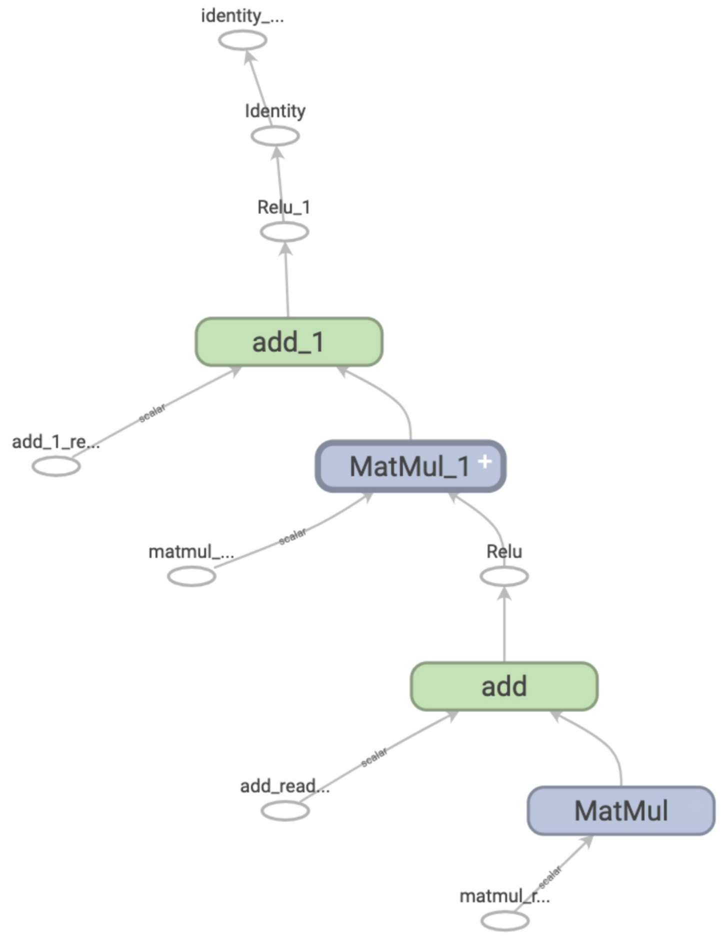
Answer: It is a bit complicated

Here is some helpful information:
https://www.tensorflow.org/guide/intro_to_graphs

Can use
- **tf.function**
- **Tf.graph**

To visualize and understand graph structure



Last thing – matrix and vector derivatives

Here's a review:

$$\mathbf{u} = \mathbf{W}\mathbf{v}$$

$$\frac{d\mathbf{u}}{d\mathbf{v}} =$$

$$\mathbf{u}_3 = W_{3,1}v_1 + W_{3,2}v_2 + \ldots + W_{3,M}v_M$$

$$\frac{\partial u_3}{\partial v_2} = \frac{\partial}{\partial v_2}(W_{3,1}v_1 + W_{3,2}v_2 + \ldots + W_{3,M}v_M) = \frac{\partial}{\partial v_2}W_{3,2}v_2 = W_{3,2}$$

$$\frac{\partial u_i}{\partial v_j} = W_{i,j}$$

$$\frac{d\mathbf{u}}{d\mathbf{v}} = \mathbf{W}$$

- When confused, write out one entry, solve derivative and generalize
- Use dimensionality to help (if **x** has N elements, and **y** has M, then d**y**/d**x** must be NxM
- Take advantage of *The Matrix Cookbook*:
  - https://www.math.uwaterloo.ca/~hwolkowi/matrixcookbook.pdf

Let's go through an example:

$$L = || \mathbf{W_2}\, \mathrm{ReLU}(\mathbf{W_1}\, \mathbf{X}) ||_2^2$$

(2-layer network with MSE where we neglect labels **y** for now)

$$dL/d\mathbf{W}_1 = ? \quad dL/d\mathbf{W}_2 = ?$$

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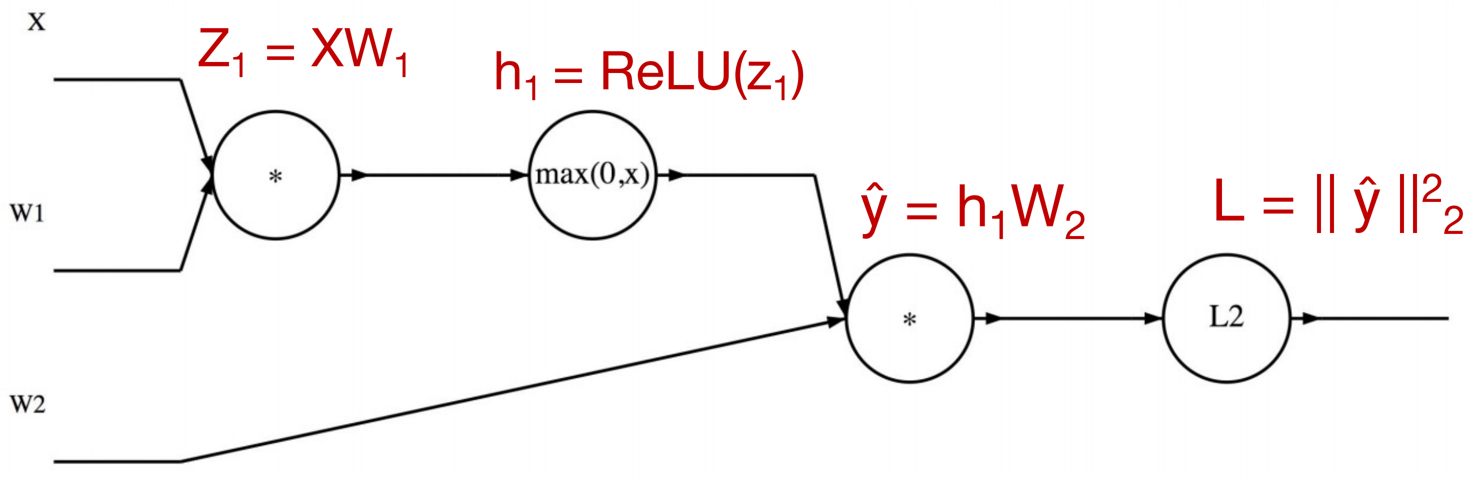
(2-layer network with MSE where we neglect labels **y** for now)

$$dL/d\mathbf{W}_1 = ? \quad dL/d\mathbf{W}_2 = ?$$

$$z_1 = XW_1$$
$$h_1 = \mathrm{ReLU}(z_1)$$
$$\hat{y} = h_1 W_2$$
$$L = ||\hat{y}||_2^2$$



Forward pass: solve for z_1, h_1, $\hat{y}$ and L

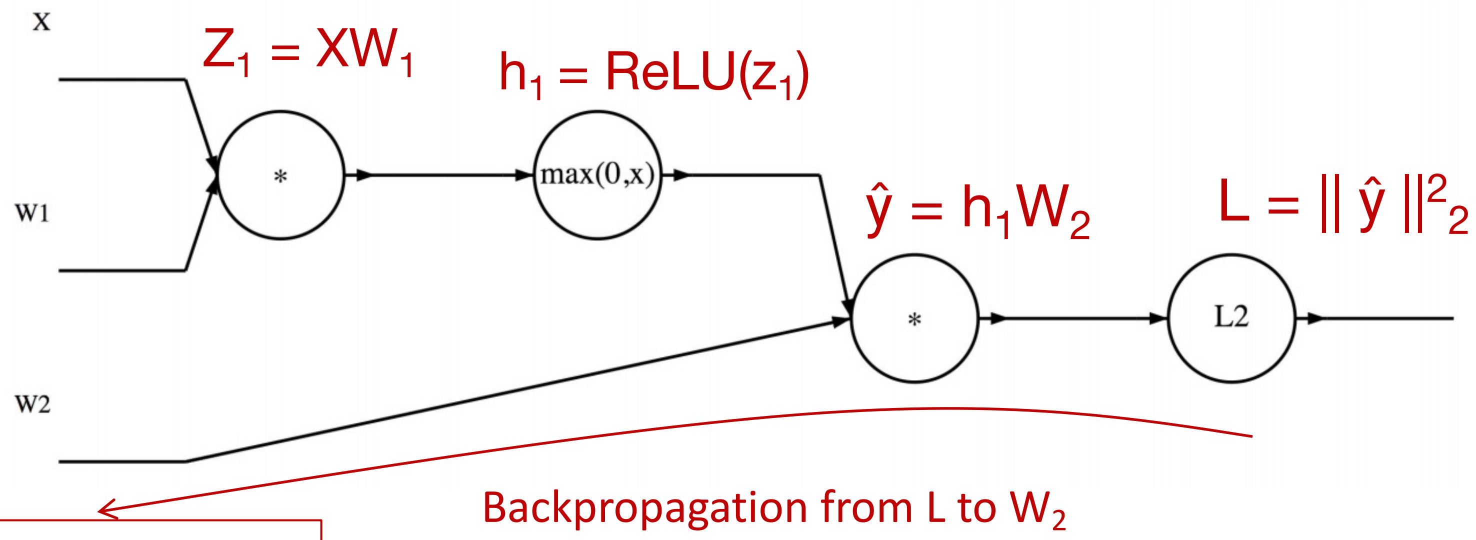
Let's go through an example:

$$L = \| \mathbf{W_2}\, \mathrm{ReLU}(\mathbf{W_1}\, \mathbf{X}) \|_2^2$$

(2-layer network with MSE where we neglect labels **y** for now)

$dL/d\mathbf{W}_1 = ?$ $\boxed{dL/d\mathbf{W}_2 = ?}$

$$z_1 = XW_1$$
$$h_1 = \mathrm{ReLU}(z_1)$$
$$\hat{y} = h_1 W_2$$
$$L = ||\hat{y}||_2^2$$



$$\boxed{\frac{\partial L}{\partial W_2} = \frac{\partial \hat{y}}{\partial W_2} \frac{\partial L}{\partial \hat{y}}}$$

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Let's go through an example:

$$L = \|\, \mathbf{W_2}\ \mathrm{ReLU}(\mathbf{W_1}\, \mathbf{X})\, \|_2^2$$

(2-layer network with MSE where we neglect labels **y** for now)

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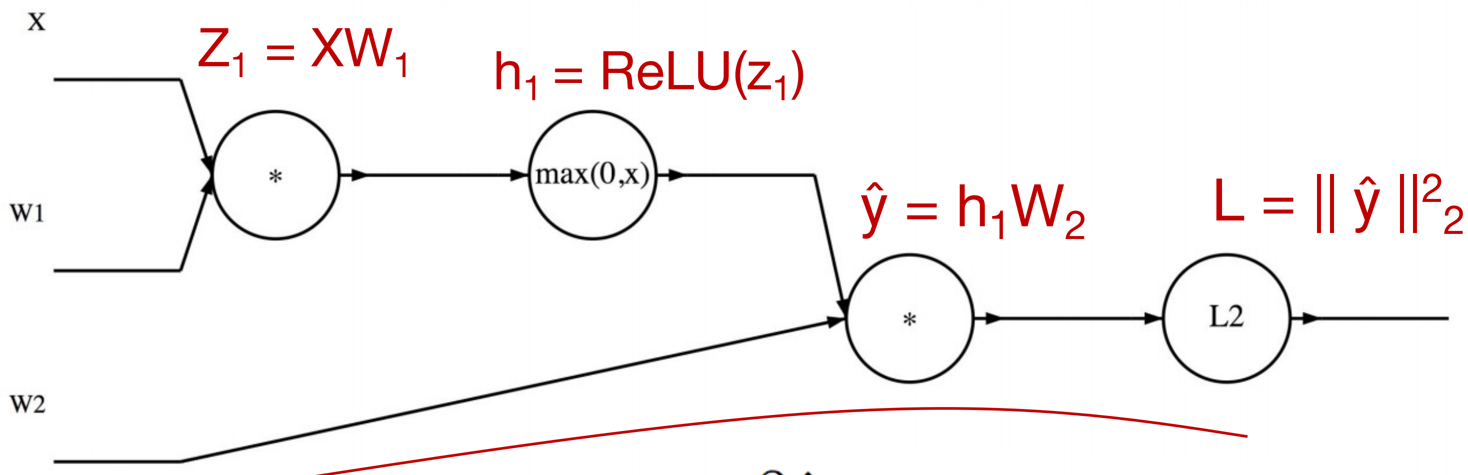

$$\frac{\partial \hat{y}}{\partial W_2} = h_1^T \qquad \frac{\partial L}{\partial \hat{y}} = 2\hat{y}$$

$$\boxed{\frac{\partial L}{\partial W_2} = \frac{\partial \hat{y}}{\partial W_2} \frac{\partial L}{\partial \hat{y}}}$$

Gradients for scalar *L* will have same shape as denominator

Let's go through an example:

$$L = \|\, \mathbf{W_2}\, \mathrm{ReLU}(\mathbf{W_1}\, \mathbf{X})\, \|_2^2$$

(2-layer network with MSE where we neglect labels **y** for now)

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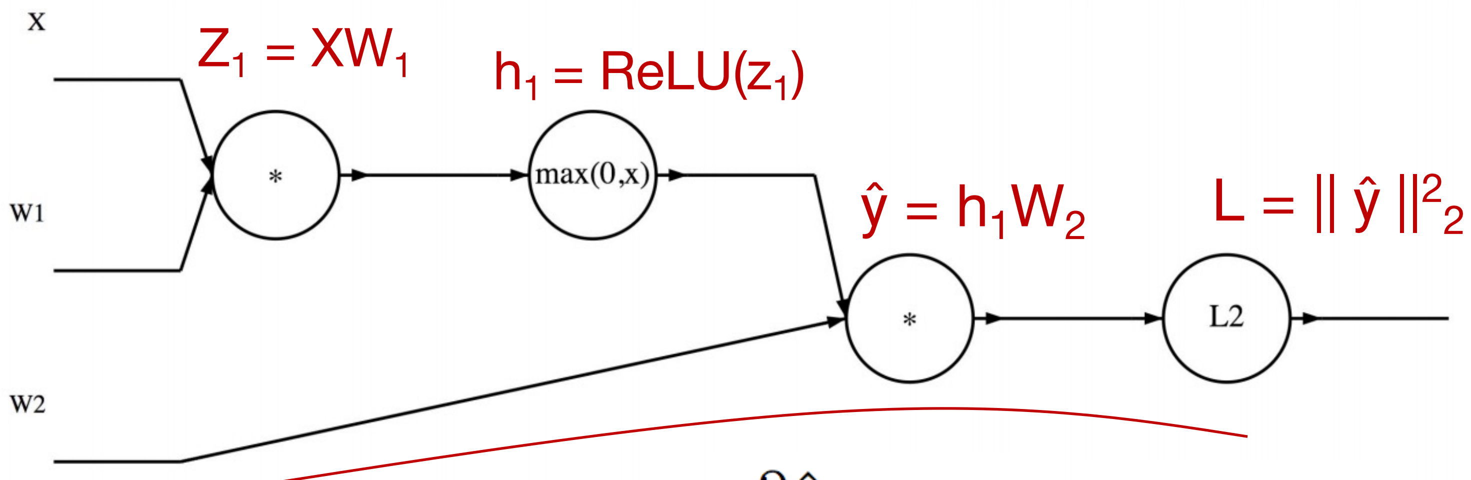
$$L = ||\hat{y}||_2^2$$



$$\frac{\partial \hat{y}}{\partial W_2} = h_1^T \qquad \frac{\partial L}{\partial \hat{y}} = 2\hat{y}$$

$$\boxed{\frac{\partial L}{\partial W_2} = \frac{\partial \hat{y}}{\partial W_2}\frac{\partial L}{\partial \hat{y}} = 2h_1^T\hat{y}}$$

Let's go through an example:

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$$L = || \mathbf{W_2}\, \mathrm{ReLU}(\mathbf{W_1}\, \mathbf{X})\, ||_2^2$$

(2-layer network with MSE where we neglect labels **y** for now)

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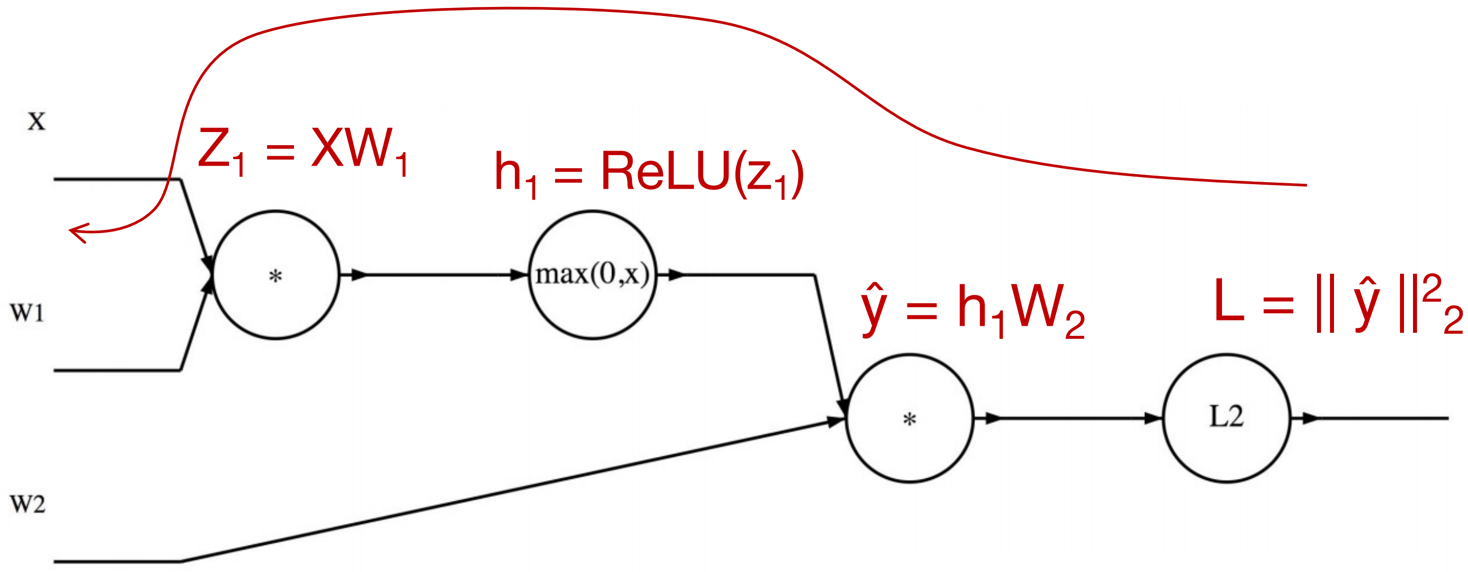
$$\hat{y} = h_1 W_2$$
$$L = ||\hat{y}||_2^2$$

$\boxed{dL/d\mathbf{W}_1 = ?}$ $dL/d\mathbf{W}_2 = ?$



$$\frac{\partial \hat{y}}{dh_1} = W_2^{T} \qquad \frac{\partial L}{\partial \hat{y}} = 2\hat{y}$$

Let's go through an example:

$$L = ||\ \mathbf{W_2}\ \mathrm{ReLU}(\mathbf{W_1}\ \mathbf{X})\ ||_2^2$$

(2-layer network with MSE where we neglect labels **y** for now)

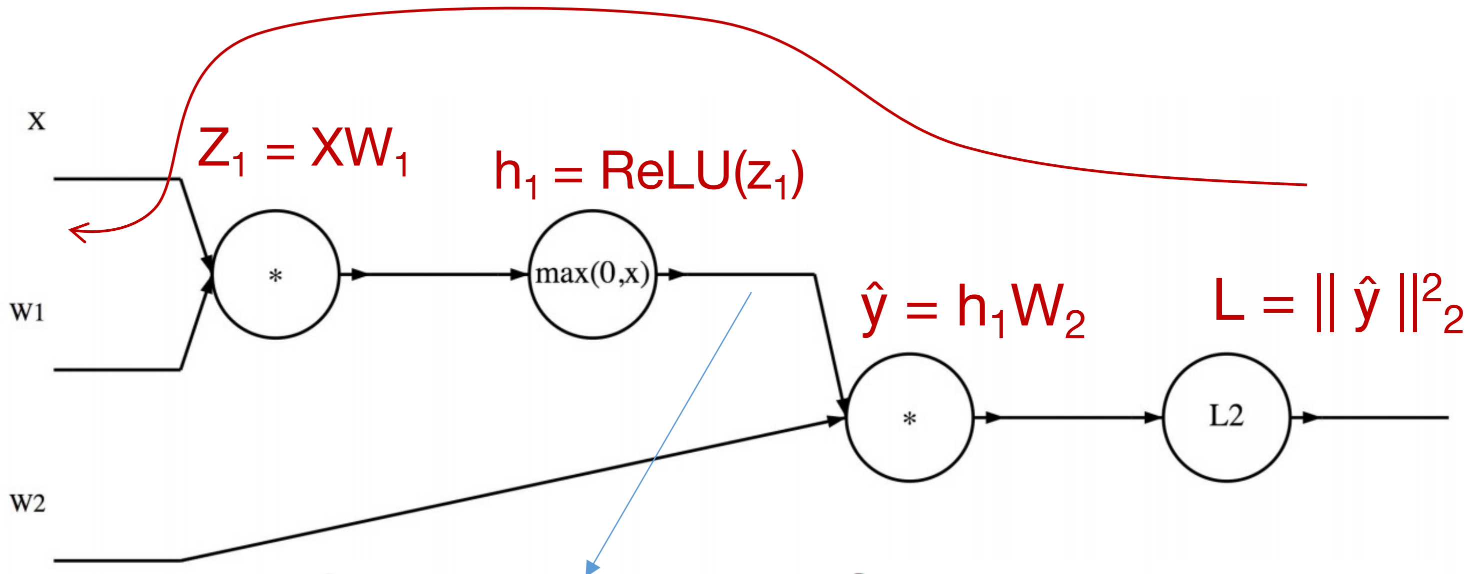
$$\boxed{dL/d\mathbf{W}_1 = ?} \quad dL/d\mathbf{W}_2 = ?$$

$$z_1 = XW_1$$

$$h_1 = \mathrm{ReLU}(z_1)$$

$$\hat{y} = h_1 W_2$$

$$L = ||\hat{y}||_2^2$$



$$\frac{\partial L}{\partial h_1} = \frac{\partial L}{\partial \hat{y}} \frac{\partial \hat{y}}{dh_1} = 2\hat{y}W_2^T \leftarrow \frac{\partial \hat{y}}{dh_1} = W_2^T \quad \frac{\partial L}{\partial \hat{y}} = 2\hat{y}$$

Let's go through an example:

$$L = \| \mathbf{W_2}\, \mathrm{ReLU}(\mathbf{W_1}\, \mathbf{X}) \|_2^2$$

(2-layer network with MSE where we neglect labels **y** for now)

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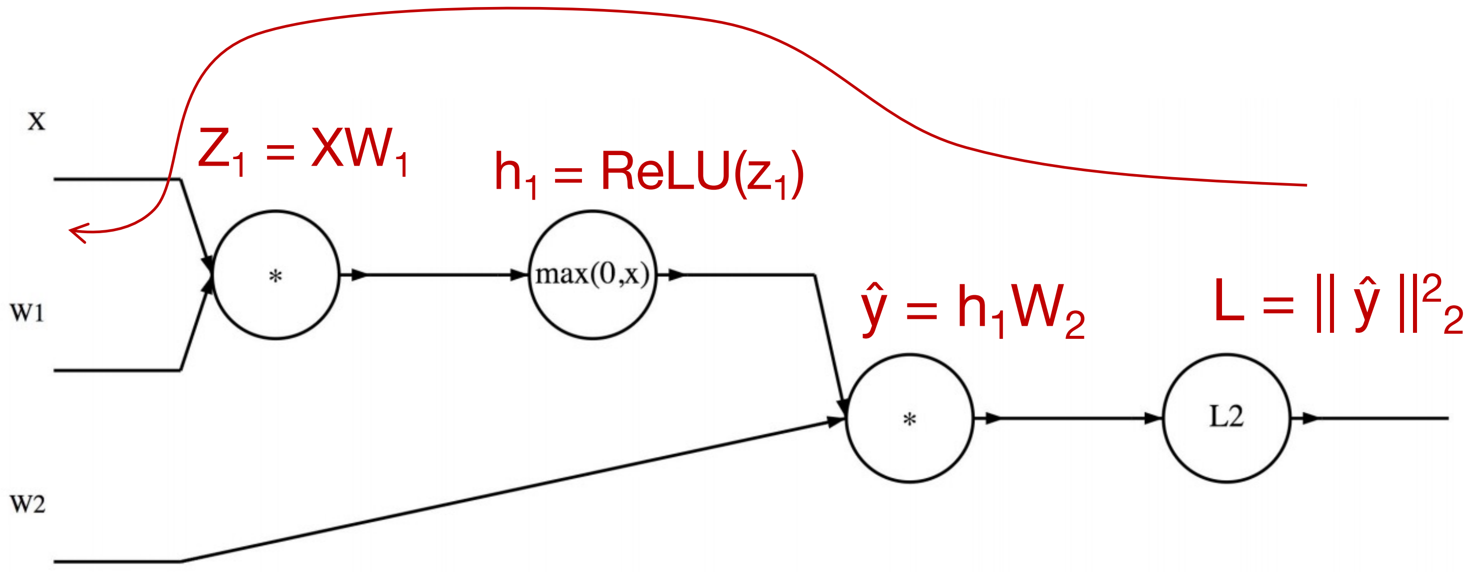
$$L = ||\hat{y}||_2^2$$

$\boxed{dL/d\mathbf{W}_1 = ?}$ $dL/d\mathbf{W}_2 = ?$



$$\boxed{\frac{\partial L}{\partial h_1} = 2\hat{y}W_2^T}$$

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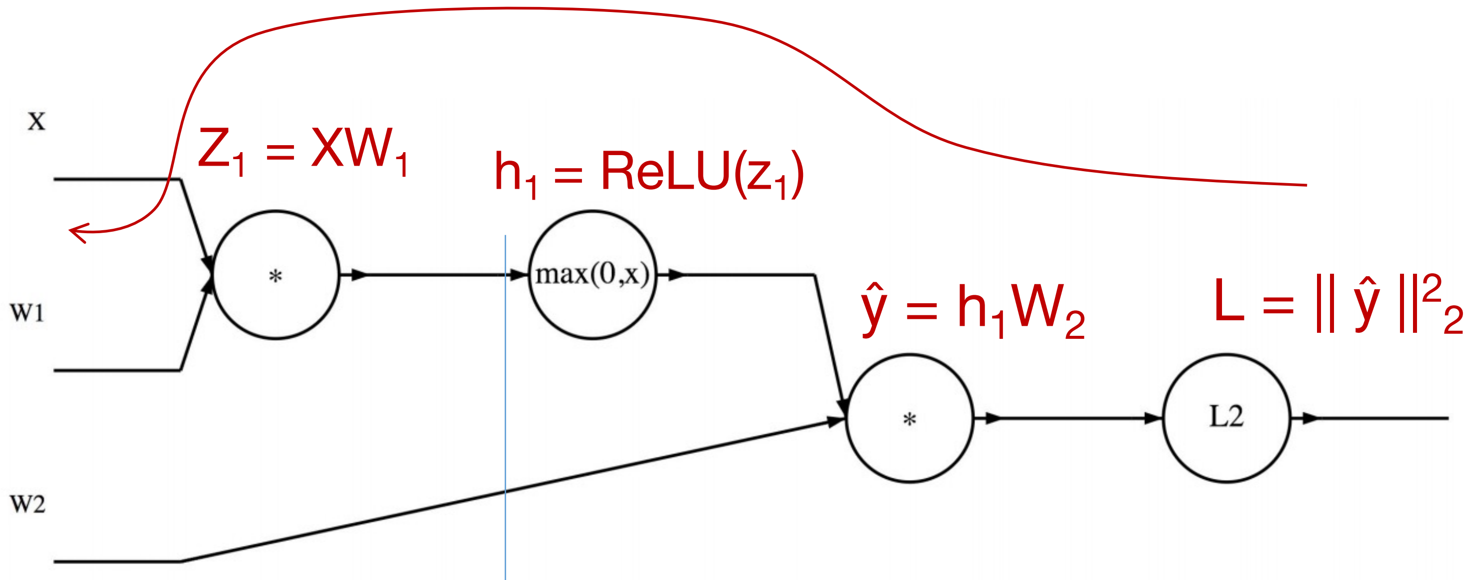
Let’s go through an example:

$$z_1 = XW_1$$
$$h_1 = \mathrm{ReLU}(z_1)$$
$$\hat{y} = h_1 W_2$$
$$L = ||\hat{y}||_2^2$$

$L = || \mathbf{W_2}\ \mathrm{ReLU}(\mathbf{W_1}\ \mathbf{X})\ ||_2^2$

(2-layer network with MSE where we neglect labels **y** for now)

$\boxed{dL/d\mathbf{W}_1 = ?}$ $\quad dL/d\mathbf{W}_2 = ?$



$$\frac{dL}{\partial z_1} = \frac{\partial L}{\partial h_1} \frac{dh_1}{dz}$$

$$\boxed{\frac{\partial L}{\partial h_1} = 2\hat{y}W_2^T}$$

Let's go through an example:

$$L = \| \mathbf{W_2}\, \mathrm{ReLU}(\mathbf{W_1}\, \mathbf{X}) \|_2^2$$

(2-layer network with MSE where we neglect labels **y** for now)

$$z_1 = XW_1$$
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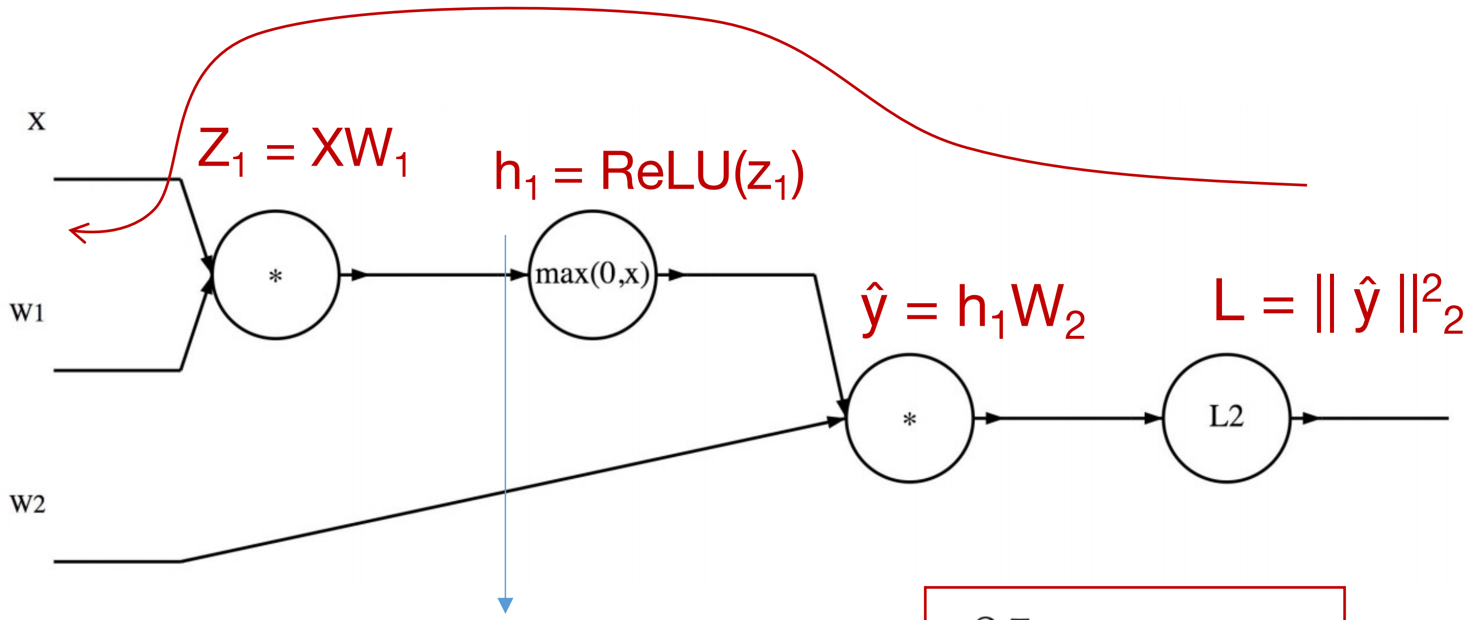
$\boxed{dL/d\mathbf{W}_1 = ?}$ $dL/d\mathbf{W}_2 = ?$



$$\frac{dL}{\partial z_1} = \frac{\partial L}{\partial h_1} \circ I[h_1 > 0]$$

$$\boxed{\frac{\partial L}{\partial h_1} = 2\hat{y}W_2^T}$$

Let's go through an example:

$L = \| \mathbf{W_2}\, \mathrm{ReLU}(\mathbf{W_1} \mathbf{X}) \|_2^2$

(2-layer network with MSE where we neglect labels **y** for now)

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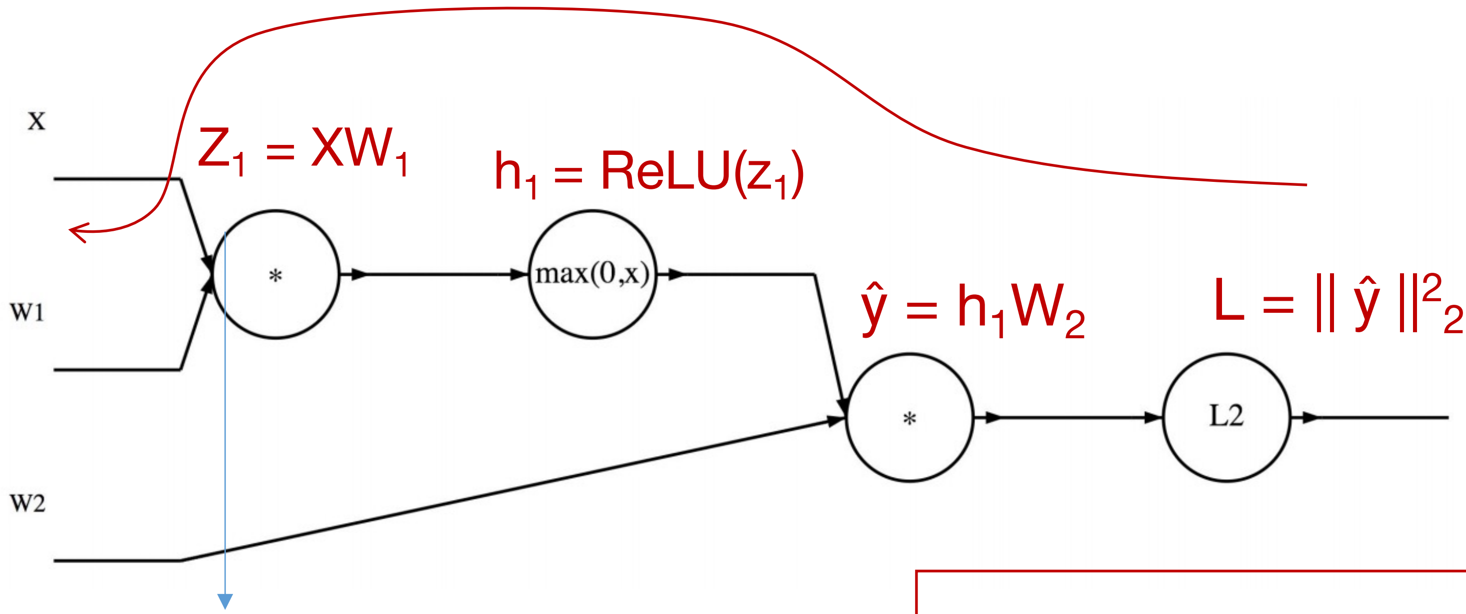
$\boxed{dL/d\mathbf{W}_1 = ?}$ $dL/d\mathbf{W}_2 = ?$



$$\frac{dL}{dW_1} = \frac{dz_1}{dW_1}\frac{dL}{dz_1}$$

$$\boxed{\frac{dL}{\partial z_1} = 2\hat{y}W_2^{T} \circ I[h_1 > 0]}$$

Let's go through an example:

$$L = \| \mathbf{W_2}\, \mathrm{ReLU}(\mathbf{W_1}\, \mathbf{X}) \|_2^2$$

(2-layer network with MSE where we neglect labels **y** for now)

$$z_1 = XW_1$$
$$h_1 = \mathrm{ReLU}(z_1)$$
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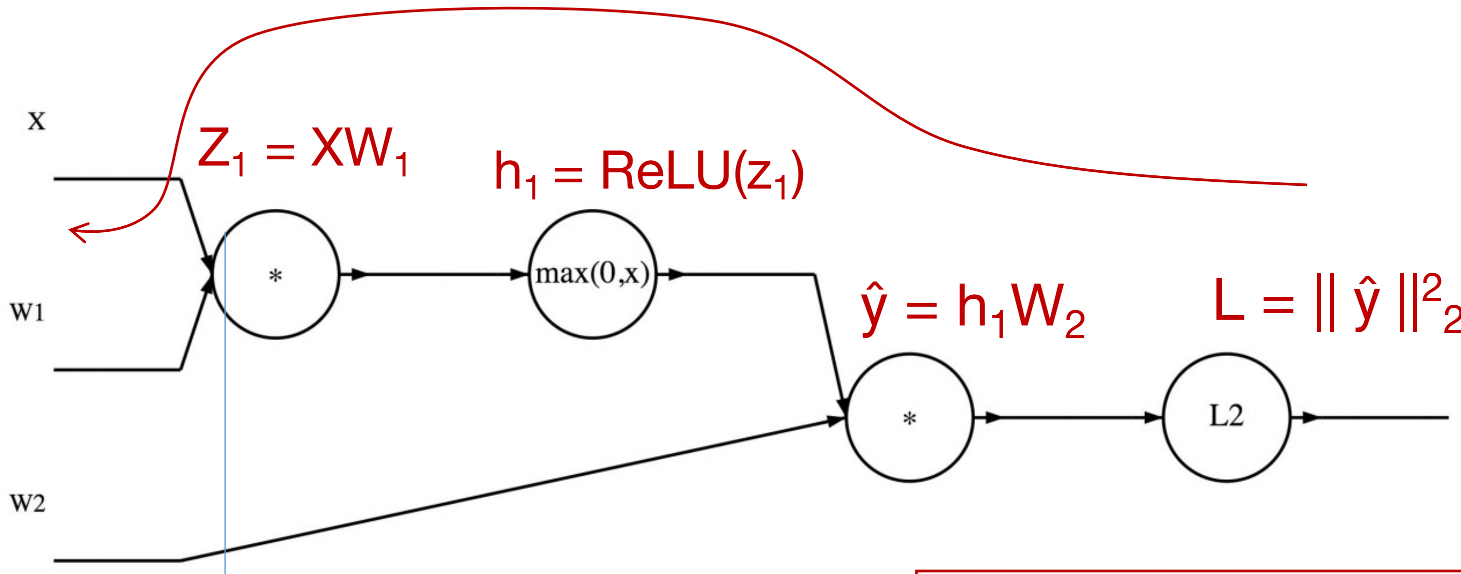
$\boxed{dL/d\mathbf{W}_1 = ?}$ $dL/d\mathbf{W}_2 = ?$



$$\frac{dL}{dW_1} = \frac{dz_1}{dW_1}\frac{dL}{dz_1}$$
$$= x^\top$$

$$\boxed{\frac{dL}{\partial z_1} = 2\hat{y}{W_2}^\top \circ I[h_1 > 0]}$$

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Let’s go through an example:

$L = ||\ \mathbf{W_2}\ \mathrm{ReLU}(\mathbf{W_1}\ \mathbf{X})\ ||_2^{\,2}$

(2-layer network with MSE where we neglect labels **y** for now)

$\boxed{dL/d\mathbf{W}_1 = ?}$ $dL/d\mathbf{W}_2 = ?$

$$z_1 = XW_1$$
$$h_1 = \mathrm{ReLU}(z_1)$$
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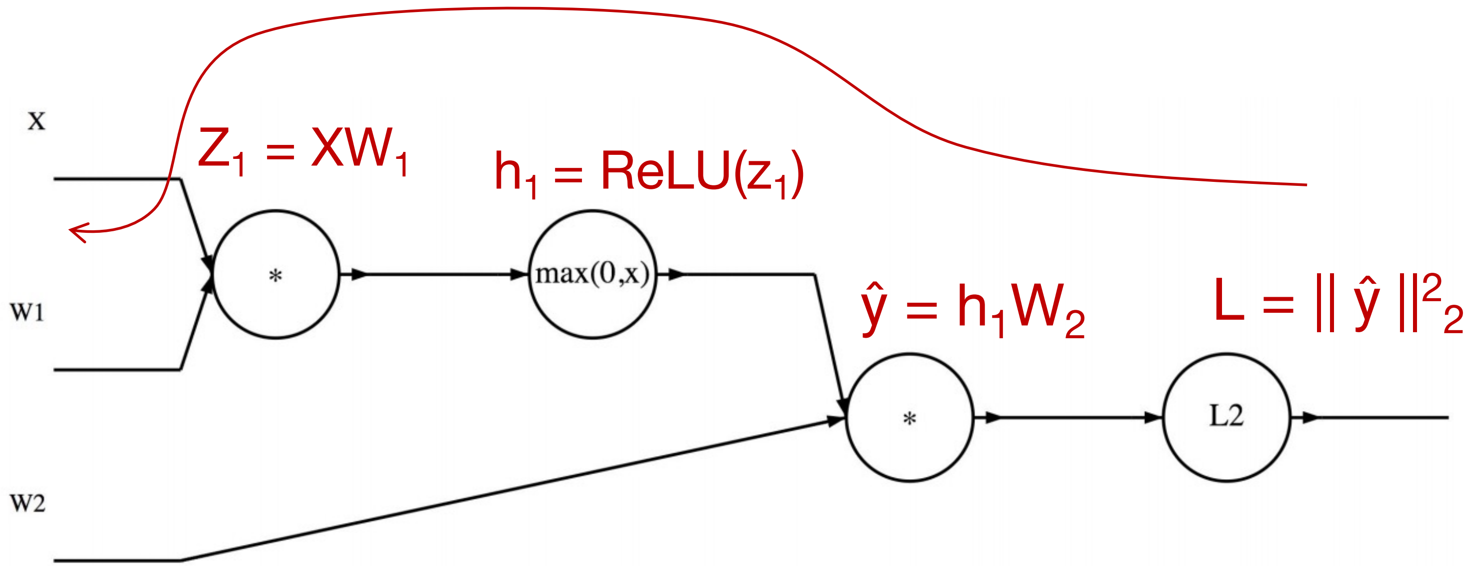

$$\boxed{\frac{dL}{dW_1} = 2x^T \hat{y} W_2^T \circ I[h_1 > 0]}$$

Let's go through an example:

$$L = || \mathbf{W_2} \, \mathrm{ReLU}(\mathbf{W_1} \, \mathbf{X}) ||_2^2$$

$$z_1 = XW_1$$
$$h_1 = \mathrm{ReLU}(z_1)$$
$$\hat{y} = h_1 W_2$$
$$L = ||\hat{y}||_2^2$$

$$\boxed{dL/d\mathbf{W}_1 = ?}$$

$$\boxed{\frac{dL}{dW_1} = 2x^T \hat{y} W_2^T \circ I[h_1 > 0]}$$

```
import numpy as np

# forward prop
z_1 = np.dot(X, W_1)
h_1 = np.maximum(z_1, 0)
y_hat = np.dot(h_1, W_2)
L = np.sum(y_hat**2)

# backward prop
dy_hat = 2.0*y_hat

dW2 = h_1.T.dot(dy_hat)

dh1 = dy_hat.dot(W_2.T)

dz1 = dh1.copy()
dz1[z1 < 0] = 0

dW1 = X.T.dot(dz1)
```

Summary

- Tensorflow: define variables, series of operations & a cost function
- When you hit enter, Tensorflow effectively forms two graphs
  - Forward graph to evaluate function at each node
  - **Backprop:** Backwards graph that includes *local* derivatives of each operation as symbolic functions, as well as connections
- Tensorflow will go through the forward graph & save numerical results, then the backwards graph, to update weights via local operations, to minimize cost function
- Uses more impressive operations to do this with vectors and matrices efficiently