

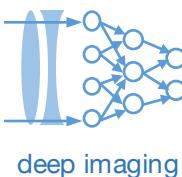
Lecture 10: Backpropagation

Machine Learning and Imaging

BME 590L
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

Architecture choices

CNN Architecture

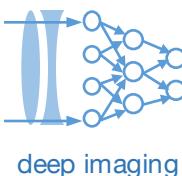
- CONV size, stride, pad, depth
- ReLU & other nonlinearities
- POOL methods
- # of layers, dimensions per layer
- Fully connected layers

Loss function & optimization

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

Optimization choices

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



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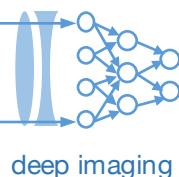
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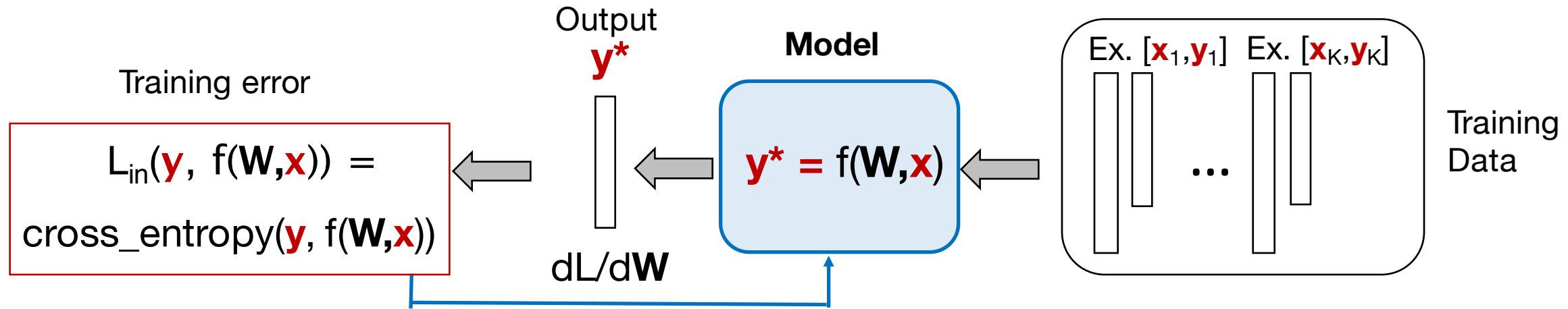
Optimization choices

How does the optimizer actually work???

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



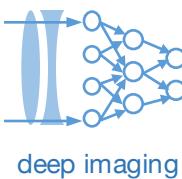
Our very basic convolutional neural network



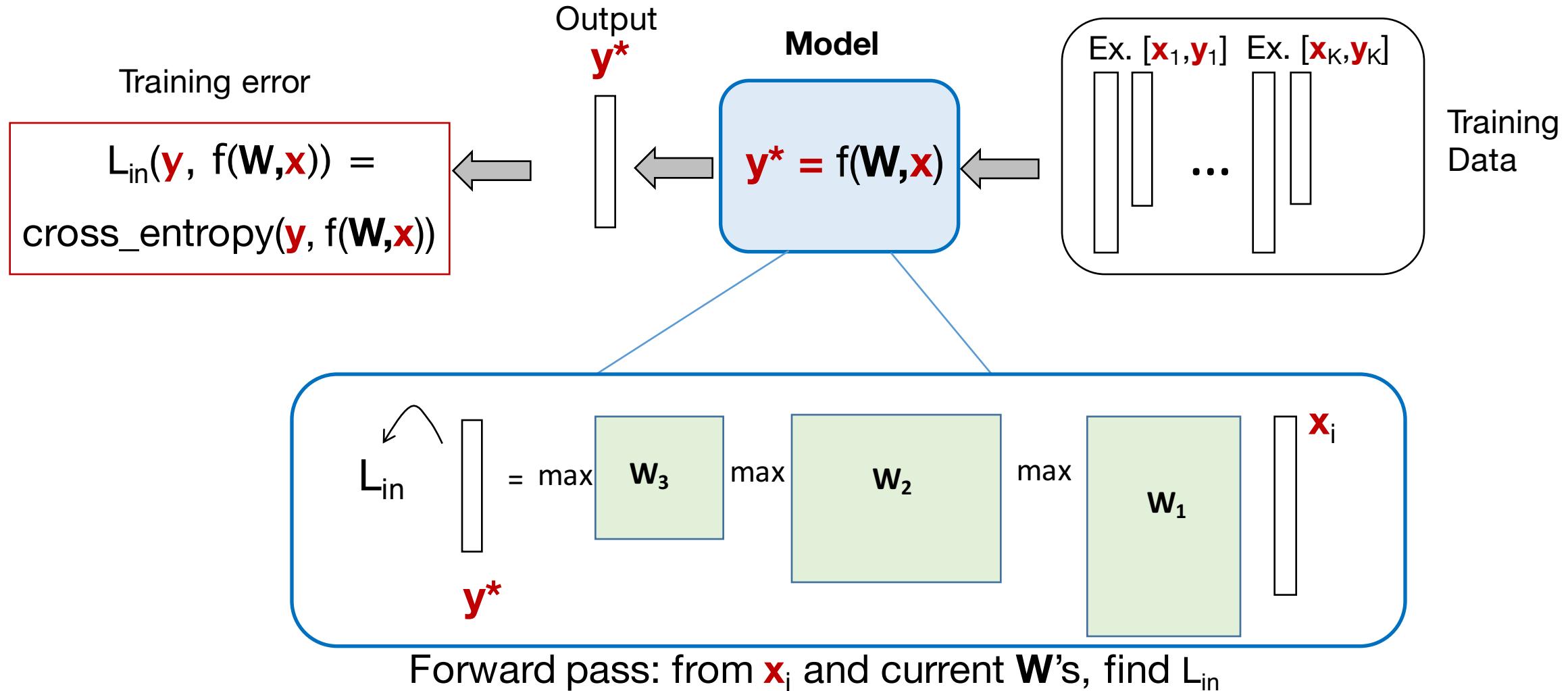
$$L(w) = \frac{1}{N} \sum_{i=1}^N \ln(1 + e^{-y_i \max(0, \mathbf{W}_3 \max(0, \mathbf{W}_2 \max(0, \mathbf{W}_1 x_i))))})$$

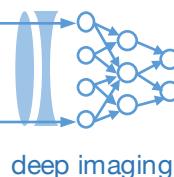
\mathbf{W}_1 and \mathbf{W}_2 are banded Toeplitz matrices, \mathbf{W}_3 is a full matrix

3-layer network

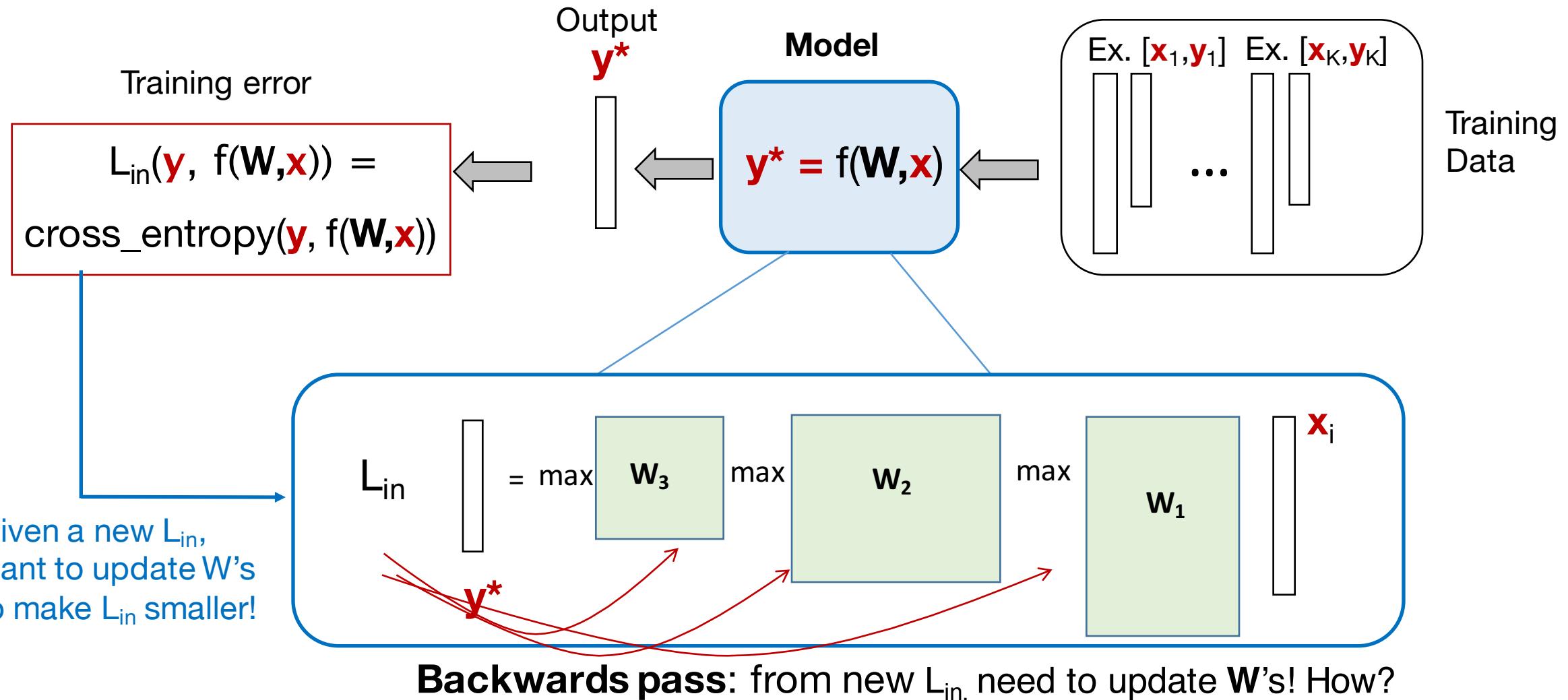


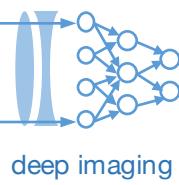
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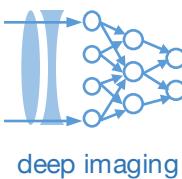
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Review: how can we determine the optimal W?

- 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 \mathbf{W} 's

while loss function is still decreasing:

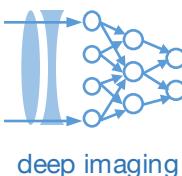
 Compute loss function $L(\mathbf{W}, \mathbf{x}_i, \mathbf{y}_i)$

 Update \mathbf{W} to make L smaller:

$dL/d\mathbf{W} = \text{evaluate_gradient}(\mathbf{W}, \mathbf{x}_i, \mathbf{y}_i, L)$

$\mathbf{W} = \mathbf{W} - \text{step_size} * dL/d\mathbf{W}$

```
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)
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```



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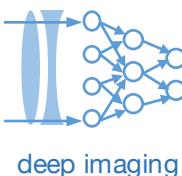
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Options to evaluate $dL/d\mathbf{W}$:

1. Numerical gradient
2. Analytic gradient
3. Automatic differentiation

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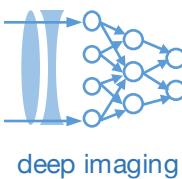
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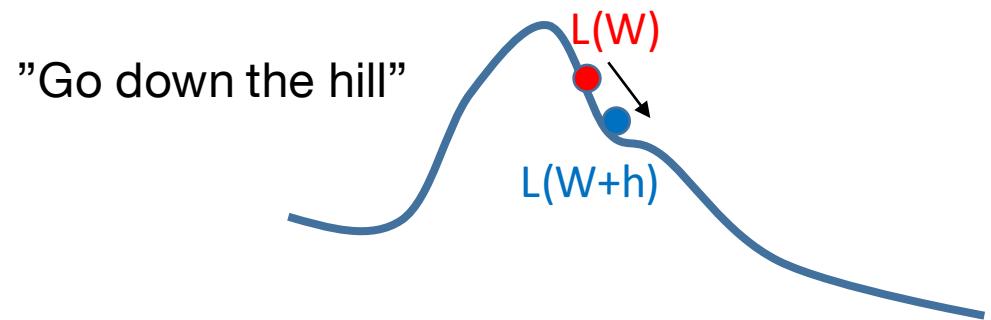
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```

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



1. Numerical gradient, a simple example



With a matrix, compute this for each entry:

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

Example:

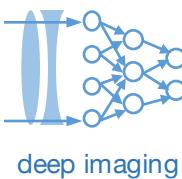
$$W = [1, 2, 3, 4]$$
$$L(W, x, y) = 12.79$$

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

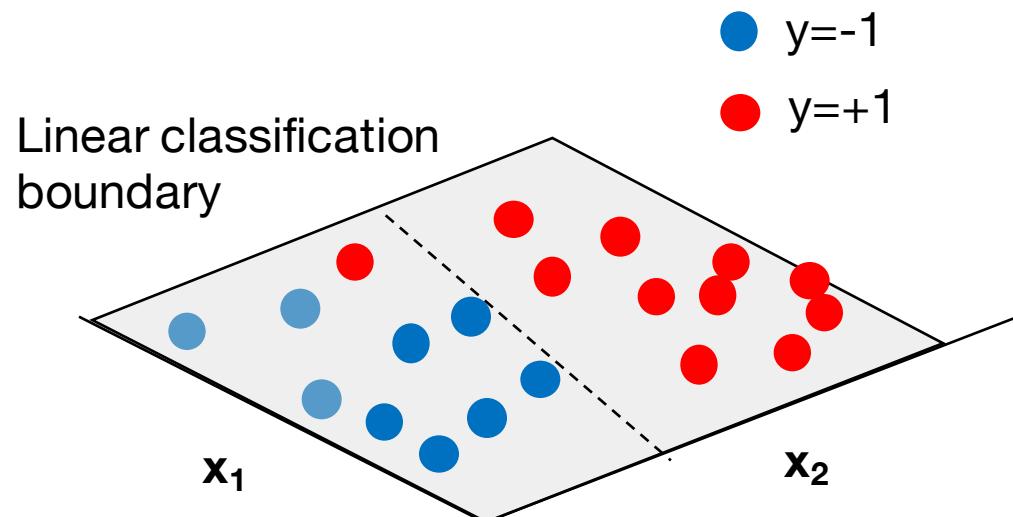
$$\frac{dL(W_1)}{dW_1} = \frac{12.8 - 12.79}{.001}$$
$$\frac{dL(W_1)}{dW_1} = 10$$

Pros: Simple! Easy to code up!

Cons: Slow...really slow. And approximate



2. Analytic gradient, a simple example



● $y=-1$
● $y=+1$

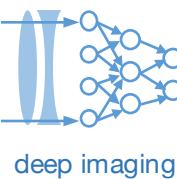
$$L = \frac{1}{N} \sum_{i=1}^N (w^T x_i - y_i)^2$$

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

Evaluate and use to update W

Pros: Fast and exact

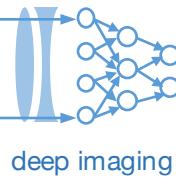
Cons: Error prone, especially with deep networks...



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>



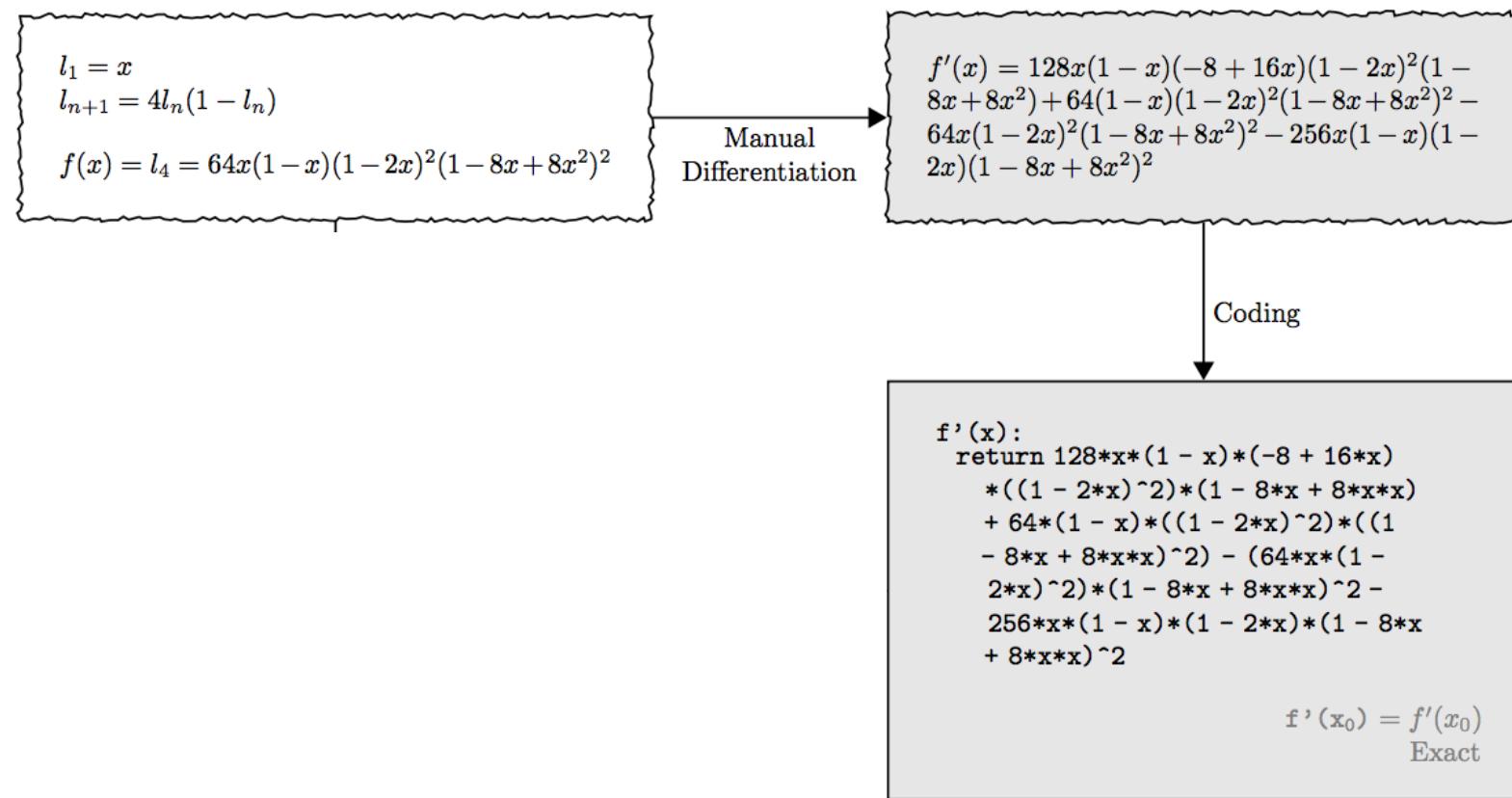
3. Automatic differentiation – what is it?

- 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*

A. Baydin et al., Automatic Differentiation in Machine Learning: a Survey

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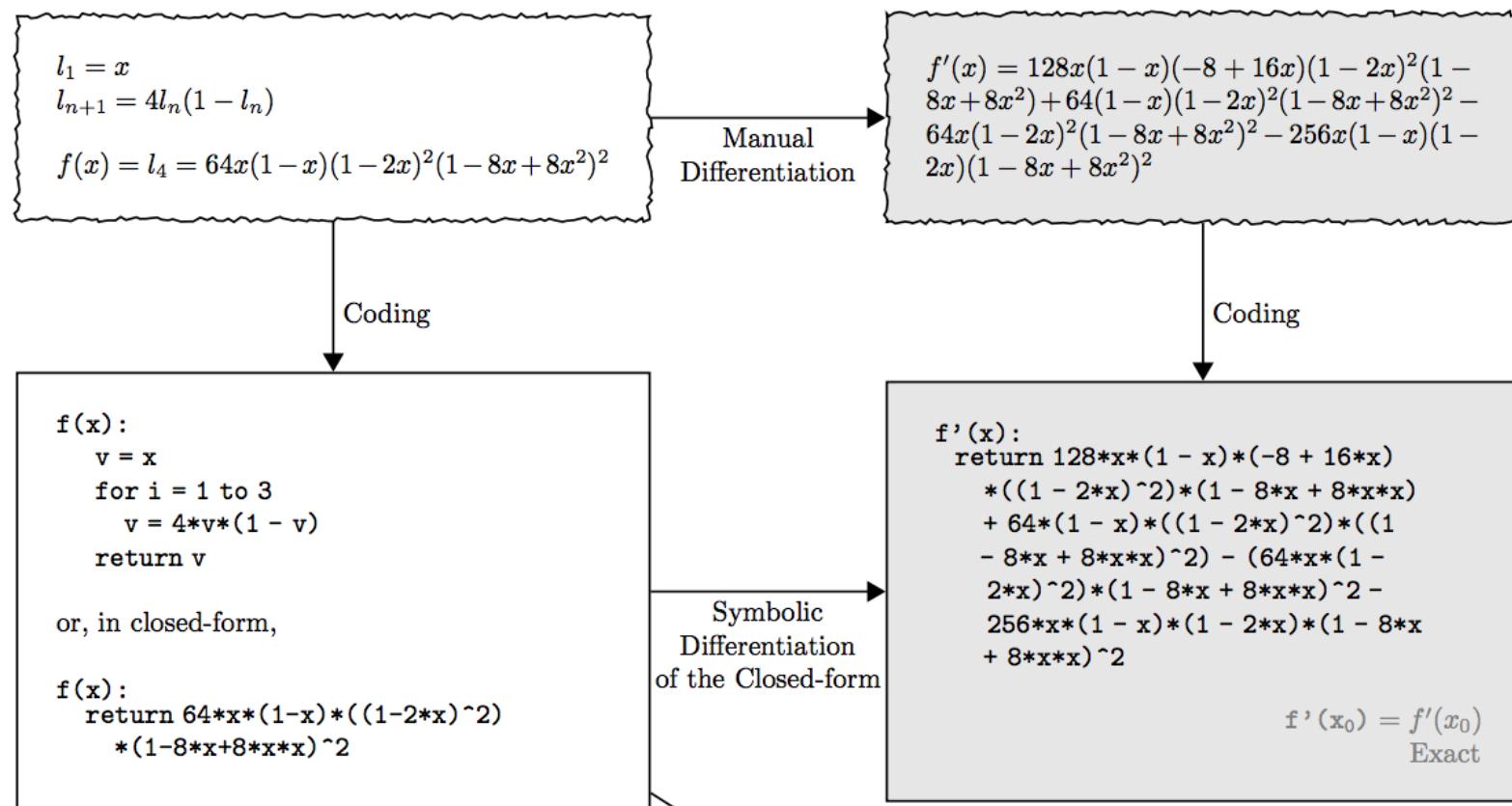
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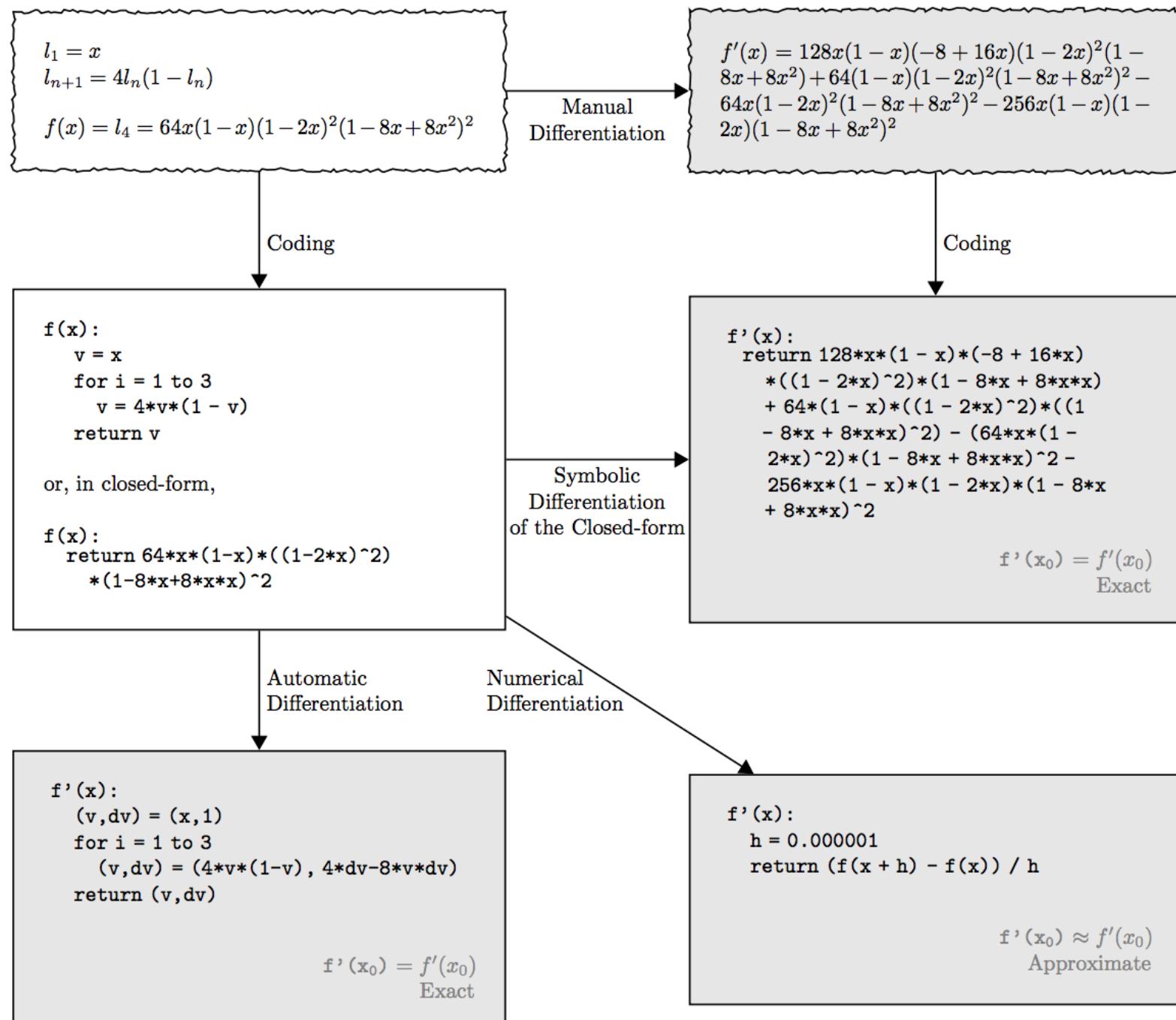
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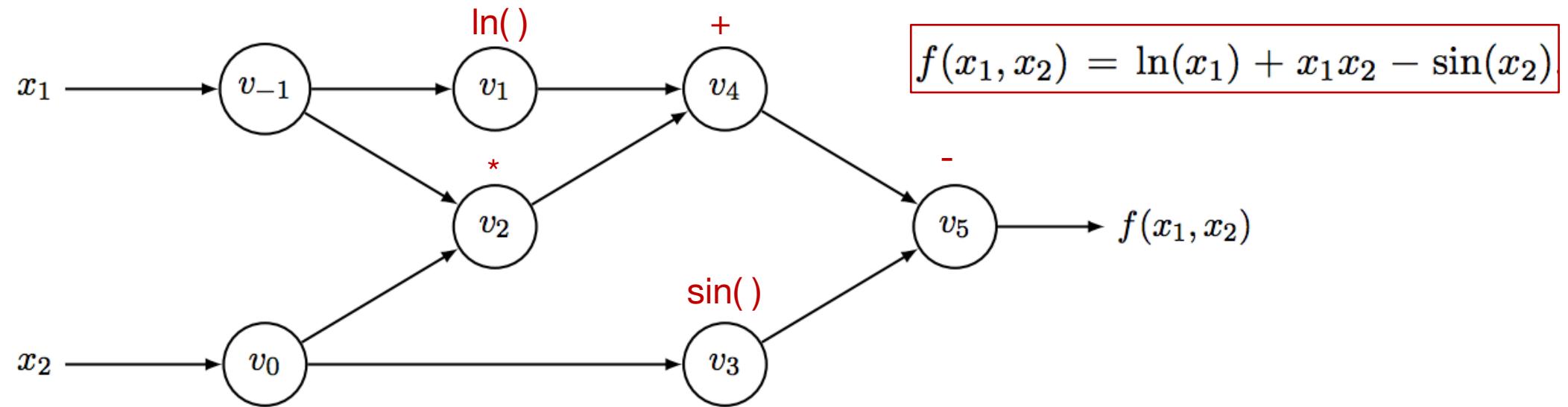
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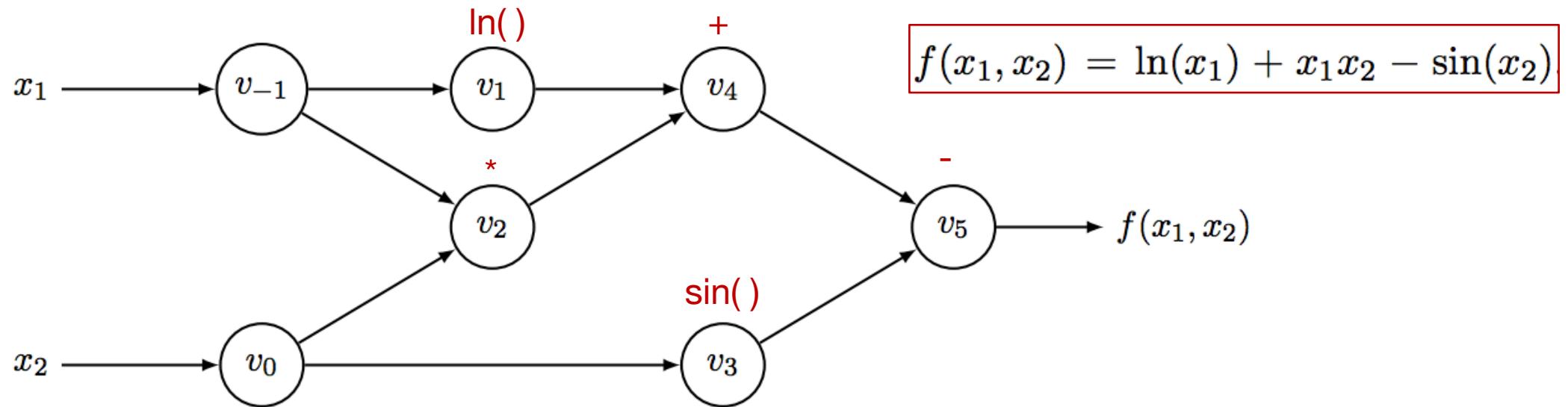
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Automatic differentiation on computational graphs



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in Machine Learning: a Survey

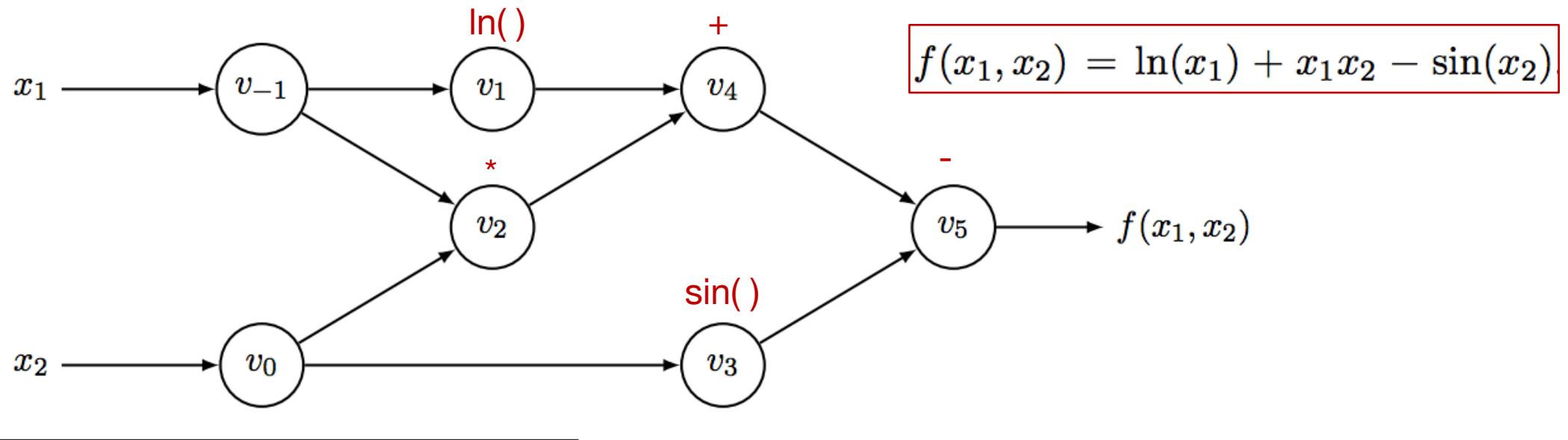
Automatic differentiation on computational graphs



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

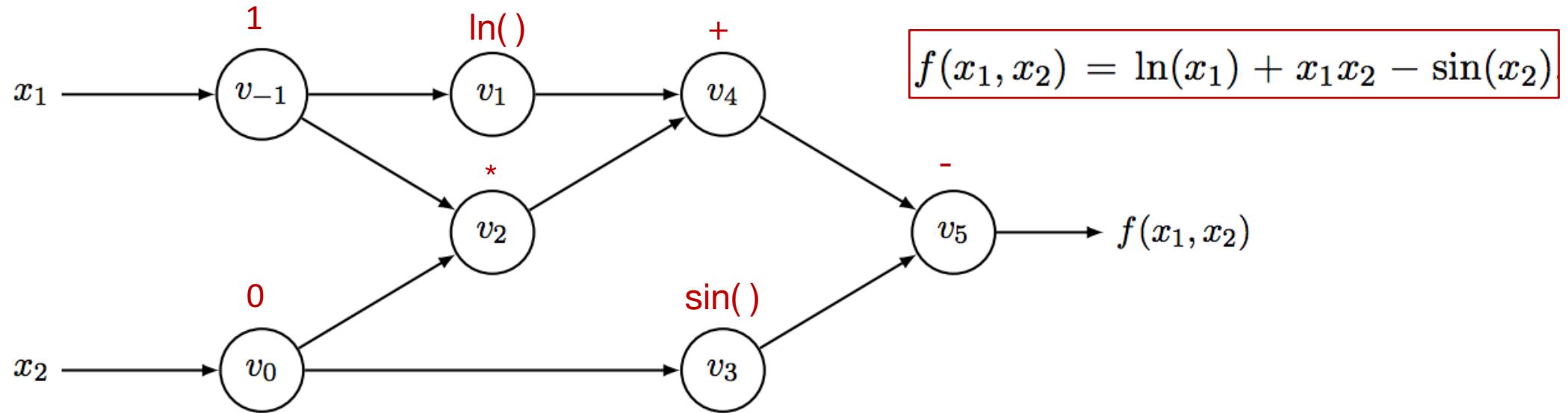
Automatic differentiation on computational graphs



Forward Primal Trace

$v_{-1} = x_1$	$= 2$
$v_0 = x_2$	$= 5$
<hr/>	
$v_1 = \ln v_{-1}$	$= \ln 2$
$v_2 = v_{-1} \times v_0$	$= 2 \times 5$
$v_3 = \sin v_0$	$= \sin 5$
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<hr/>	
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Forward automatic differentiation



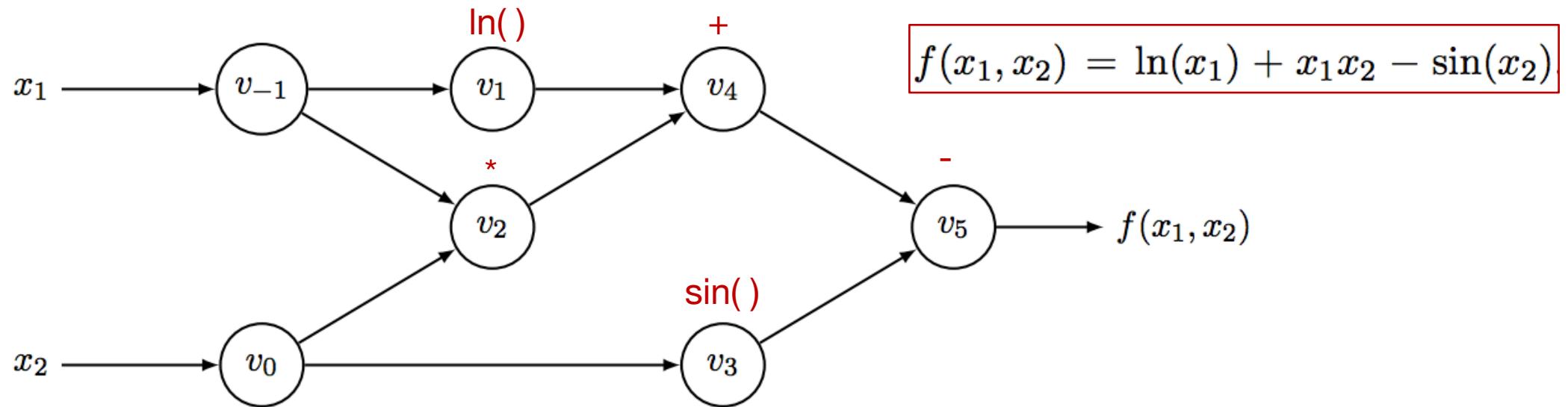
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Forward Tangent (Derivative) Trace

$$\begin{aligned}
\dot{v}_{-1} &= \dot{x}_1 &= 1 &\xleftarrow{\text{Set to 1 because we want } df/dx_1} \\
\dot{v}_0 &= \dot{x}_2 &= 0 \\
\\
\dot{v}_1 &= \dot{v}_{-1}/v_{-1} &= 1/2 \\
\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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Forward automatic differentiation



Forward Primal Trace

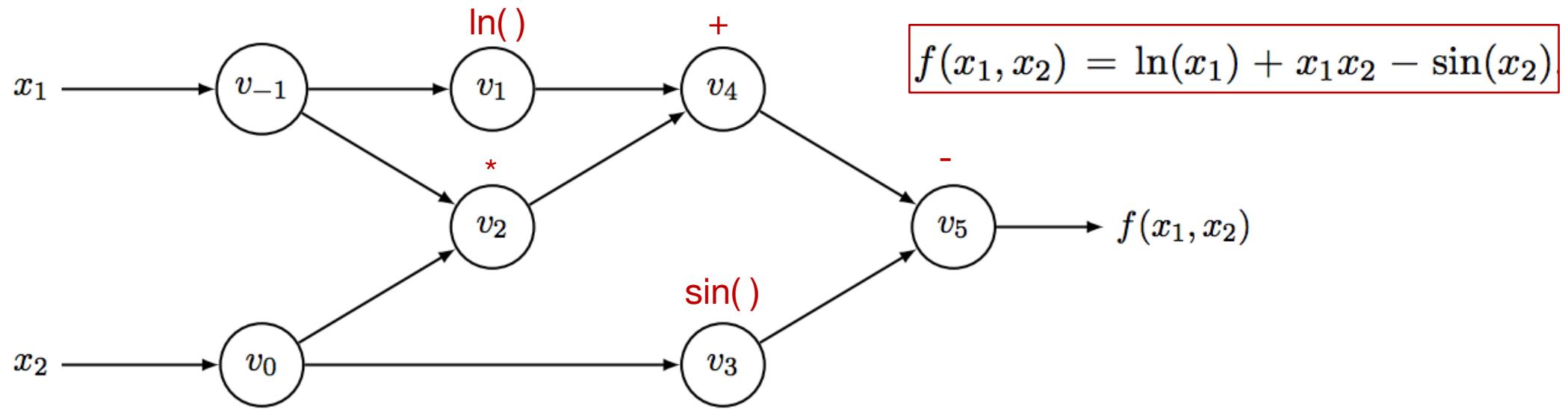
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Compute local derivative for all inputs and accumulate with chain rule

Forward automatic differentiation



Forward Primal Trace

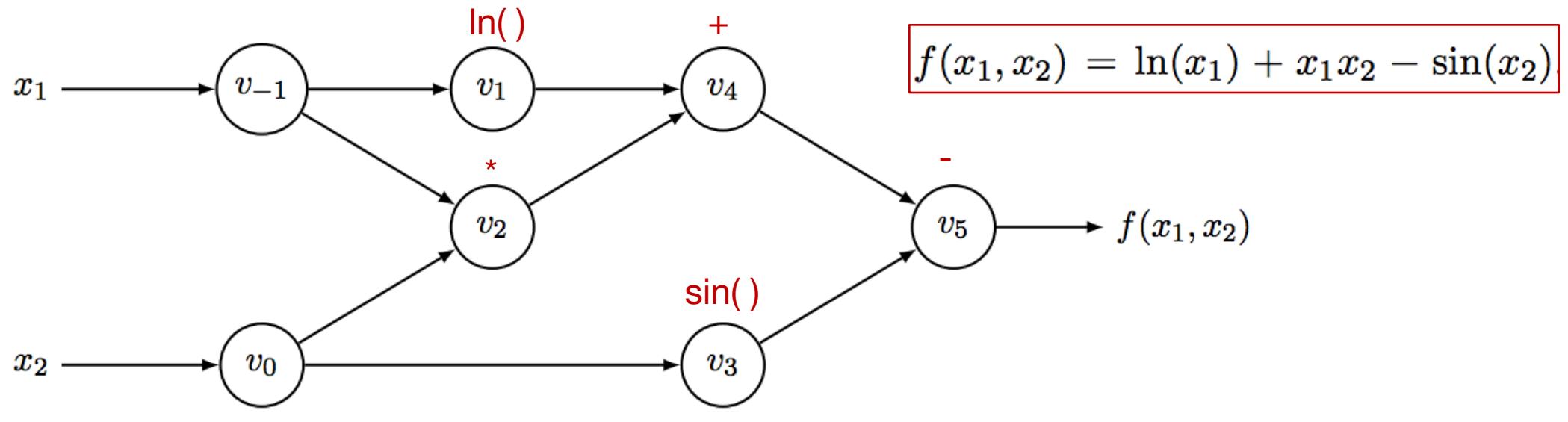
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Leads to final
desired df/dx_1

Forward automatic differentiation



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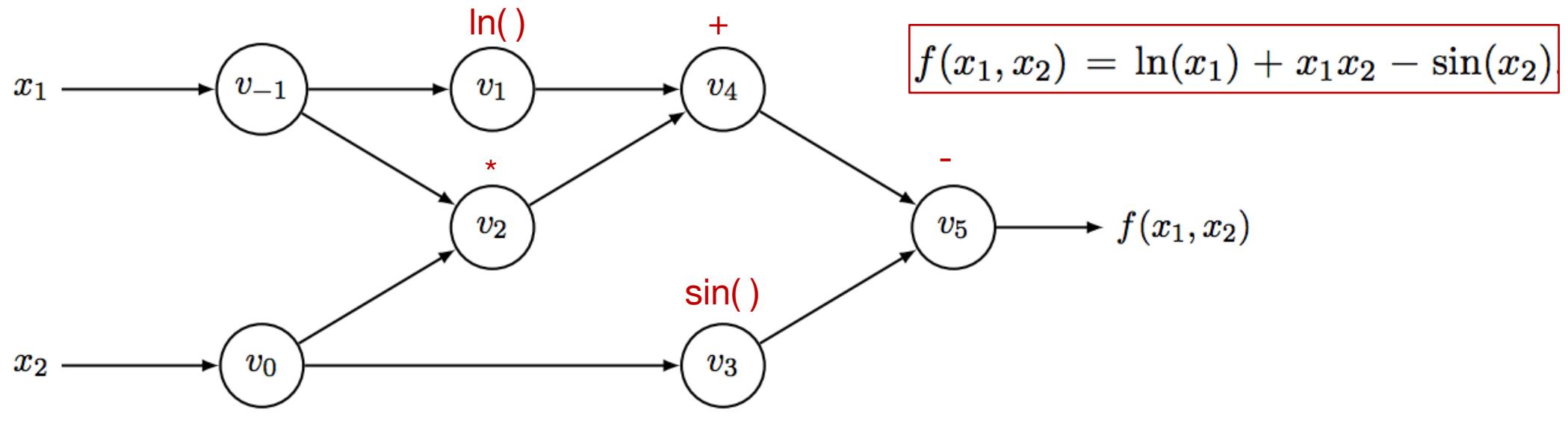
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Problem:

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

Forward automatic differentiation



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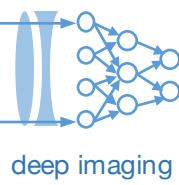
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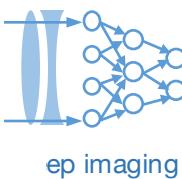
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Solution:

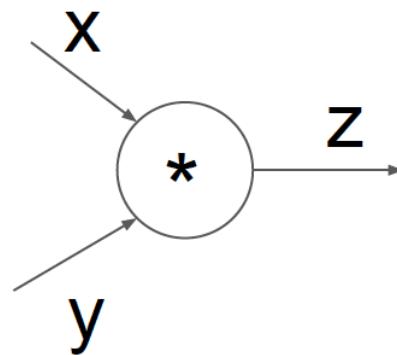
Work backwards from end to start with back-propagation



Backpropagation explanation from Stanford CS231N Slides



Modularized implementation: forward / backward API



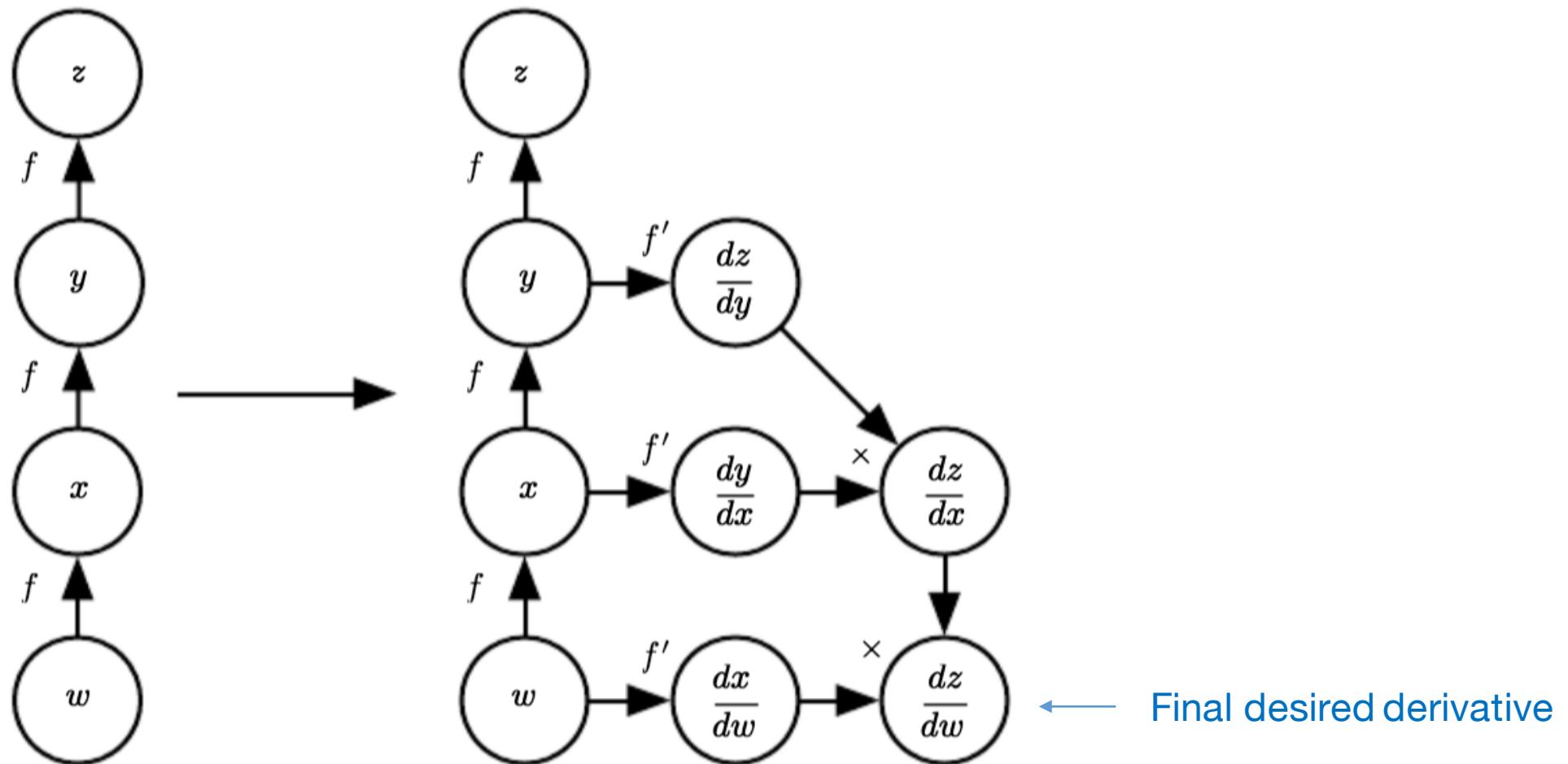
(x, y, z are scalars)

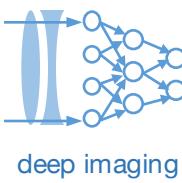
```
class MultiplyGate(object):
    def forward(x,y):
        z = x*y
        self.x = x # must keep these around!
        self.y = y
        return z
    def backward(dz):
        dx = self.y * dz # [dz/dx * dL/dz]
        dy = self.x * dz # [dz/dy * dL/dz]
        return [dx, dy]
```

Local gradient

Upstream gradient variable

How Tensorflow actually works: create a whole extra new graph





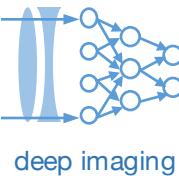
Last thing – matrix and vector derivatives

Here's a review:

$$\mathbf{u} = \mathbf{Wv}$$

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

Last thing – matrix and vector derivatives



Here's a review:

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

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

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

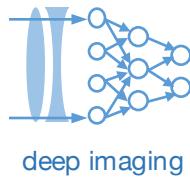
$$\frac{\partial u_3}{\partial v_2} = \frac{\partial}{\partial v_2}(W_{3,1}v_1 + W_{3,2}v_2 + \dots + W_{3,M}v_M) = \frac{\partial}{\partial v_2}W_{3,2}v_2 = W_{3,2}$$

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

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

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

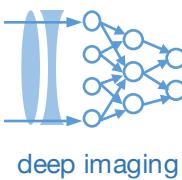
Let's go through an example:



$$L = \| \mathbf{W}_2 \text{ReLU}(\mathbf{W}_1 \mathbf{X}) \|_2^2$$

(2-layer network with MSE where we neglect labels \mathbf{y} for now)

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



Let's go through an example:

$$L = \| \mathbf{W}_2 \text{ReLU}(\mathbf{W}_1 \mathbf{X}) \|_2^2$$

(2-layer network with MSE where we neglect labels \mathbf{y} for now)

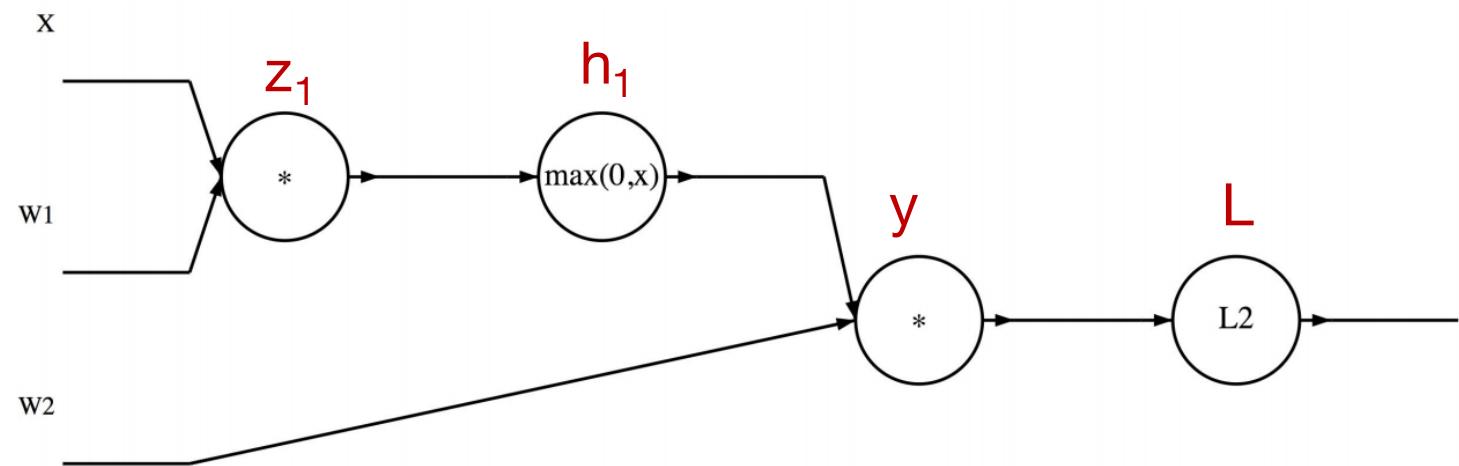
$$\frac{dL}{d\mathbf{W}_1} = ? \quad \frac{dL}{d\mathbf{W}_2} = ?$$

$$z_1 = \mathbf{X}\mathbf{W}_1$$

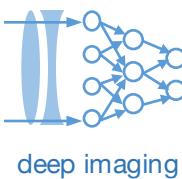
$$h_1 = \text{ReLU}(z_1)$$

$$\hat{\mathbf{y}} = h_1 \mathbf{W}_2$$

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



Forward pass: solve for z_1 , h_1 , y and L



Let's go through an example:

$$L = \| \mathbf{W}_2 \text{ReLU}(\mathbf{W}_1 \mathbf{X}) \|_2^2$$

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

(2-layer network with MSE where we neglect labels \mathbf{y} for now)

$$z_1 = \mathbf{X}\mathbf{W}_1$$

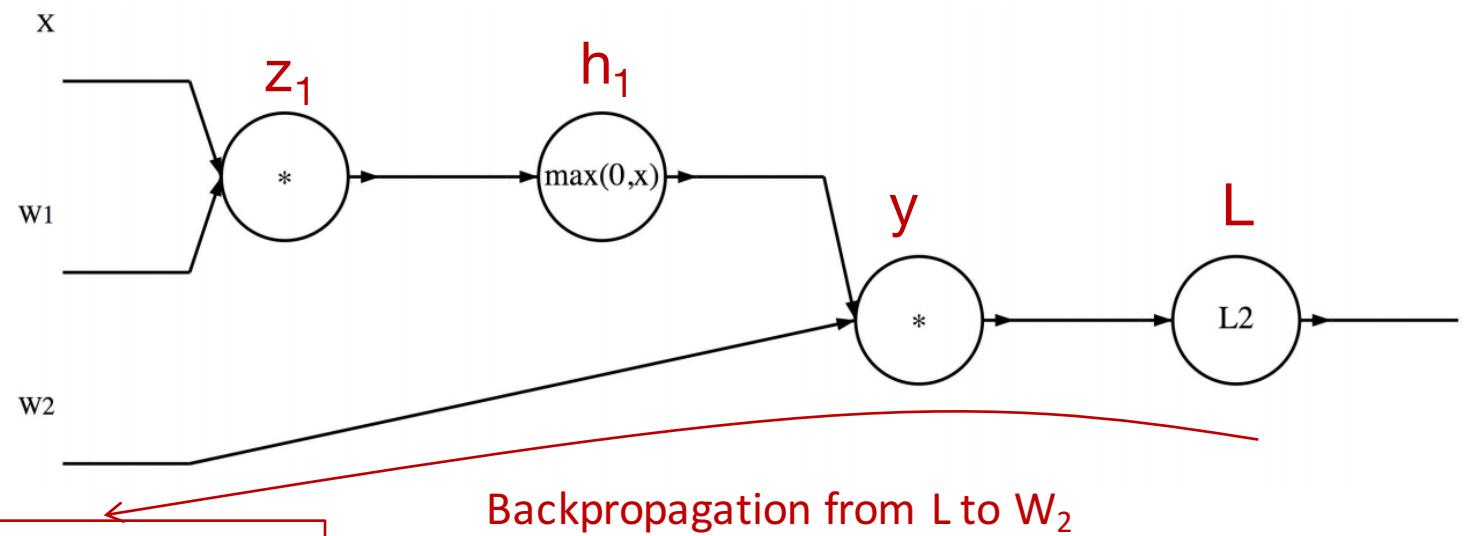
$$h_1 = \text{ReLU}(z_1)$$

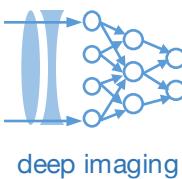
$$\hat{\mathbf{y}} = h_1 \mathbf{W}_2$$

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

Gradients for scalar L will have same shape as denominator

$$\frac{\partial L}{\partial \mathbf{W}_2} = \frac{\partial \hat{\mathbf{y}}}{\partial \mathbf{W}_2} \frac{\partial L}{\partial \hat{\mathbf{y}}}$$





Let's go through an example:

$$L = \| \mathbf{W}_2 \text{ReLU}(\mathbf{W}_1 \mathbf{X}) \|_2^2$$

(2-layer network with MSE where we neglect labels \mathbf{y} for now)

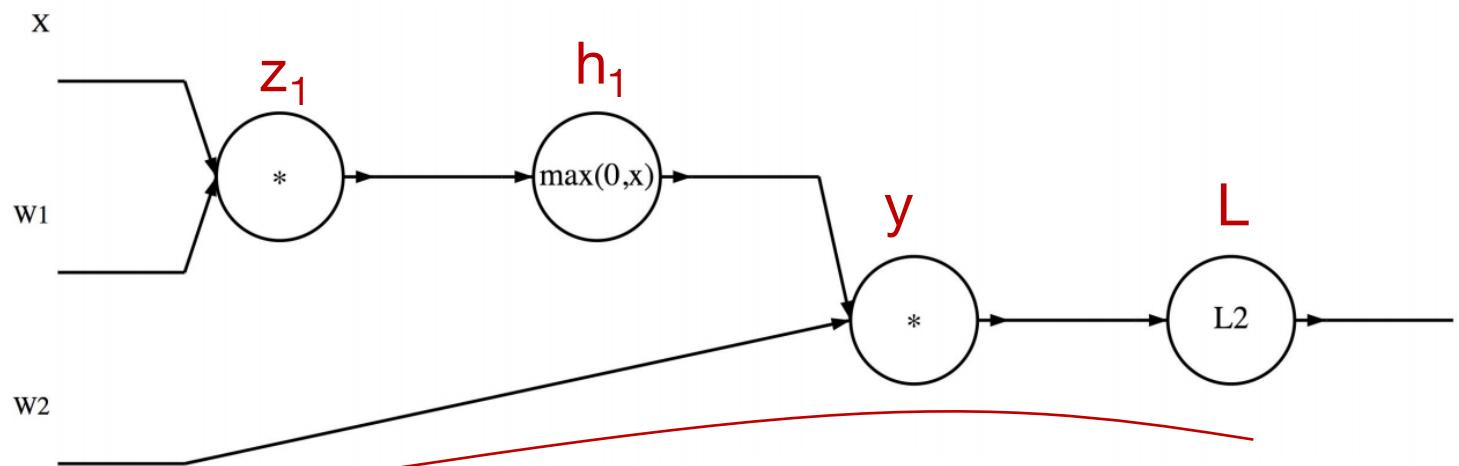
$$\frac{dL}{d\mathbf{W}_1} = ? \quad \boxed{\frac{dL}{d\mathbf{W}_2} = ?}$$

$$z_1 = \mathbf{X}\mathbf{W}_1$$

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

$$\hat{y} = h_1 \mathbf{W}_2$$

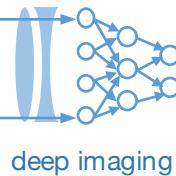
$$L = \|\hat{y}\|_2^2$$



Gradients for scalar L will have same shape as denominator

$$\boxed{\frac{\partial L}{\partial \mathbf{W}_2} = \frac{\partial \hat{y}}{\partial \mathbf{W}_2} \frac{\partial L}{\partial \hat{y}}}$$

$$\frac{\partial \hat{y}}{\partial \mathbf{W}_2} = h_1^T \quad \frac{\partial L}{\partial \hat{y}} = 2\hat{y}$$



Let's go through an example:

$$L = \| \mathbf{W}_2 \text{ReLU}(\mathbf{W}_1 \mathbf{X}) \|_2^2$$

(2-layer network with MSE where we neglect labels \mathbf{y} for now)

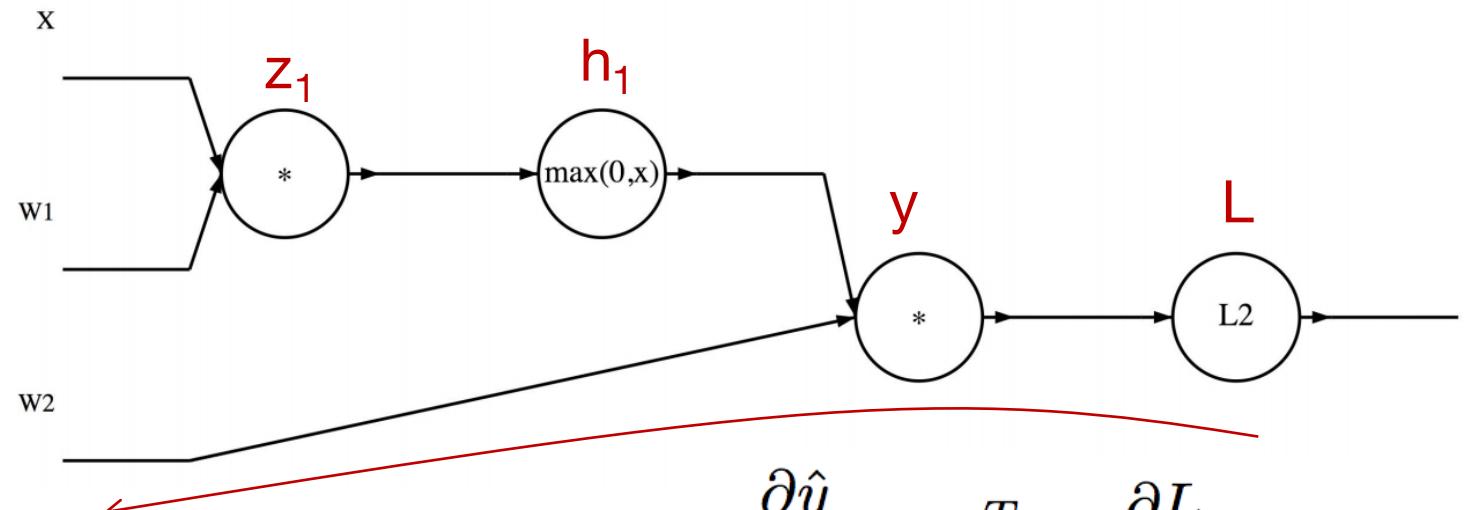
$$\frac{dL}{d\mathbf{W}_1} = ? \quad \boxed{\frac{dL}{d\mathbf{W}_2} = ?}$$

$$z_1 = \mathbf{X}\mathbf{W}_1$$

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

$$\hat{y} = h_1 \mathbf{W}_2$$

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



$$\boxed{\frac{\partial L}{\partial \mathbf{W}_2} = \frac{\partial \hat{y}}{\partial \mathbf{W}_2} \frac{\partial L}{\partial \hat{y}} = 2h_1^T \hat{y}}$$

$$\frac{\partial \hat{y}}{\partial \mathbf{W}_2} = h_1^T \quad \frac{\partial L}{\partial \hat{y}} = 2\hat{y}$$

Let's go through an example:

$$z_1 = XW_1$$

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

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

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

$$\frac{\partial L}{\partial h_1} = \frac{\partial L}{\partial \hat{y}} W_2^\top$$

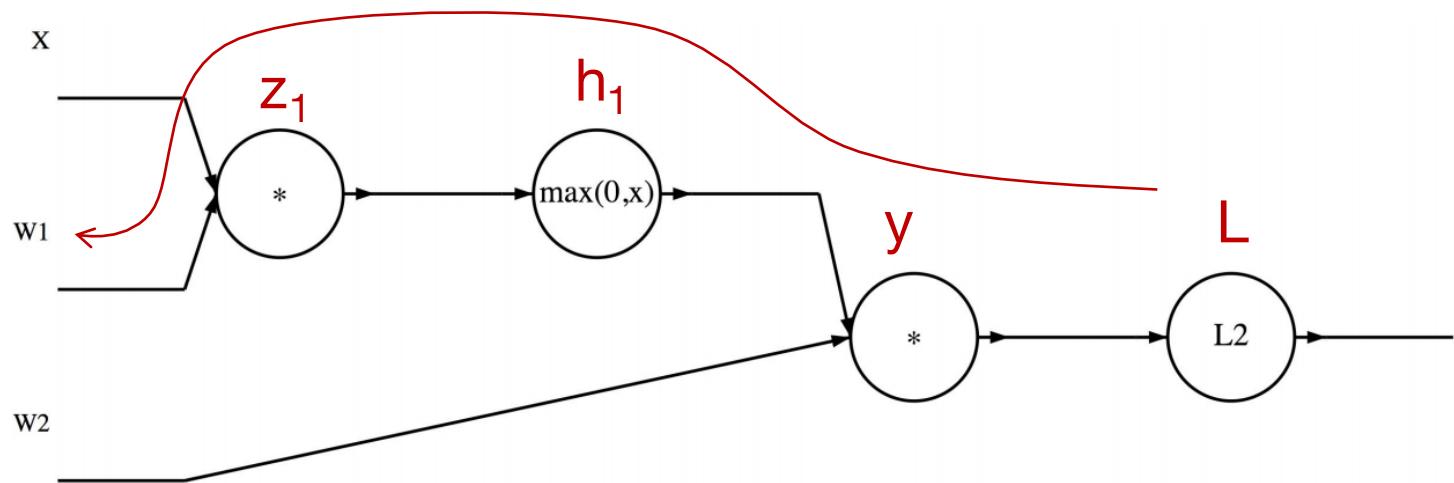
$$\frac{\partial h_1}{\partial z_1} = \frac{\partial L}{\partial h_1} \circ I[h_1 > 0]$$

$$\boxed{\frac{\partial z_1}{\partial W_1} = x^\top \frac{\partial h_1}{\partial z_1}}$$

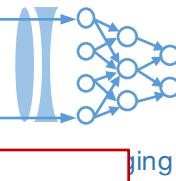
$$L = \| \mathbf{W}_2 \text{ReLU}(\mathbf{W}_1 \mathbf{X}) \|_2^2$$

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

(2-layer network with MSE where we neglect labels \mathbf{y} for now)



Rely on dimensional analysis to select order of operations



Let's go through an example:

$$z_1 = XW_1$$

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

$$\hat{y} = h_1W_2$$

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

$$\frac{\partial L}{\partial h_1} = \frac{\partial L}{\partial \hat{y}} W_2^\top$$

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

$$\frac{\partial z_1}{\partial W_1} = x^\top \frac{\partial h_1}{\partial z_1}$$

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

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

```
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

