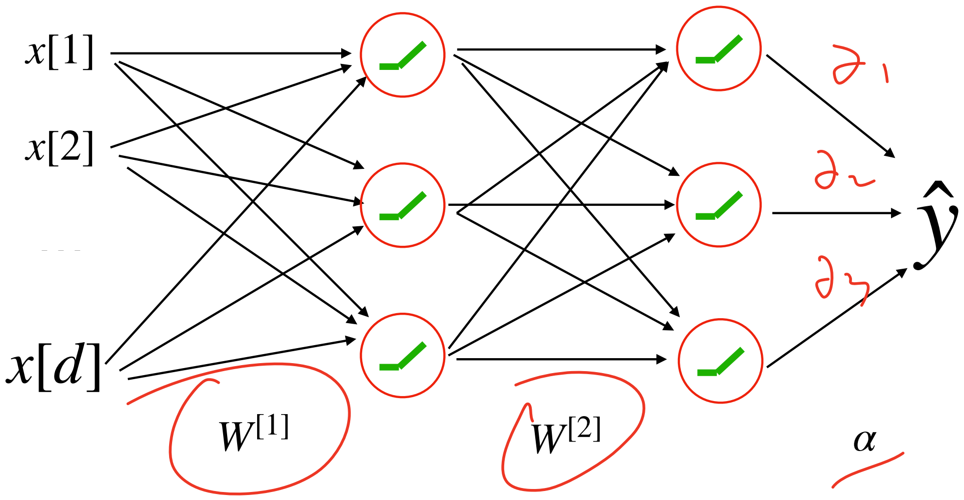
Neural Network:
Training & Backpropagation

Recap

A two layer fully connected feedforward NN:



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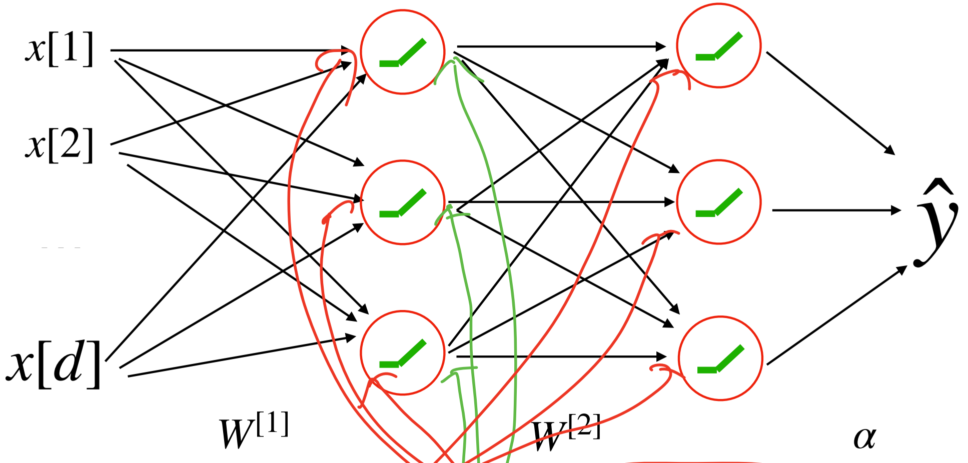
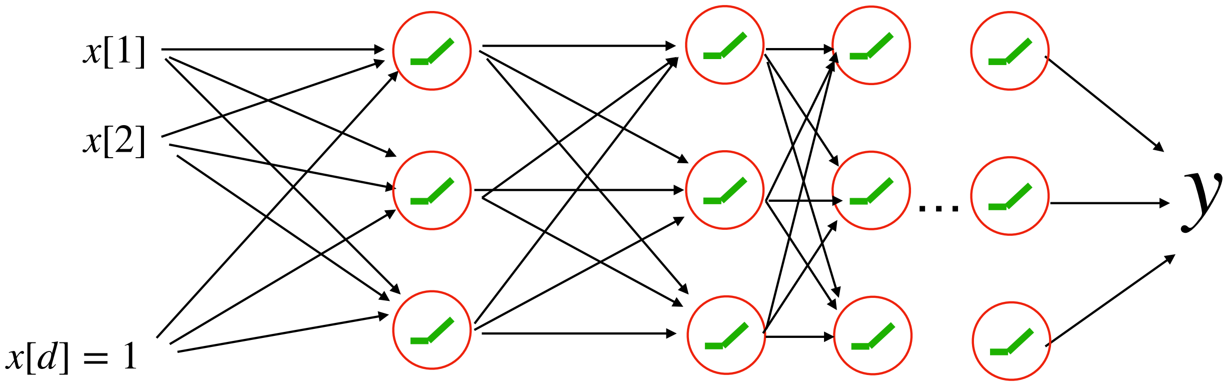


$$h(x) := \alpha^\top \text{ReLU}\left(W^{[2]}\text{ReLU}\left(W^{[1]}x\right)\right) + b$$

A multi-layer fully connected neural network



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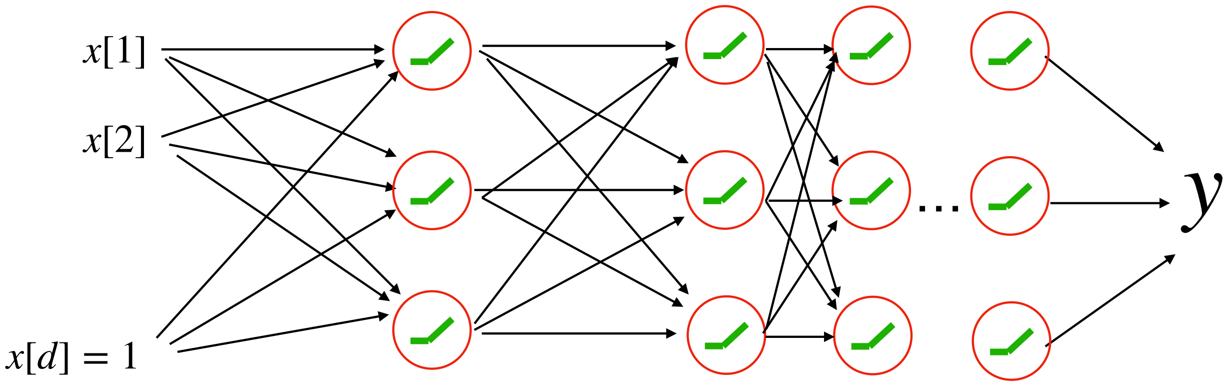

Define it by a forward pass:

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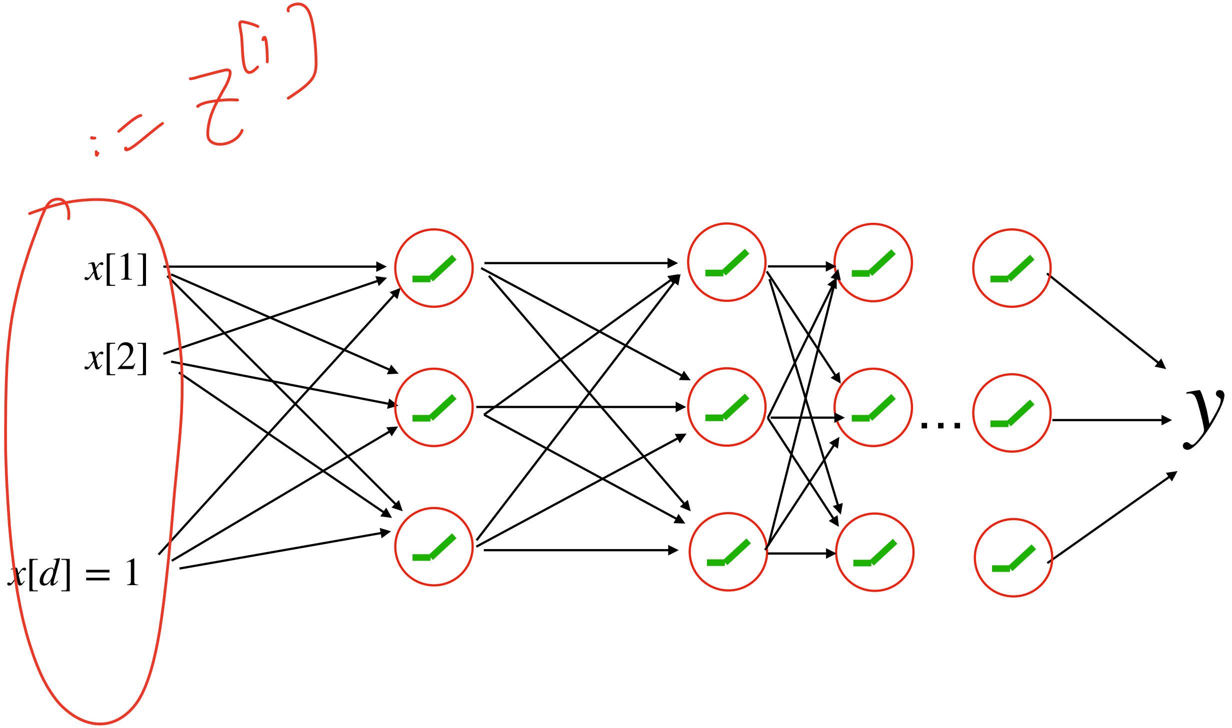

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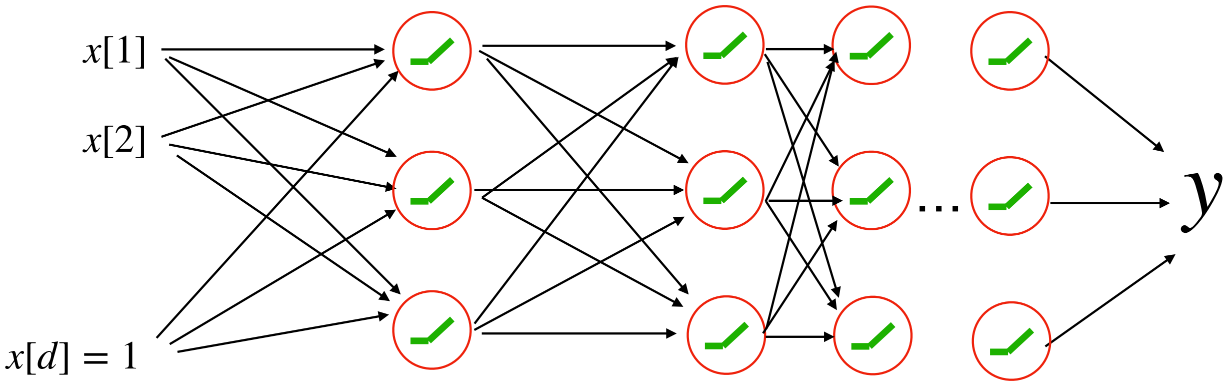

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depth

For t = 1 to T-1:

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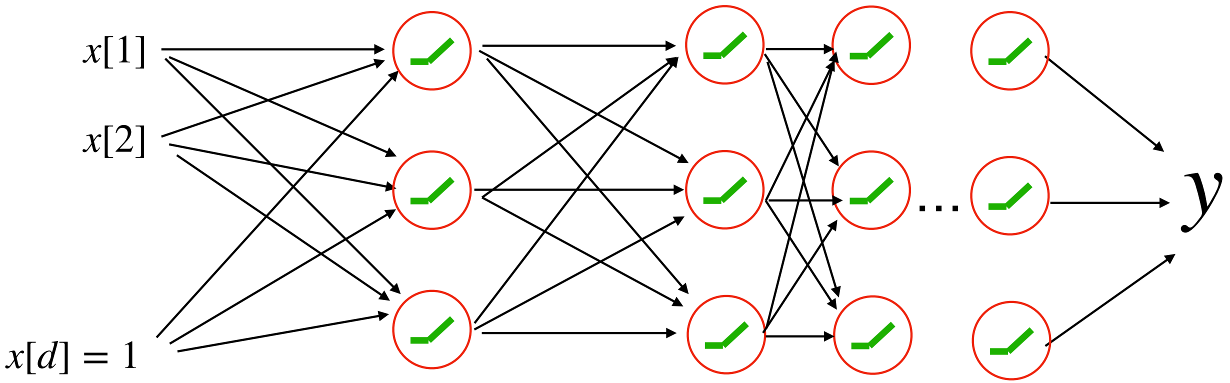

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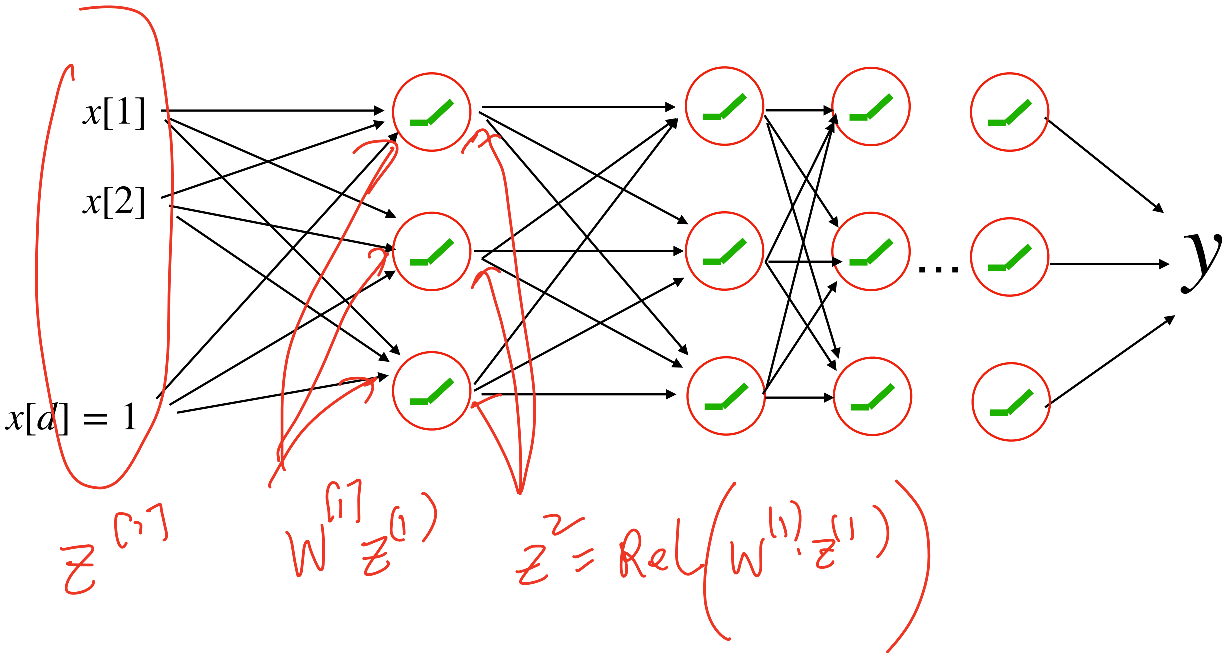
$$z^{[t+1]} = \text{ReLU}\left(W^{[t]} z^{t}\right)$$

A multi-layer fully connected neural network

One-layer: width ≈ exp(d)



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$$y = \alpha^{\top} z^{[T]} + b$$

Outline of Today

1. Training NNs via SGD

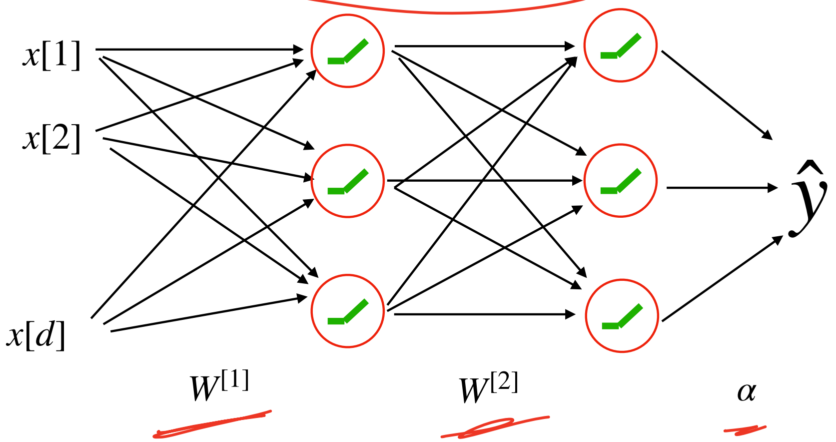
2. A Naive approach of computing gradients

3. Backpropagation: efficient way of computing gradients

Training neural network via SGD

Square loss on training example (x, y)

$$h(x) := \alpha^\top \text{ReLU}\left(W^{[2]}\text{ReLU}\left(W^{[1]}x\right)\right) + b$$



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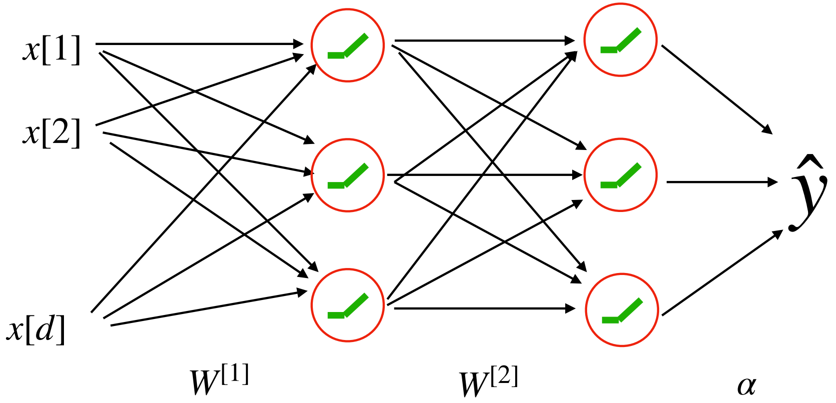

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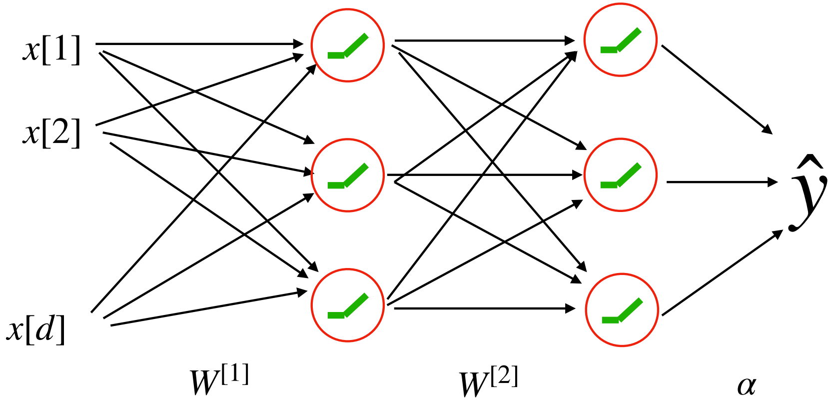

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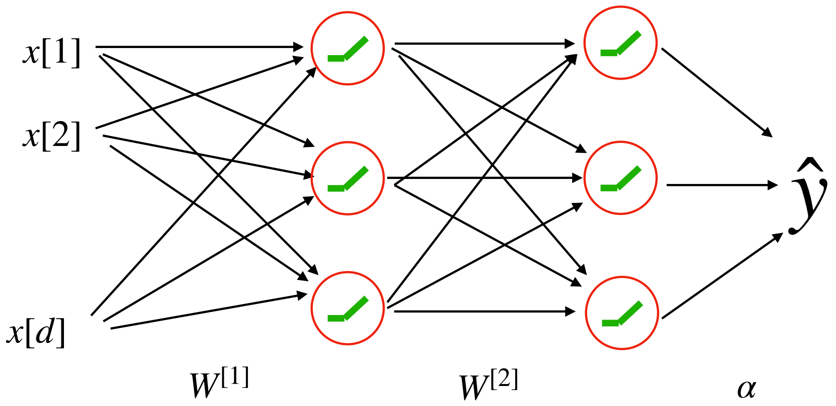

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Compute gradients:

$$\frac{\partial \ell(h(x), y)}{\partial W^{[1]}} \quad \frac{\partial \ell(h(x), y)}{\partial W^{[2]}}$$

$$\frac{\partial \ell(h(x), y)}{\partial \alpha} \quad \frac{\partial \ell(h(x), y)}{\partial b}$$

Training neural network via SGD

Mini-batch Stochastic gradient descent

$\theta = [W^{[1]}, W^{[2]}, \alpha, b]$

For epoc $t = 1$ to T:

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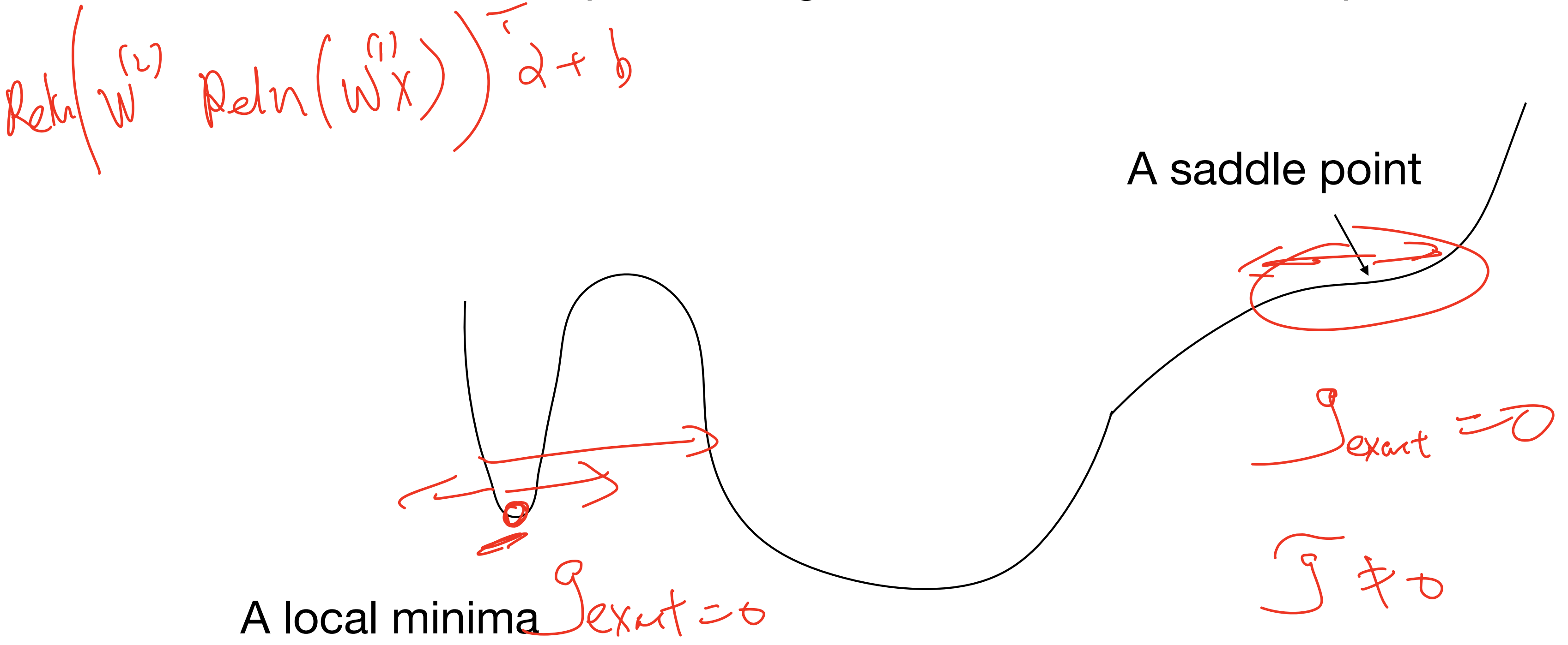
$\theta = \theta - \eta g$

Adam or AdaGrad

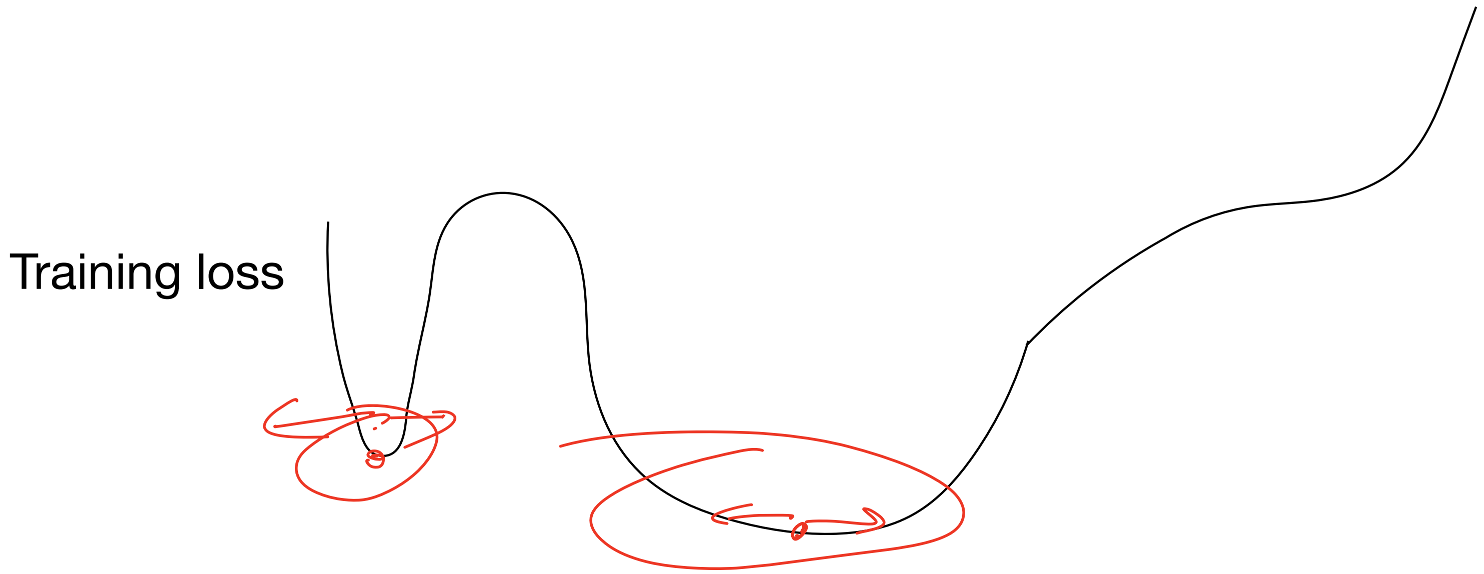
Training neural network via SGD

SGD helps avoiding local minima and saddle point



Training neural network via SGD

SGD tends to converge to a flat region



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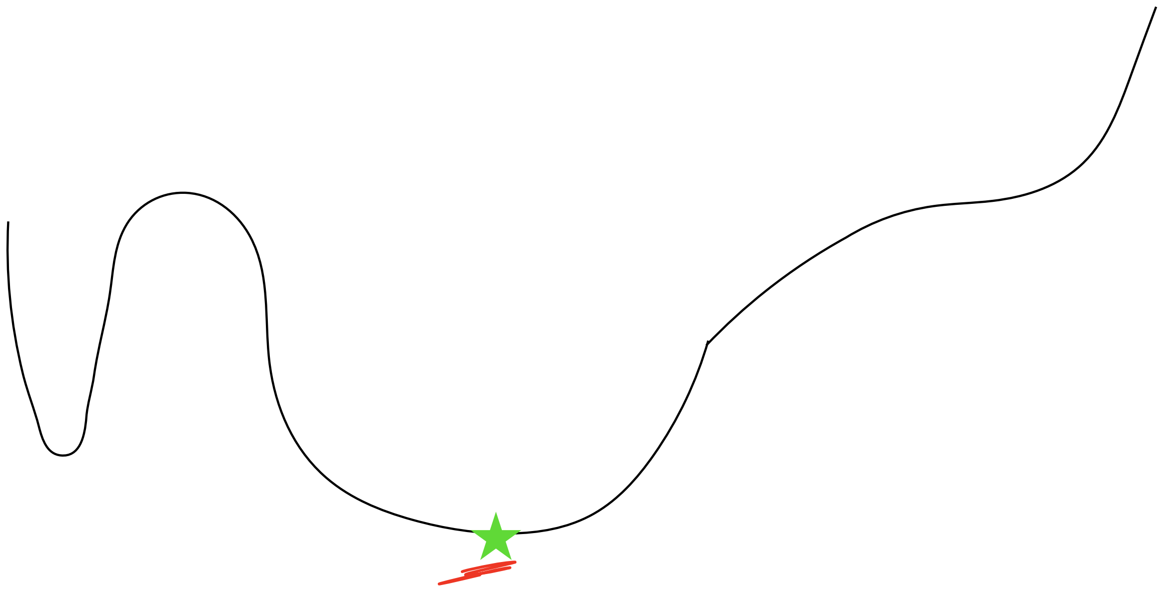

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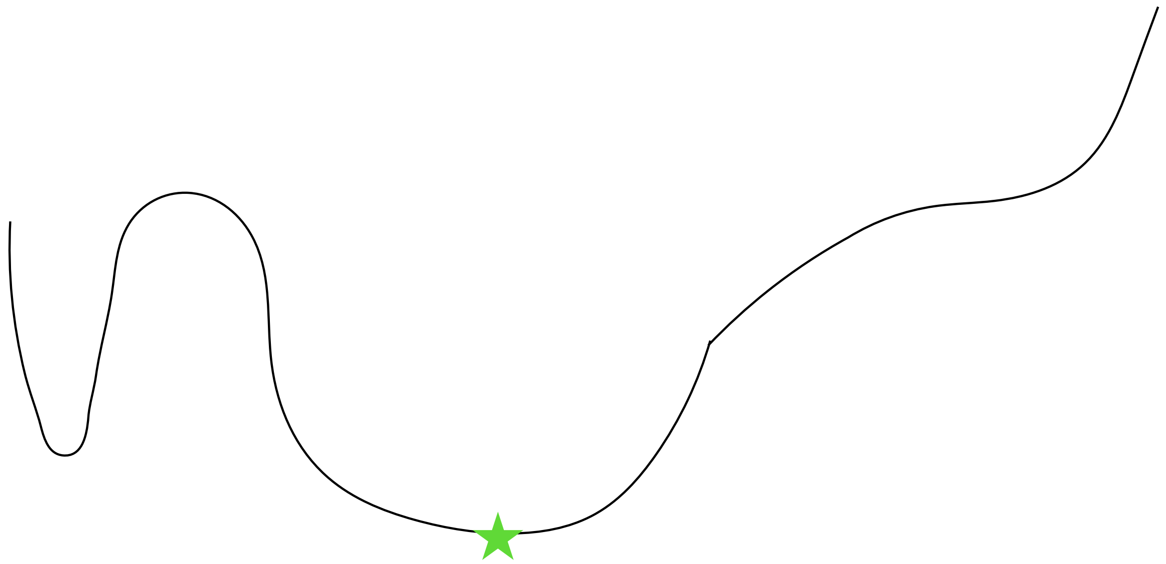

A flat local minima solution can help generalizes better to test data

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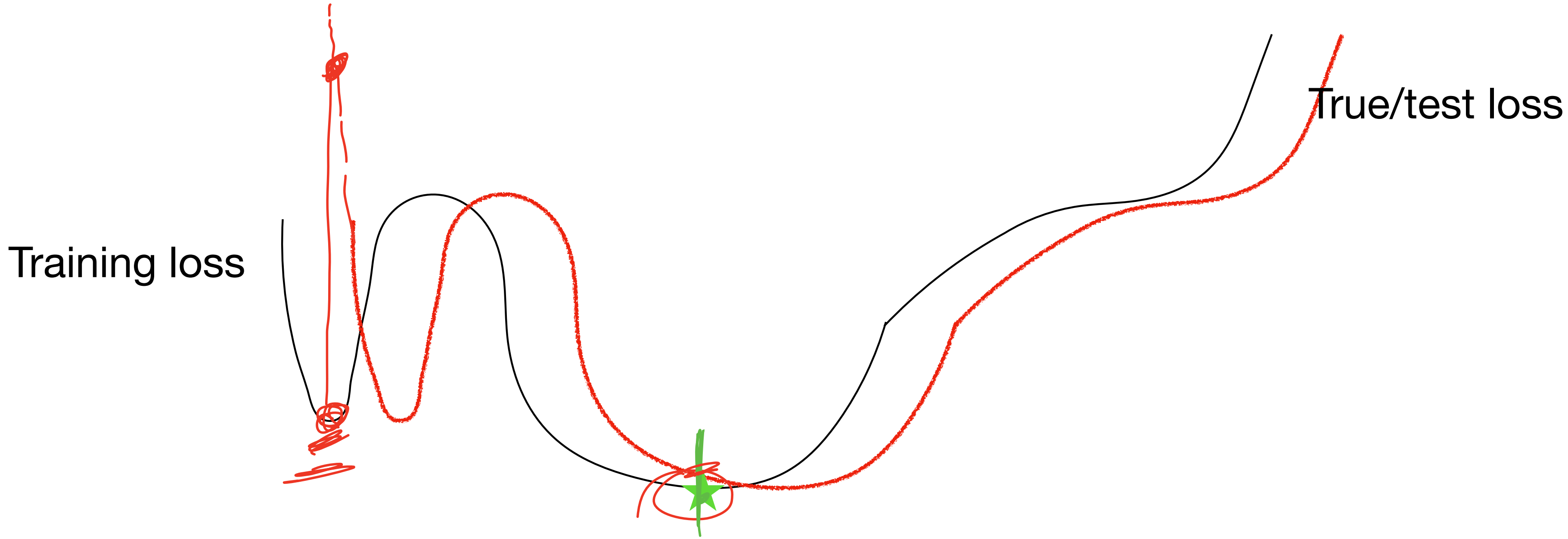

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Outline of Today

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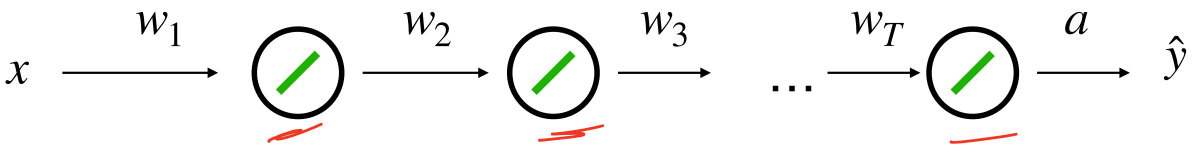
2. A Naive approach of computing gradients

3. Backpropagation: efficient way of computing gradients

A naive algorithm

Consider the following one-dim case with identity transformation



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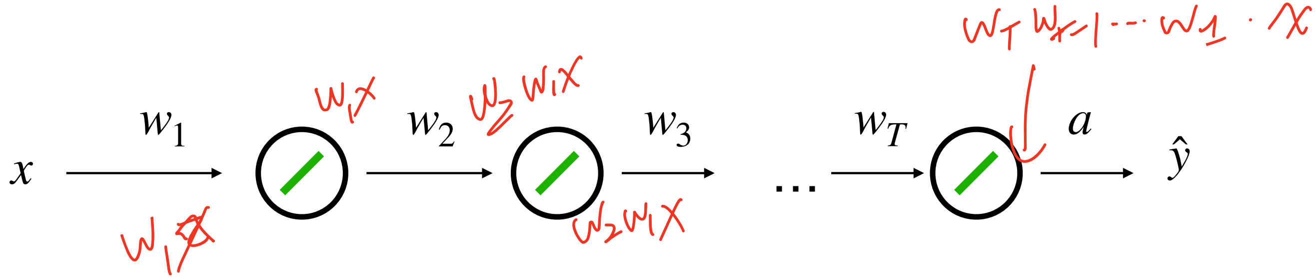

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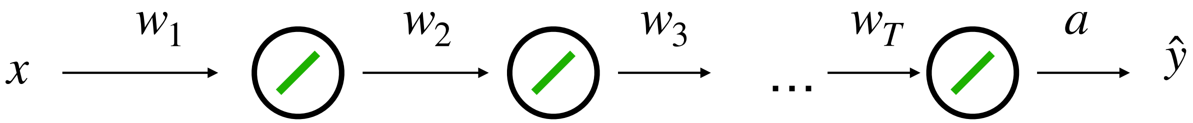

$$\hat{y} = a w_T \ldots w_2 w_1 x$$

Let's compute derivatives $\partial \hat{y} / \partial w_i, \forall i = 1, \ldots T$

$$\nabla = \begin{bmatrix} \frac{\partial l}{\partial w_1} \\ \vdots \\ \frac{\partial l}{\partial w_T} \end{bmatrix}$$

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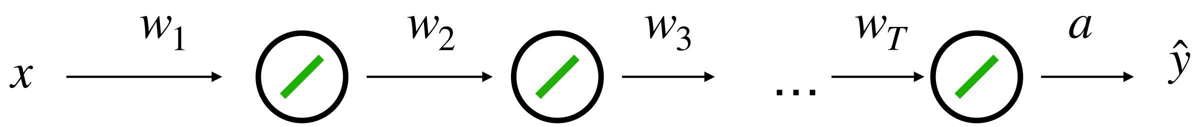


$$\ell(\hat{y}, y) = (\hat{y} - y)^2$$

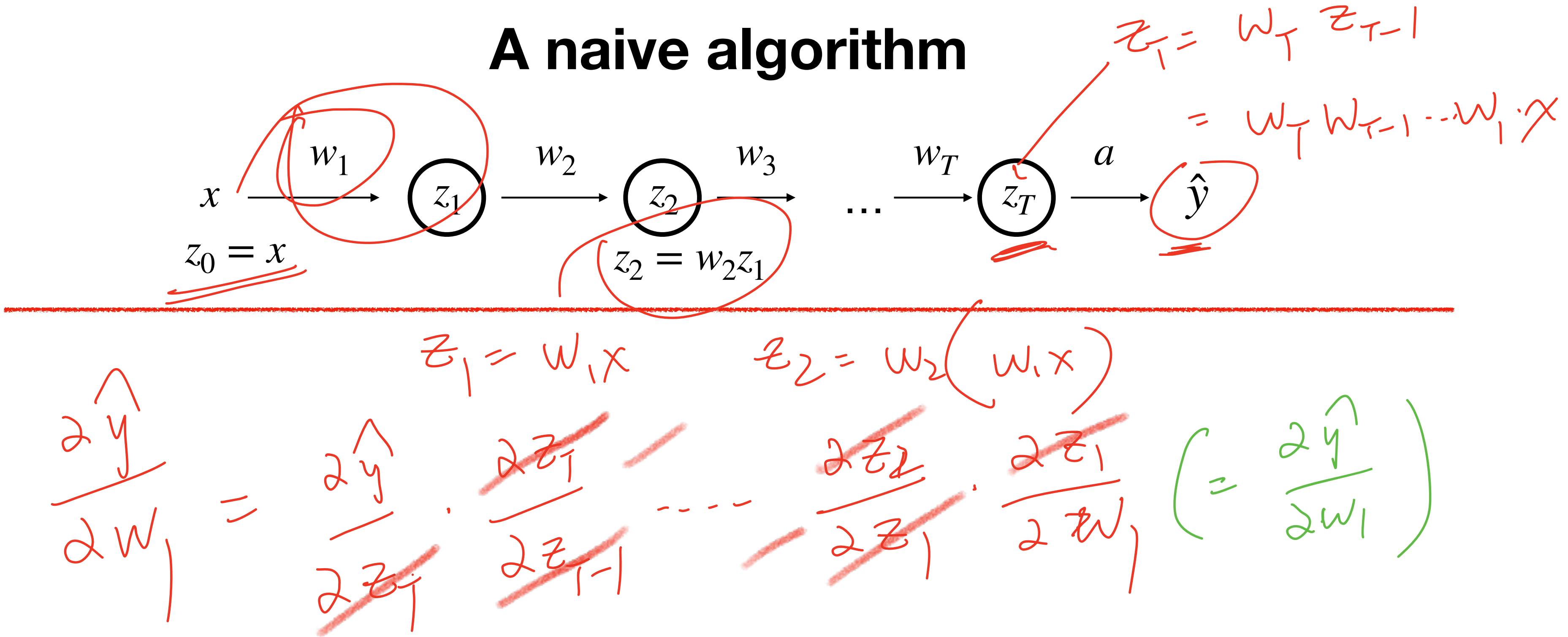
$$\frac{\partial \ell}{\partial \hat{y}} = 2(\hat{y} - y)$$

$$\hat{y} = a w_T \ldots w_2 w_1 x$$

Let's compute derivatives $\partial \hat{y} / \partial w_i, \forall i = 1, \ldots T$

Via chain rule: $\frac{\partial \ell}{\partial w_i} = \frac{\partial \ell}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial w_i}$

A naive algorithm



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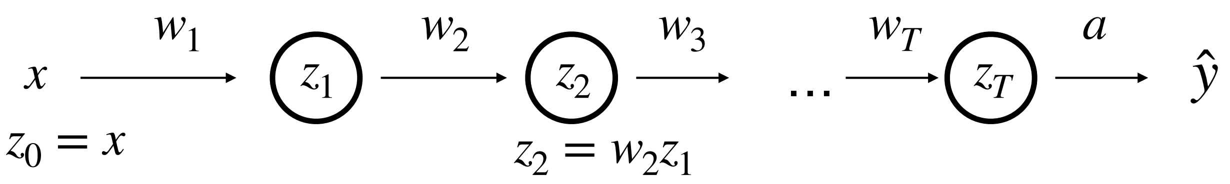

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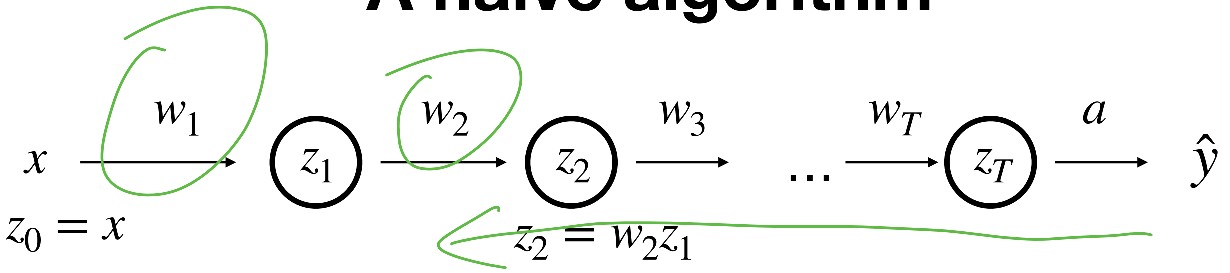

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$$\frac{\partial \hat{y}}{\partial w_1} = \frac{\partial \hat{y}}{\partial z_T} \frac{\partial z_T}{\partial z_{T-1}} \dots \frac{\partial z_2}{\partial z_1} \frac{\partial z_1}{\partial w_1}$$

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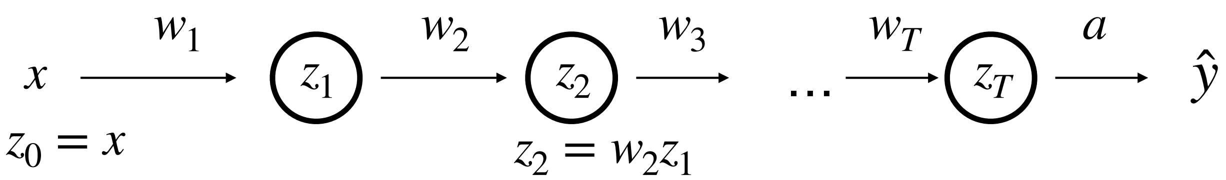

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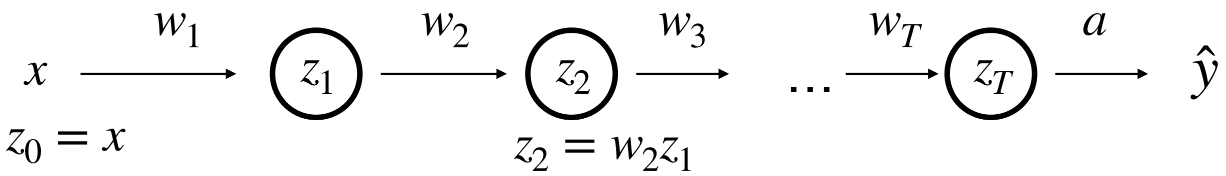

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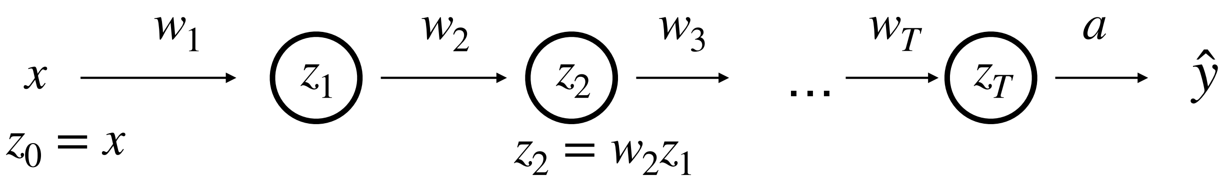

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$\frac{\partial \hat{y}}{\partial w_3}$ ← T-3

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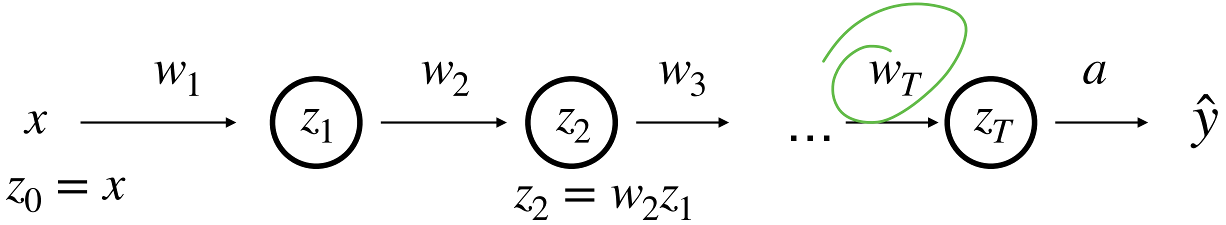

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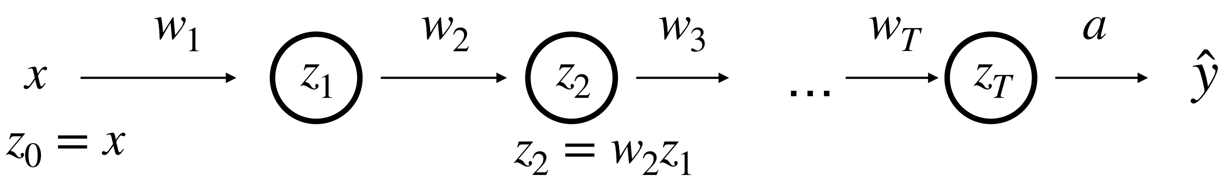

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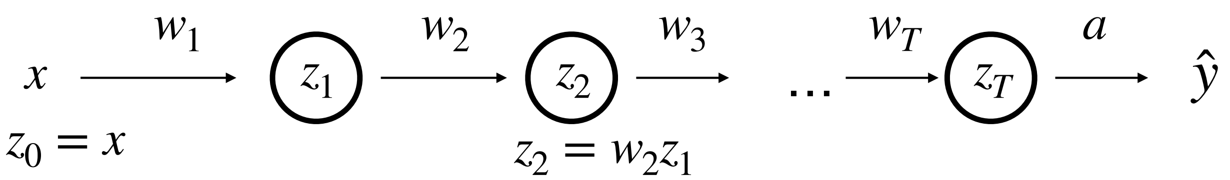

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Total complexity:

$$1 + 2 + \ldots + T = O(T^2)$$

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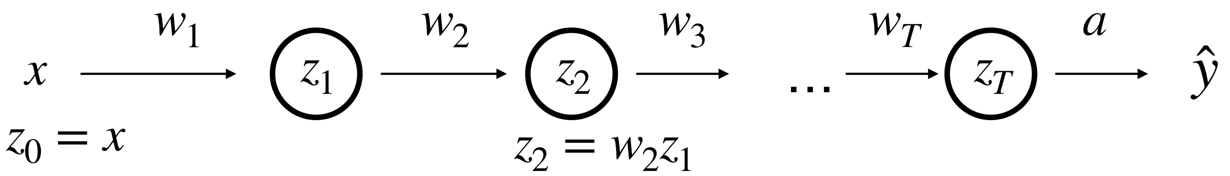

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Quadratic in size of the graph!

Summary so far

What we did:

for each edge weight w_i, apply chain rule to calculate $\partial\hat{y}/\partial w_i$

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Can we do better in running time?

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3. Backpropagation: efficient way of computing gradients

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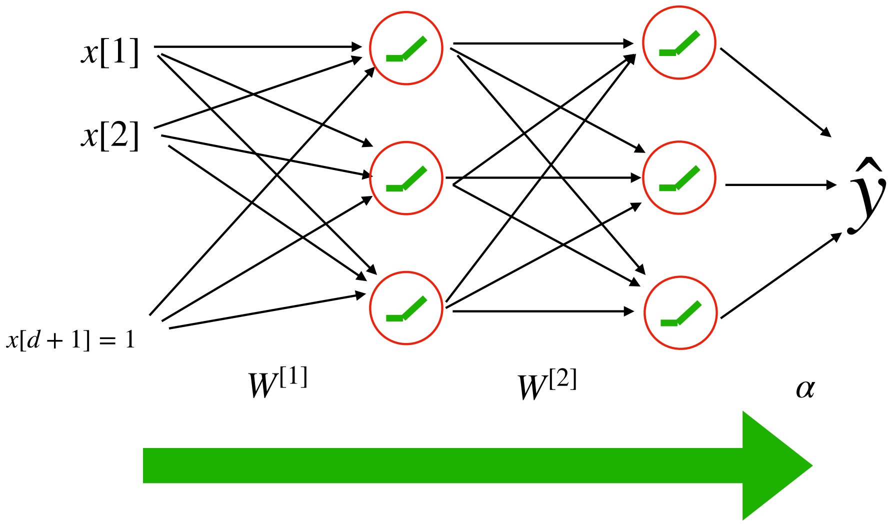
This allowed networks with intermediate "hidden" neurons between input and output layers to **learn efficiently,** overcoming the limitations noted by Minsky and Papert.

Overview of backpropagation

Forward pass followed by a backward pass

Forward pass:



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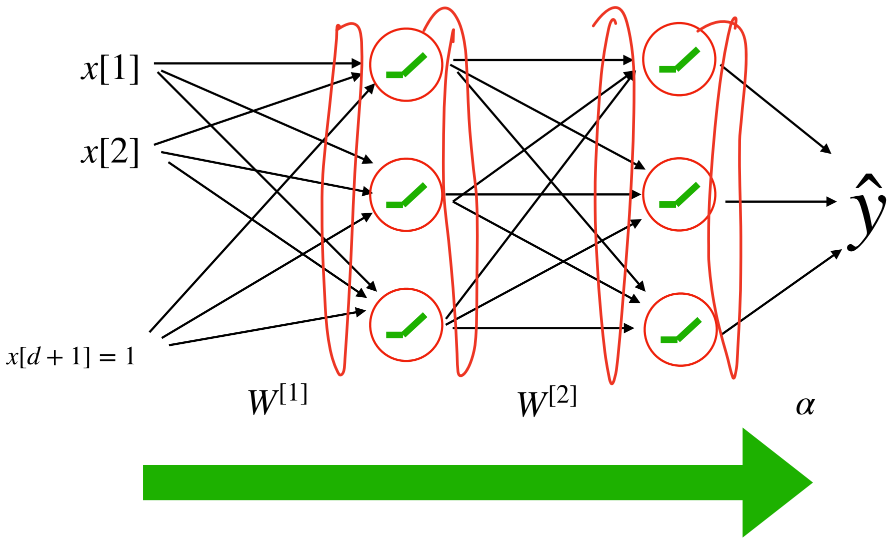

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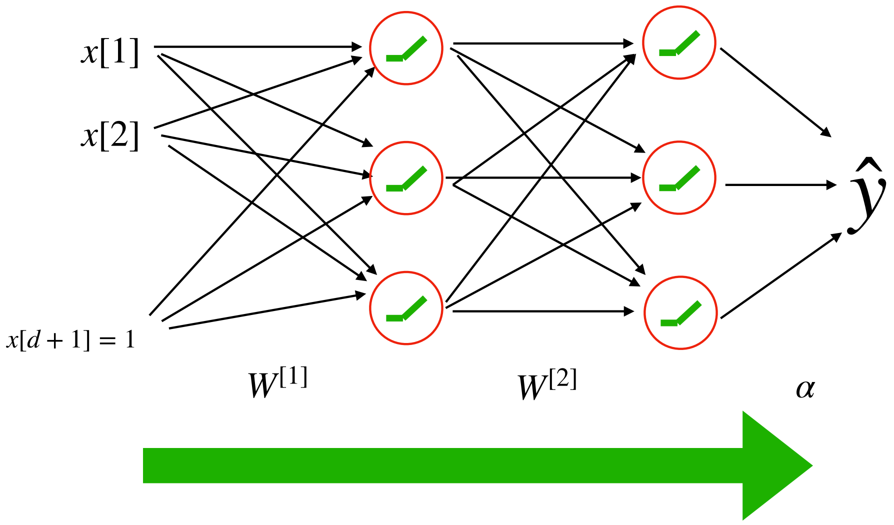

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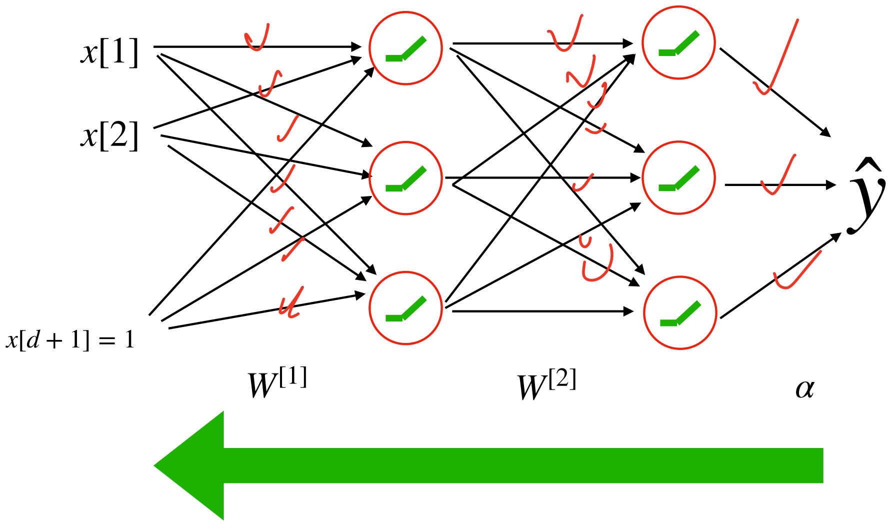

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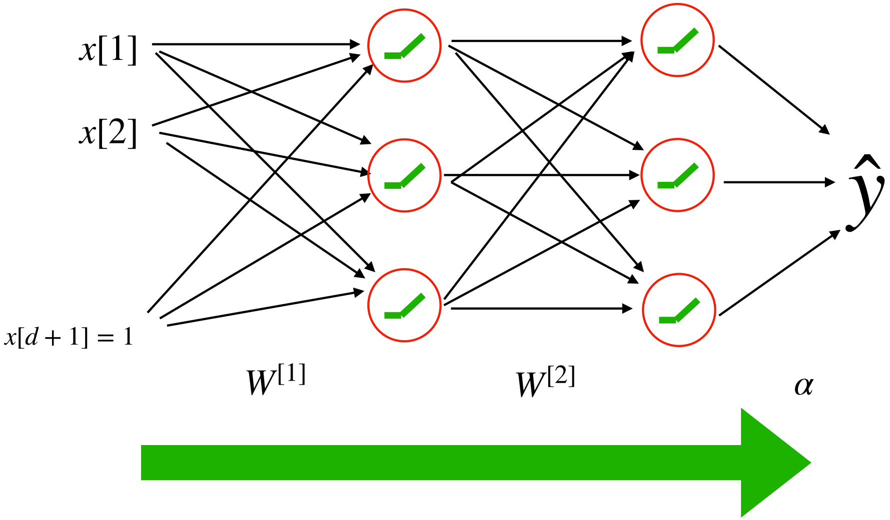

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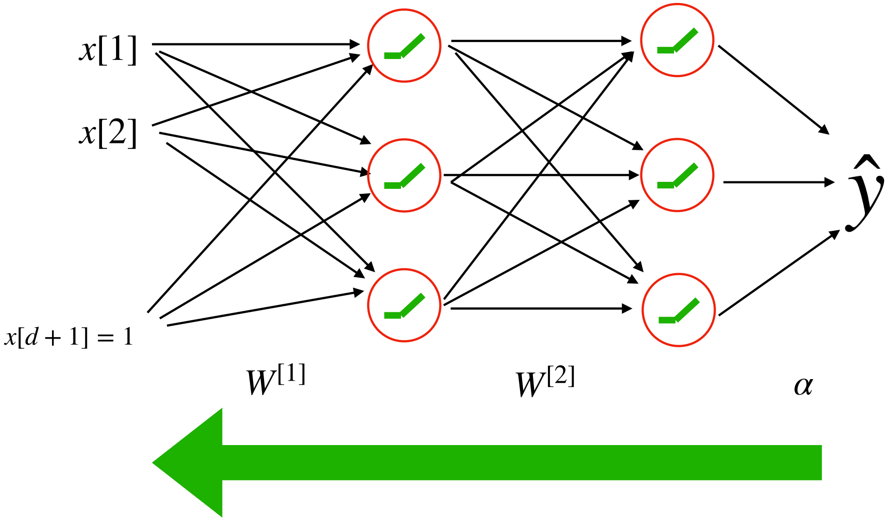
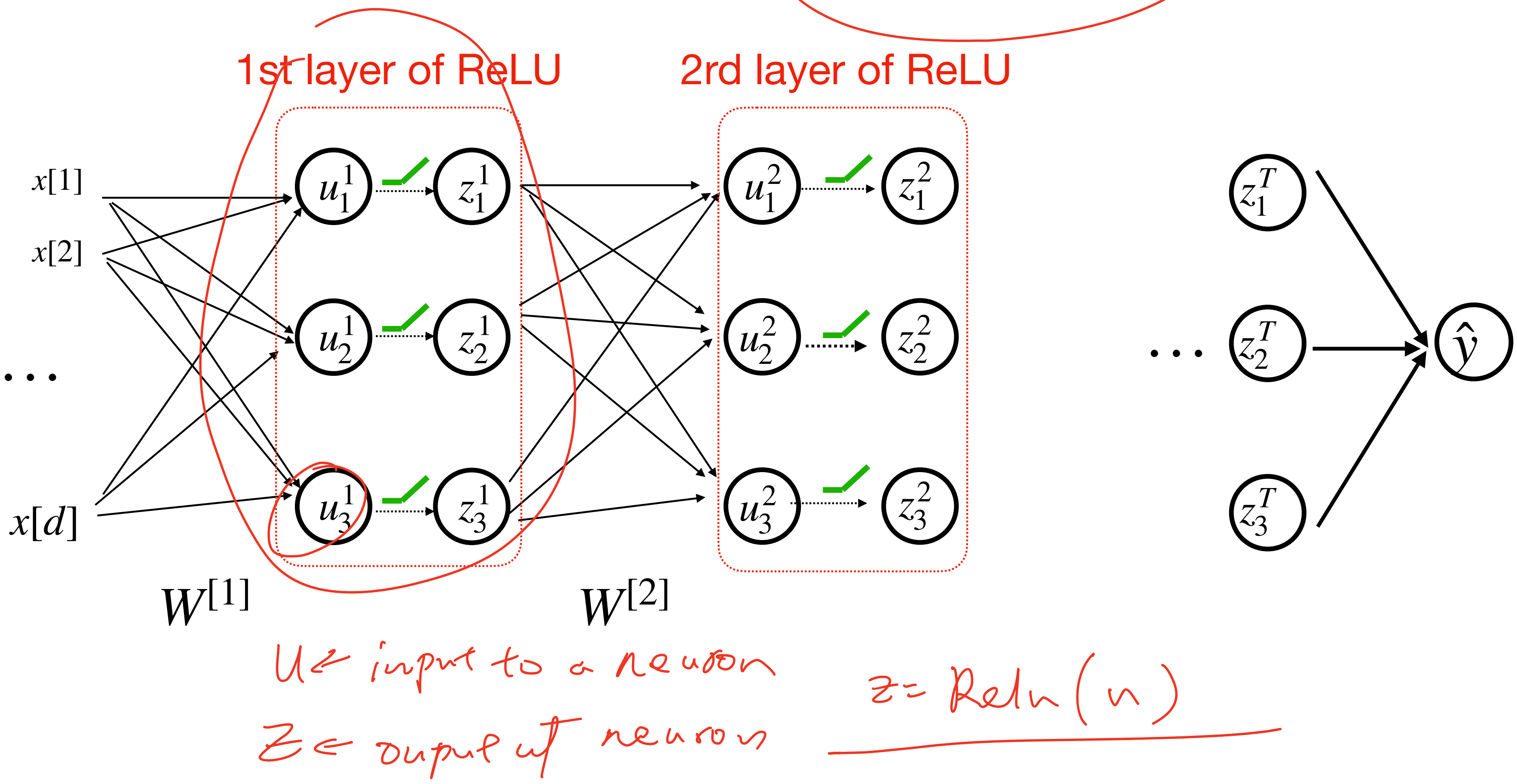
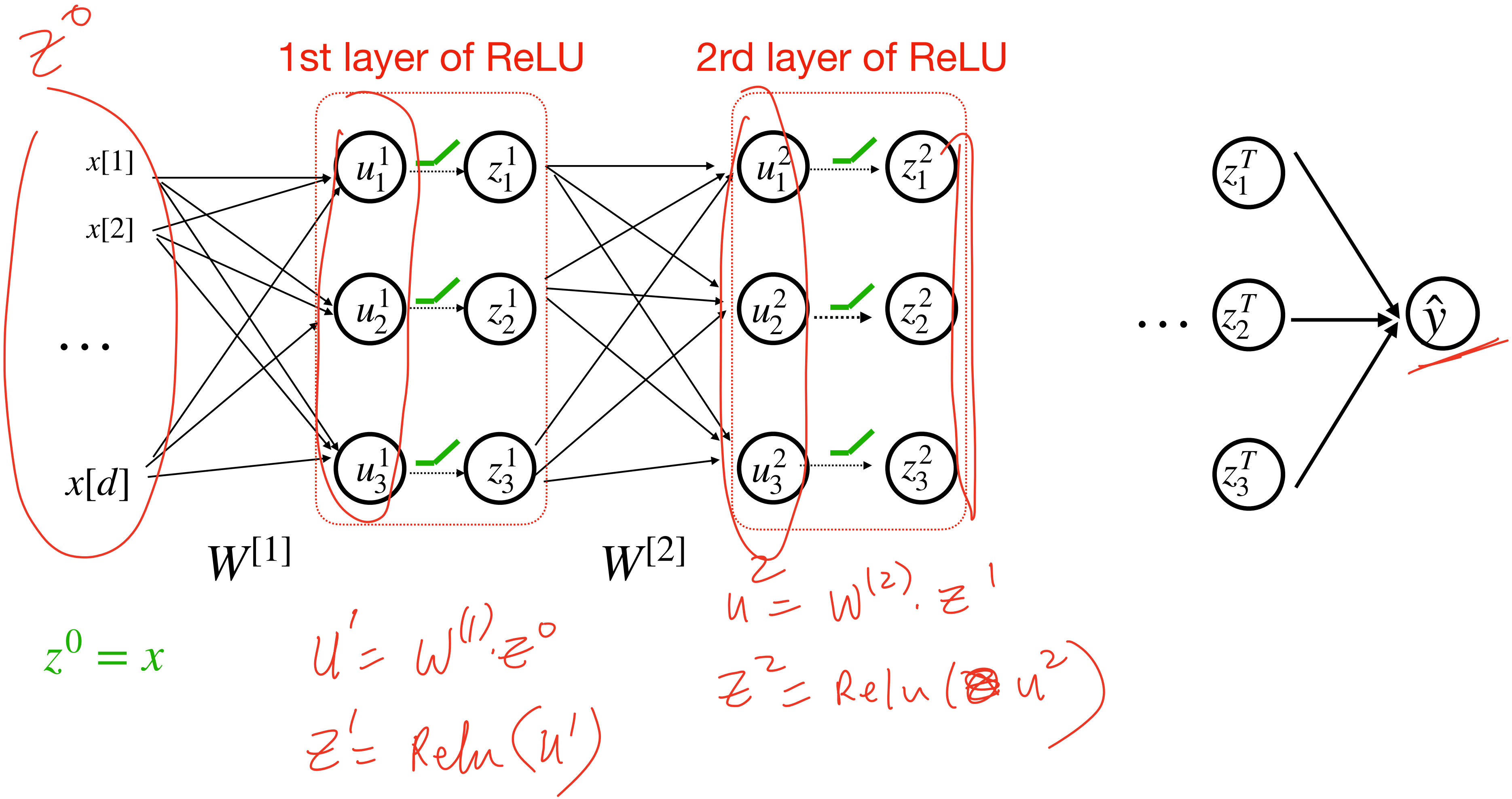


Compute derivatives

A Forward Pass: from $t = 0$ to T



A Forward Pass: from $t = 0$ to T



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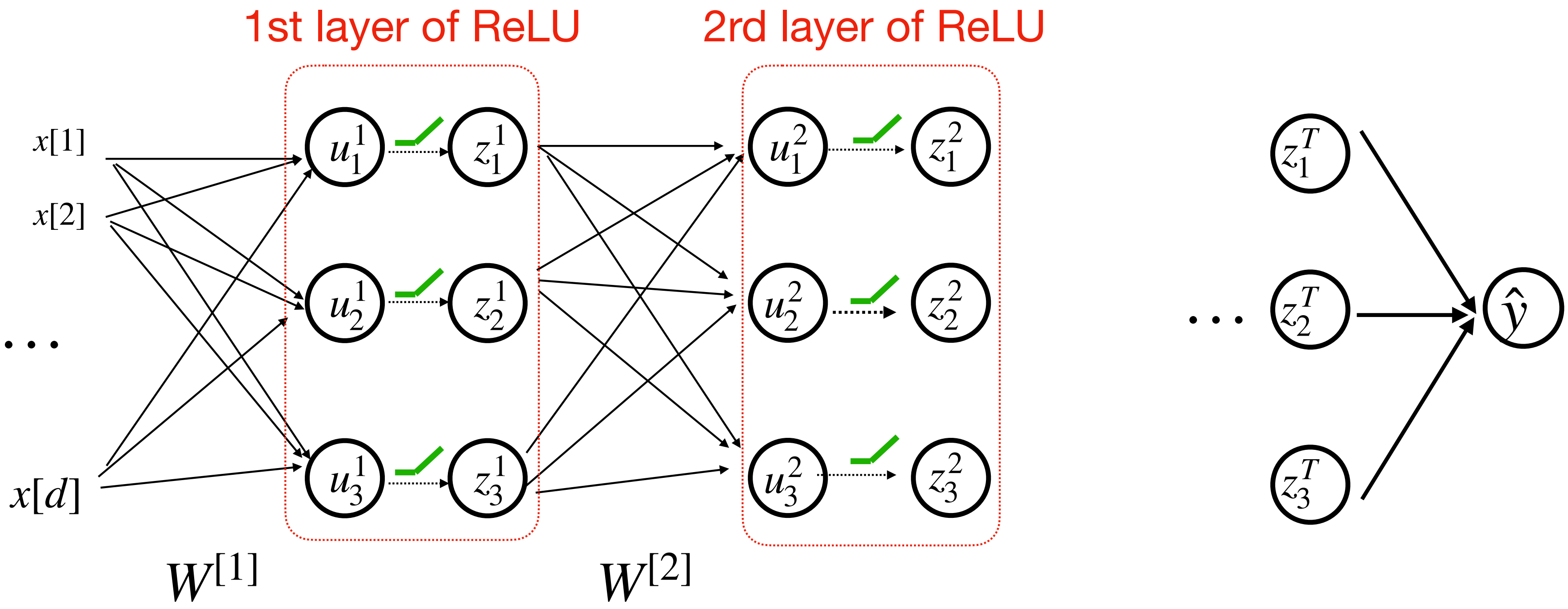
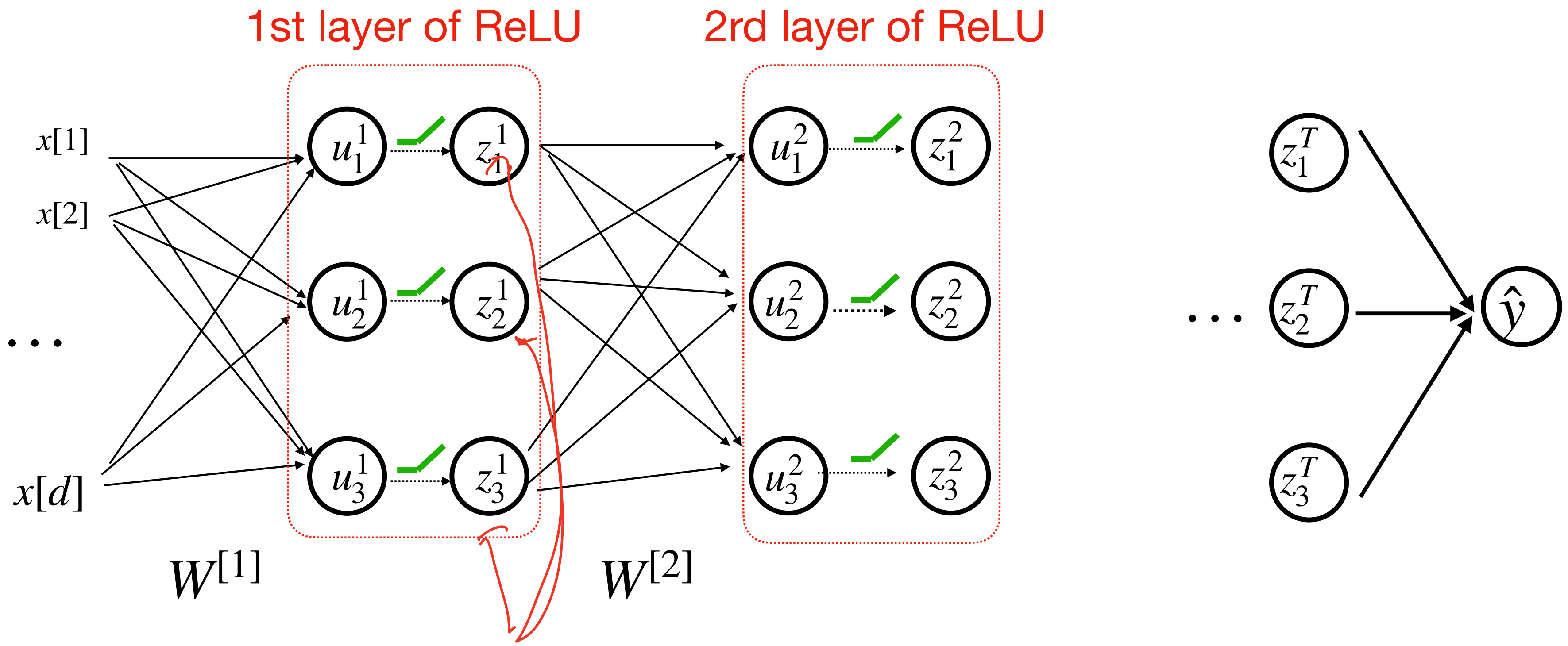


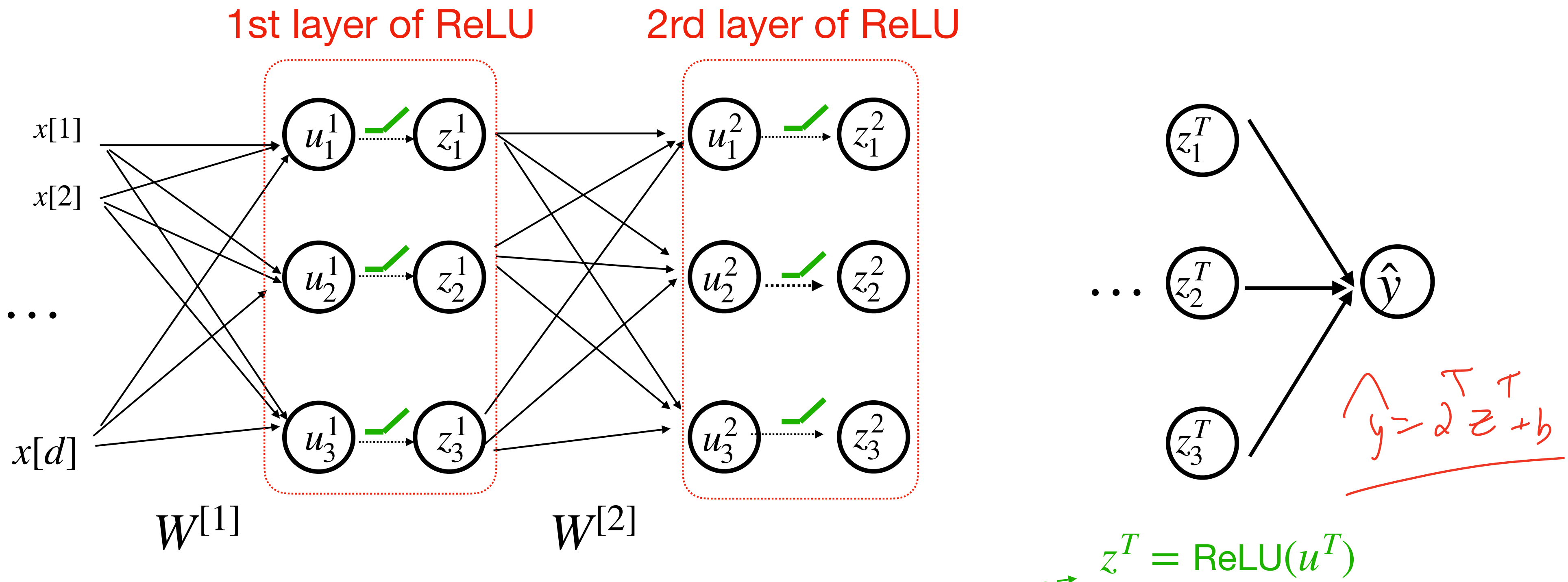
$z^0 = x$ $\quad$ $u^1 = W^{[1]} z^0$

A Forward Pass: from $t = 0$ to T



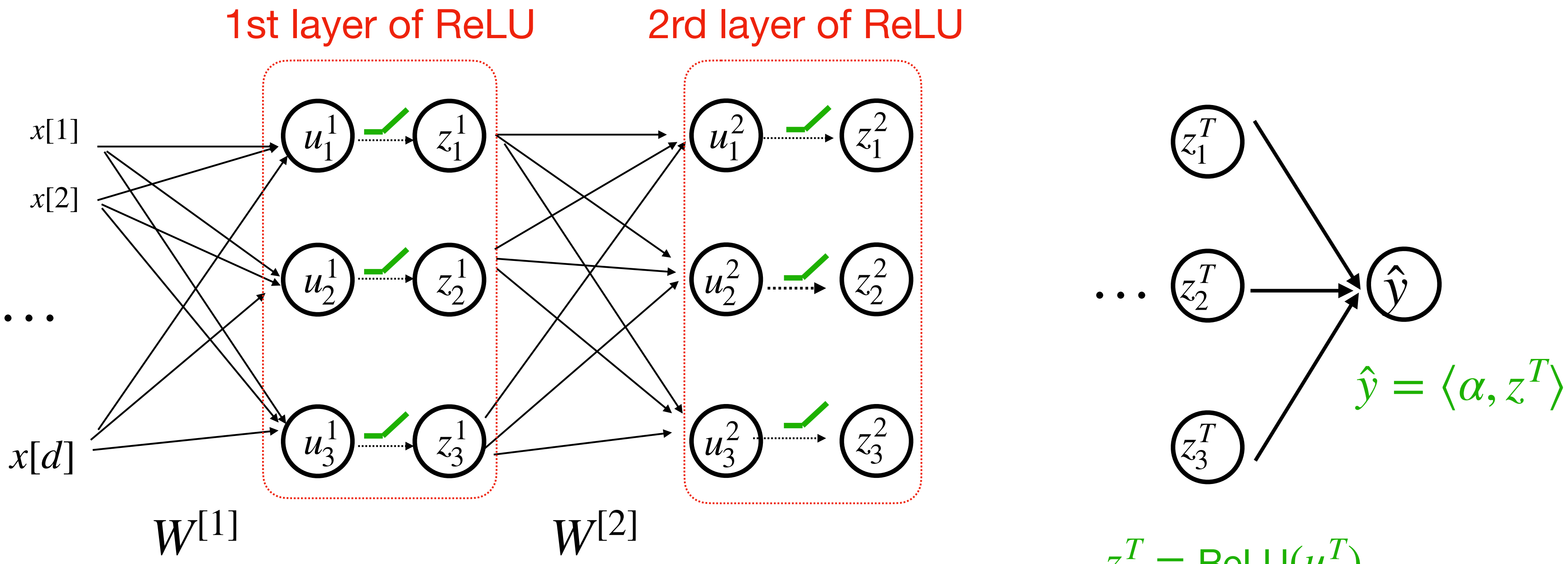
$z^0 = x$ $\quad u^1 = W^{[1]} z^0 \quad z^1 = \text{ReLU}(u^1)$

A Forward Pass: from $t = 0$ to T



$z^0 = x$ $u^1 = W^{[1]} z^0$ $z^1 = \text{ReLU}(u^1)$

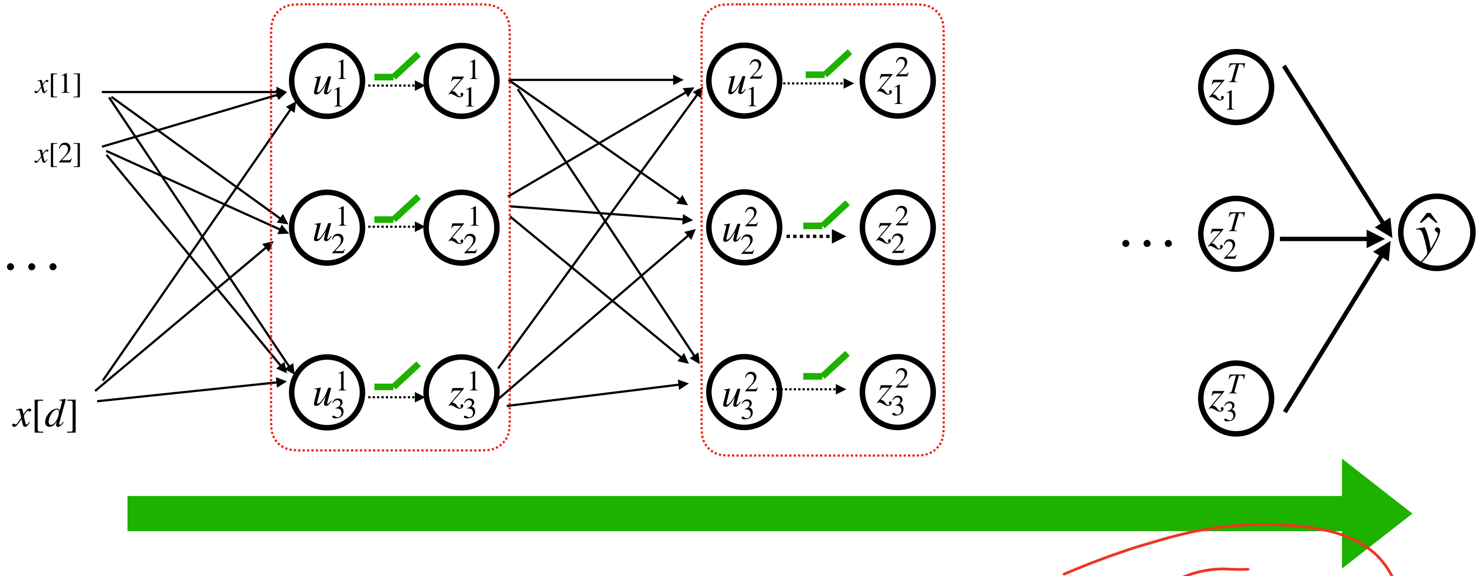
A Forward Pass: from $t = 0$ to T



$z^T = \mathrm{ReLU}(u^T)$

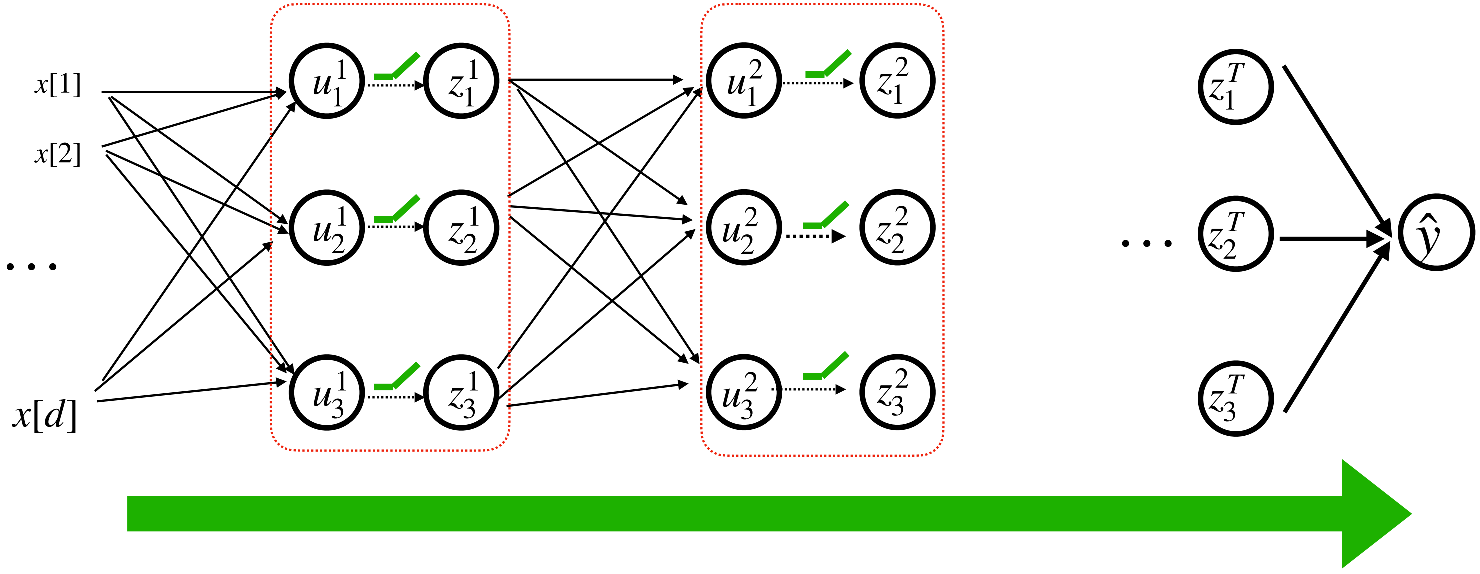
$z^0 = x$ $\quad u^1 = W^{[1]} z^0$ $\quad z^1 = \mathrm{ReLU}(u^1)$

Summary of the forward pass



All nodes' values (i.e., z, u, $\hat{y}$) are computed and stored

Summary of the forward pass



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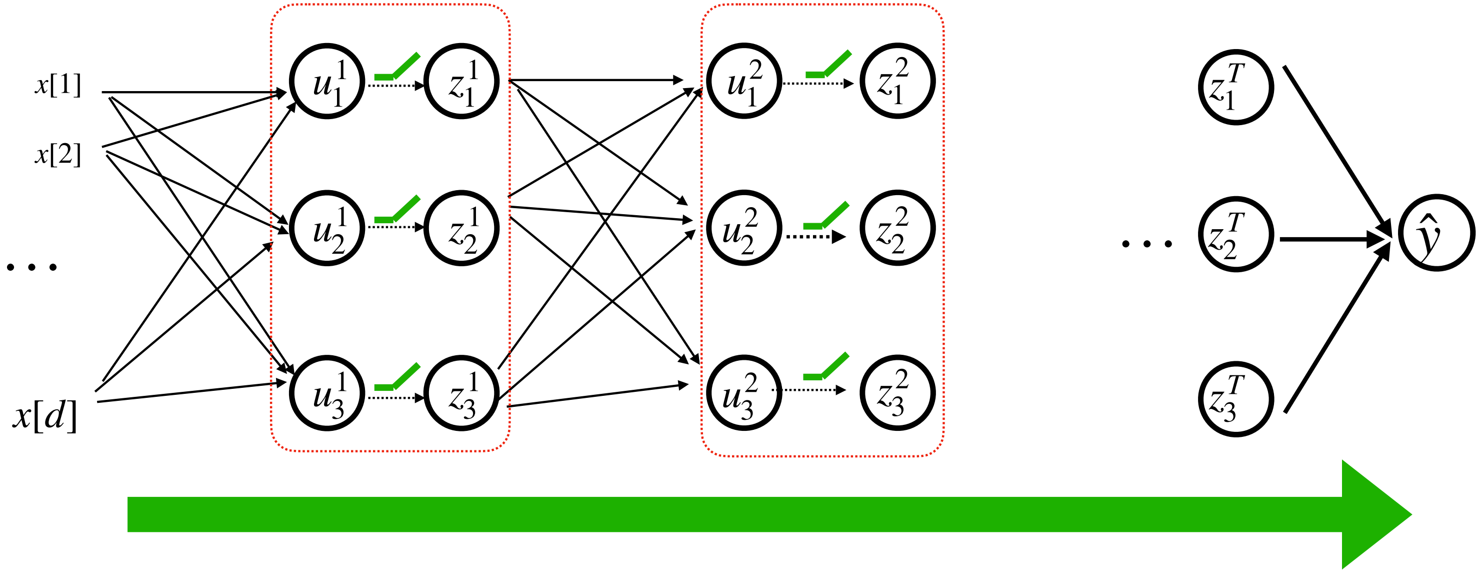
Summary of the forward pass



All nodes' values (i.e., z, u, $\hat{y}$) are computed and stored

Q: what is the computation complexity of the forward pass?

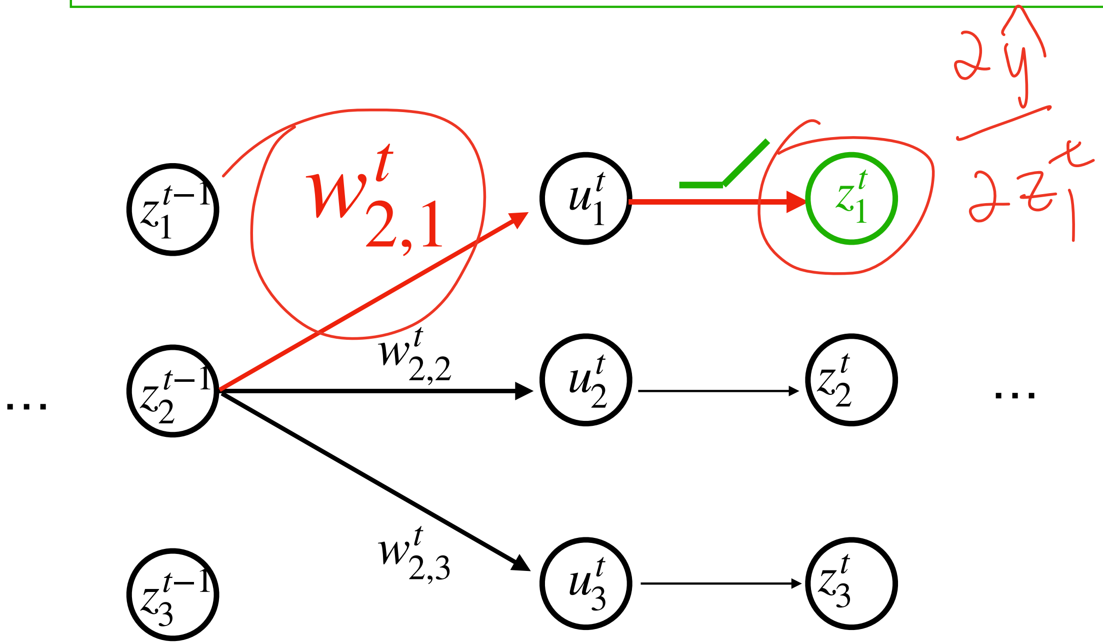
A: linear in # of Edges + # of nodes

The backward Pass

Claim: to compute $\partial \hat{y} / \partial w$, $\forall$ edge w, it suffices to compute $\partial \hat{y} / \partial z$, $\forall$ node z.

The backward Pass

Claim: to compute $\partial\hat{y}/\partial w, \forall$ edge w, it suffices to compute $\partial\hat{y}/\partial z, \forall$ node z.



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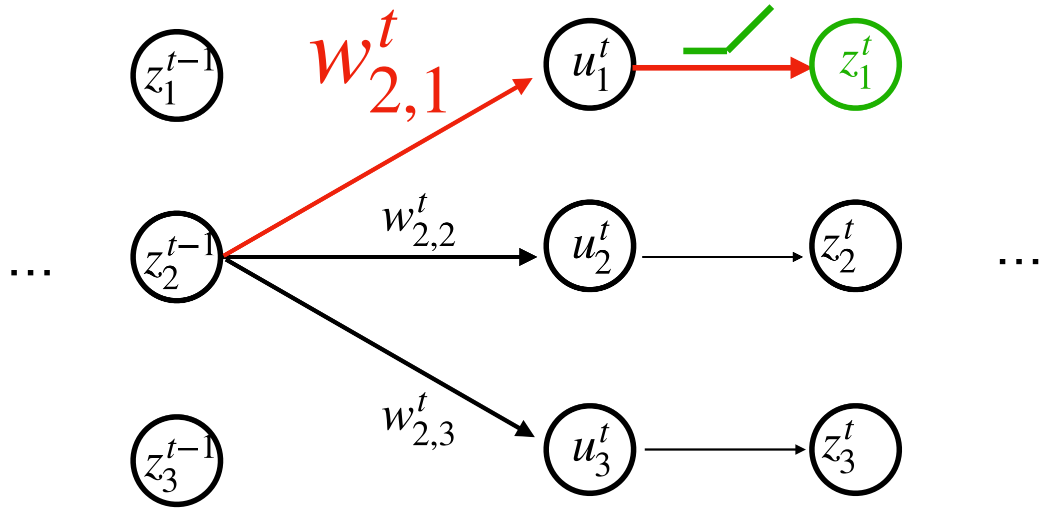

Proof:

WLOG consider $\partial \hat{y} / \partial w_{2,1}^t$

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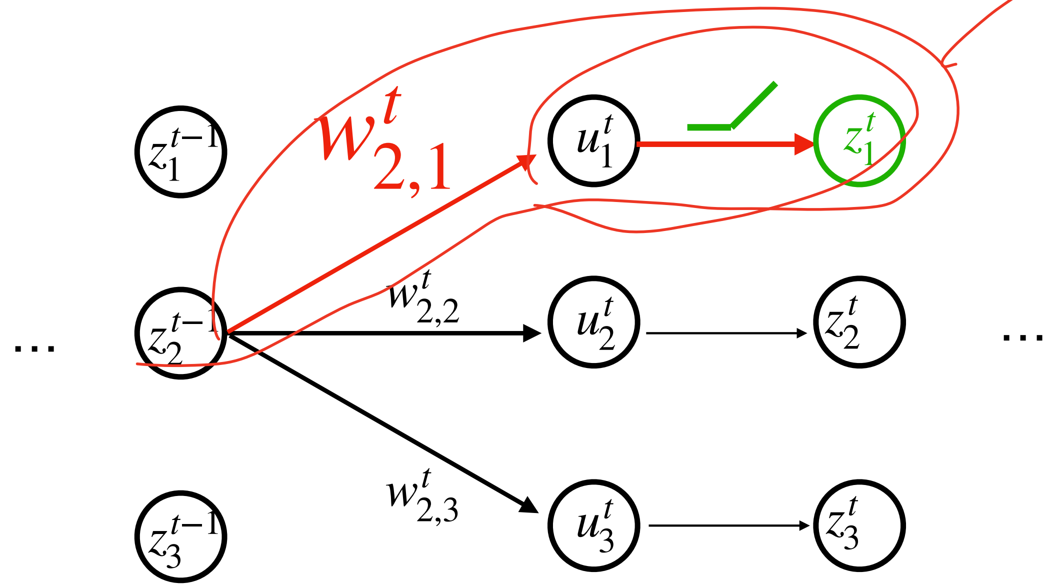
Claim: to compute $\partial\hat{y}/\partial w, \forall$ edge w, it suffices to compute $\partial\hat{y}/\partial z, \forall$ node z.



Proof:

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$$\partial\hat{y}/\partial w_{2,1}^t = \frac{\partial \hat{y}}{\partial z_1^t} \cdot \frac{\partial z_1^t}{\partial u_1^t} \cdot \frac{\partial u_1^t}{\partial w_{2,1}^t}$$

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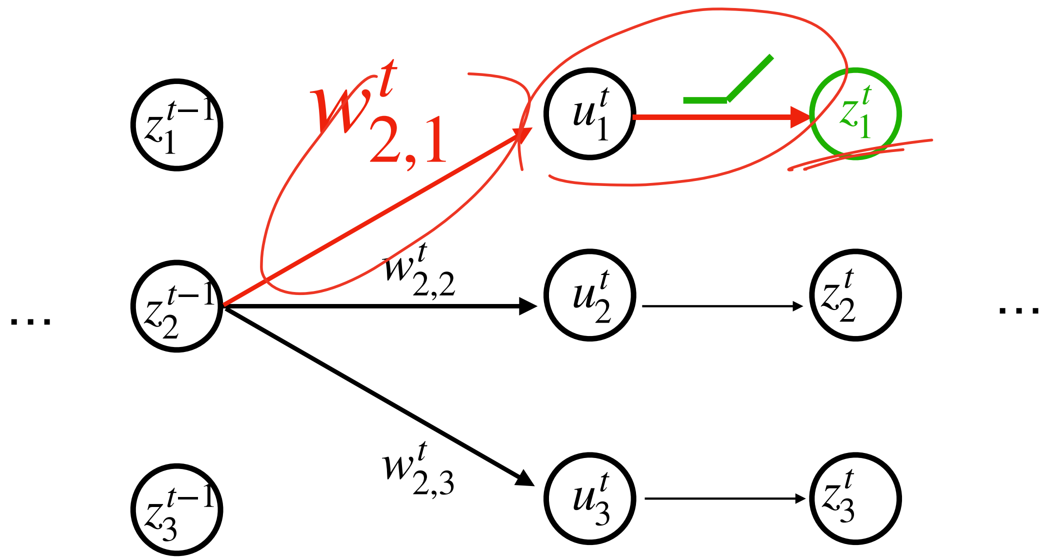

Proof:

WLOG consider $\partial\hat{y}/\partial w^t_{2,1}$

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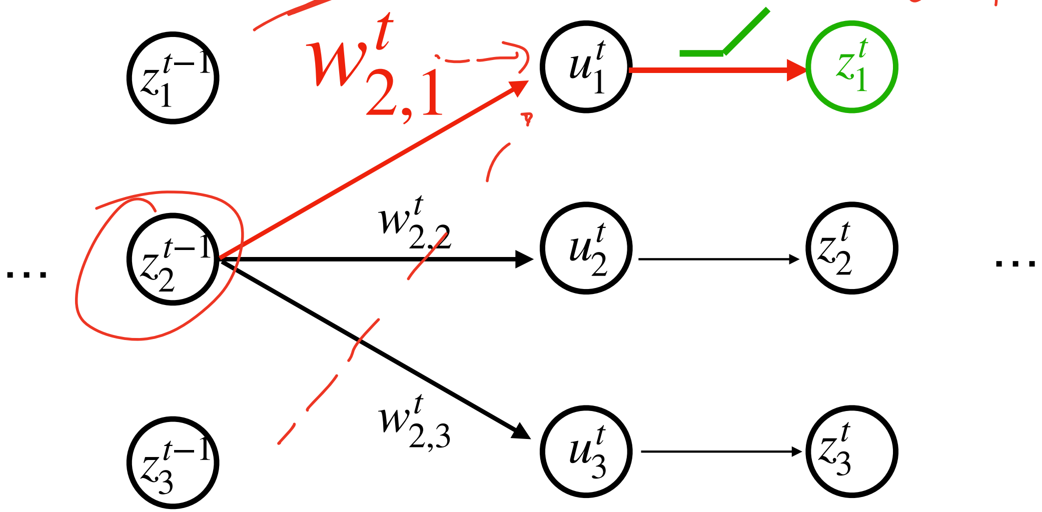
The backward Pass

$z_1^t = \mathrm{Relu}(u_1^t) := \sigma(u_1^t)$

Claim: to compute $\partial \hat{y} / \partial w, \forall$ edge w, it suffices to compute $\partial \hat{y} / \partial z, \forall$ node z.

$u_1^t = \sum \cdots + w_{2,1}^t z_2^{t-1} + \cdots \Rightarrow \frac{\partial u_1^t}{\partial w_{2,1}^t} = z_2^{t-1} \quad \frac{\partial z_1^t}{\partial u_1^t}$



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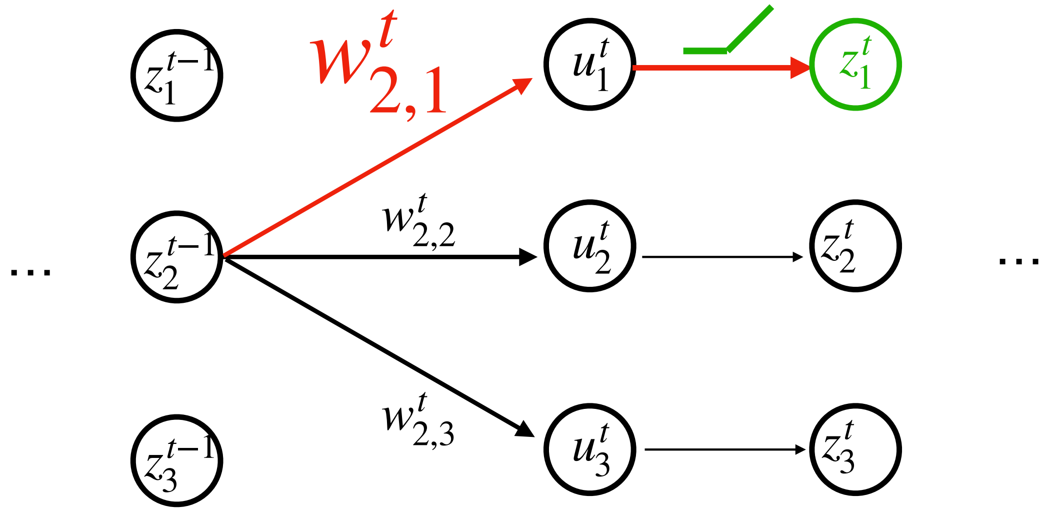
The backward Pass

Claim: to compute $\partial \hat{y}/\partial w, \forall$ edge w, it suffices to compute $\partial \hat{y}/\partial z, \forall$ node z.



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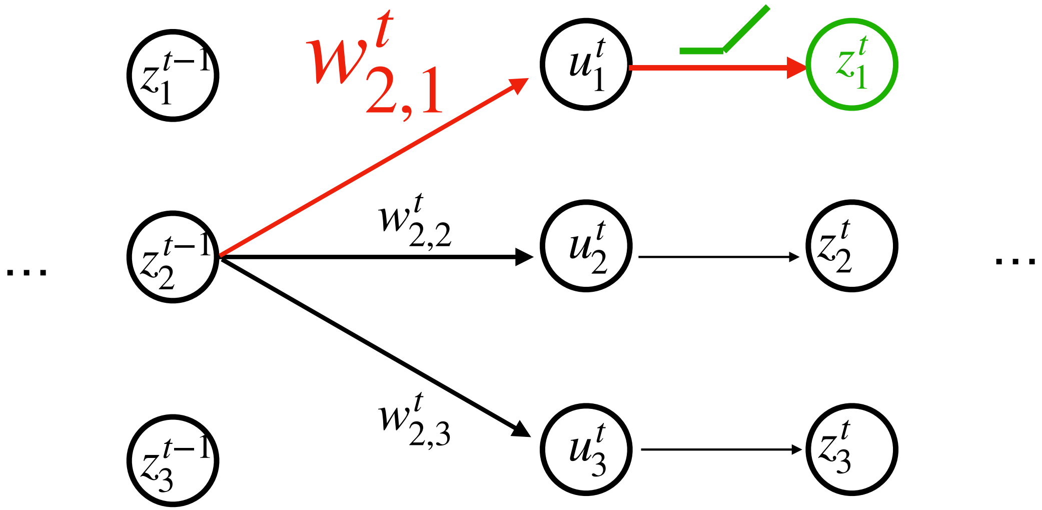
Given by assumption

The backward Pass

Claim: to compute $\partial \hat{y} / \partial w, \forall$ edge w, it suffices to compute $\partial \hat{y} / \partial z, \forall$ node z.



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Derivative of ReLU

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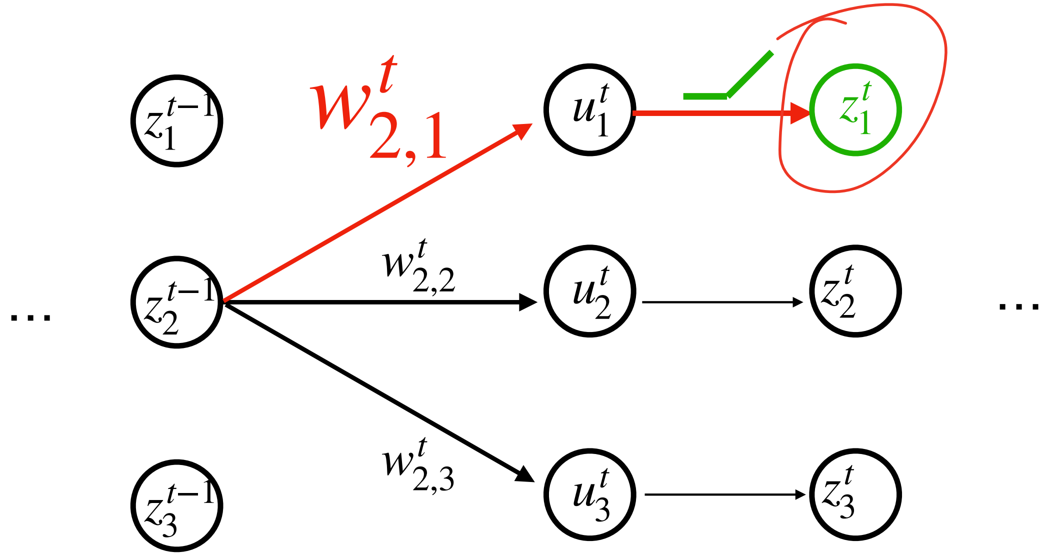


Proof:

WLOG consider $\partial \hat{y} / \partial w_{2,1}^t$

$$\partial \hat{y} / \partial w_{2,1}^t = \frac{\partial \hat{y}}{\partial z_1^t} \cdot \frac{\partial z_1^t}{\partial u_1^t} \cdot \frac{\partial u_1^t}{\partial w_{2,1}^t}$$

$$= \frac{\partial \hat{y}}{\partial z_1^t} \cdot \sigma'(u_1^t) \cdot z_2^{t-1}$$

Given by assumption

Derivative of ReLU

Known from forward pass

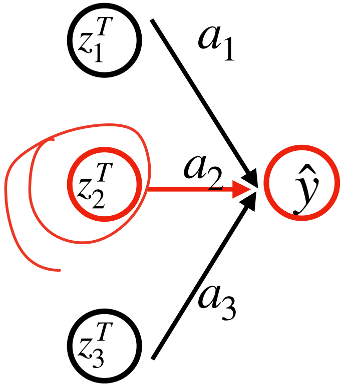
The backward Pass

We compute $\partial \hat{y}/\partial z^t$ backwards in time from $t = T$ to $t = 1$:

The backward Pass: base case

Base case: compute $\partial\hat{y}/\partial z^T$, for all node z at T-th Layer

$$\frac{\partial \hat{y}}{\partial z_2^T}$$



$$\hat{y} = z_1^T \cdot a_1 + z_2^T \cdot a_2 + z_3^T \cdot a_3$$

$$\frac{\partial \hat{y}}{\partial z_2^T} = a_2$$

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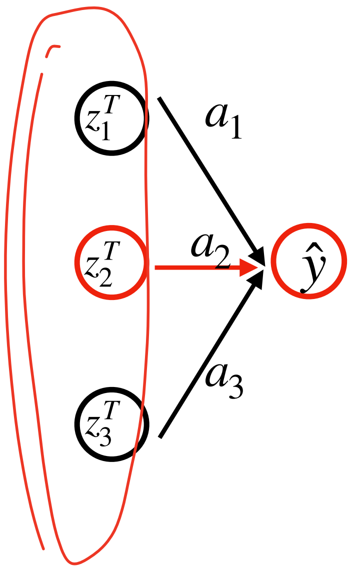
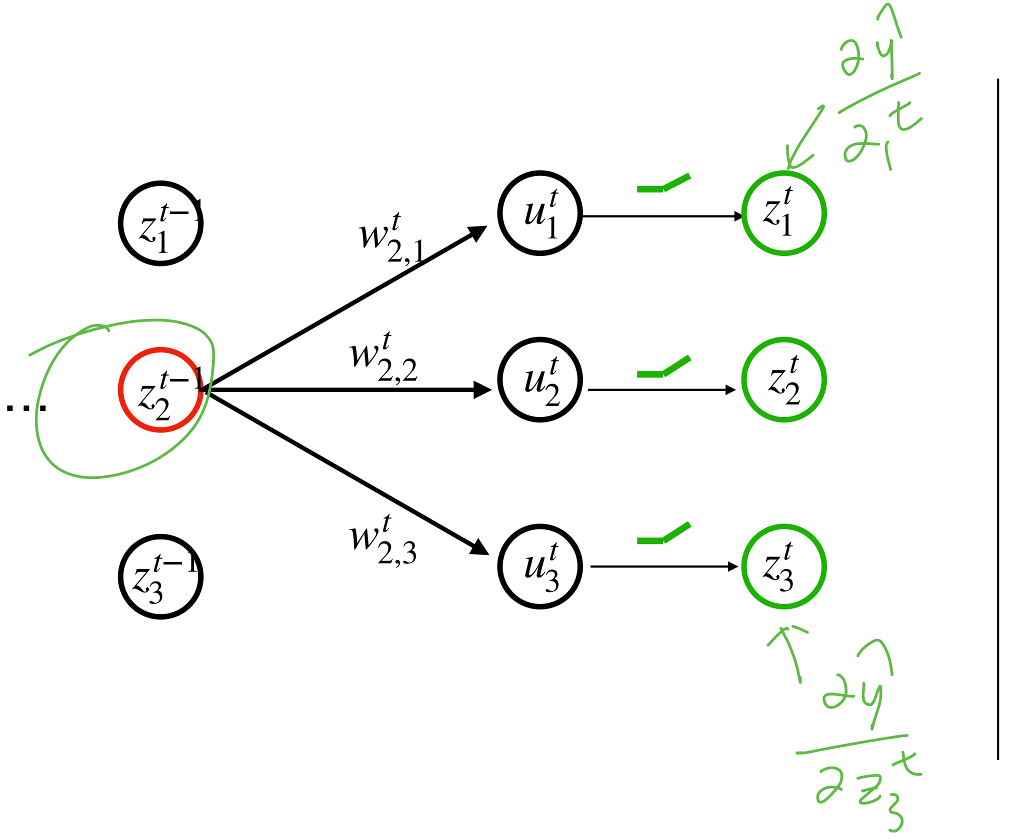
Base case: compute $\partial \hat{y} / \partial z^T$, for all node z at T-th Layer



$$\partial \hat{y} / \partial z_i^T = a_i$$

The backward Pass: induction step

Assume that we have computed $\partial \hat{y} / \partial z_i^t, \forall i$



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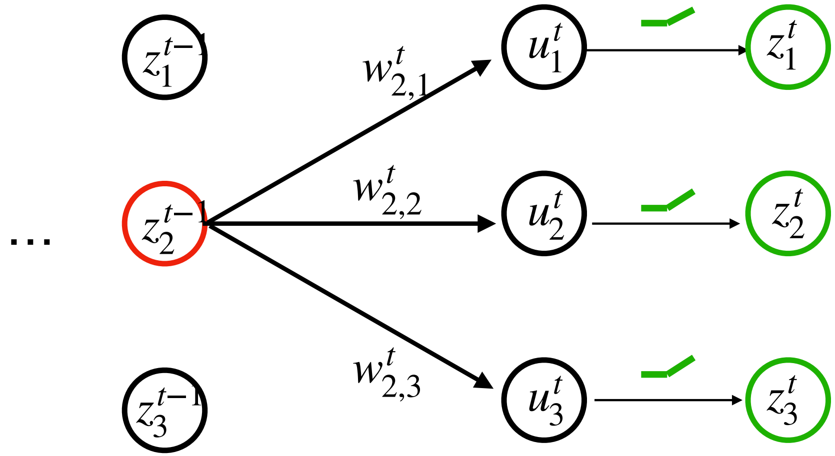

WLOG, consider $\partial \hat{y} / \partial z_2^{t-1}$

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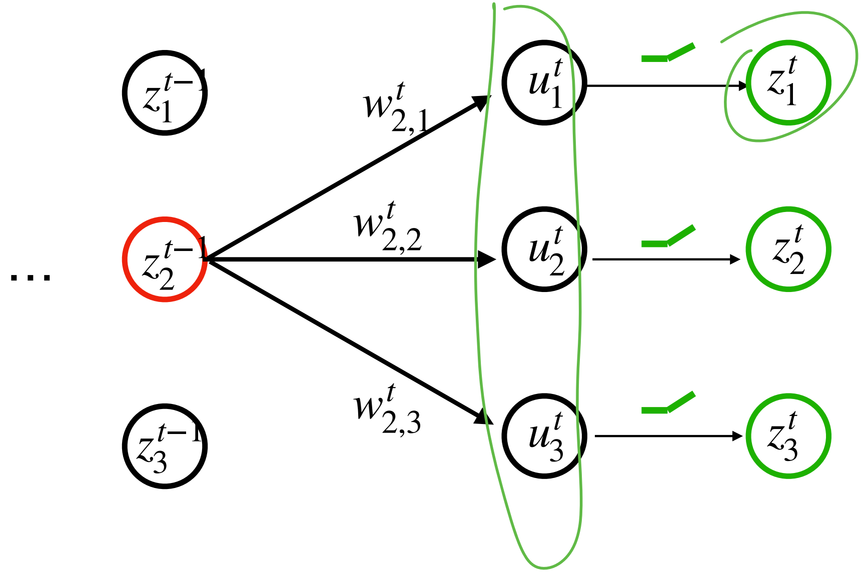

WLOG, consider $\partial \hat{y} \, / \partial z_2^{t-1}$

Step 1: for all i, $\dfrac{\partial \hat{y}}{\partial u_i^t} = \dfrac{\partial \hat{y}}{\partial z_i^t} \dfrac{\partial z_i^t}{\partial u_i^t}$

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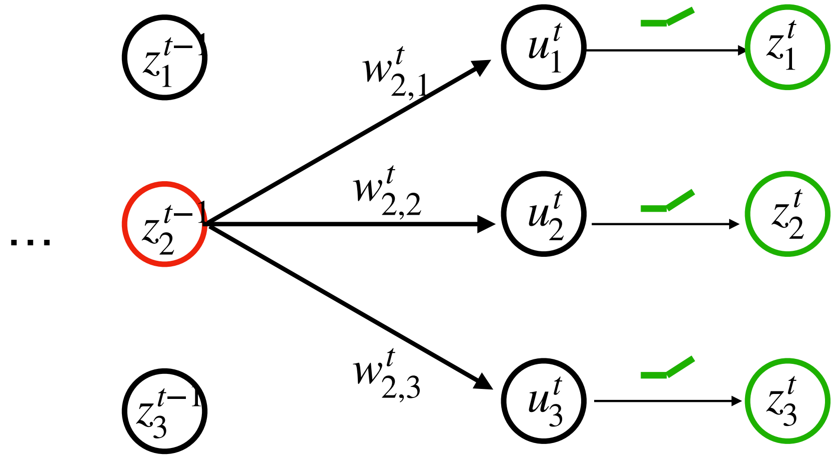

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$$= \frac{\partial \hat{y}}{\partial z_i^t} \cdot \sigma'(u_i^t)$$

(ReLU'(u_i^t))

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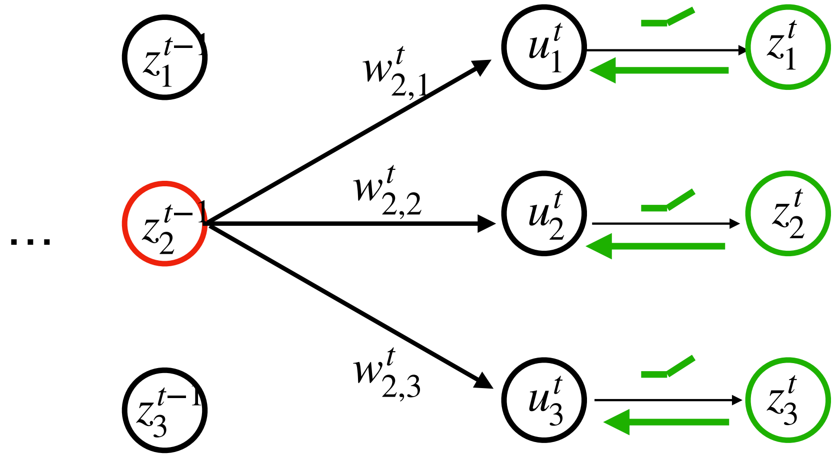

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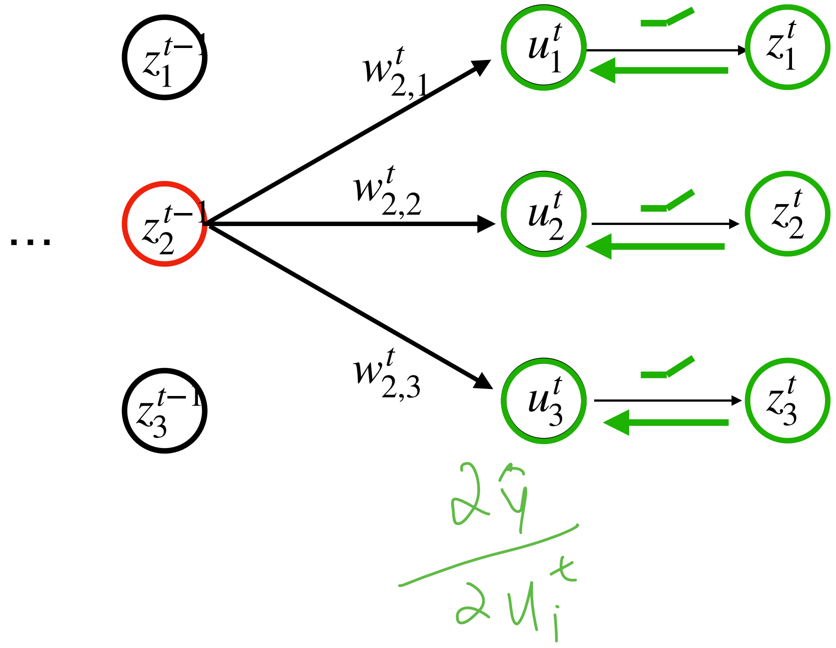

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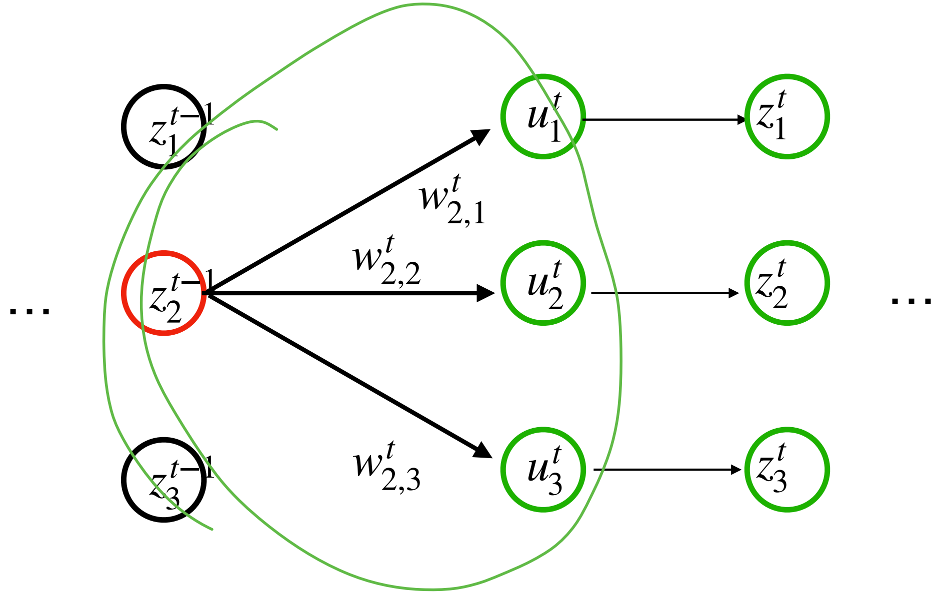

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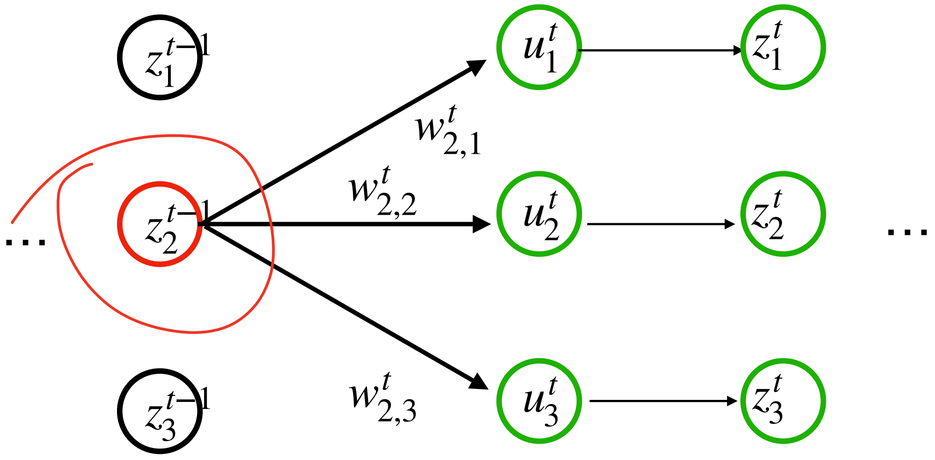


After step 1, we have $\partial \hat{y} / \partial u_i^t, \forall i$

Via multivariate chain rule:

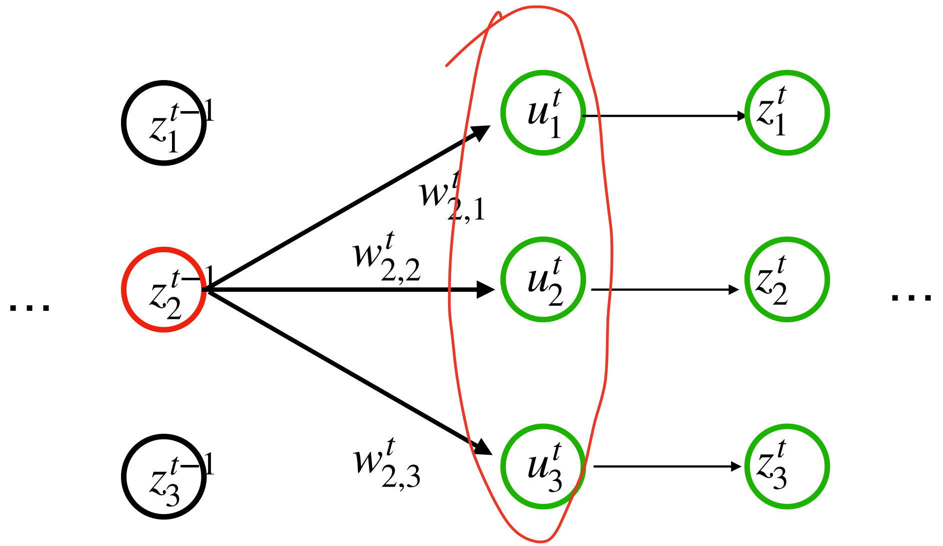
$$\hat{y} = f(u_1(x), u_2(x), u_3(x))$$

$$\frac{\partial \hat{y}}{\partial x} = \frac{\partial \hat{y}}{\partial u_1} \cdot \frac{\partial u_1}{\partial x} + \frac{\partial \hat{y}}{\partial u_2} \cdot \frac{\partial u_2}{\partial x} + \frac{\partial \hat{y}}{\partial u_3} \cdot \frac{\partial u_3}{\partial x}$$

The backward Pass: induction step

Assume that we have computed $\partial \ell / \partial z_i^t, \forall i$

$K=3$



After step 1, we have $\partial \hat{y} / \partial u_i^t, \forall i$

Via multivariate chain rule:

Step 2: $$\frac{\partial \hat{y}}{\partial z_2^{t-1}} = \sum_{i=1}^{K} \frac{\partial \hat{y}}{\partial u_i^t} \frac{\partial u_i^t}{\partial z_2^{t-1}}$$

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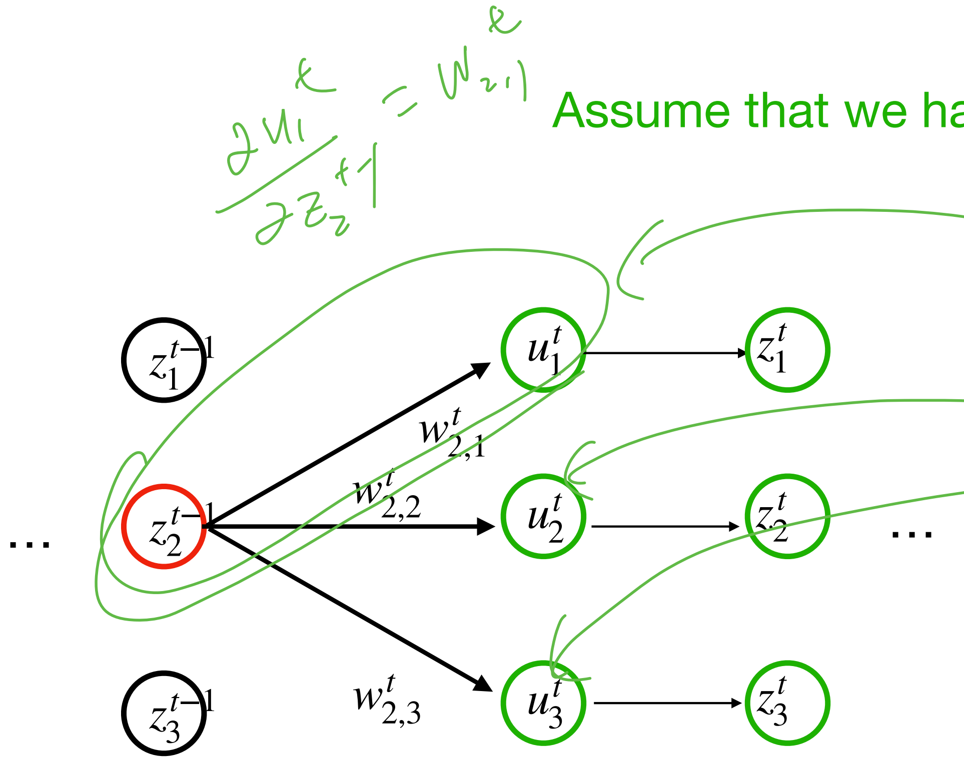
The backward Pass: induction step

Assume that we have computed $\partial \ell / \partial z_i^t, \forall i$



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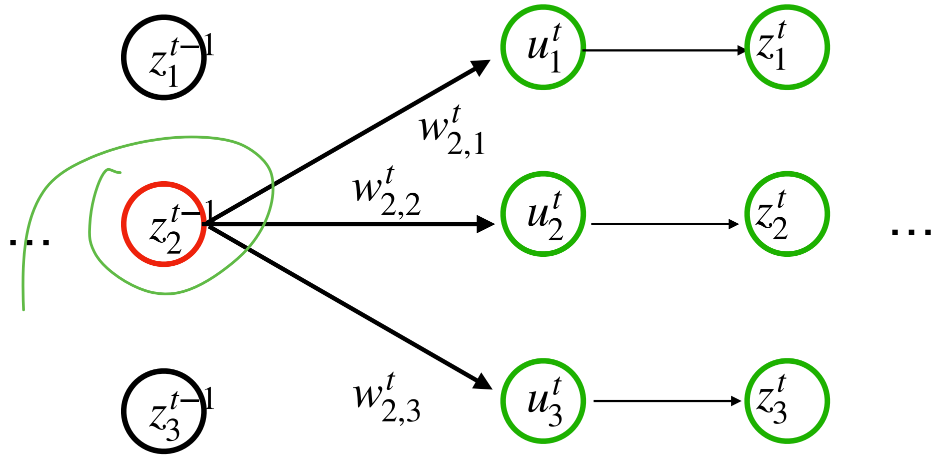
The backward Pass: induction step

Assume that we have computed $\partial \ell / \partial z_i^t, \forall i$



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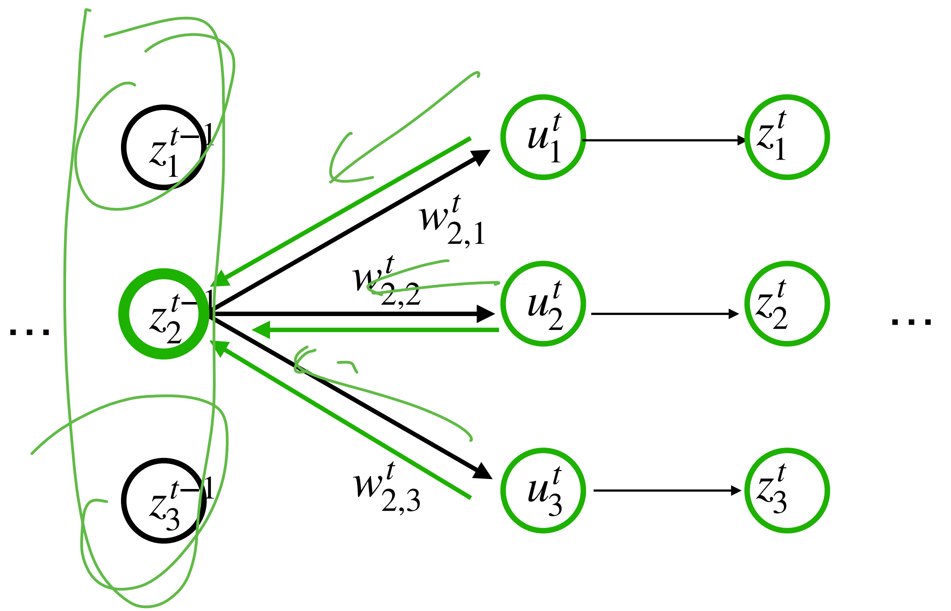
$$= \sum_{i=1}^{K} \frac{\partial \hat{y}}{\partial u_i^t} \cdot w_{2,i}^t$$

We are done at node z_2^{t-1}!

The backward Pass: induction step

Assume that we have computed $\partial \ell / \partial z_i^t, \forall i$



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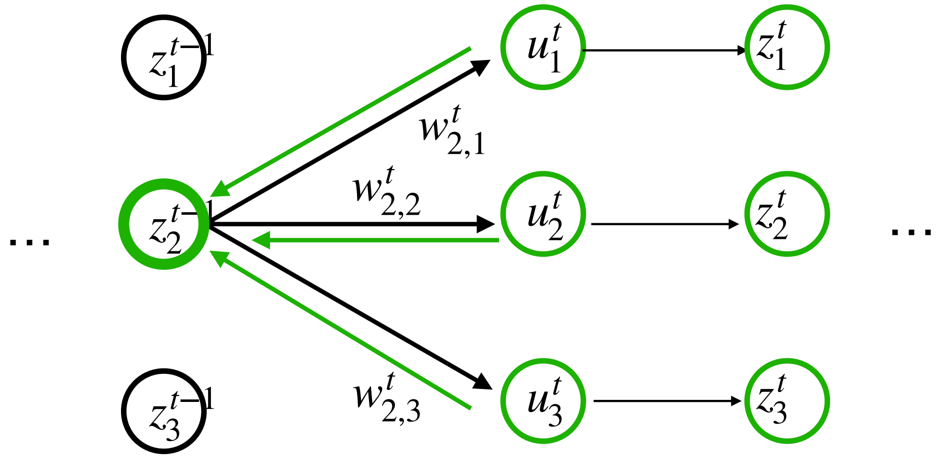

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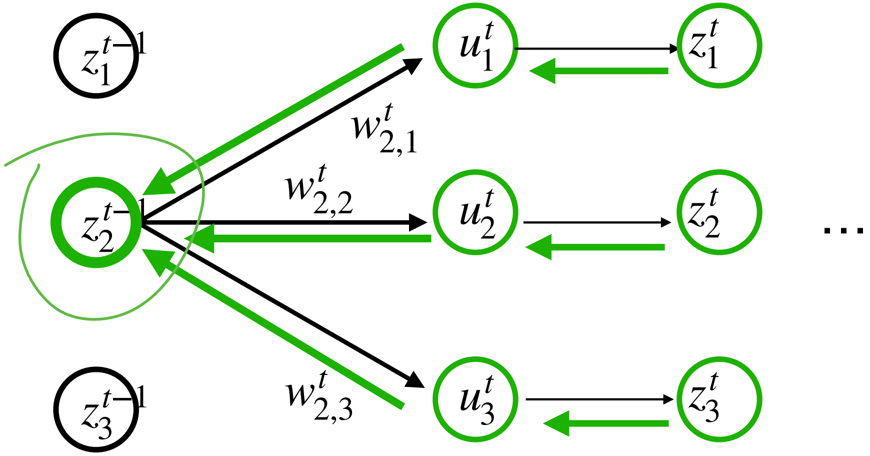
Repeat this for all $z_i^{t-1}, \forall i$

Summary of backward pass



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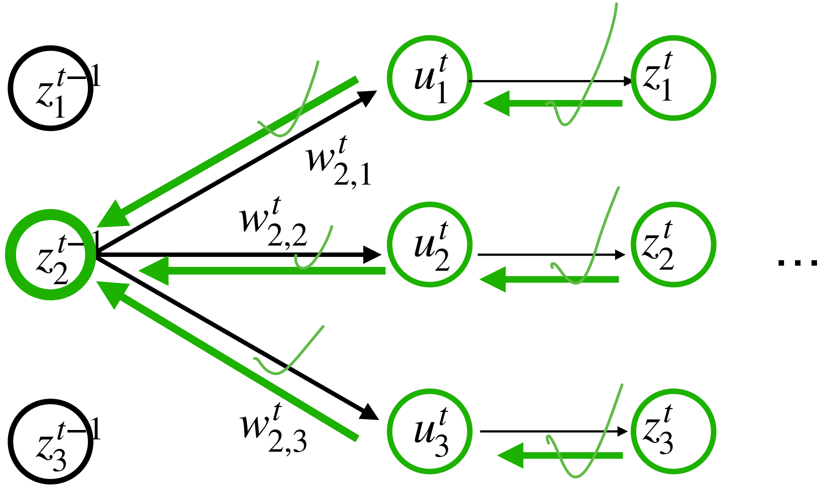

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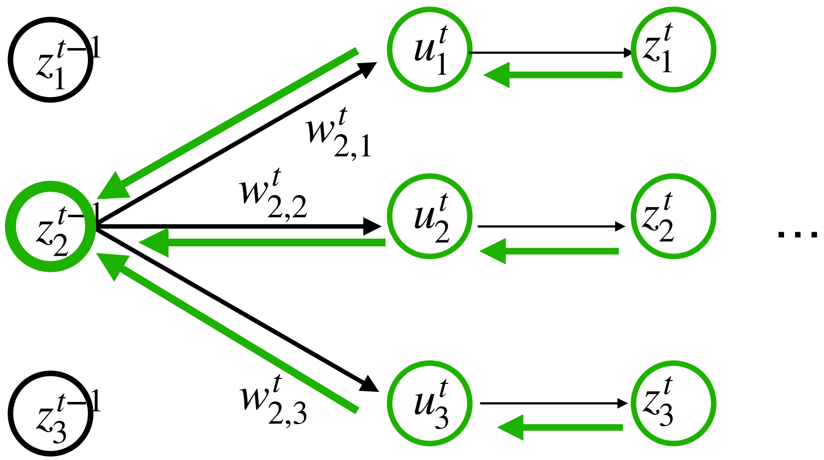

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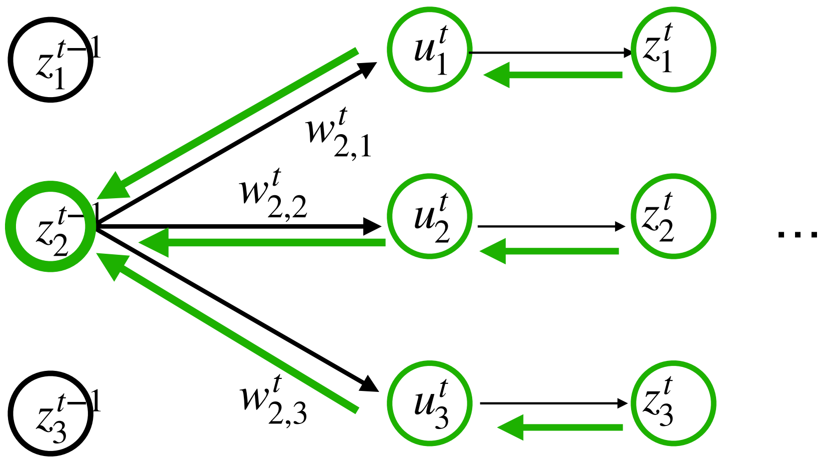

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Total computation: # of edges + # of nodes!

Exercise: can you express backward pass in matrix-vector format?

Summary for today

1. **Naively compute all derivatives wrt edges using chain rule takes $(E + V)^2$ time**

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2. Backpropagation: forward pass & backward pass takes $O(E+V)$ time

Forward pass: $x = z^0 \to u^1 \to z^1 \to \ldots \to z^t \to u^{t+1} \to z^{t+1} \ldots \to z^T \to \hat{y}$

Backward pass: $\frac{\partial \hat{y}}{\partial z^T} \to \frac{\partial \hat{y}}{\partial z^{T-1}} \to \ldots \frac{\partial \hat{y}}{\partial z^1}$