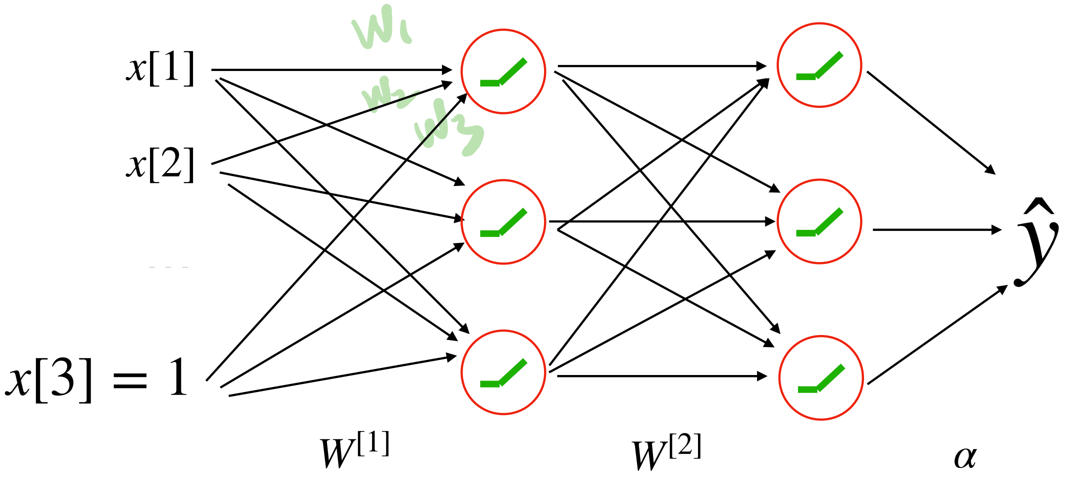
Neural Network:
Training & Backpropagation

Announcements

Recap

A two layer fully connected feedforward NN:



$$W^{[1]} = \begin{bmatrix} w_1 & w_2 & w_3 \\ & & \end{bmatrix}$$

$Relu(x) = \max\{x, 0\}$

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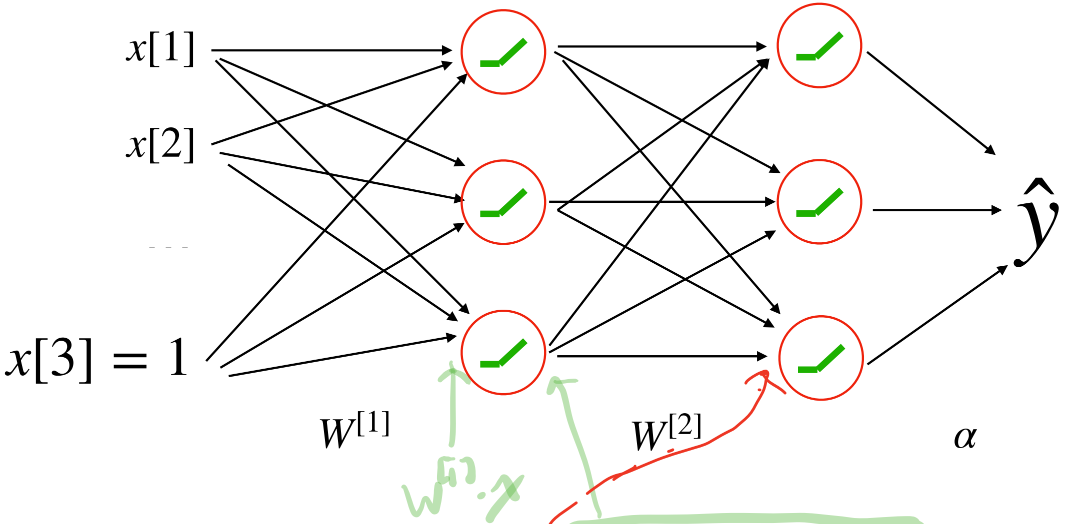

$$h(x) := \alpha^\top \mathrm{ReLU}\left(W^{[2]}\mathrm{ReLU}\left(W^{[1]}x\right)\right) + b$$

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)

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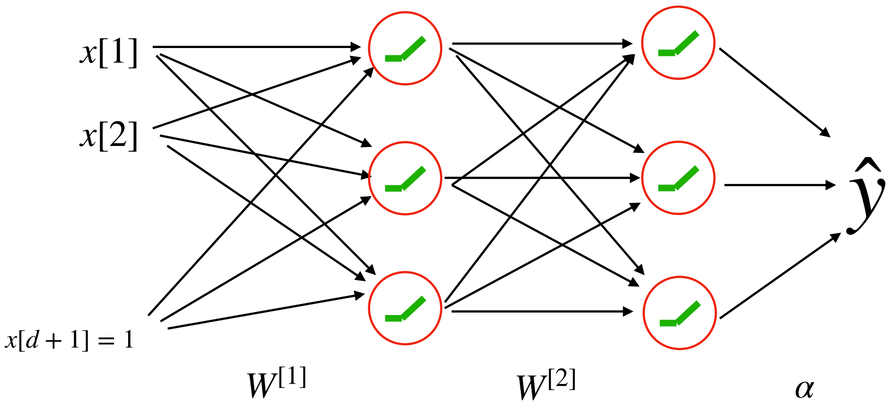

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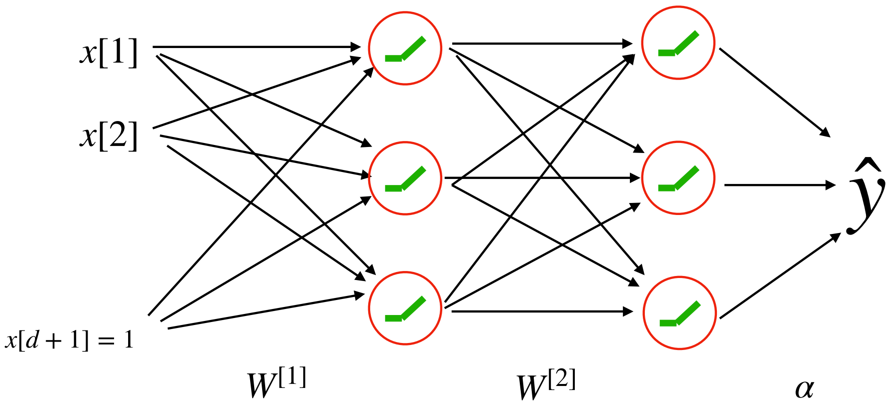

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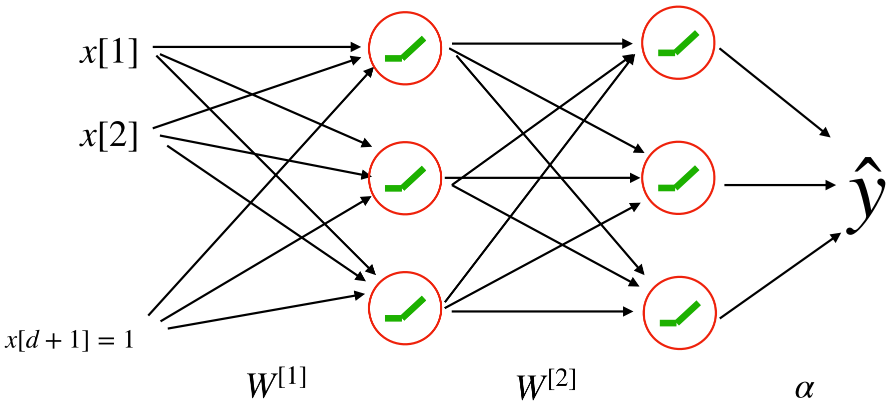

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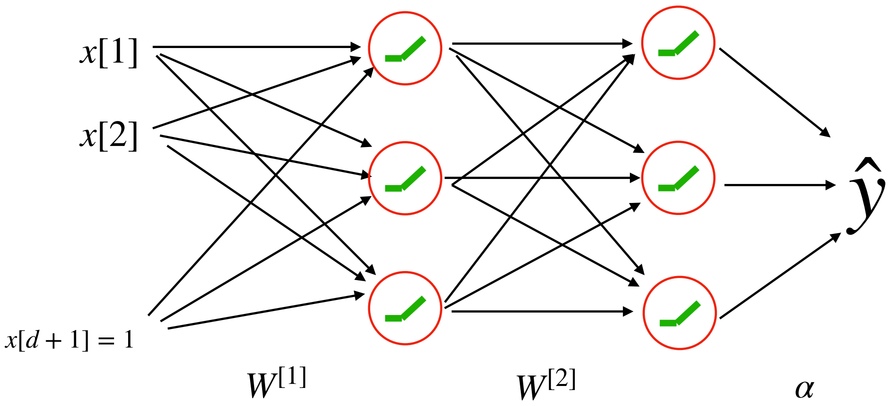

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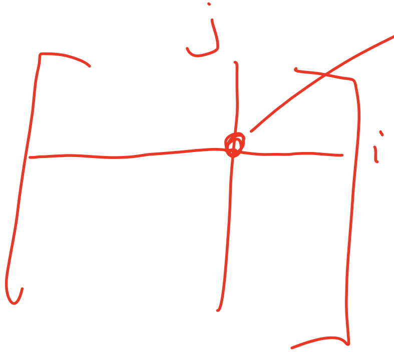
Compute gradients:

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

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

$\frac{\partial l}{\partial W^{[1]}} =$



$\frac{\partial l}{\partial W^{[1]}_{ij}}$

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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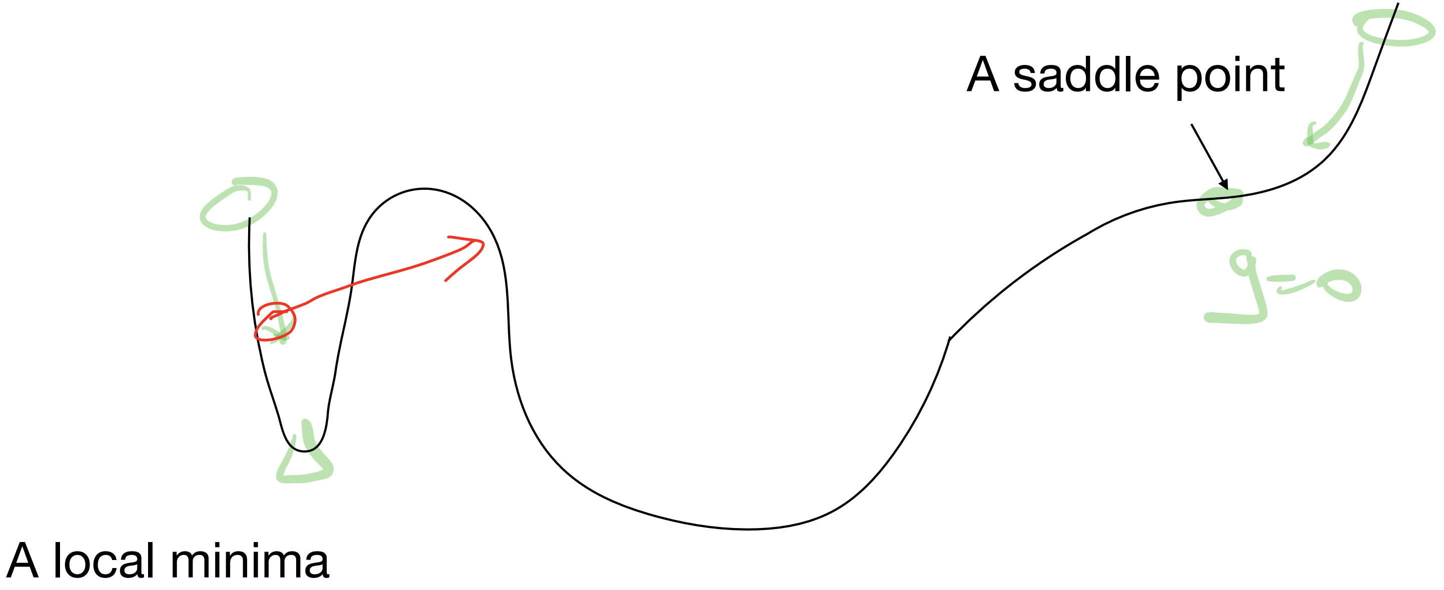
$\theta = \theta - \eta g$

Training neural network via SGD

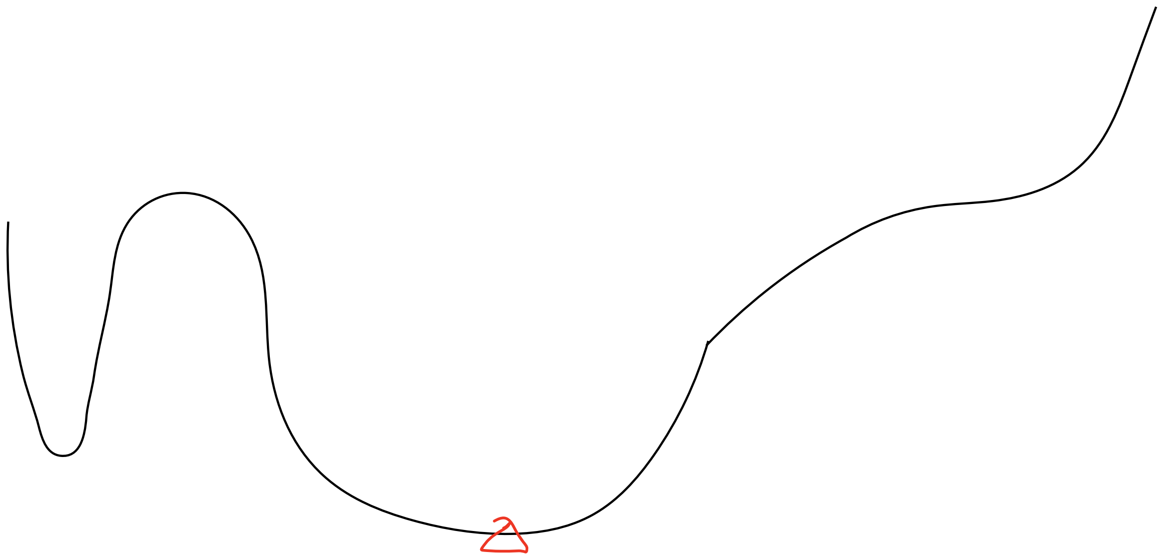
SGD helps avoiding local minima and saddle point



Training neural network via SGD

SGD tends to converge to a flat region

Training loss



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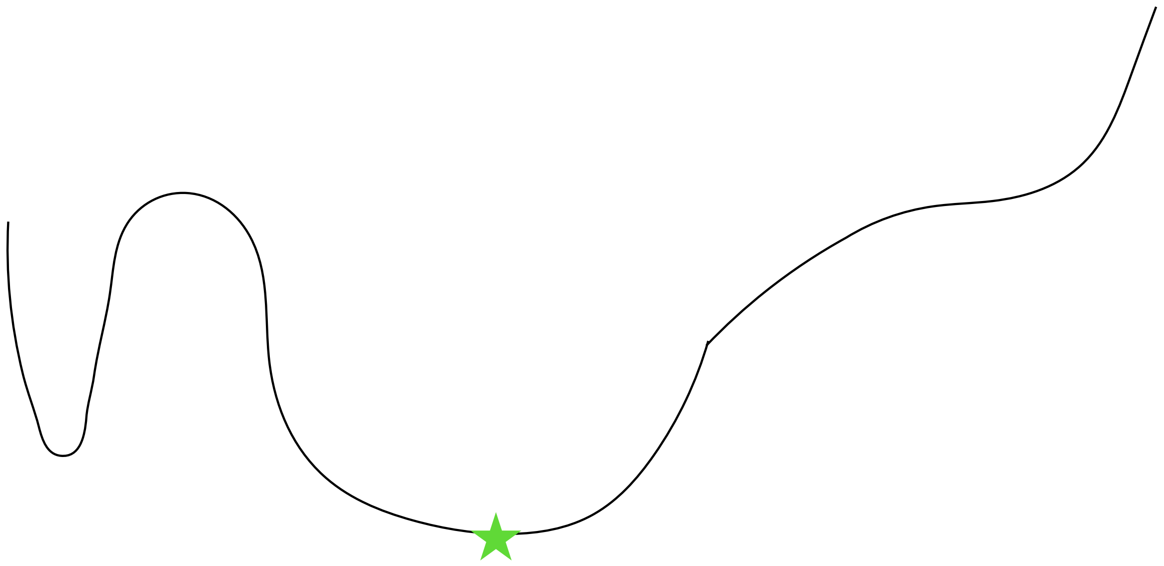

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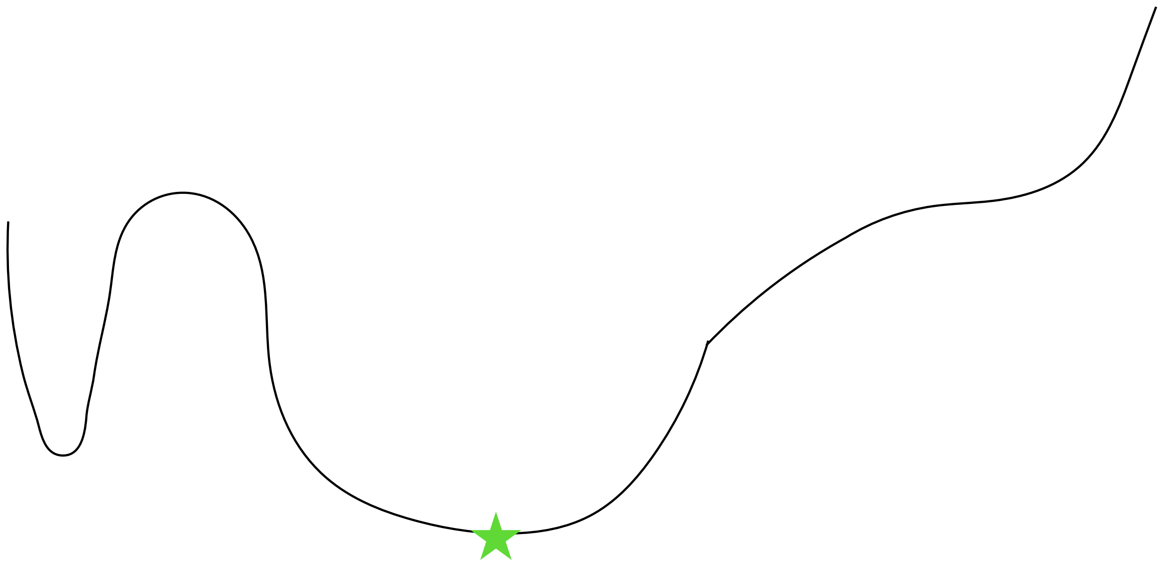

A flat local minima solution can help generalizes better to test data

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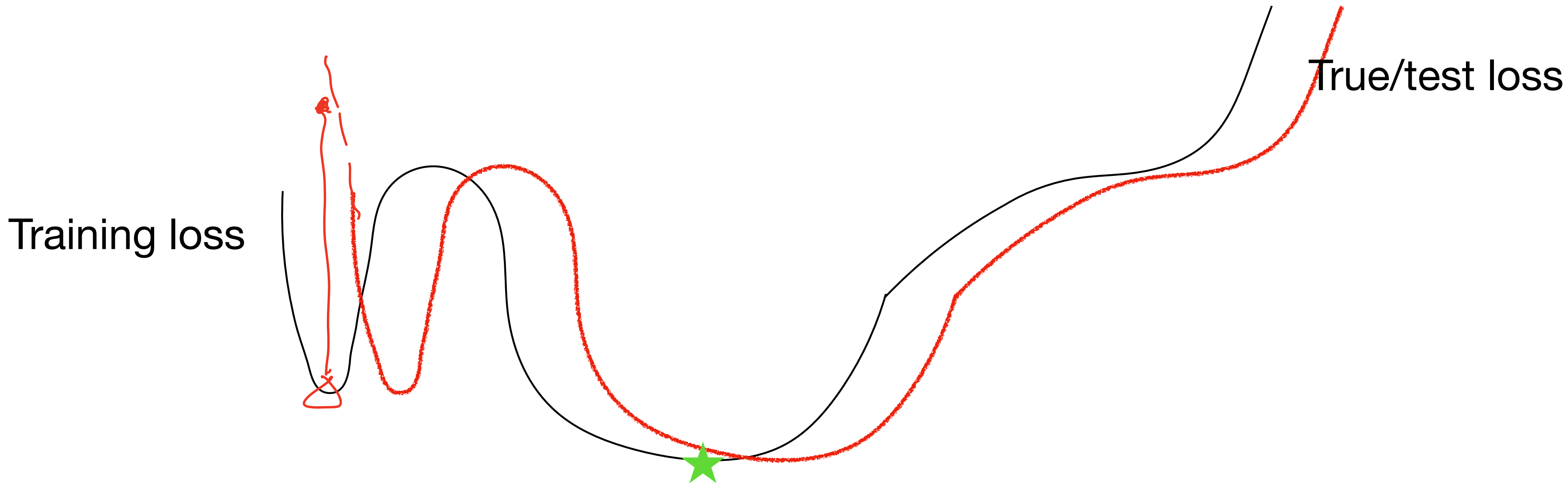

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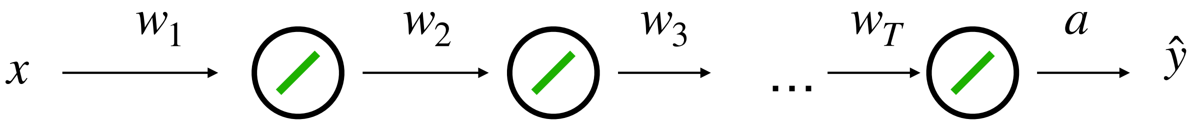
A naive algorithm

Consider the following one-dim case with identity transformation



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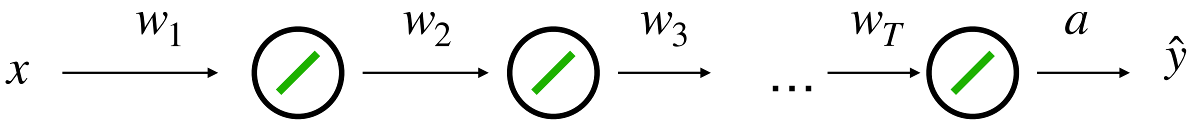

$$\hat{y} = a w_T \dots w_2 w_1 x$$

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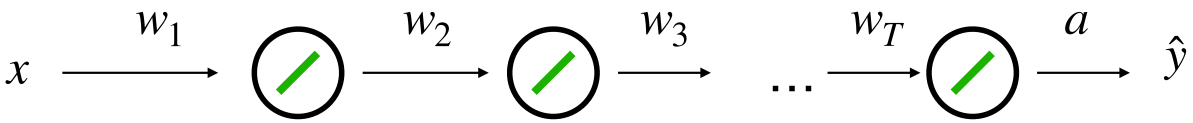

$l(\hat{y}, y)$

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

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

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

$\dfrac{\partial l}{\partial w_i}$

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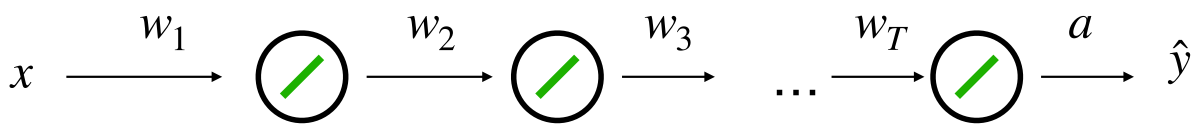

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Via chain rule: $\dfrac{\partial \ell}{\partial w_i} = \dfrac{\partial \ell}{\partial \hat{y}} \cdot \dfrac{\partial \hat{y}}{\partial w_i}$

A naive algorithm

$$x \xrightarrow{w_1} z_1 \xrightarrow{w_2} z_2 \xrightarrow{w_3} \cdots \xrightarrow{w_T} z_T \xrightarrow{a} \hat{y}$$

$z_0 = x$

$z_2 = w_2 z_1$

$z_1 = w_1 x = w_1 z_0$

A naive algorithm

$$
\begin{tikzcd}
x \arrow[r, "w_1"] & \boxed{z_1} \arrow[r, "w_2"] & \boxed{z_2} \arrow[r, "w_3"] & \cdots \arrow[r, "w_T"] & \boxed{z_T} \arrow[r, "a"] & \hat{y}
\end{tikzcd}
$$

$z_0 = x$ $\qquad$ $z_2 = w_2 z_1$

Via chain rule:

$$\frac{\partial \hat{y}}{\partial w_1} = \frac{\partial \hat{y}}{\cancel{\partial z_T}} \cdot \frac{\cancel{\partial z_T}}{\cancel{\partial z_{T-1}}} \cdot \frac{\cancel{\partial z_{T-1}}}{\cancel{\partial z_{T-2}}} \cdots \frac{\cancel{\partial z_1}}{\partial w_1}$$

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$$\frac{\partial \hat{y}}{\partial w_T}$$

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Total complexity:

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

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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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What we got:

Able to compute gradient in running time $O\left((\text{size of graph})^2\right)$

Can we do better in running time?

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3. Backpropagation: efficient way of computing gradients

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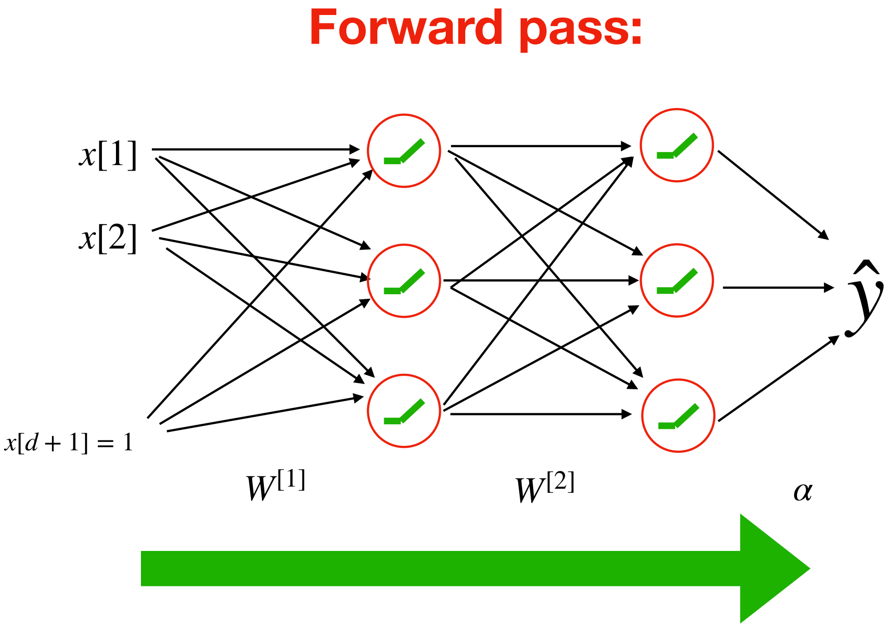
…the algorithm propagated measures of the errors produced by the network's guesses **backwards through its neurons, starting with those directly connected to the outputs.**

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



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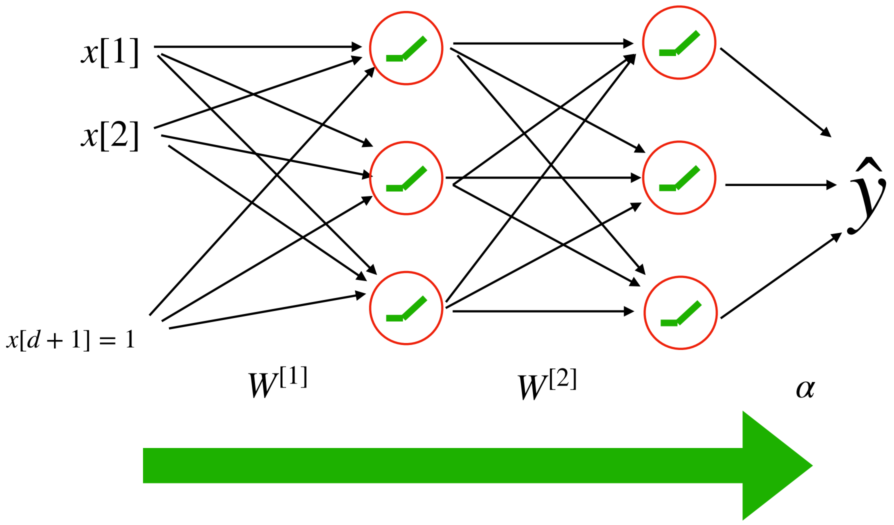

Store input & output of all neurons

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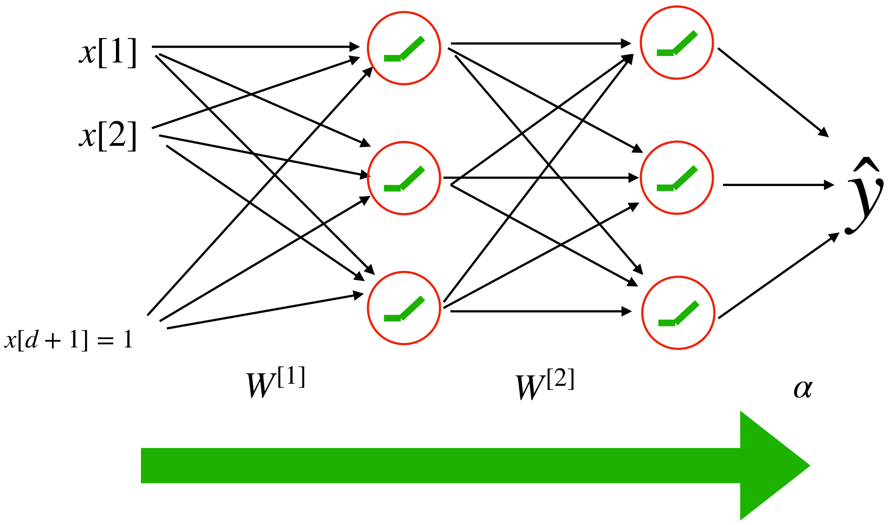

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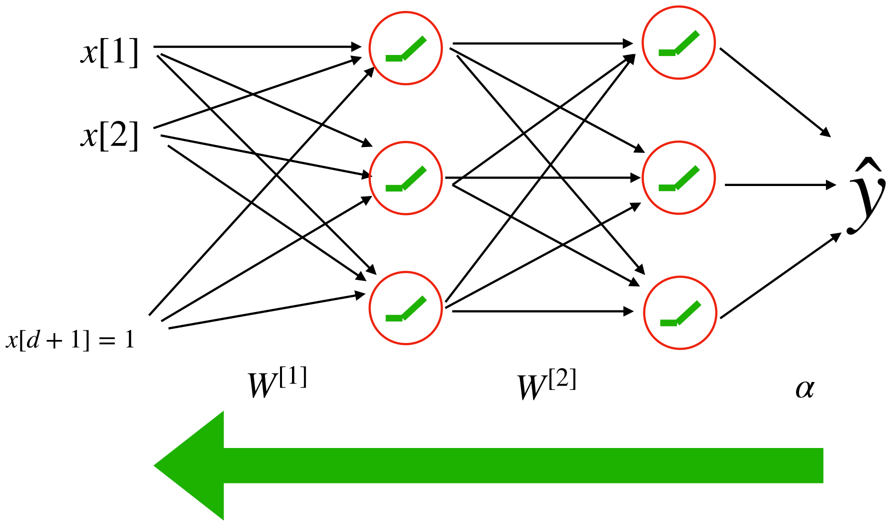

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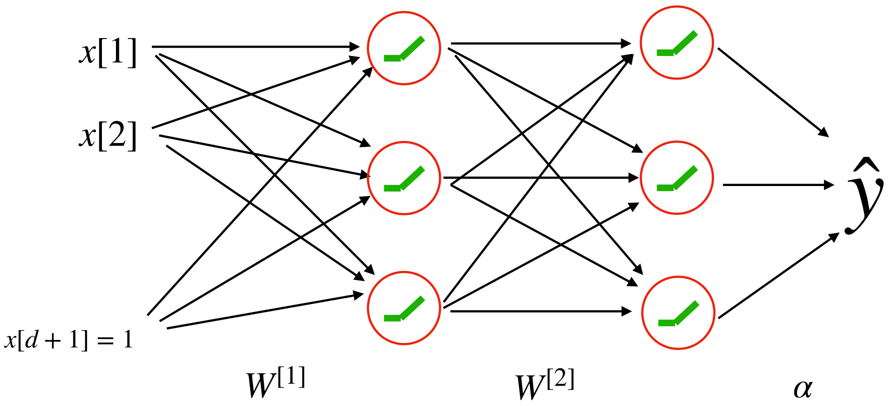

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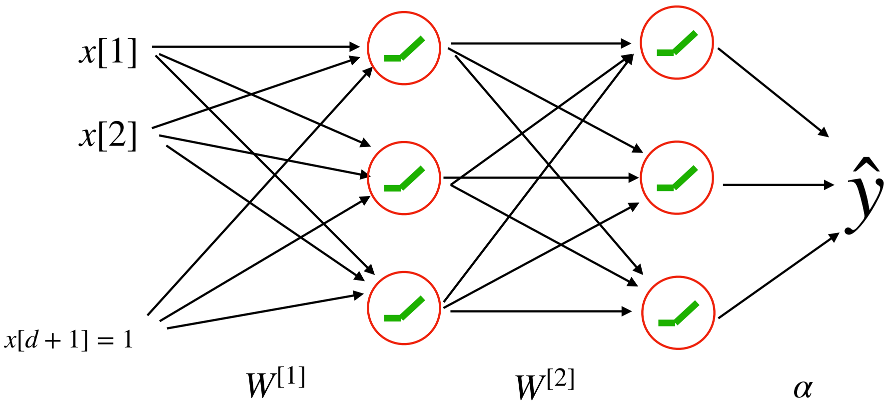
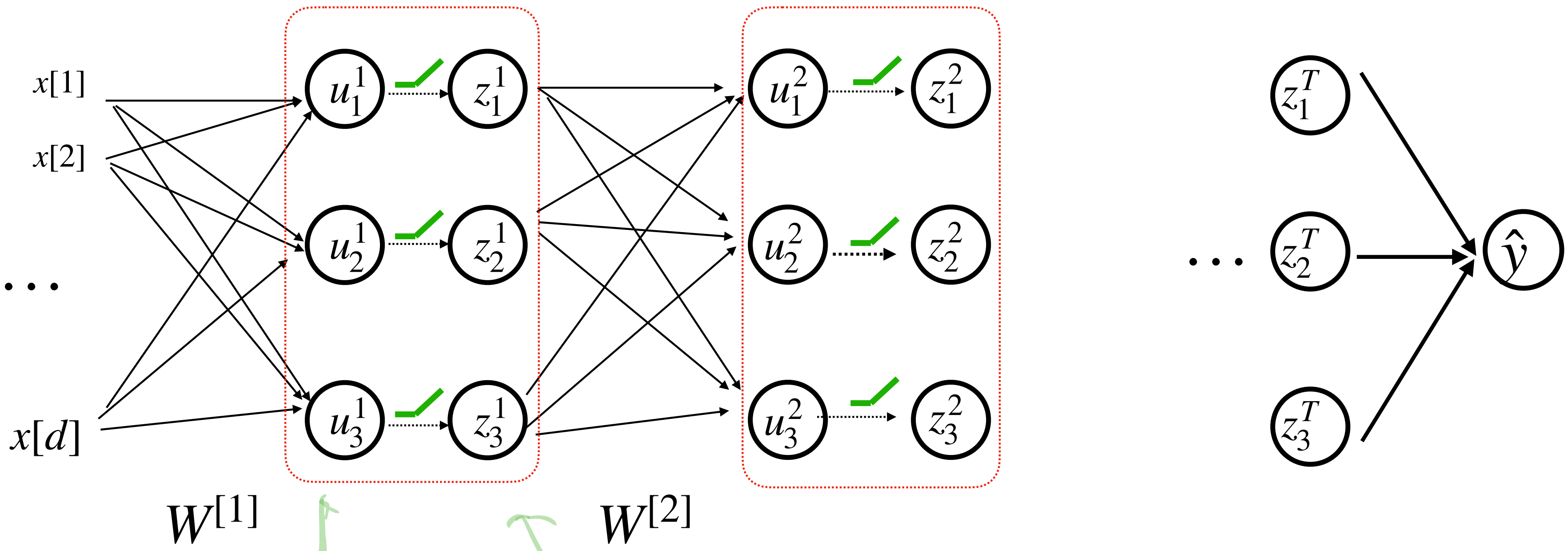


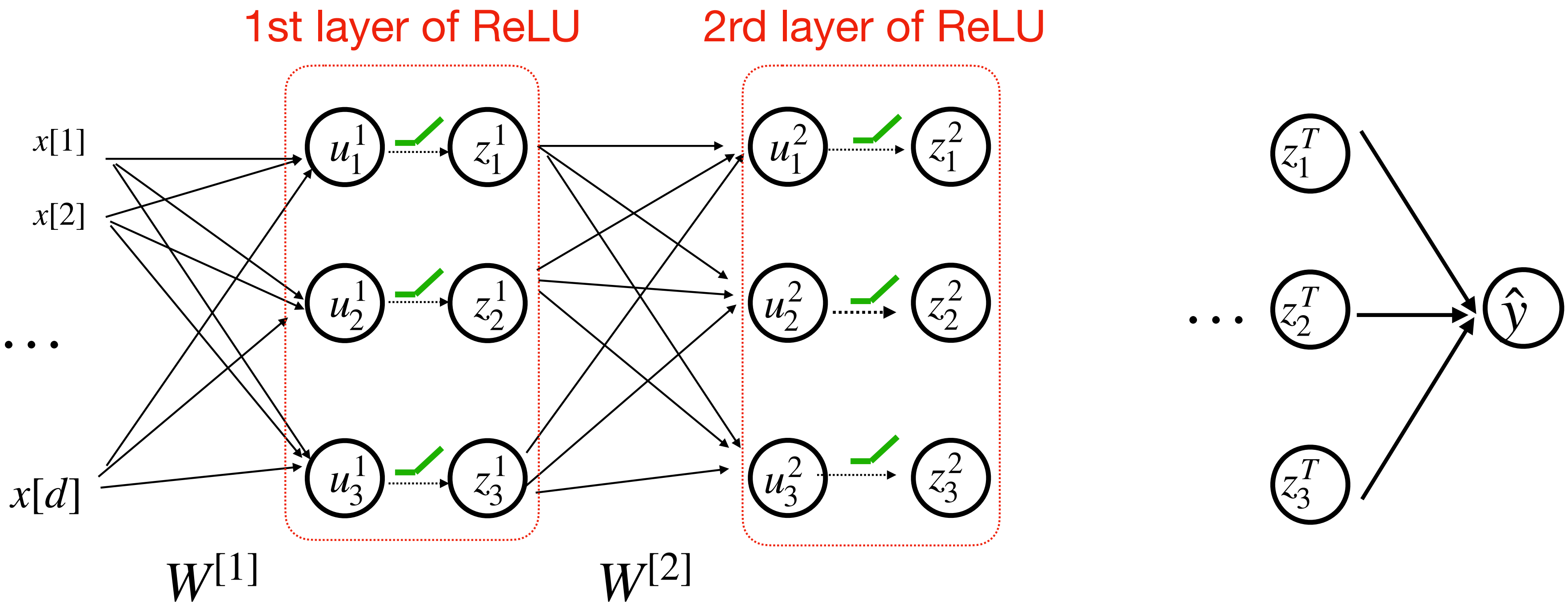
Compute derivatives

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



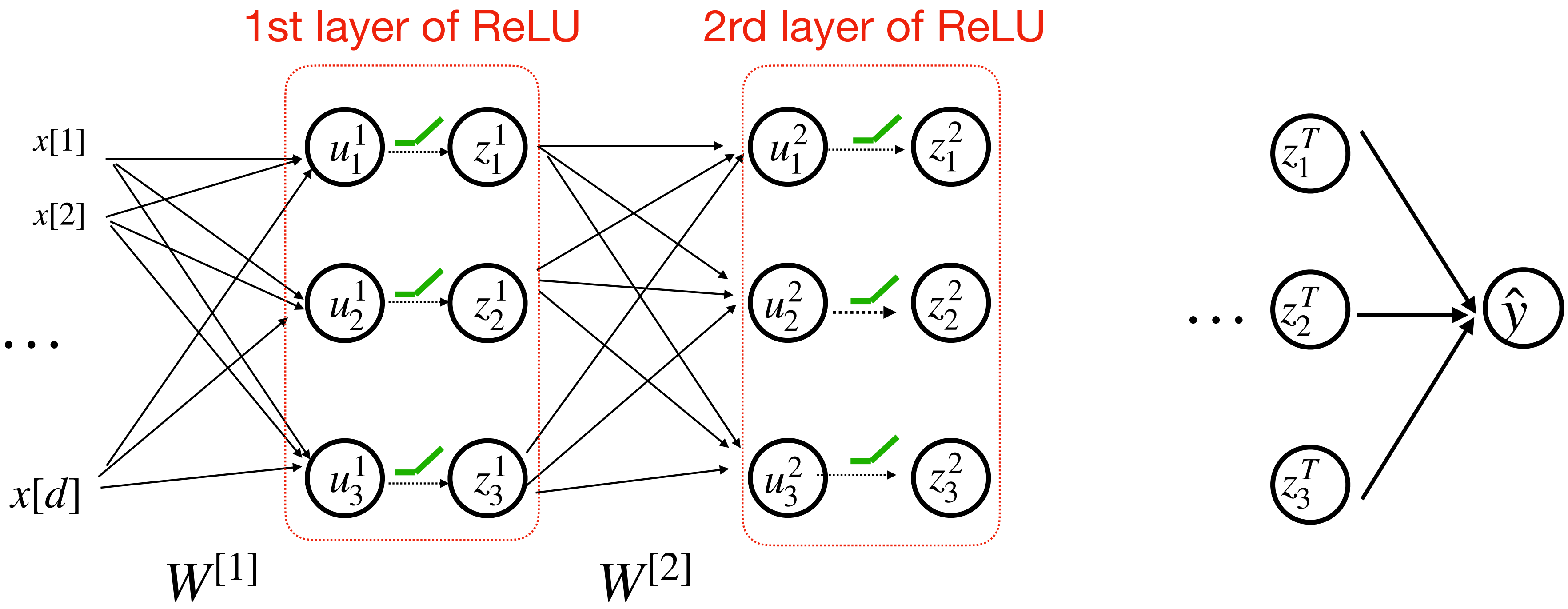
$u = W^{[1]} x$ $\quad$ $z = \mathrm{Relu}(u)$

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



$z^0 = x$

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



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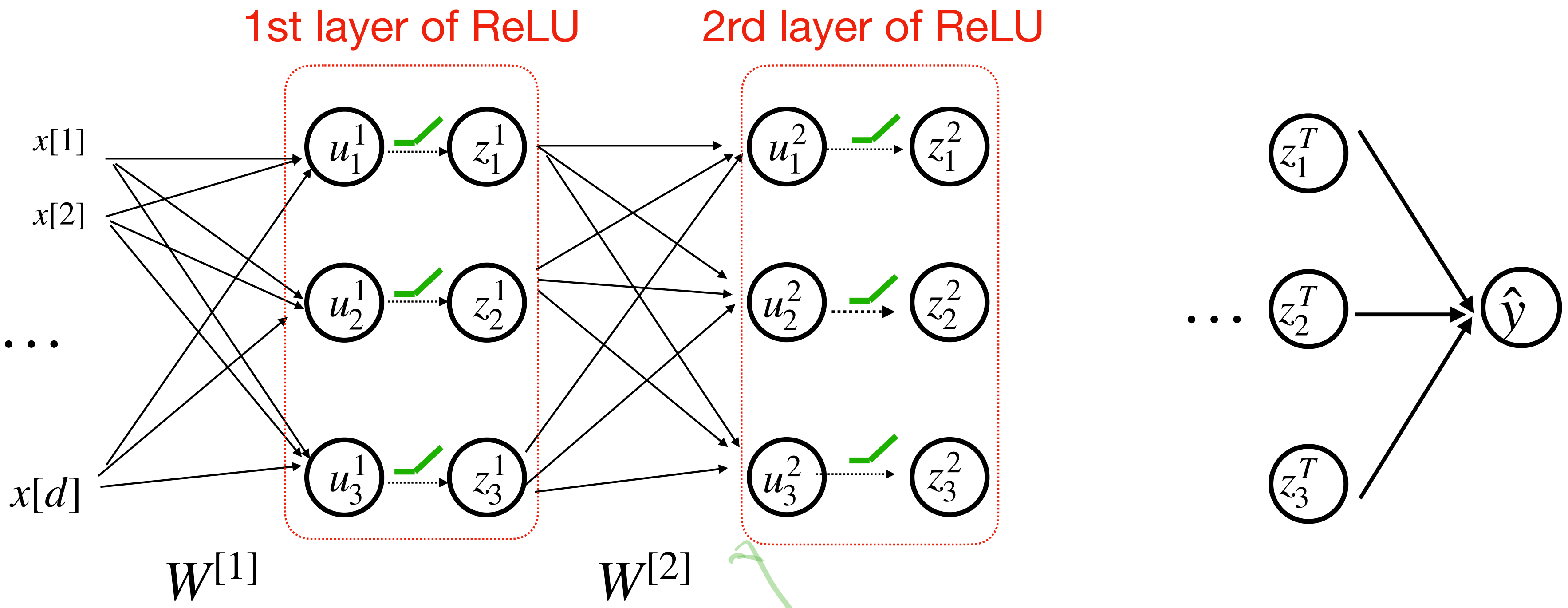
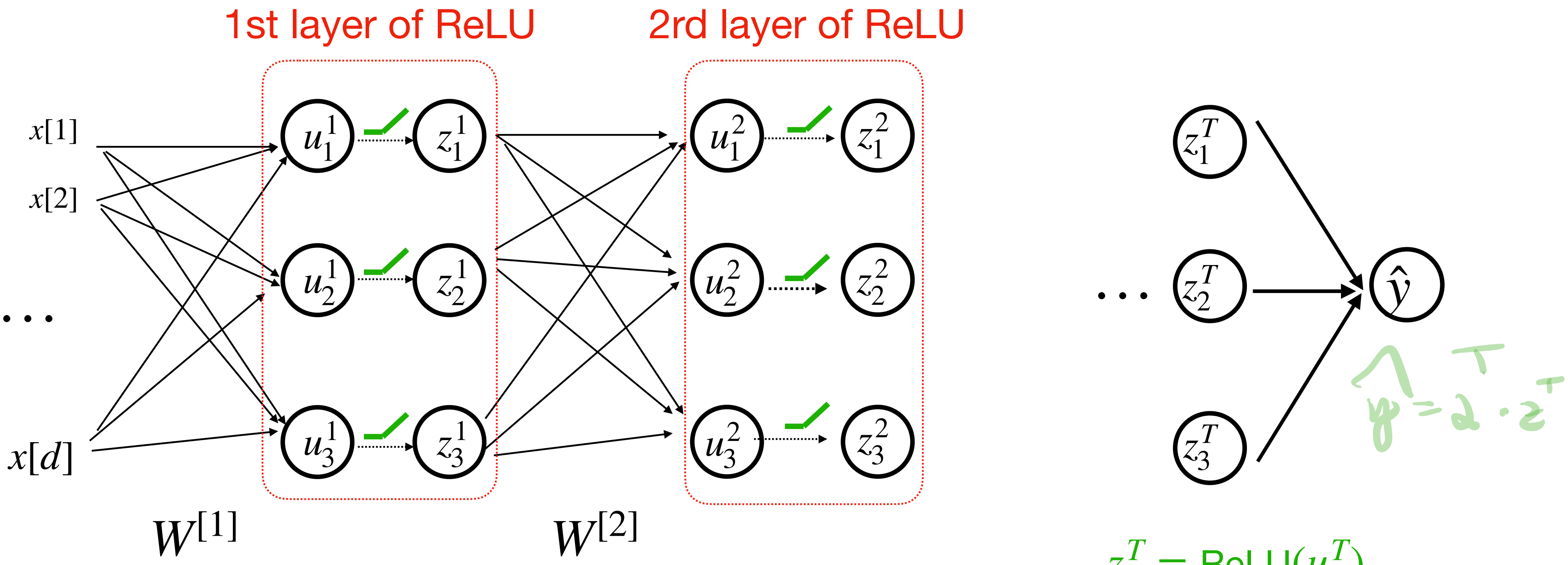


$z^0 = x$ $\quad u^1 = W^{[1]} z^0$ $\quad z^1 = \text{ReLU}(u^1)$

$u^2 = W^{[2]} \cdot z^1$

$z^2 = \text{Relu}[u^2]$

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



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

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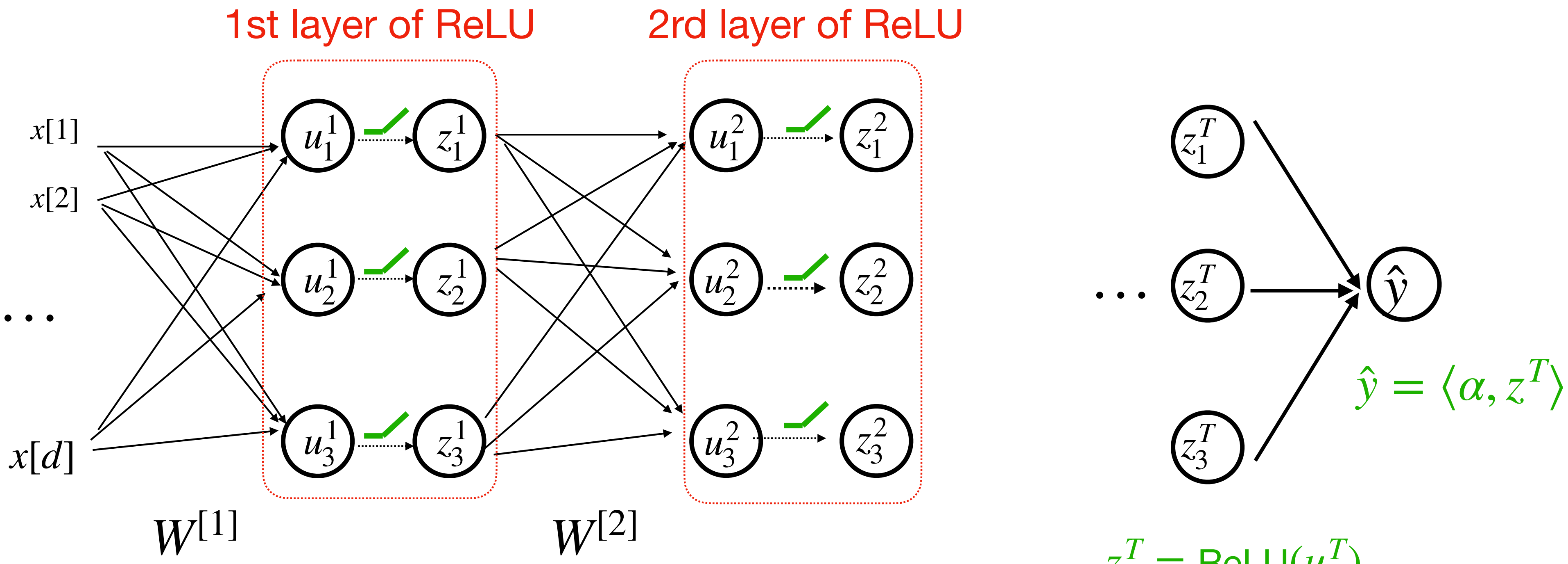
A Forward Pass: from $t = 0$ to T



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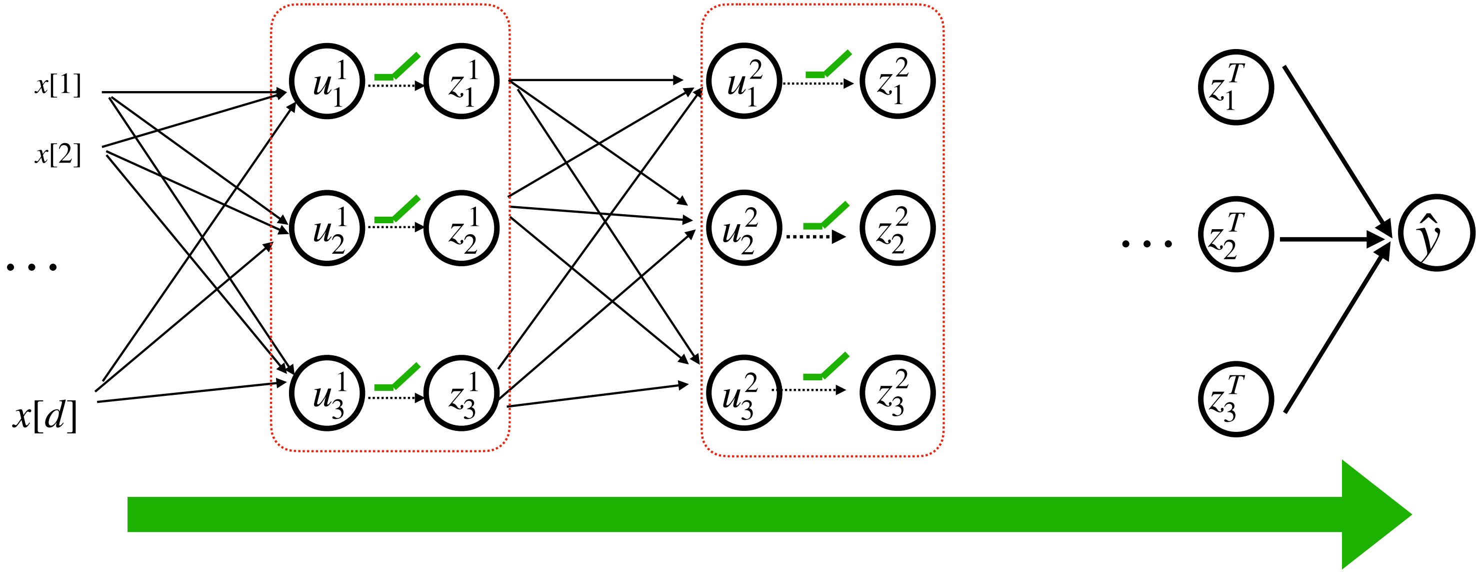
$z^0 = x$ $\quad u^1 = W^{[1]} z^0$ $\quad z^1 = \text{ReLU}(u^1)$

Summary of the forward pass



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

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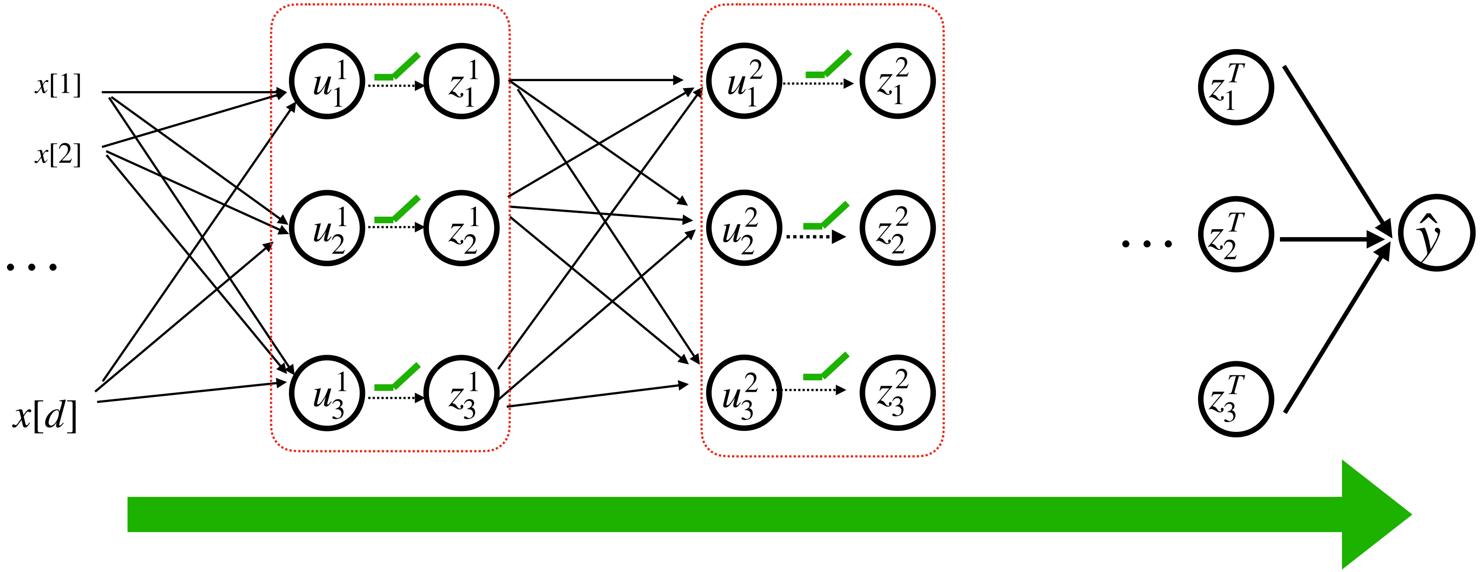

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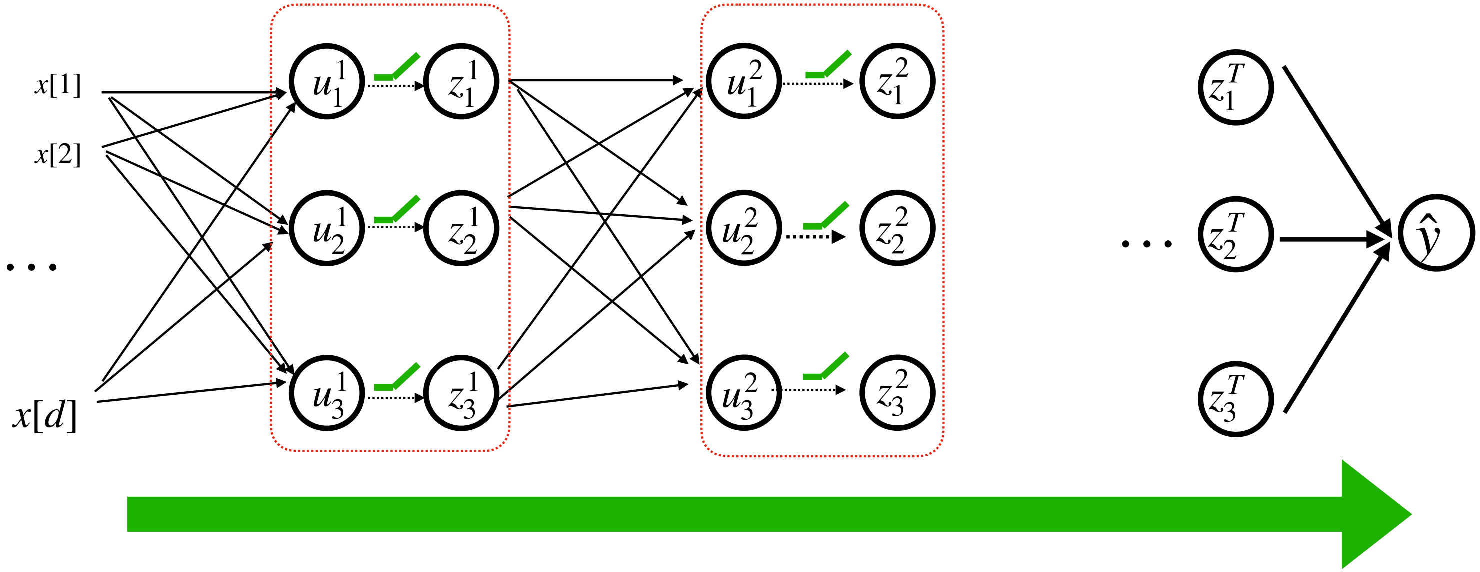
Summary of the forward pass



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

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

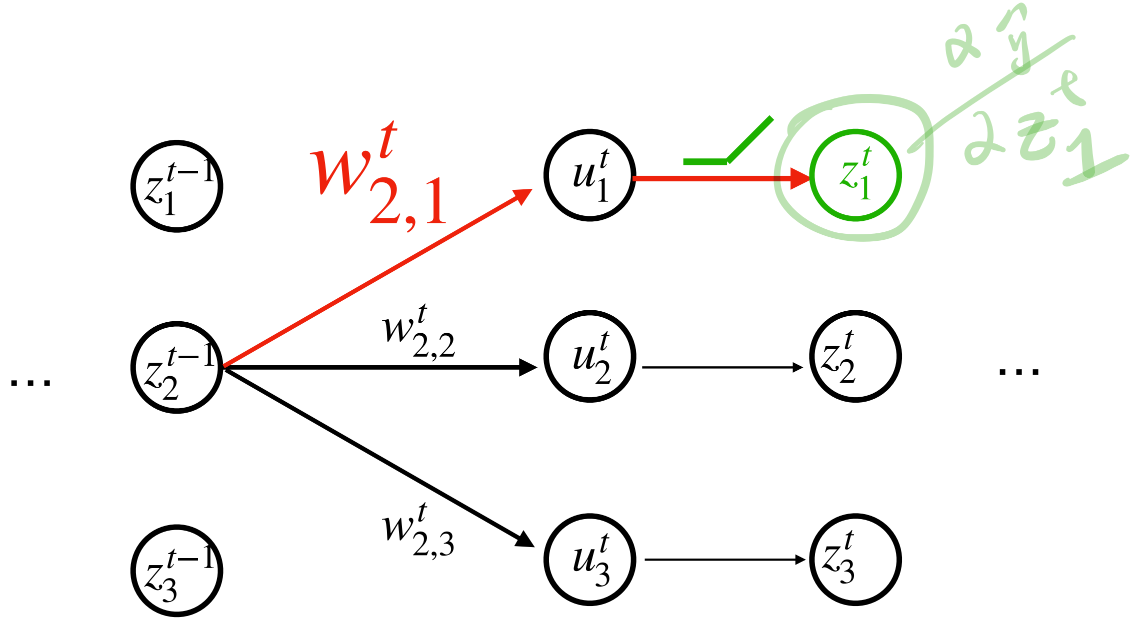
A: linear in # of Edges + # of nodes

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.

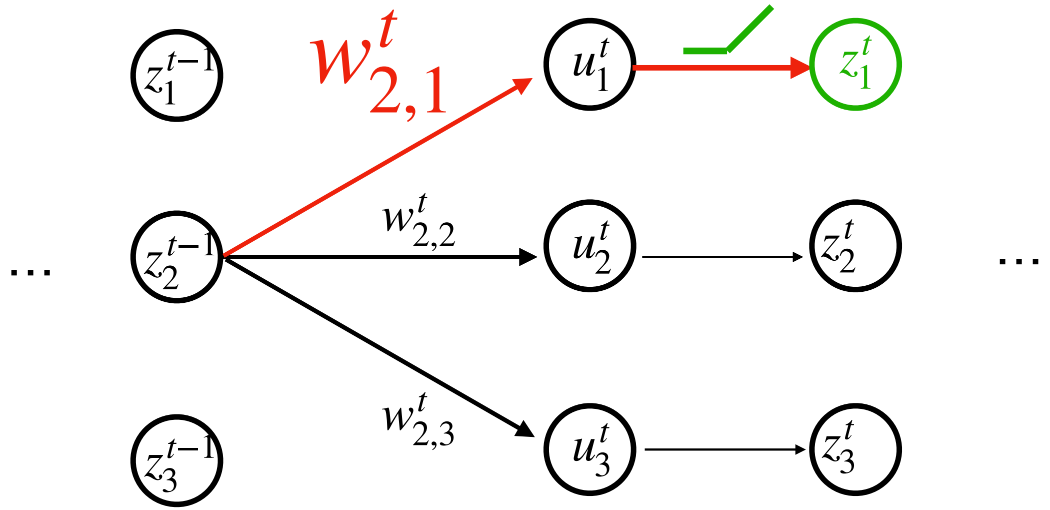
The backward Pass

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



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.



Proof:

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

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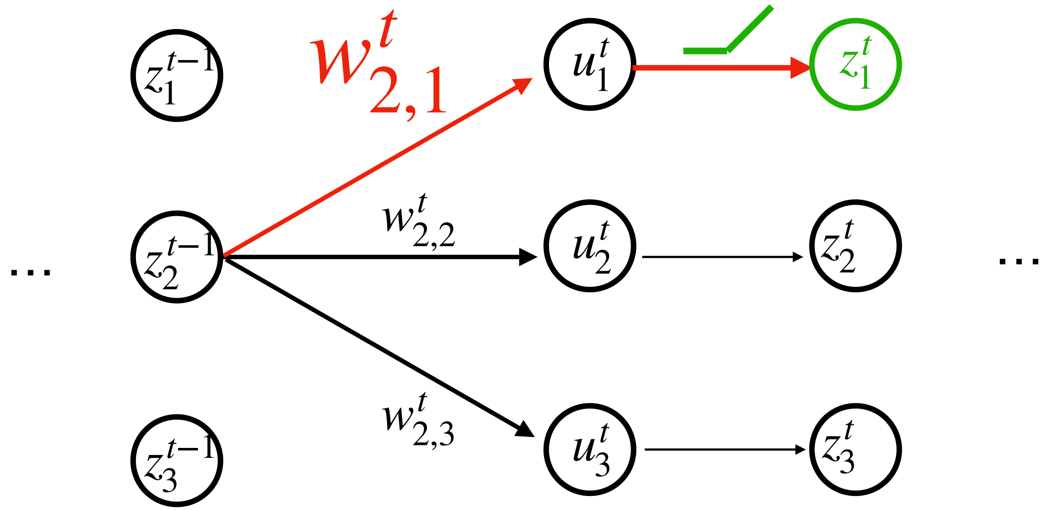
Claim: to compute $\partial\hat{y}/\partial w, \forall$ edge w, it suffices to compute $\partial\hat{y}/\partial z, \forall$ node z.



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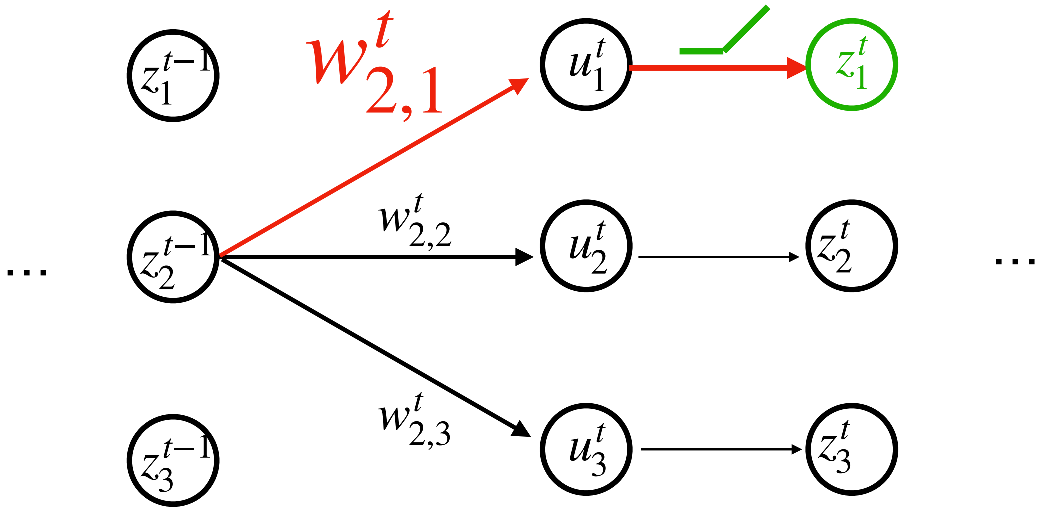

Proof:

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

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

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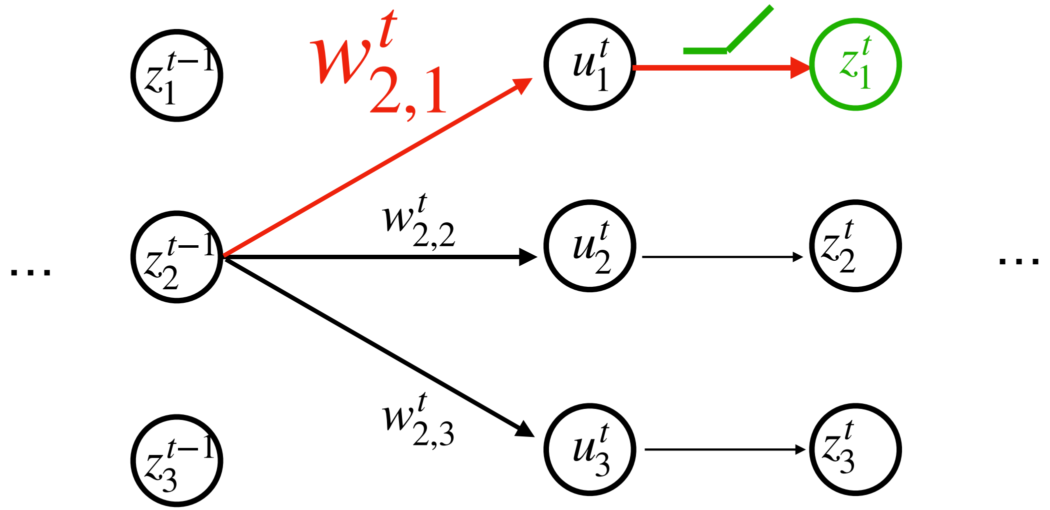

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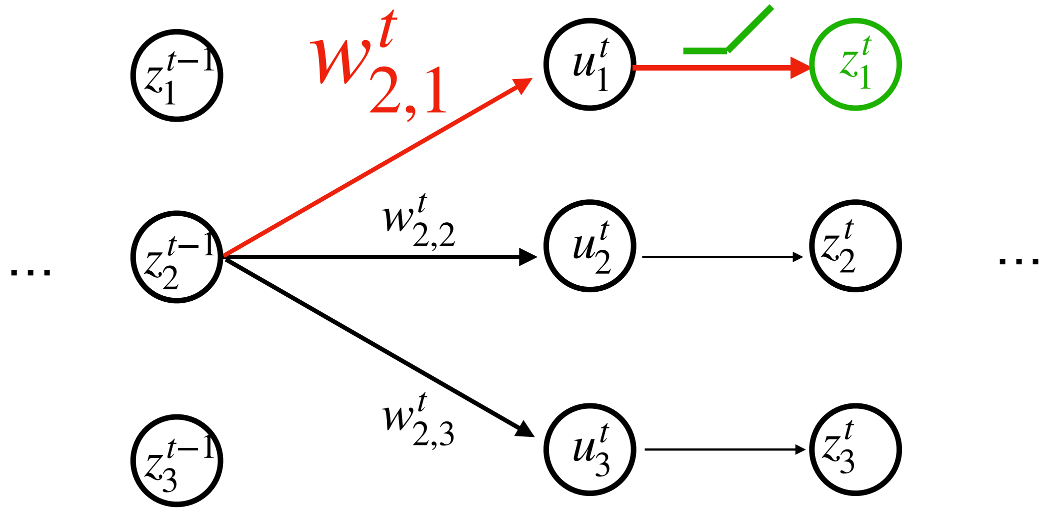

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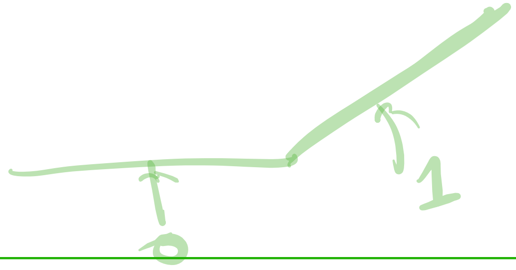
Given by assumption

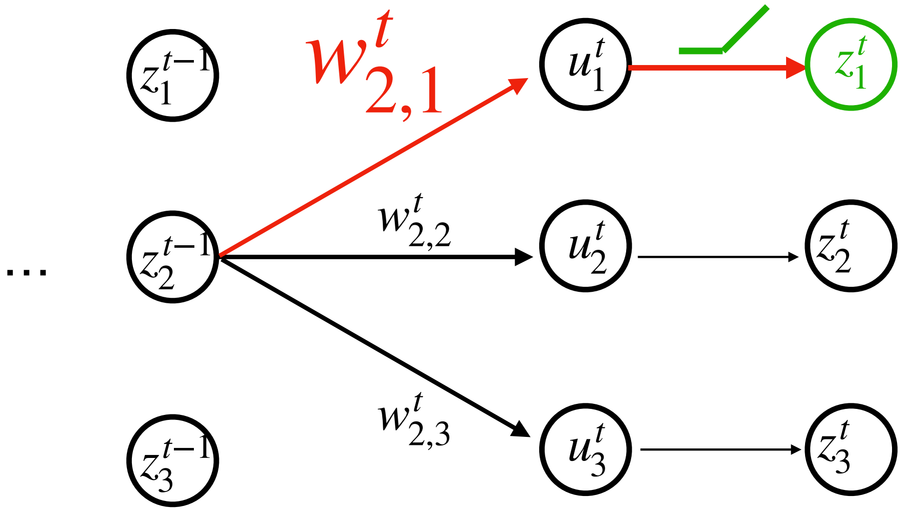


The backward Pass

$\sigma(x) = \max\{x, 0\}$

$\sigma'(x) = \begin{cases} 1, & \text{if } x \geq 0 \\ 0, & \text{else} \end{cases}$

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



Proof:

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

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

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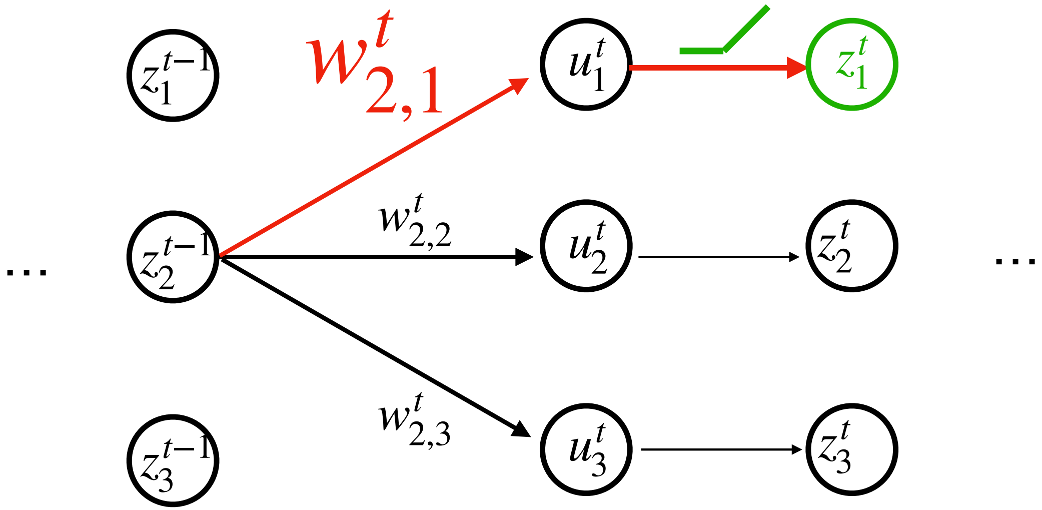
Given by assumption

Derivative of ReLU

The backward Pass

$u_1^t = \cdots + z_2^{t-1} \cdot w_{2,1}^t + \cdots$

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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Known from forward pass

Given by assumption

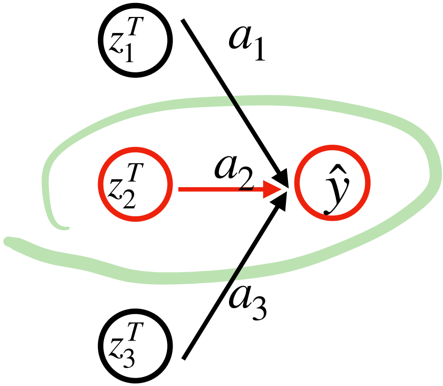
Derivative of ReLU

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

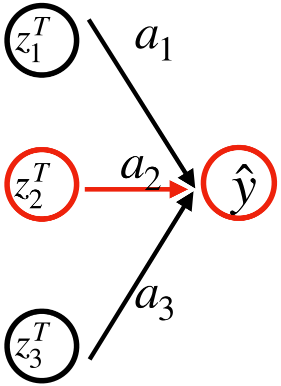
Base case: compute $\partial \hat{y} / \partial z^T$, for all node z at T-th Layer



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

The backward Pass: base case

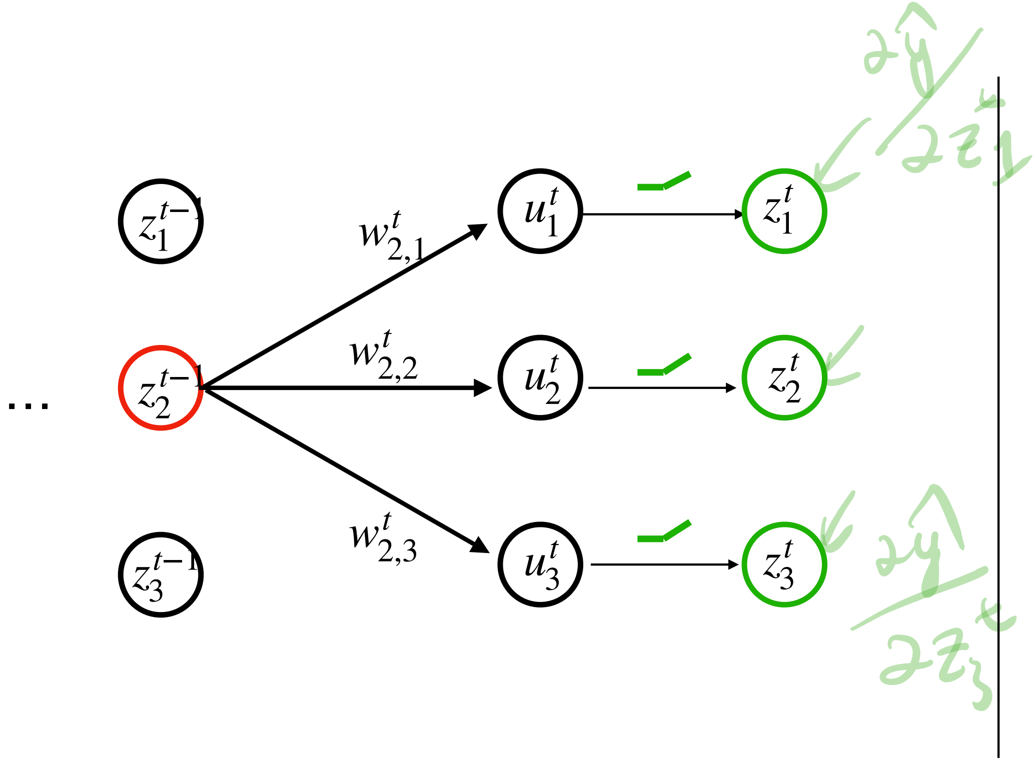
Base case: compute $\partial \hat{y} / \partial z^T$, for all node z at T-th Layer



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

The backward Pass: induction step

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



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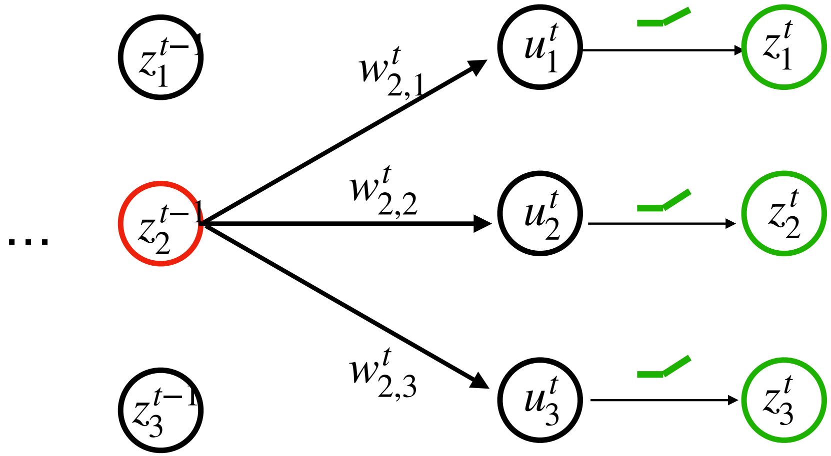

WLOG, consider $\partial \hat{y} / \partial z_2^{t-1}$

The backward Pass: induction step

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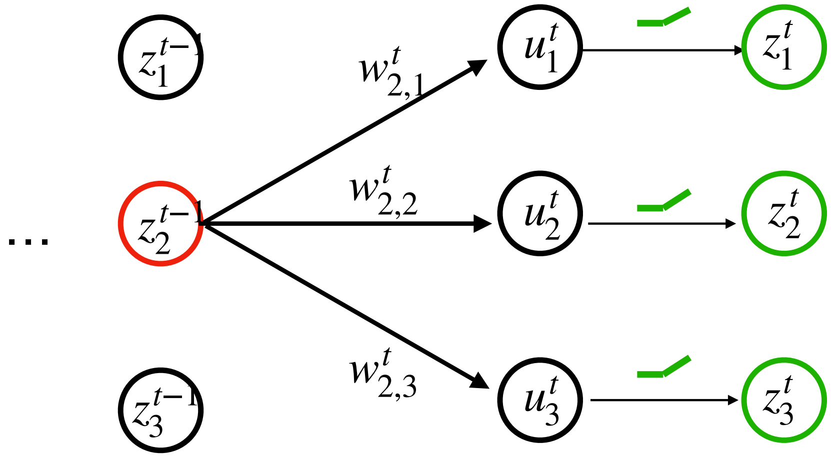

WLOG, consider $\partial \hat{y} / \partial z_2^{t-1}$

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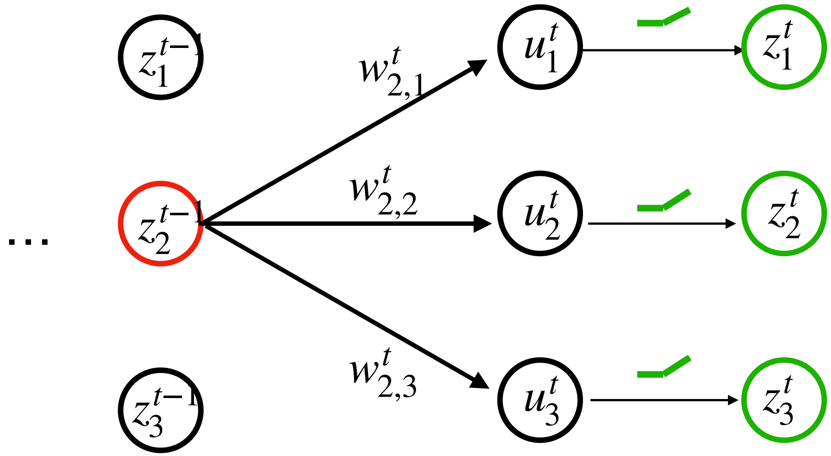

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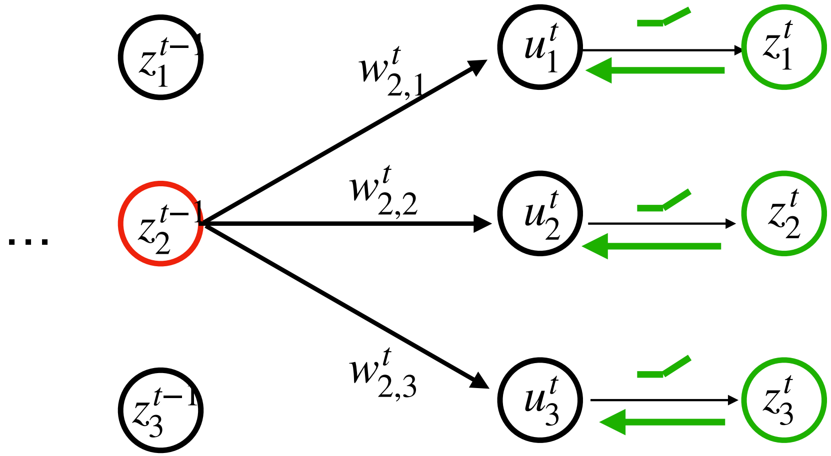

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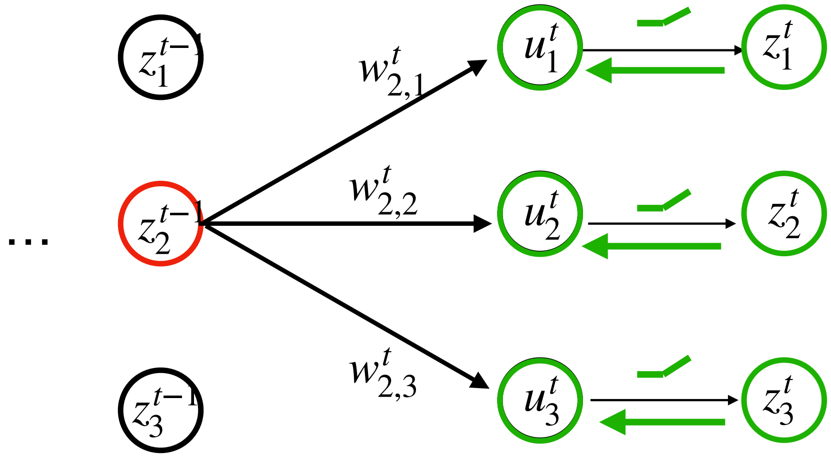

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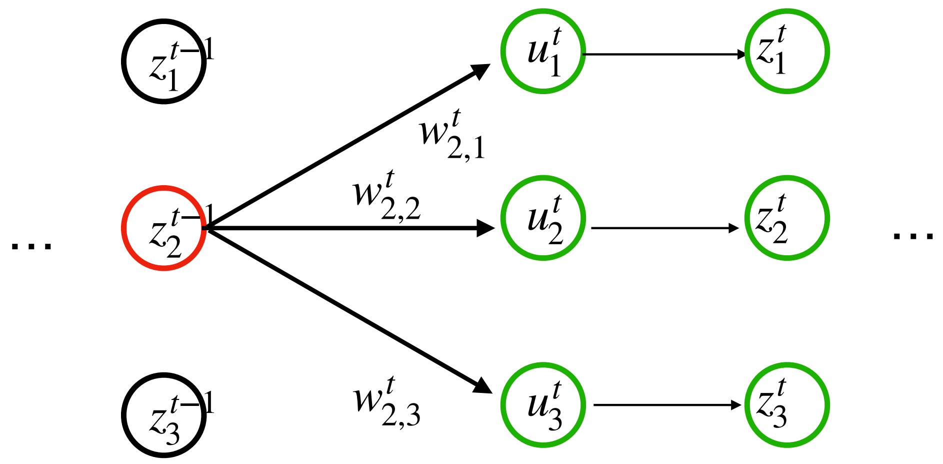

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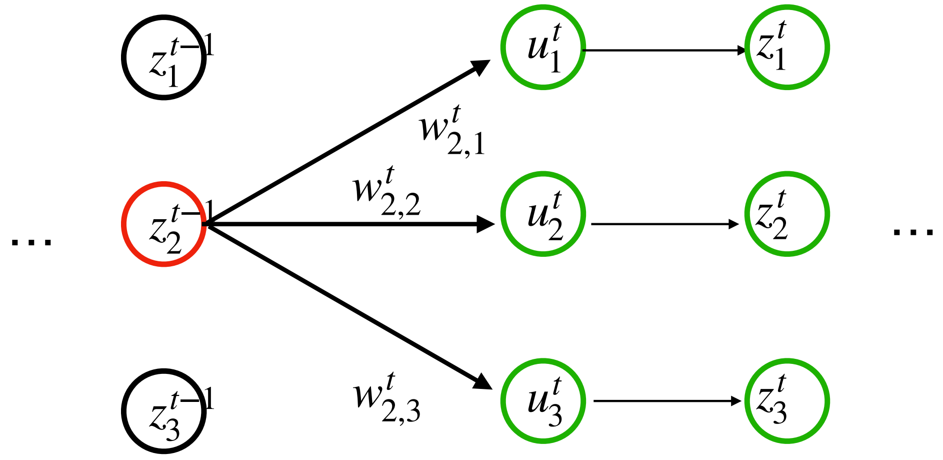
The backward Pass: induction step

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



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

Via multivariate chain rule:

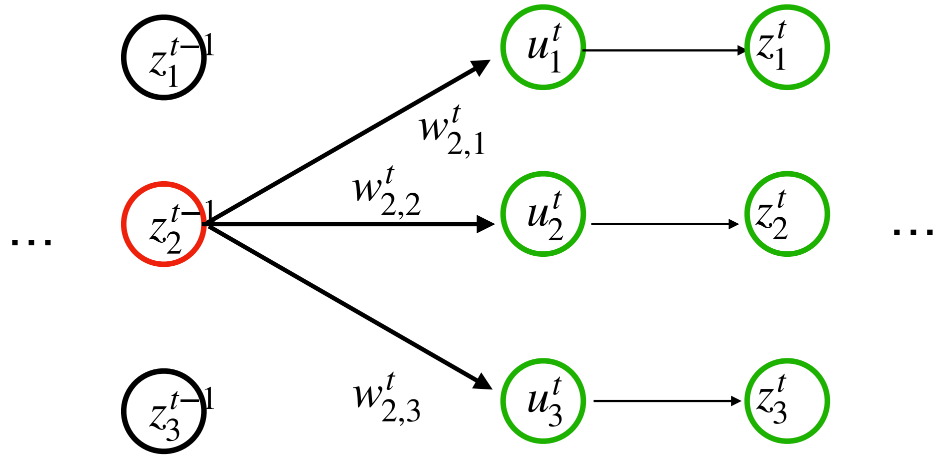
$$\hat{y} = f(u_1(x), u_2(x), u_3(x))$$

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

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:

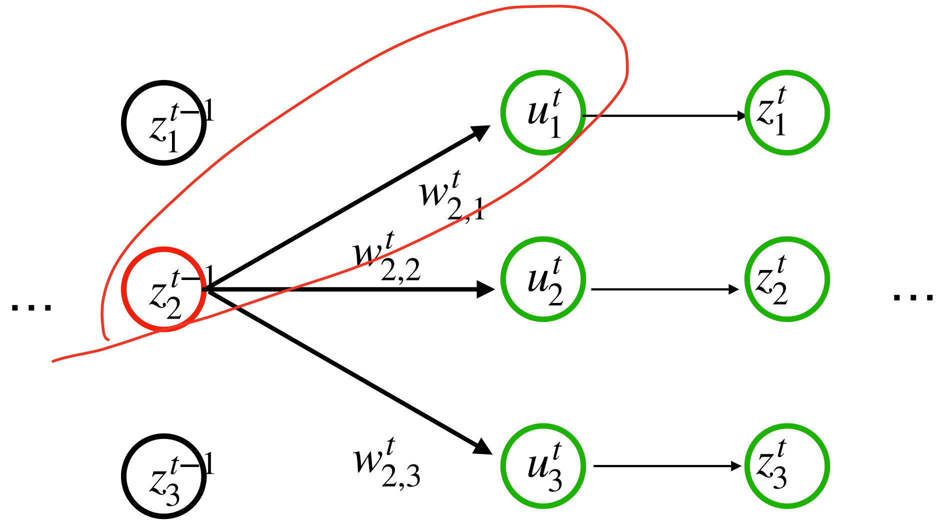
Step 2: $$\frac{\partial \hat{y}}{\partial z_2^{t-1}} = \sum_{i=1}^{K} \frac{\partial \hat{y}}{\partial u_i^t} \frac{\partial u_i^t}{\partial z_2^{t-1}}$$

Computed after step 1

The backward Pass: induction step

$\frac{\partial u_i^t}{\partial z_2^{t-1}}$

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



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The backward Pass: induction step

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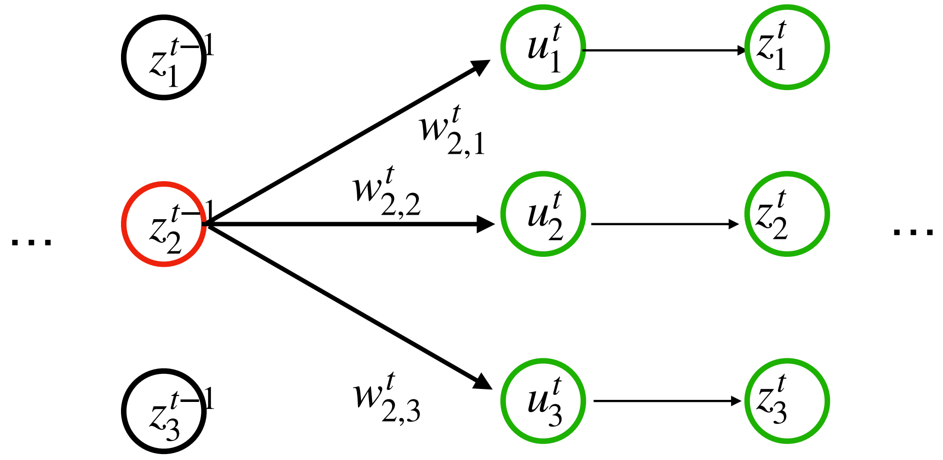

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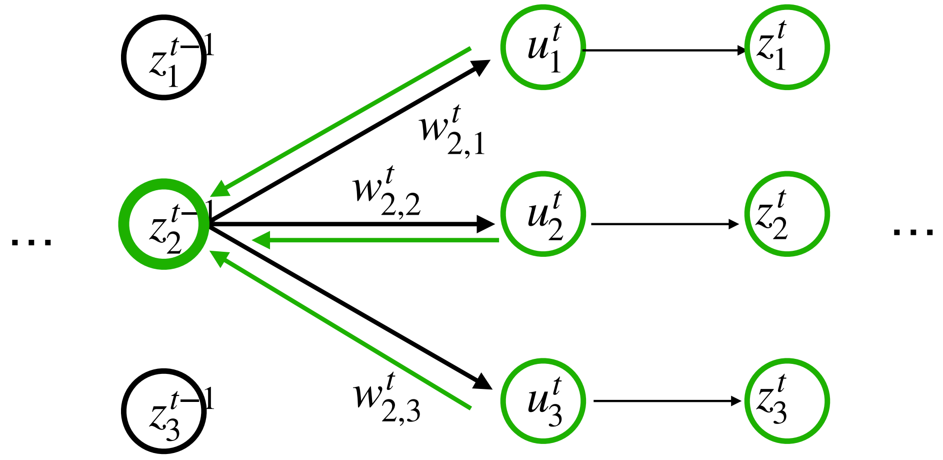
We are done at node z_2^{t-1}!

The backward Pass: induction step

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



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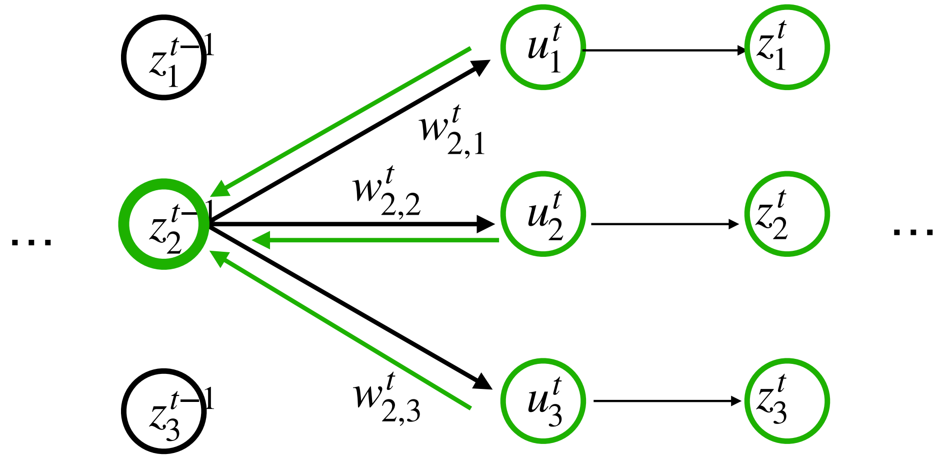

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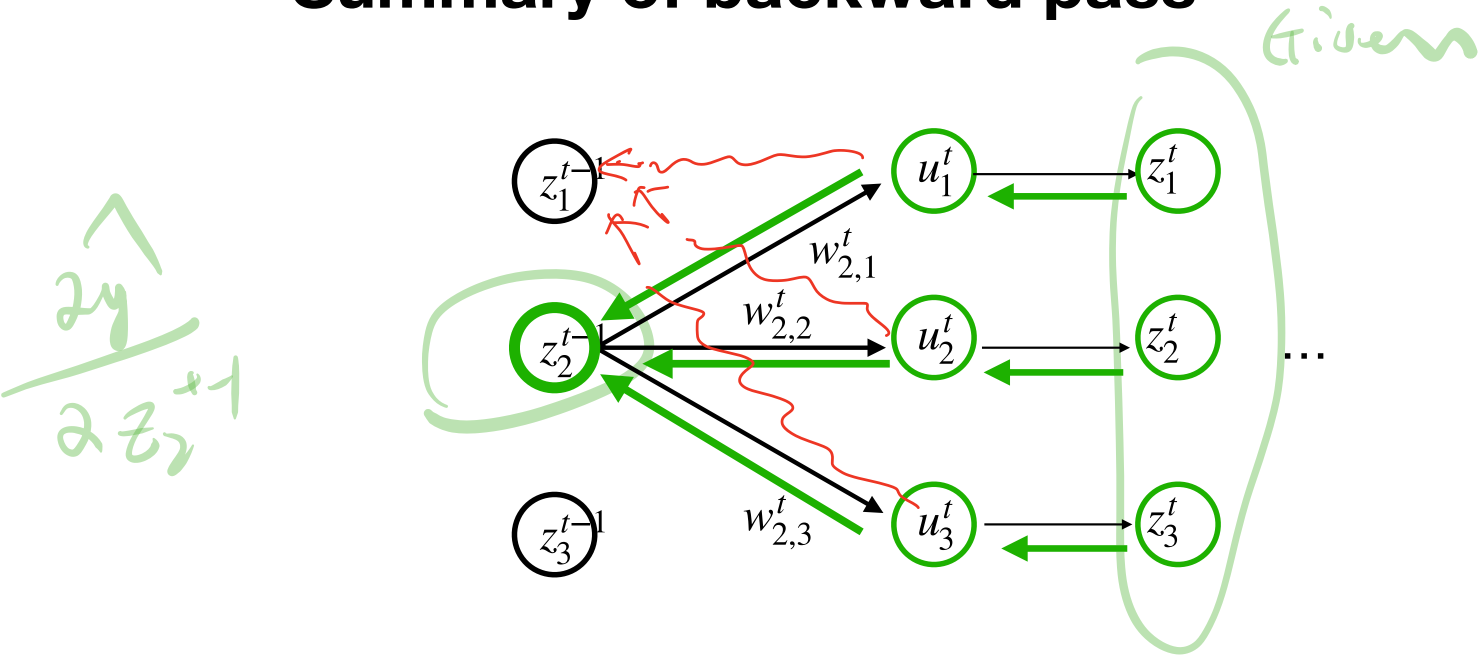
We are done at node z_2^{t-1}!

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

Summary of backward pass



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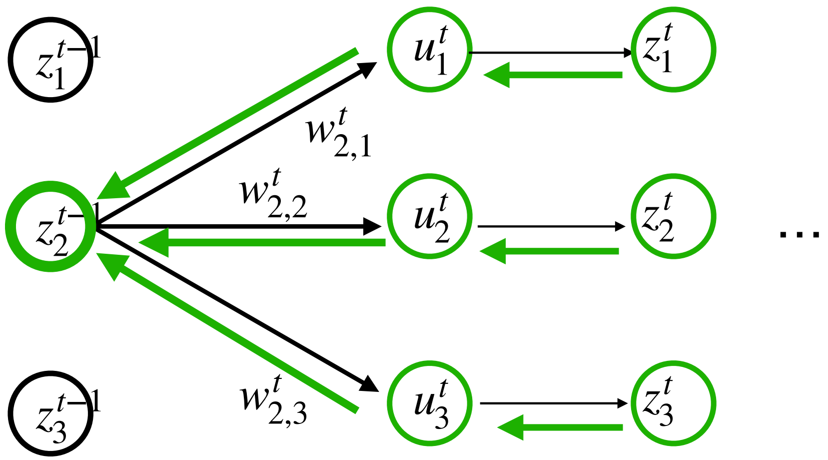

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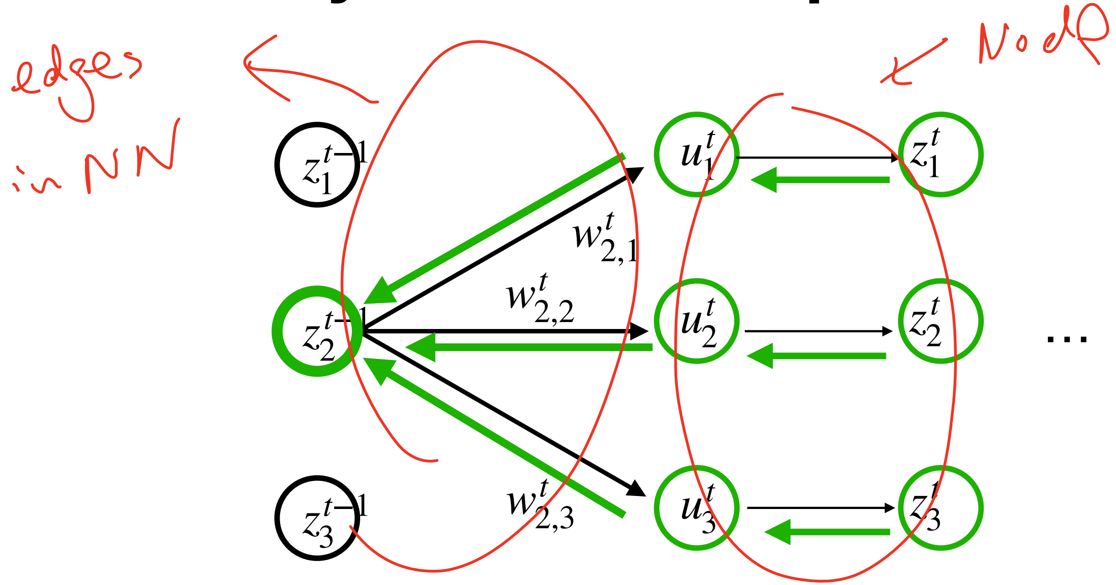

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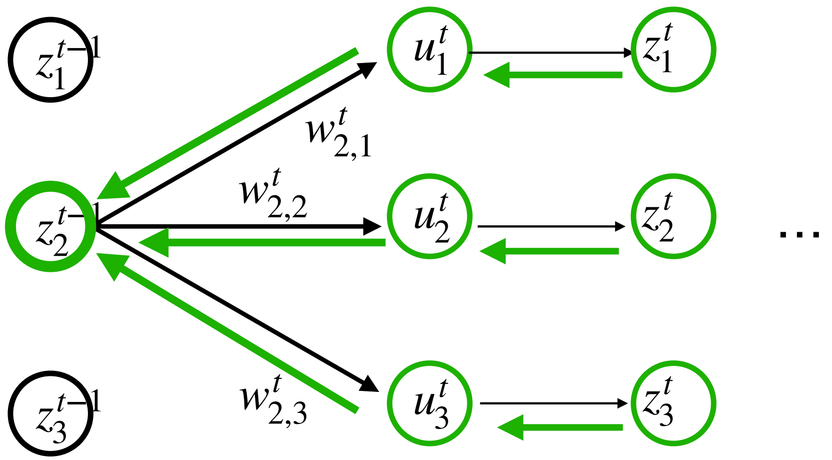

The computation from $\partial \hat{y} / z^t$ to $\partial \hat{y} / z^{t-1}$ is the # of all edges in the sub-graph

Total computation: # of edges + # of nodes!

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

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

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

$\Rightarrow \frac{\partial \hat{y}}{\partial w}$