CPEN 455: Deep Learning

Lecture 4: Backpropagation I

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University of British Columbia Winter, Term 2, 2024

Outline

- Learning Algorithm for Feedforward Neural Networks:
 - Backpropagation
 - Weight Initialization
 - Learning Rate & Momentum & Adam
 - Weight Decay & Early Stopping

Learning Algorithm

• Learning algorithms are just optimization algorithms and are about **credit assignment**!

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Stochastic gradient descent (SGD) [1], introduced in 1951 by Herbert Robbins and Sutton Monro

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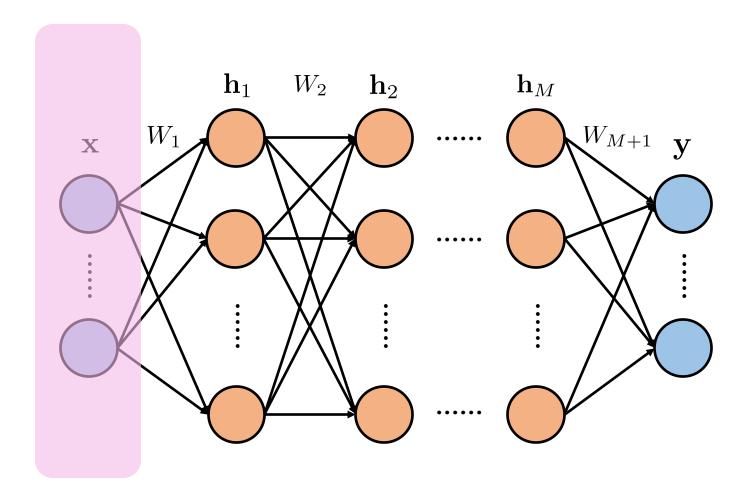
Stochastic gradient descent (SGD) [1], introduced in 1951 by Herbert Robbins and Sutton Monro

- Back-propagation (BP) = an efficient SGD in the context of deep learning
 - o BP has been independently discovered many times (see the history of deep learning in the 1st lecture)
 - o BP was first shown to successfully train neural networks and learn useful representations in 1986 [2] by David Rumelhart, Geoffrey Hinton, and Ronald Williams
 - o BP is the most successful learning algorithm so far for training feedforward neural networks

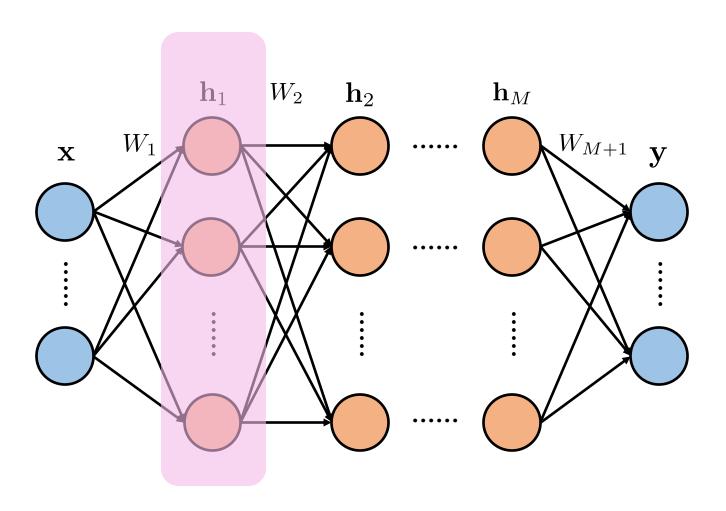
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Consider a MLP as follows. Recall what we do in the forward pass:

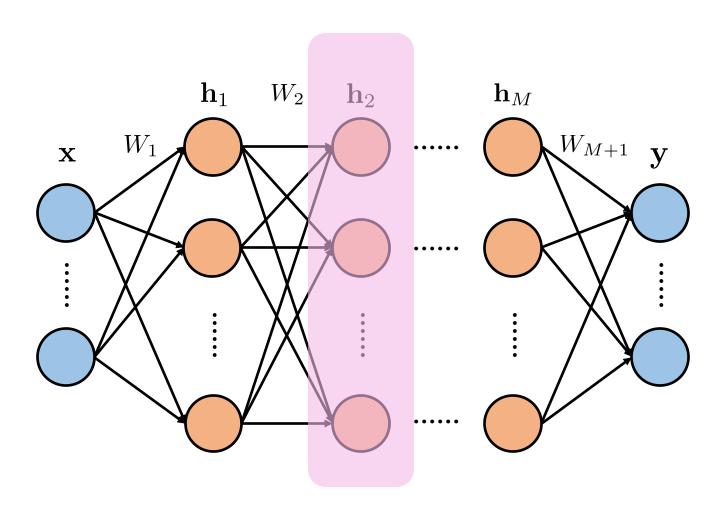


Consider a MLP as follows. Recall what we do in the forward pass:



$$\mathbf{h}_1 = \sigma\left(W_1\mathbf{x}\right)$$

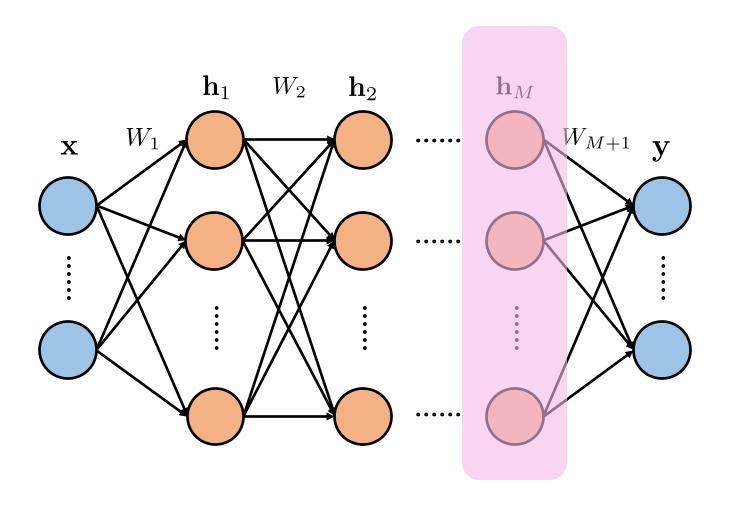
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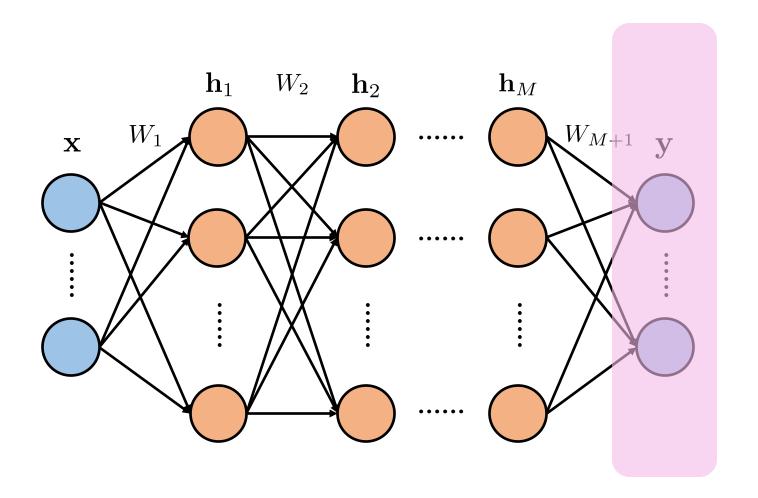
$$\mathbf{h}_{1} = \sigma (W_{1}\mathbf{x})$$

$$\mathbf{h}_{2} = \sigma (W_{2}\mathbf{h}_{1})$$

$$\vdots$$

$$\mathbf{h}_{M} = \sigma (W_{M}\mathbf{h}_{M-1})$$

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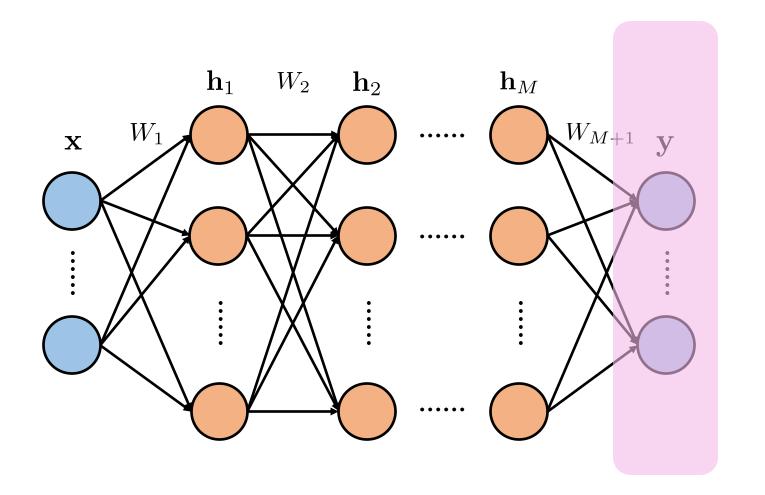
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$$\mathbf{h}_{M} = \sigma \left(W_{M} \mathbf{h}_{M-1} \right)$$

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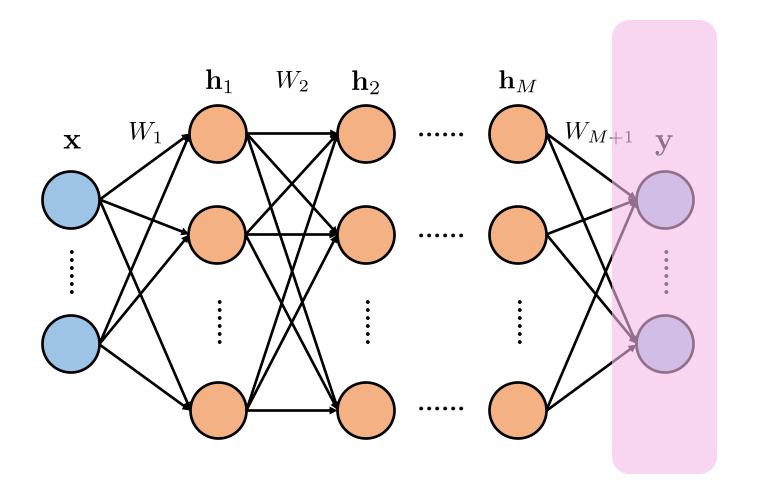


$$\mathbf{h}_M = \sigma\left(W_M \mathbf{h}_{M-1}\right)$$

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Loss:
$$L = \ell(\mathbf{y}, \bar{\mathbf{y}})$$

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Input Sample

$$\mathbf{h}_1 = \sigma\left(W_1\mathbf{x}\right)$$

$$\mathbf{h}_2 = \sigma\left(W_2\mathbf{h}_1\right)$$



$$\mathbf{h}_M = \sigma\left(W_M \mathbf{h}_{M-1}\right)$$

$$\mathbf{y} = W_{M+1}\mathbf{h}_M$$

Loss:
$$L = \ell(\mathbf{y}, \bar{\mathbf{y}})$$

Mini-batch version:

$$L = \frac{1}{B} \sum_{i=1}^{B} \ell(\mathbf{y}_i, \bar{\mathbf{y}}_i)$$

Before we introduce backpropagation, let us review several concepts in vector calculus.

Gradient: for a scalar-valued differentiable function $f: \mathbb{R}^n \to \mathbb{R}$ of multiple variables, the gradient $\nabla f: \mathbb{R}^n \to \mathbb{R}^n$ evaluated at $\mathbf{p} = [\mathbf{p}_1, \mathbf{p}_2, \dots, \mathbf{p}_n]^\top$ is

$$\nabla f(\mathbf{p}) = \begin{bmatrix} \frac{\partial f}{\partial x_1}(\mathbf{p}) \\ \vdots \\ \frac{\partial f}{\partial x_n}(\mathbf{p}) \end{bmatrix}$$

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Jacobian: for a vector-valued differentiable function $f: \mathbb{R}^n \to \mathbb{R}^m$ of multiple variables, the Jacobian matrix evaluated at $\mathbf{p} = [\mathbf{p}_1, \mathbf{p}_2, \dots, \mathbf{p}_n]^{\top}$ is

$$\mathbf{J}_{f}(\mathbf{p}) = \begin{bmatrix} \nabla^{\mathrm{T}} f_{1}(\mathbf{p}) \\ \vdots \\ \nabla^{\mathrm{T}} f_{m}(\mathbf{p}) \end{bmatrix} = \begin{bmatrix} \frac{\partial f_{1}}{\partial x_{1}}(\mathbf{p}) & \cdots & \frac{\partial f_{1}}{\partial x_{n}}(\mathbf{p}) \\ \vdots & \ddots & \vdots \\ \frac{\partial f_{m}}{\partial x_{1}}(\mathbf{p}) & \cdots & \frac{\partial f_{m}}{\partial x_{n}}(\mathbf{p}) \end{bmatrix}$$

Before we introduce backpropagation, let us review several concepts in vector calculus.

Chain Rule: the derivative of the composition of two differentiable functions in terms of the derivatives of individual functions

• Scalar-valued & single variable $f: \mathbb{R} o \mathbb{R}$ $g: \mathbb{R} o \mathbb{R}$

$$g: \mathbb{R} \to \mathbb{R}$$

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$$\frac{df(g(x))}{dx} = \frac{df(g(x))}{dg(x)} \frac{dg(x)}{dx}$$

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We can derive it from the single variable case!

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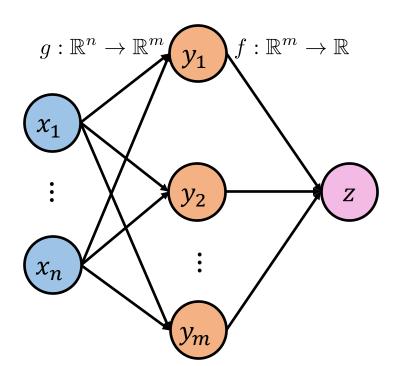
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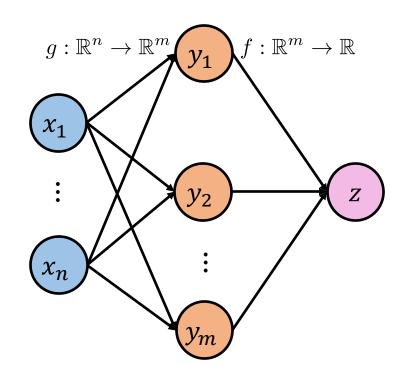


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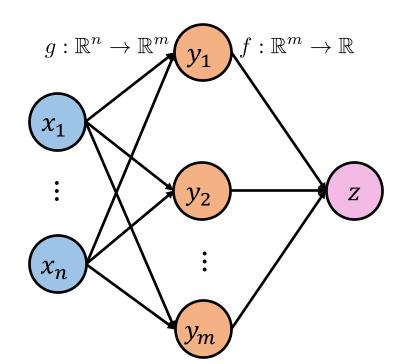
$$\frac{\partial z}{\partial x_1} = \sum_{i=1}^m \frac{\partial z}{\partial y_i} \frac{\partial y_i}{\partial x_1} = \begin{bmatrix} \frac{\partial z}{\partial y_1} \dots \frac{\partial z}{\partial y_m} \end{bmatrix} \begin{bmatrix} \frac{\partial y_1}{\partial x_1} \\ \vdots \\ \frac{\partial y_m}{\partial x_1} \end{bmatrix}$$

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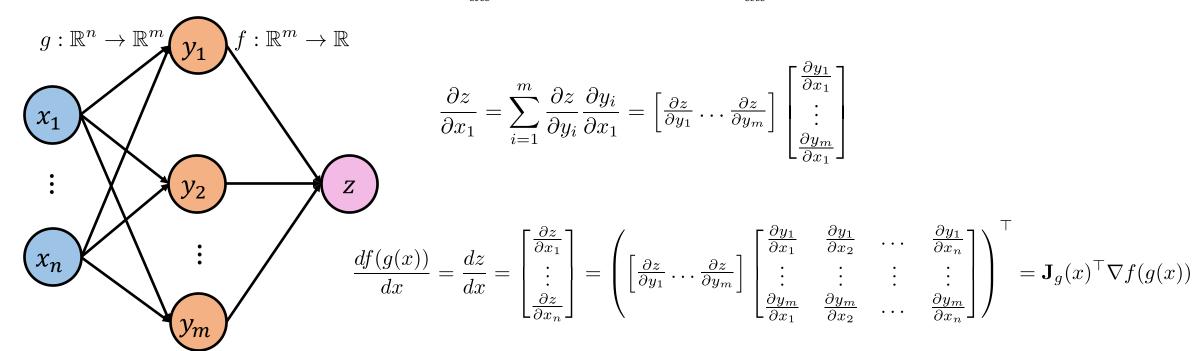
Consider all possible paths from x_1 to z!

Before we introduce backpropagation, let us review several concepts in vector calculus.

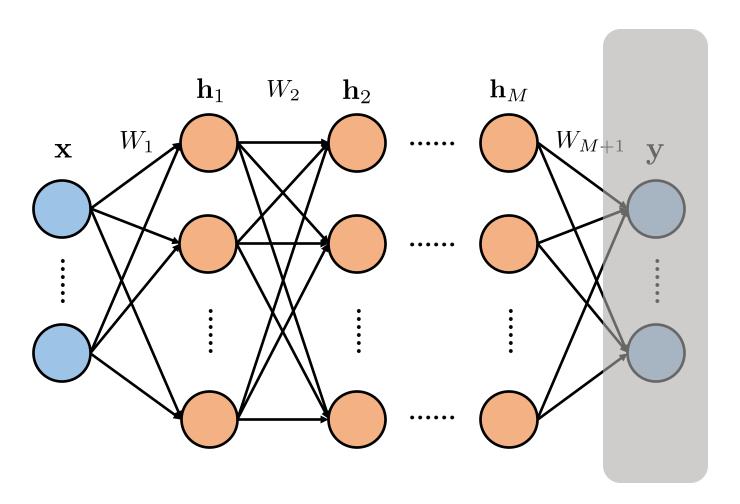
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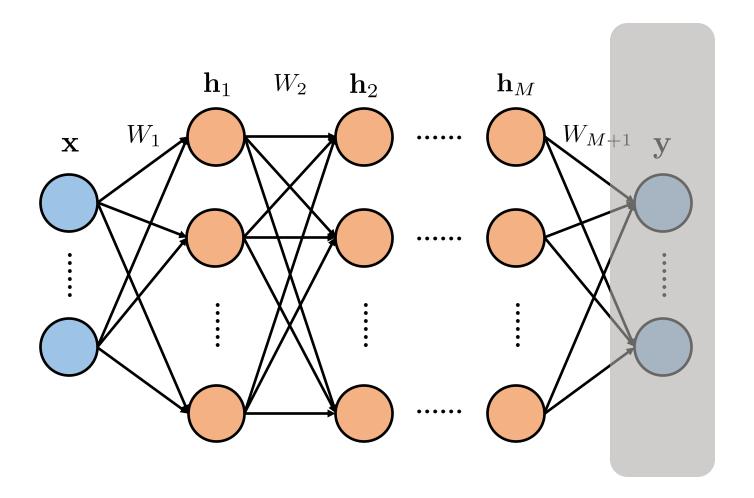


During the backward pass:



Loss: $L = \ell(\mathbf{y}, \bar{\mathbf{y}})$

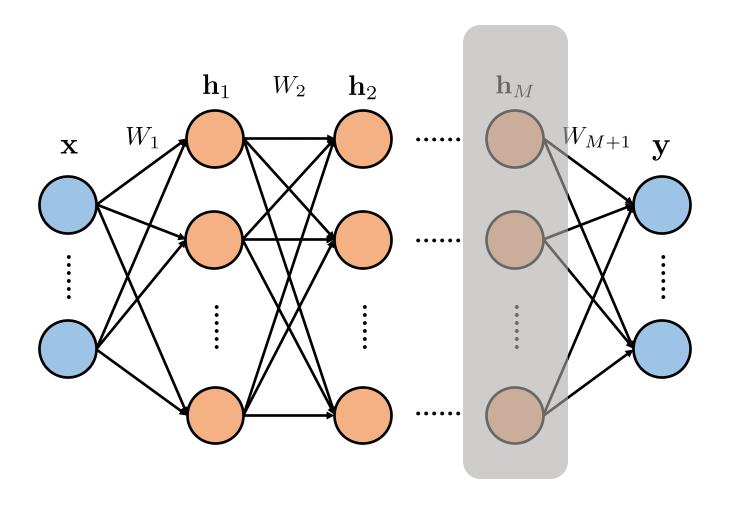
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Gradient of loss w.r.t. $\mathbf{y}: \frac{\partial L}{\partial \mathbf{y}}$

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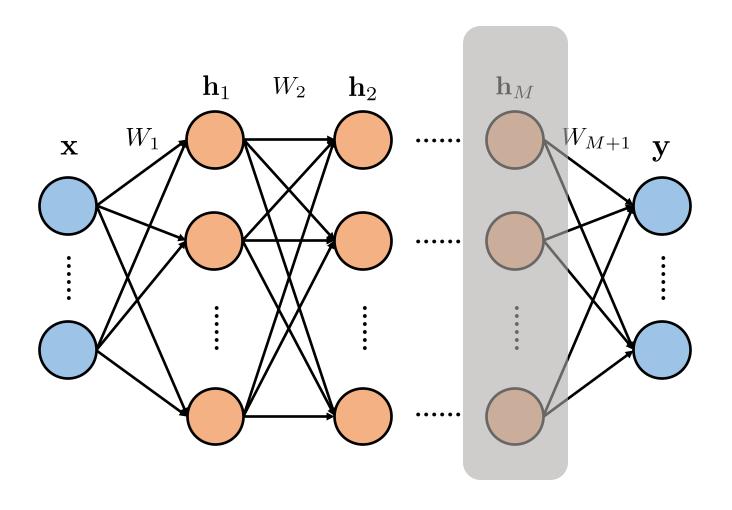


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Gradient of loss w.r.t. $\mathbf{y}: \frac{\partial L}{\partial \mathbf{y}}$

Gradient of loss w.r.t. \mathbf{h}_M :

During the backward pass:



Loss:
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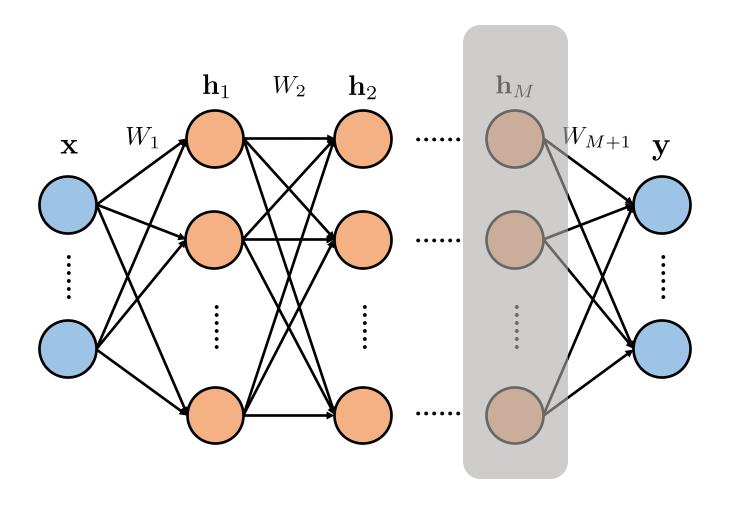
Gradient of loss w.r.t.
$$\mathbf{y}: \frac{\partial L}{\partial \mathbf{y}}$$

Gradient of loss w.r.t. \mathbf{h}_M :

Apply the chain rule we learned before:

$$\frac{\partial L}{\partial \mathbf{h}_M} = \left(\frac{\partial \mathbf{y}}{\partial \mathbf{h}_M}\right)^\top \frac{\partial \mathbf{L}}{\partial \mathbf{y}}$$

During the backward pass:



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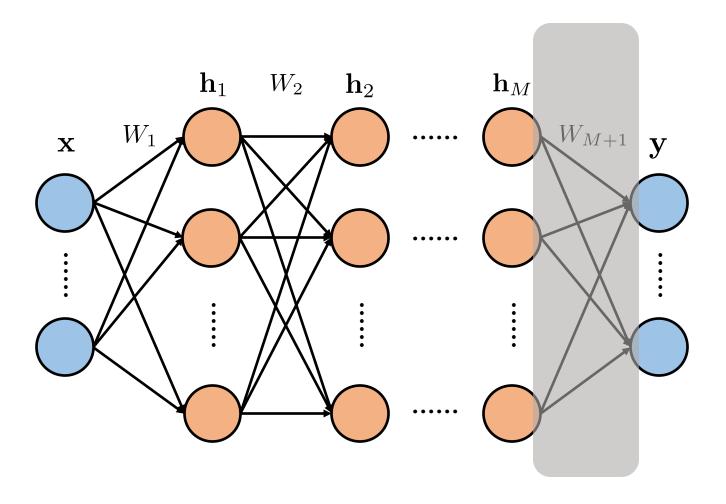
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Recall $\mathbf{y} = W_{M+1}\mathbf{h}_M$

We have
$$\frac{\partial \mathbf{y}}{\partial \mathbf{h}_M} = W_{M+1}$$

During the backward pass:

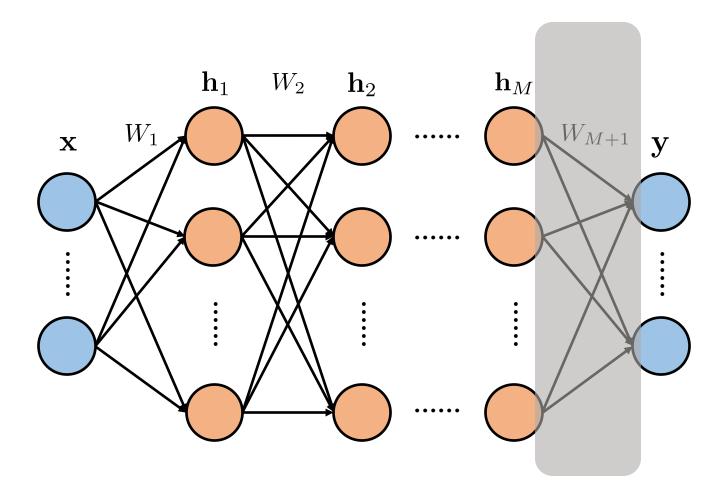


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Gradient of loss w.r.t. $\mathbf{y}: \frac{\partial L}{\partial \mathbf{y}}$

Gradient of loss w.r.t. W_{M+1} :

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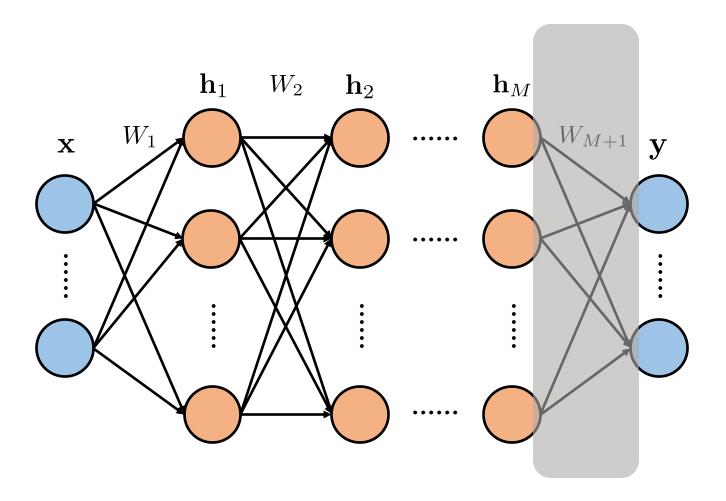
Gradient of loss w.r.t. $\mathbf{y}: \frac{\partial L}{\partial \mathbf{y}}$

Gradient of loss w.r.t. W_{M+1} :

Ideally, chain rule should be something like

$$\frac{\partial L}{\partial W_{M+1}} = \frac{\partial L}{\partial \mathbf{y}} \frac{\partial \mathbf{y}}{\partial W_{M+1}}$$

During the backward pass:



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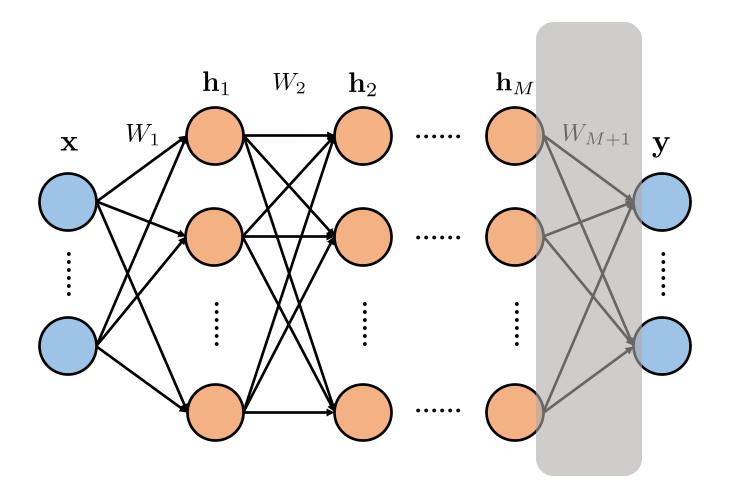
Ideally, chain rule should be something like

$$\frac{\partial L}{\partial W_{M+1}} = \frac{\partial L}{\partial \mathbf{y}} \frac{\partial \mathbf{y}}{\partial W_{M+1}}$$

But this is wrong, since $\frac{\partial \mathbf{y}}{\partial W_{M+1}}$ is the

derivative of a vector w.r.t. a matrix, shapes do not work out!

During the backward pass:



Loss: $L = \ell(\mathbf{y}, \bar{\mathbf{y}})$

Gradient of loss w.r.t. $\mathbf{y}: \frac{\partial L}{\partial \mathbf{y}}$

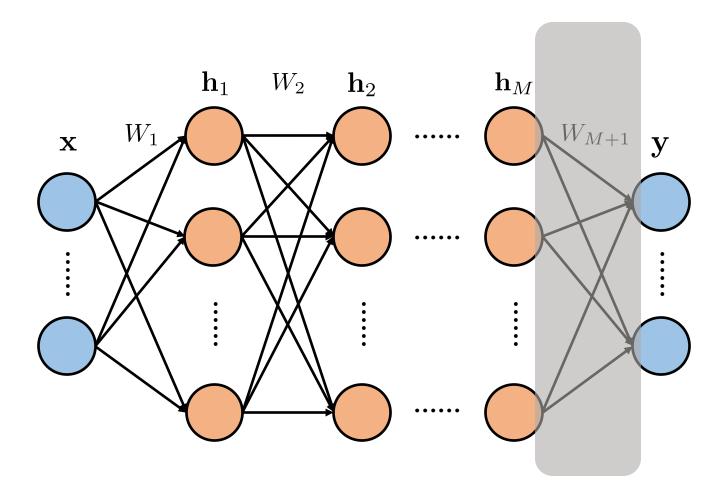
Gradient of loss w.r.t. W_{M+1} :

Note $\mathbf{y}[i]$ only depends on $W_{M+1}[i,:]$

does not depend on $W_{M+1}[j,:] \quad \forall j \neq i$

$$\mathbf{y}[i] = \sum_{j} W_{M+1}[i,j]\mathbf{h}[j]$$

During the backward pass:



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Gradient of loss w.r.t. $\mathbf{y}: \frac{\partial L}{\partial \mathbf{y}}$

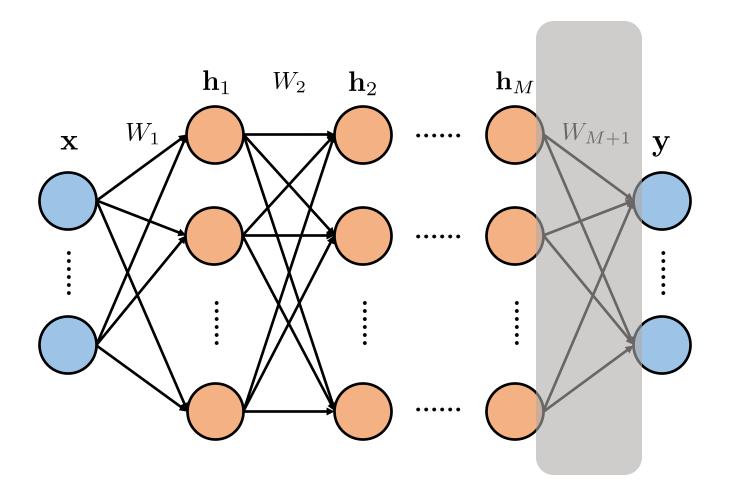
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$$\frac{\partial \mathbf{y}[i]}{\partial W_{M+1}[i, j]} = \mathbf{h}[j]$$

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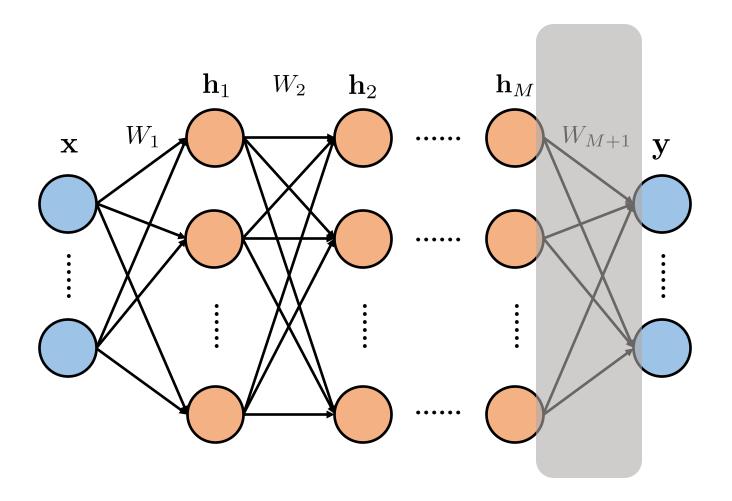
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We have

$$\frac{\partial L}{\partial W_{M+1}[i,j]} = \frac{\partial L}{\partial \mathbf{y}[i]} \frac{\partial \mathbf{y}[i]}{\partial W_{M+1}[i,j]} = \frac{\partial L}{\partial \mathbf{y}[i]} \mathbf{h}[j]$$

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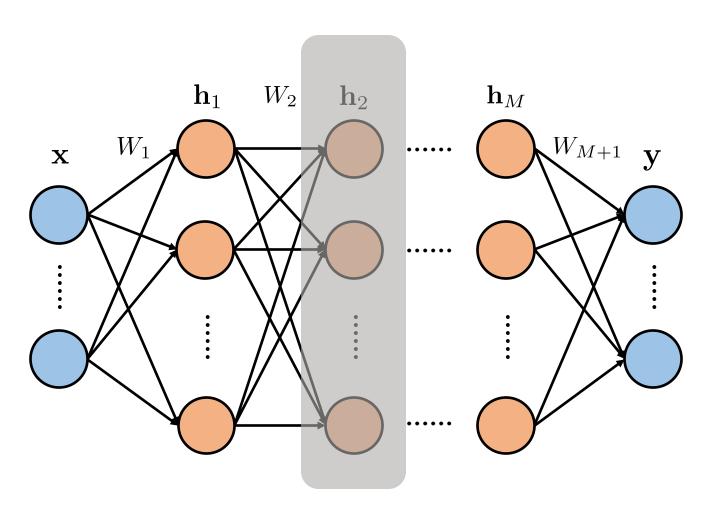
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$$\frac{\partial L}{\partial W_{M+1}} = \frac{\partial L}{\partial \mathbf{y}} \mathbf{h}^{\top}$$

During the backward pass:

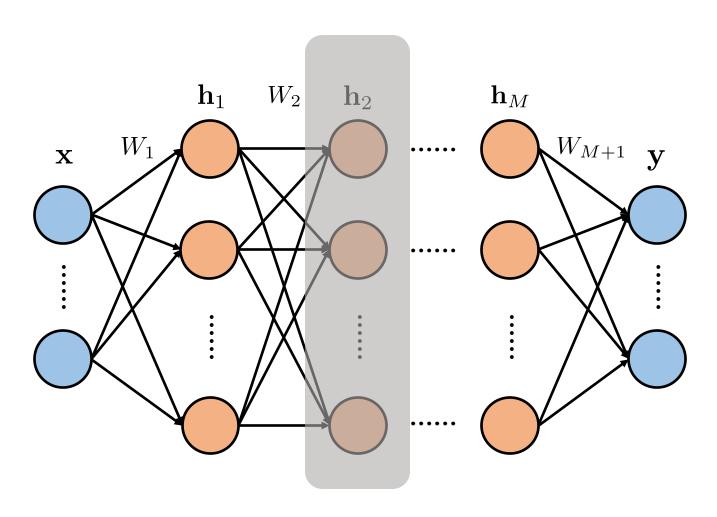


Loss: $L = \ell(\mathbf{y}, \bar{\mathbf{y}})$

Gradient of loss w.r.t. $\mathbf{y}: \frac{\partial L}{\partial \mathbf{y}}$

Gradient of loss w.r.t. h_2 :

During the backward pass:



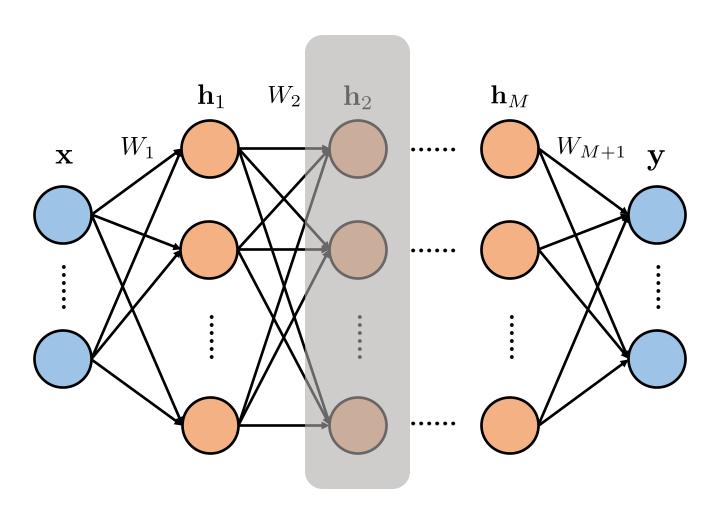
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Gradient of loss w.r.t. $\mathbf{y}: \frac{\partial L}{\partial \mathbf{y}}$

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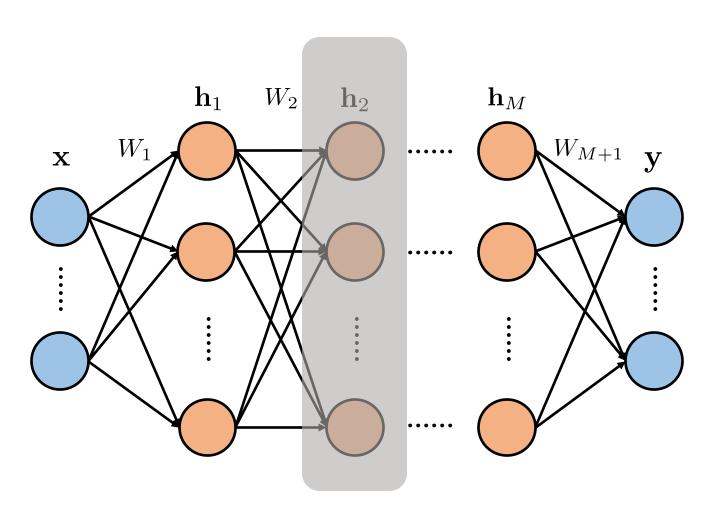
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$$\frac{\partial L}{\partial \mathbf{h}_{M-1}} = \left(\frac{\partial \mathbf{h}_{M}}{\partial \mathbf{h}_{M-1}}\right)^{\top} \frac{\partial L}{\partial \mathbf{h}_{M}}$$

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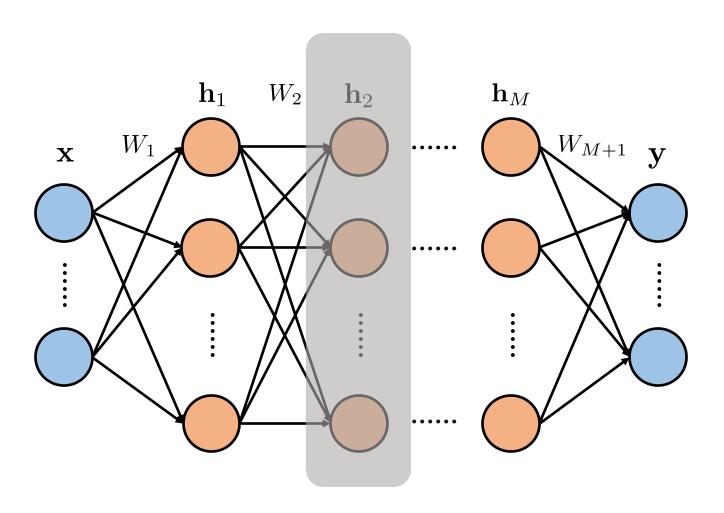
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$$\vdots$$

$$\frac{\partial L}{\partial \mathbf{h}_2} = \left(\frac{\partial \mathbf{h}_3}{\partial \mathbf{h}_2}\right)^{\top} \cdots \left(\frac{\partial \mathbf{h}_M}{\partial \mathbf{h}_{M-1}}\right)^{\top} \left(\frac{\partial \mathbf{y}}{\partial \mathbf{h}_M}\right)^{\top} \frac{\partial L}{\partial \mathbf{y}}$$

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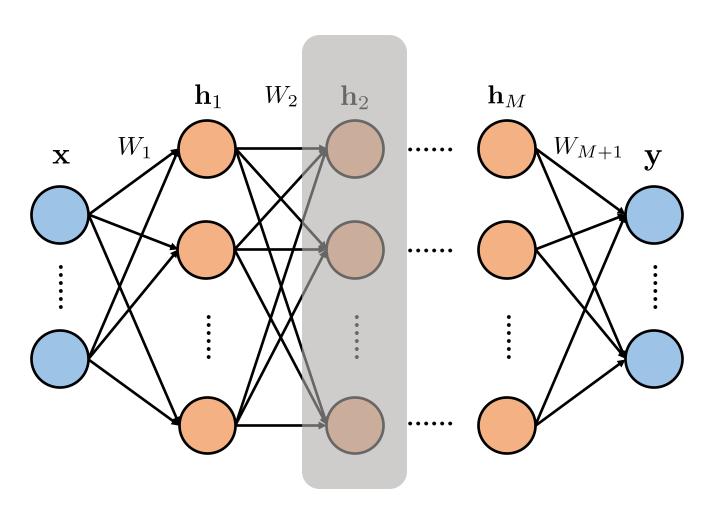
$$\vdots$$

$$\frac{\partial L}{\partial \mathbf{h}_2} = \left(\frac{\partial \mathbf{h}_3}{\partial \mathbf{h}_2}\right)^{\top} \cdots \left(\frac{\partial \mathbf{h}_M}{\partial \mathbf{h}_{M-1}}\right)^{\top} \left(\frac{\partial \mathbf{y}}{\partial \mathbf{h}_M}\right)^{\top} \frac{\partial L}{\partial \mathbf{y}}$$

General form:

$$rac{\partial L}{\partial \mathbf{h}_i} = \mathbf{J}_{i+1}^{ op} \cdots \mathbf{J}_M^{ op} rac{\partial L}{\partial \mathbf{y}} \quad ext{where} \quad egin{matrix} \mathbf{J}_{i+1} \equiv rac{\partial \mathbf{h}_{i+1}}{\partial \mathbf{h}_i} \\ \mathbf{h}_{M+1} \equiv \mathbf{y} \end{split}$$

During the backward pass:

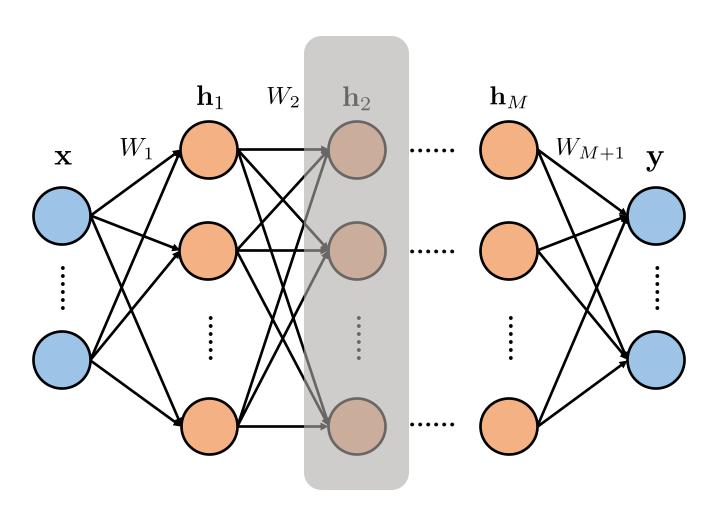


Loss: $L = \ell(\mathbf{y}, \bar{\mathbf{y}})$

Gradient of loss w.r.t. $\mathbf{y}: \frac{\partial L}{\partial \mathbf{y}}$

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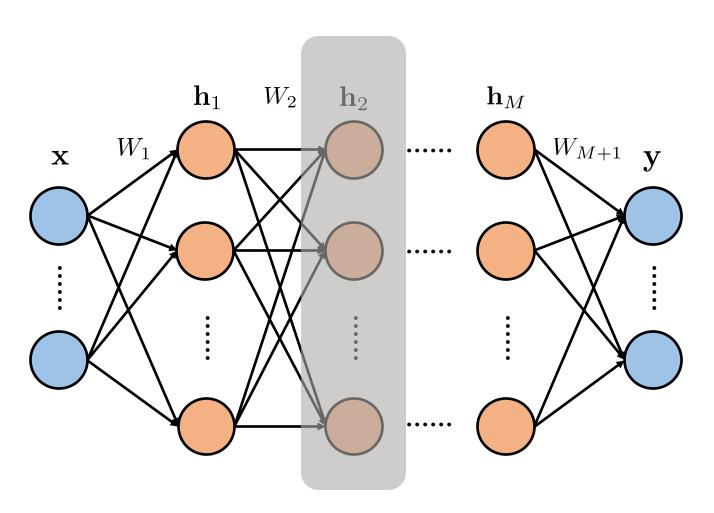
Recall
$$\mathbf{h}_2 = \sigma\left(W_2\mathbf{h}_1\right)$$

Denoting
$$\mathbf{z}_2 = W_2 \mathbf{h}_1$$

We have

$$\frac{\partial \mathbf{h}_2}{\partial \mathbf{h}_1} = \frac{\partial \mathbf{h}_2}{\partial \mathbf{z}_2} \frac{\partial \mathbf{z}_2}{\partial \mathbf{h}_1}$$

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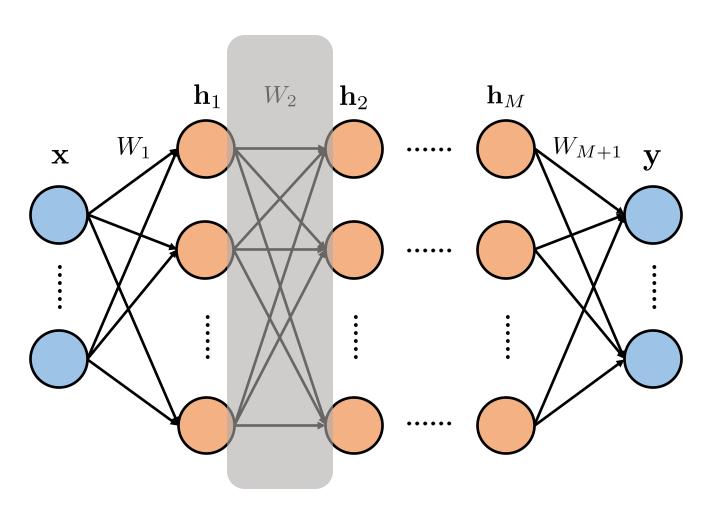
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The Jacobian of element-wise nonlinearity is a diagonal matrix!

During the backward pass:

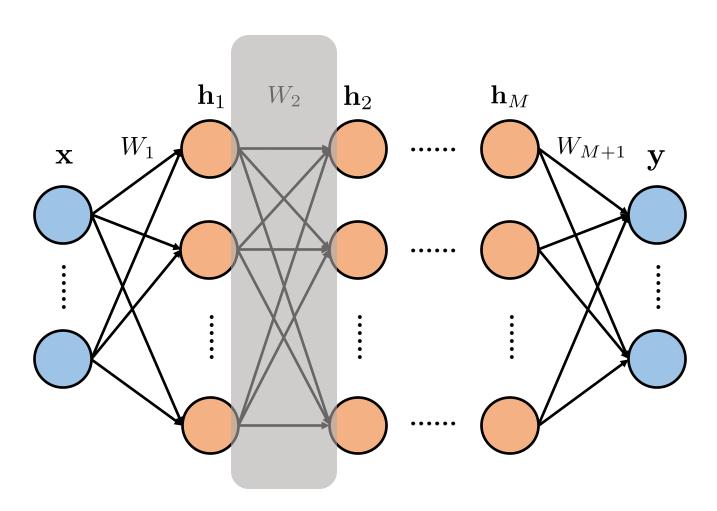


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Gradient of loss w.r.t. W_2 :

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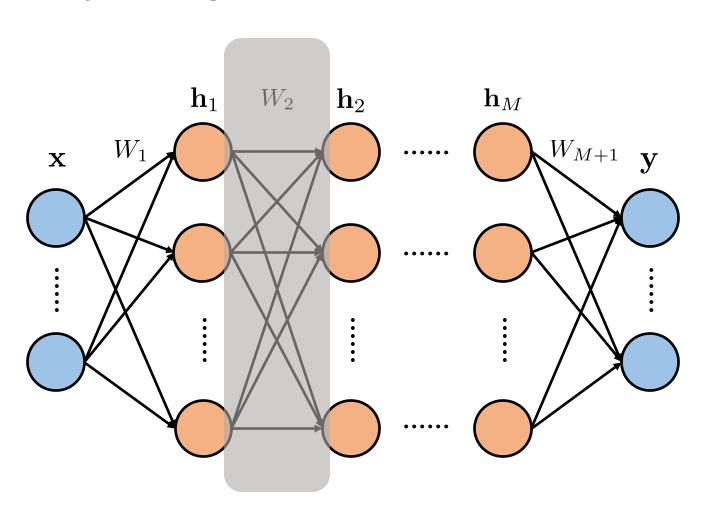
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$$\frac{\partial L}{\partial \mathbf{z}_2} = \left(\frac{\partial \mathbf{h}_2}{\partial \mathbf{z}_2}\right)^{\top} \frac{\partial L}{\partial \mathbf{h}_2}$$

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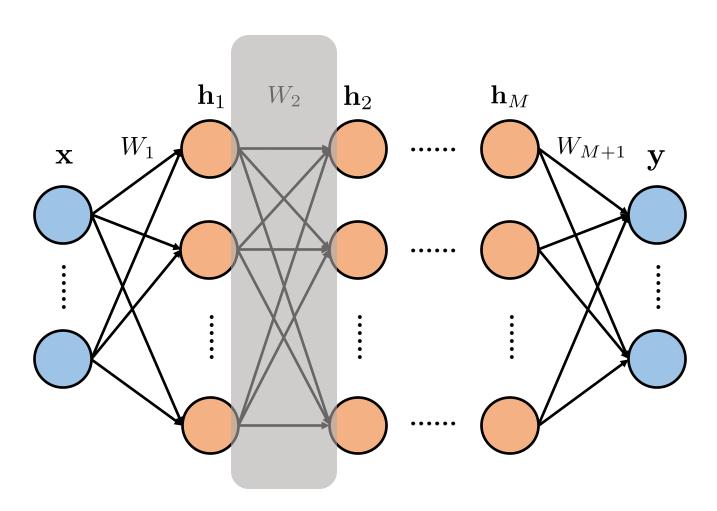
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Why?

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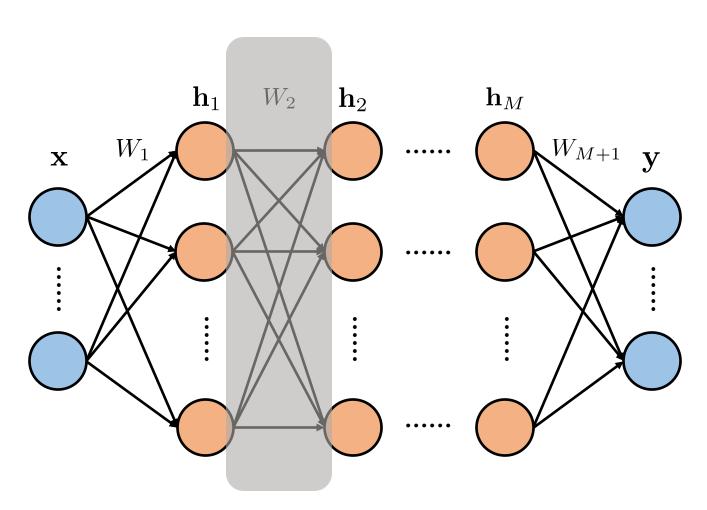
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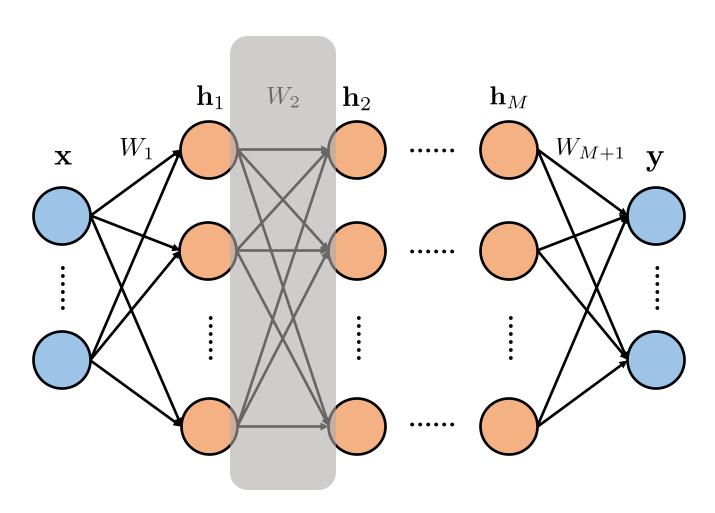
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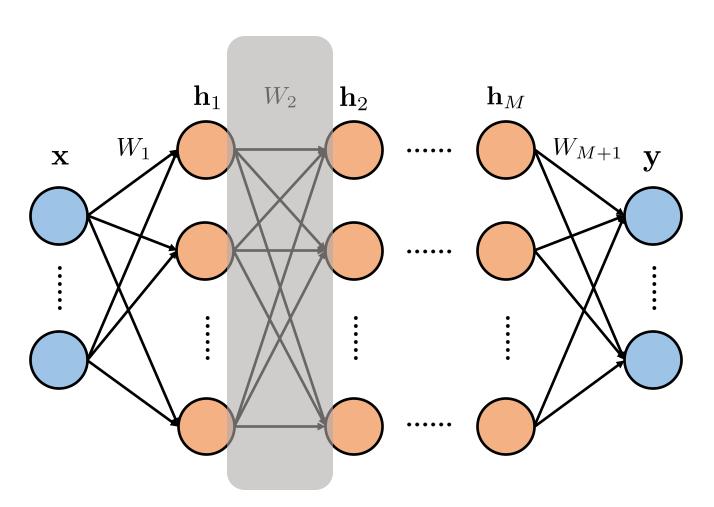
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Note
$$\mathbf{z}_2[i] = \sum_j W_2[i,j]\mathbf{h}_1[j]$$

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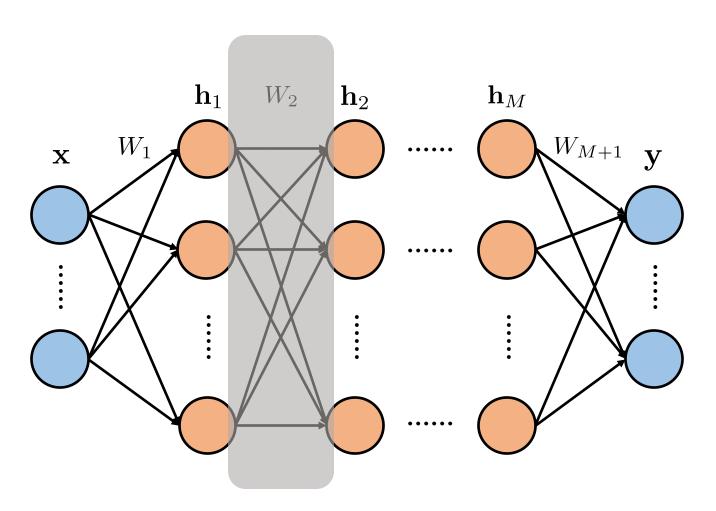
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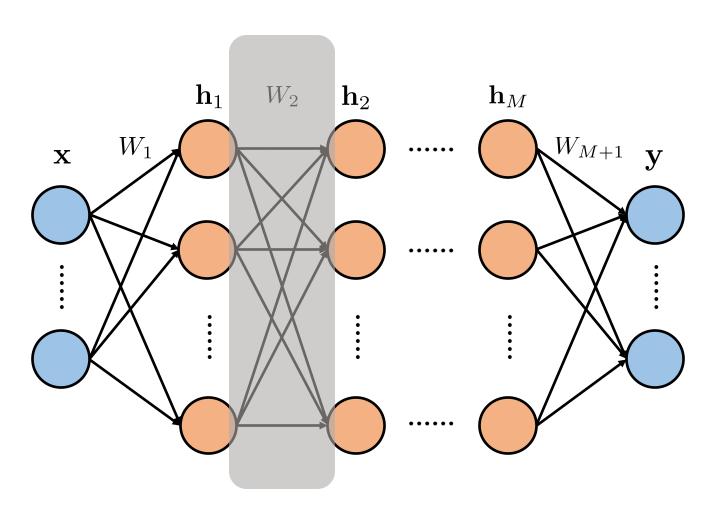
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$$\frac{\partial L}{\partial W_2} = \left(\sigma'(\mathbf{z}_2) \odot \frac{\partial L}{\partial \mathbf{h}_2}\right) \mathbf{h}_1^{\top}$$

During the backward pass:



In summary:

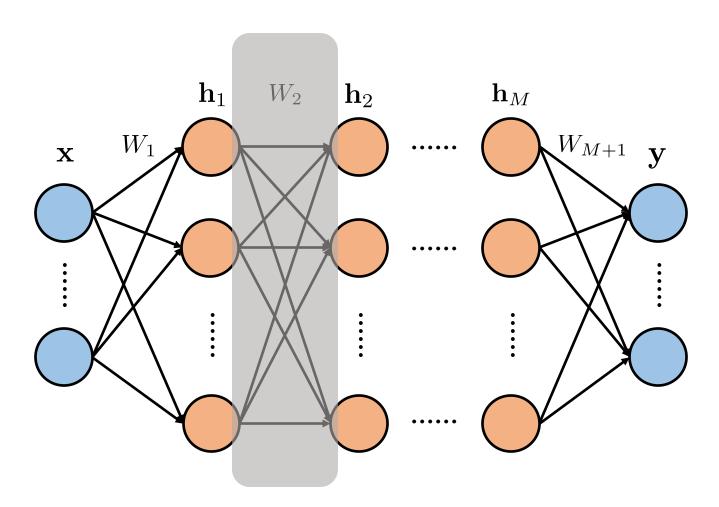
$$\mathbf{z}_i = W_i \mathbf{h}_{i-1}$$

$$\mathbf{J}_i = \operatorname{diag}(\sigma'(\mathbf{z}_i))W_i$$

$$\frac{\partial L}{\partial \mathbf{h}_i} = \mathbf{J}_{i+1}^{\top} \cdots \mathbf{J}_M^{\top} \frac{\partial L}{\partial \mathbf{y}}$$

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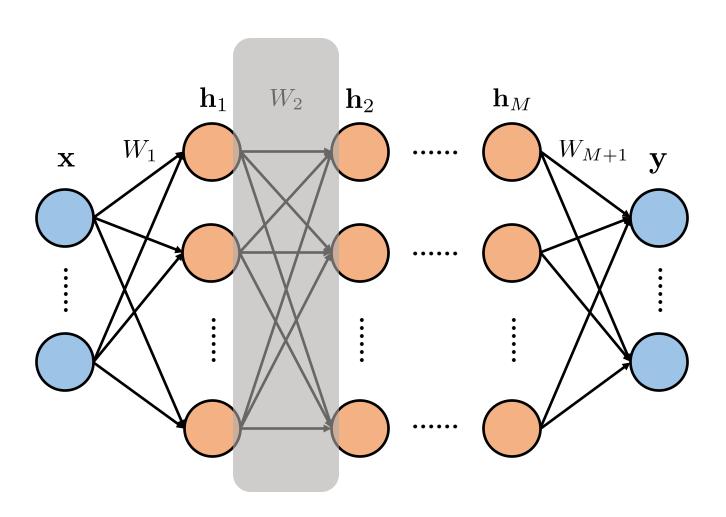
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We can cache these tensors in the forward pass to avoid duplicated computation in the backward pass!

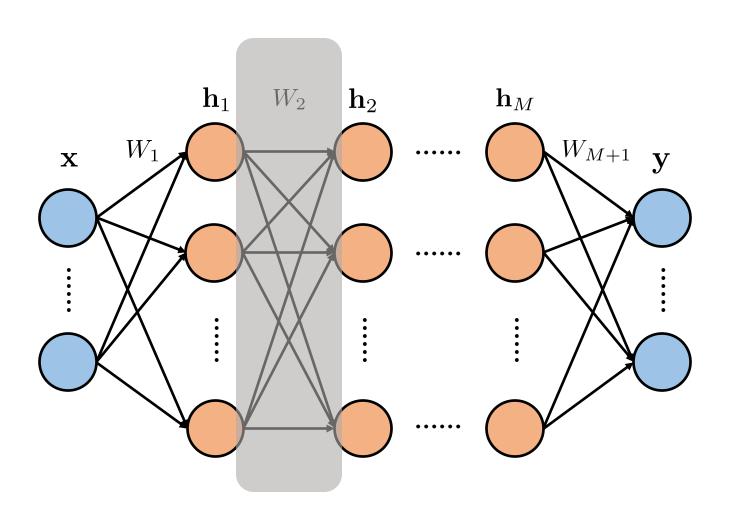
Forward vs. Backward



Computation in Forward Pass:

$$\mathbf{h}_2 = \sigma\left(W_2\mathbf{h}_1\right)$$

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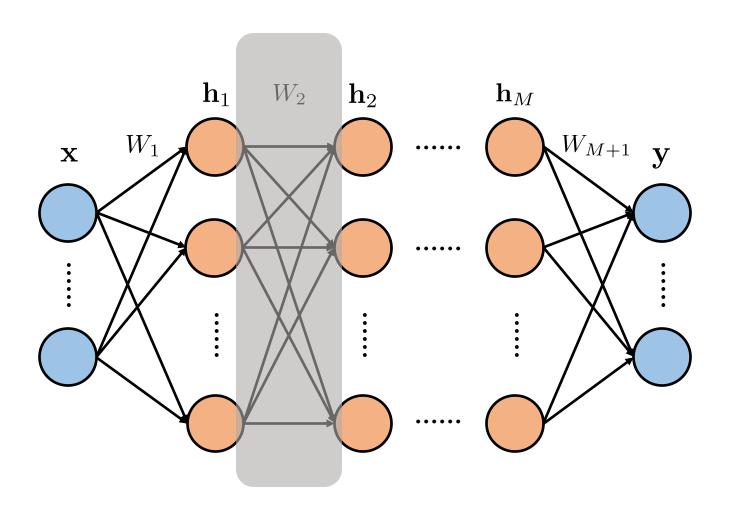
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Computation in Backward Pass:

$$\frac{\partial L}{\partial \mathbf{h}_1} = \mathbf{J}_2^{\top} \frac{\partial L}{\partial \mathbf{h}_2}$$
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$$\mathbf{z}_2 = W_2 \mathbf{h}_1$$
 (cached)

Forward vs. Backward



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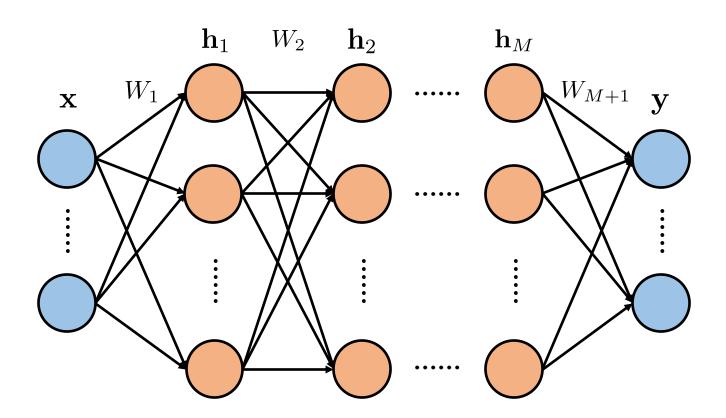
$$\mathbf{z}_2 = W_2 \mathbf{h}_1$$
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Backward pass is roughly twice as computationally expensive as Forward pass!

Outline

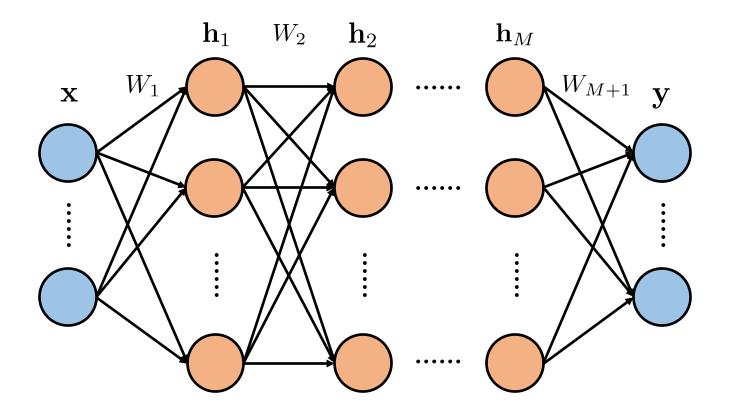
- Learning Algorithm for Feedforward Neural Networks:
 - Backpropagation
 - Weight Initialization
 - Learning Rate & Momentum & Adam
 - Weight Decay & Early Stopping

How should we initialize the neural network?



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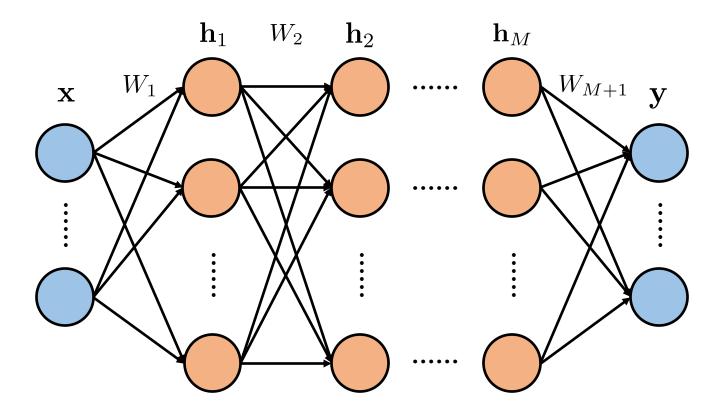
A lot of criterions for good initialization exist, e.g., be close to some local optima, have a higher chance to reach a global optima.



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A lot of criterions for good initialization exist, e.g., *be close to some local optima*, *have a higher chance to reach a global optima*. But most of them are not easily computable before training the neural networks!

 W_2 \mathbf{h}_2 \mathbf{h}_{M} $\mathbf{v}^{W_{M+1}}$ \mathbf{y} \mathbf{X}

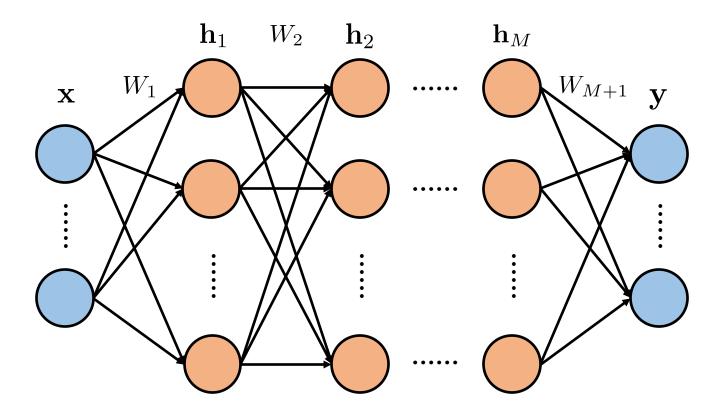
One computable criterion is:

We want to start with some **stable** initial neural network!

How should we initialize the neural network?

A lot of criterions for good initialization exist, e.g., be close to some local optima, have a higher chance to reach a global optima.

But most of them are not easily computable before training the neural networks!



One computable criterion is:

We want to start with some **stable** initial neural network!

There are also many stability notions. Let us look at the variance of the activations and gradients.

Let us recap some basic facts about expectation

Linearity

$$\mathbb{E}[x+y] = \mathbb{E}[x] + \mathbb{E}[y]$$

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Linearity

$$\mathbb{E}[x+y] = \mathbb{E}[x] + \mathbb{E}[y]$$

For two independent random variables

$$\mathbb{E}[xy] = \mathbb{E}[x]\mathbb{E}[y]$$
$$\mathbb{E}[x^2y^2] = \mathbb{E}[x^2]\mathbb{E}[y^2]$$

Let us recap some basic facts about variance

$$\mathbb{V}[x] = \mathbb{E}\left[(x - \mathbb{E}[x])^2\right] = \mathbb{E}[x^2] - (\mathbb{E}[x])^2$$

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$$= \mathbb{E}[x^2 + y^2 + 2xy] - (\mathbb{E}[x] + \mathbb{E}[y])^2$$

$$= \mathbb{E}[x^2] + \mathbb{E}[y^2] + 2\mathbb{E}[xy] - \mathbb{E}[x]^2 - \mathbb{E}[y]^2 - 2\mathbb{E}[x]\mathbb{E}[y]$$

$$= \mathbb{V}[x] + \mathbb{V}[y] + 2(\mathbb{E}[xy] - \mathbb{E}[x]\mathbb{E}[y])$$

$$= \mathbb{V}[x] + \mathbb{V}[y] + 2\text{Cov}(x, y)$$

Let us recap some basic facts about variance

$$\mathbb{V}[x] = \mathbb{E}\left[(x - \mathbb{E}[x])^2\right] = \mathbb{E}[x^2] - (\mathbb{E}[x])^2$$

$$V[x + y] = \mathbb{E}[(x + y)^{2}] - \mathbb{E}[x + y]^{2}$$

$$= \mathbb{E}[x^{2} + y^{2} + 2xy] - (\mathbb{E}[x] + \mathbb{E}[y])^{2}$$

$$= \mathbb{E}[x^{2}] + \mathbb{E}[y^{2}] + 2\mathbb{E}[xy] - \mathbb{E}[x]^{2} - \mathbb{E}[y]^{2} - 2\mathbb{E}[x]\mathbb{E}[y]$$

$$= V[x] + V[y] + 2(\mathbb{E}[xy] - \mathbb{E}[x]\mathbb{E}[y])$$

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Let us recap some basic facts about variance

$$\mathbb{V}[x] = \mathbb{E}\left[(x - \mathbb{E}[x])^2\right] = \mathbb{E}[x^2] - (\mathbb{E}[x])^2$$

$$\begin{split} \mathbb{V}[xy] &= \mathbb{E}[x^2y^2] - (\mathbb{E}[xy])^2 \\ &= \mathbb{E}[x^2y^2] - \mathbb{E}[x]^2 \mathbb{E}[y]^2 \\ &= \mathbb{E}[x^2] \mathbb{E}[y^2] - \mathbb{E}[x]^2 \mathbb{E}[y^2] + \mathbb{E}[x]^2 \mathbb{E}[y^2] - \mathbb{E}[x]^2 \mathbb{E}[y]^2 \\ &= (\mathbb{E}[x^2] - \mathbb{E}[x]^2) \mathbb{E}[y^2] + \mathbb{E}[x]^2 (\mathbb{E}[y^2] - \mathbb{E}[y]^2) \\ &= \mathbb{V}[x] \mathbb{E}[y^2] + \mathbb{E}[x]^2 \mathbb{V}[y] \\ &= \mathbb{V}[x] (\mathbb{V}[y] + \mathbb{E}[y]^2) + \mathbb{E}[x]^2 \mathbb{V}[y] \\ &= \mathbb{V}[x] \mathbb{V}[y] + \mathbb{E}[y]^2 \mathbb{V}[x] + \mathbb{E}[x]^2 \mathbb{V}[y] \end{split}$$

$$\mathbb{E}[xy] = \mathbb{E}[x]\mathbb{E}[y]$$
$$\mathbb{E}[x^2y^2] = \mathbb{E}[x^2]\mathbb{E}[y^2]$$

Let us recap some basic facts about variance

$$\mathbb{V}[x] = \mathbb{E}\left[(x - \mathbb{E}[x])^2 \right] = \mathbb{E}[x^2] - (\mathbb{E}[x])^2$$

For two independent random variables, we have

If $\mathbb{E}[x] = \mathbb{E}[y] = 0$, then $\mathbb{V}[xy] = \mathbb{V}[x]\mathbb{V}[y]$

$$V[xy] = \mathbb{E}[x^2y^2] - (\mathbb{E}[xy])^2$$

$$= \mathbb{E}[x^2y^2] - \mathbb{E}[x]^2\mathbb{E}[y]^2$$

$$= \mathbb{E}[x^2]\mathbb{E}[y^2] - \mathbb{E}[x]^2\mathbb{E}[y^2] + \mathbb{E}[x]^2\mathbb{E}[y^2] - \mathbb{E}[x]^2\mathbb{E}[y]^2$$

$$= (\mathbb{E}[x^2] - \mathbb{E}[x]^2)\mathbb{E}[y^2] + \mathbb{E}[x]^2(\mathbb{E}[y^2] - \mathbb{E}[y]^2)$$

$$= \mathbb{V}[x]\mathbb{E}[y^2] + \mathbb{E}[x]^2\mathbb{V}[y]$$

$$= \mathbb{V}[x](\mathbb{V}[y] + \mathbb{E}[y]^2) + \mathbb{E}[x]^2\mathbb{V}[y]$$

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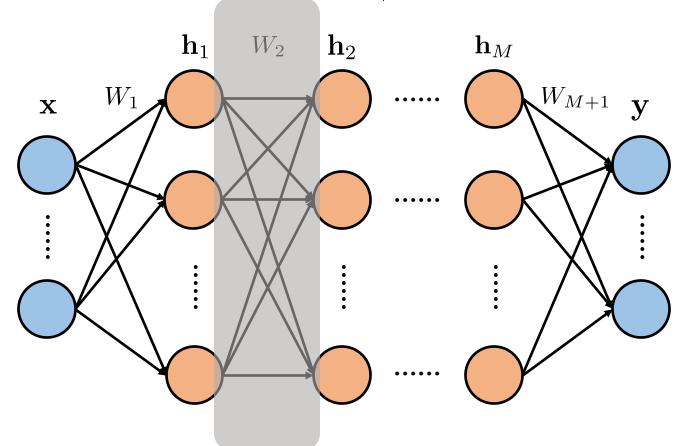
In summary, for two independent random variables, we have

$$V[x+y] = V[x] + V[y]$$
$$V[xy] = V[x]V[y] + \mathbb{E}[y]^2V[x] + \mathbb{E}[x]^2V[y]$$

If
$$\mathbb{E}[x] = \mathbb{E}[y] = 0$$
, then $\mathbb{V}[xy] = \mathbb{V}[x]\mathbb{V}[y]$

Recall $\mathbf{h}_2 = \sigma(W_2\mathbf{h}_1)$

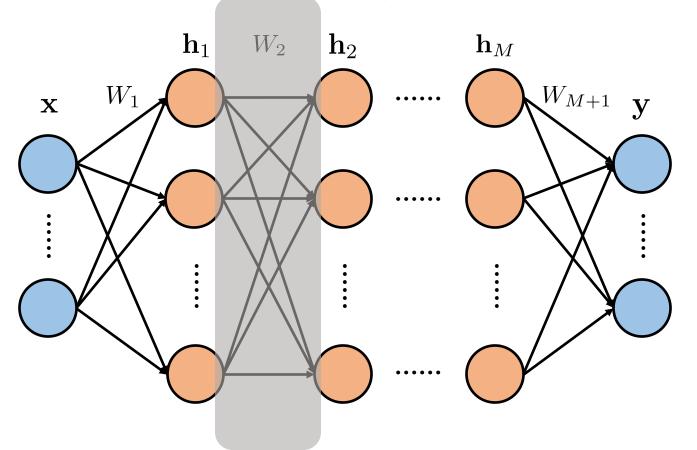
If we assume Tanh activation $\sigma(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$ and we are in the linear regime

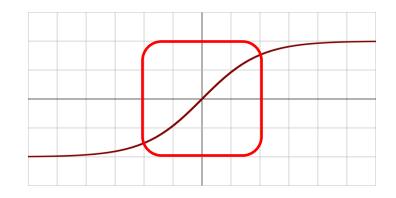




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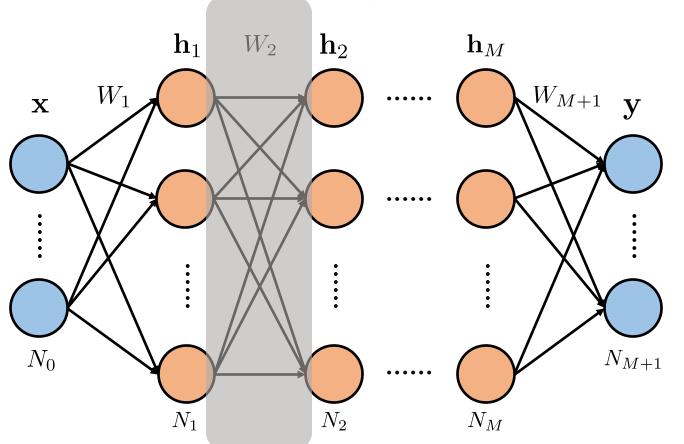
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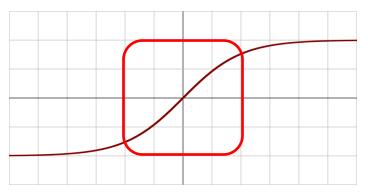




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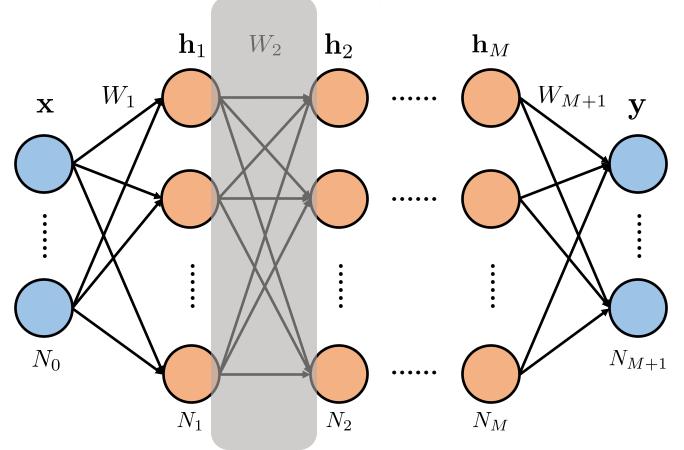


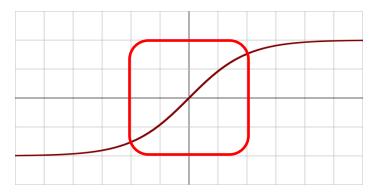
Then we have

$$\mathbf{h}_{2}[i] = \sigma(\sum_{j=1}^{N_{1}} W_{2}[i, j] \mathbf{h}_{1}[j]) \approx \sum_{j=1}^{N_{1}} W_{2}[i, j] \mathbf{h}_{1}[j]$$

Recall $\mathbf{h}_2 = \sigma\left(W_2\mathbf{h}_1\right)$

If we assume Tanh activation $\sigma(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$ and we are in the linear regime





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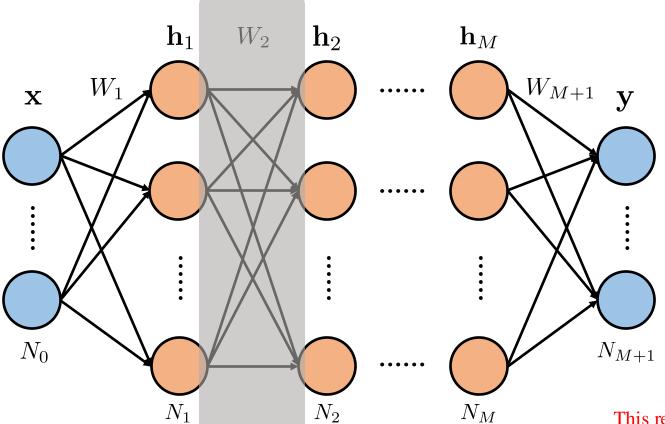
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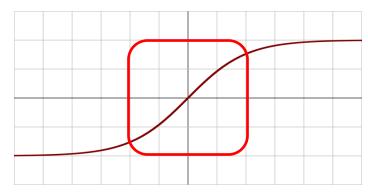
We further assume i.i.d. and zero mean with same variance for all activations $\mathbf{h}_1[j]$ and all weights $W_2[i,j]$ at all layers, then

$$\begin{split} \mathbb{V}\left[\mathbf{h}_{2}[i]\right] &\approx \mathbb{V}\left[\sum_{j=1}^{N_{1}}W_{2}[i,j]\mathbf{h}_{1}[j]\right] \\ &= \sum_{j=1}^{N_{1}}\mathbb{V}\left[W_{2}[i,j]\mathbf{h}_{1}[j]\right] \\ &= \sum_{j=1}^{N_{1}}\mathbb{V}\left[W_{2}[i,j]\right]\mathbb{V}\left[\mathbf{h}_{1}[j]\right] \\ &= N_{1}\mathbb{V}\left[W_{2}[i,j]\right]\mathbb{V}\left[\mathbf{h}_{1}[j]\right] \end{split}$$

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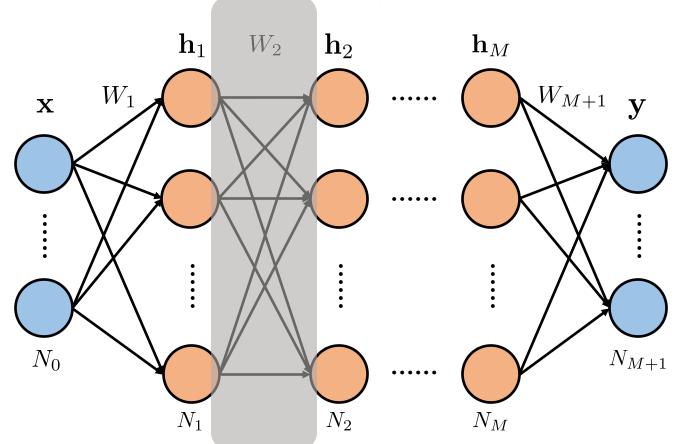
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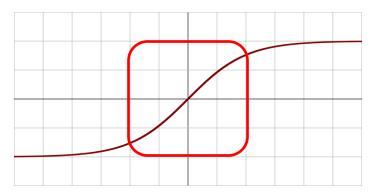
$$\begin{split} \mathbb{V}\left[\mathbf{h}_{2}[i]\right] &\approx \mathbb{V}\left[\sum_{j=1}^{N_{1}} W_{2}[i,j]\mathbf{h}_{1}[j]\right] \\ &= \sum_{j=1}^{N_{1}} \mathbb{V}\left[W_{2}[i,j]\mathbf{h}_{1}[j]\right] \\ &= \sum_{j=1}^{N_{1}} \mathbb{V}\left[W_{2}[i,j]\right] \mathbb{V}\left[\mathbf{h}_{1}[j]\right] \\ &= N_{1} \mathbb{V}\left[W_{2}[i,j]\right] \mathbb{V}\left[\mathbf{h}_{1}[j]\right] \end{split}$$

This relation holds for all layers given the assumptions!

Recall $\mathbf{h}_2 = \sigma\left(W_2\mathbf{h}_1\right)$

If we assume Tanh activation $\sigma(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$ and we are in the linear regime





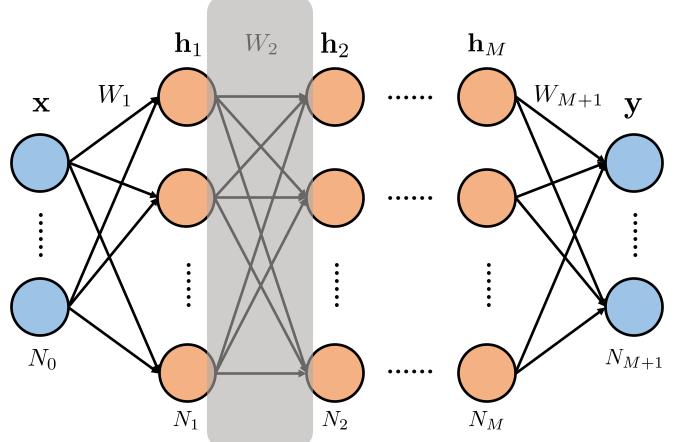
Then unroll the recursion, we have

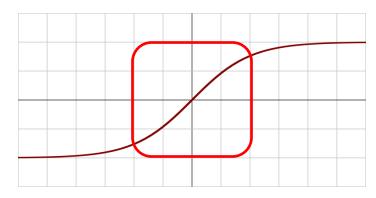
$$\mathbb{V}\left[\mathbf{h}_{l}[i]\right] \approx \mathbb{V}\left[\mathbf{x}[j]\right] \prod_{k=1}^{l} N_{k-1} \mathbb{V}\left[W_{k}[i,j]\right]$$

Note i and j here are arbitrary since we assume all activations have the same variance and all weights have the same variance as well!

Recall $\mathbf{h}_2 = \sigma\left(W_2\mathbf{h}_1\right)$

If we assume Tanh activation $\sigma(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$ and we are in the linear regime





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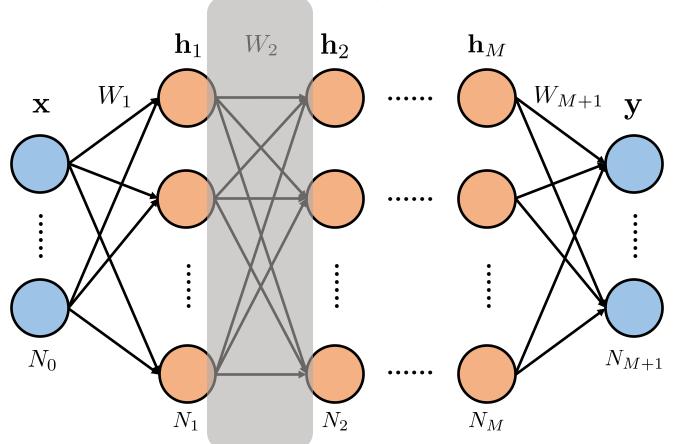
Note i and j here are arbitrary since we assume all activations have the same variance and all weights have the same variance as well!

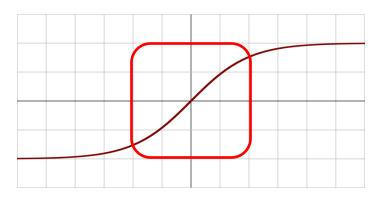
To preserve the variance of activations through forward pass, i.e.,

$$\mathbb{V}\left[\mathbf{h}_{l}[i]\right] \approx \mathbb{V}\left[\mathbf{x}[j]\right]$$

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Then unroll the recursion, we have

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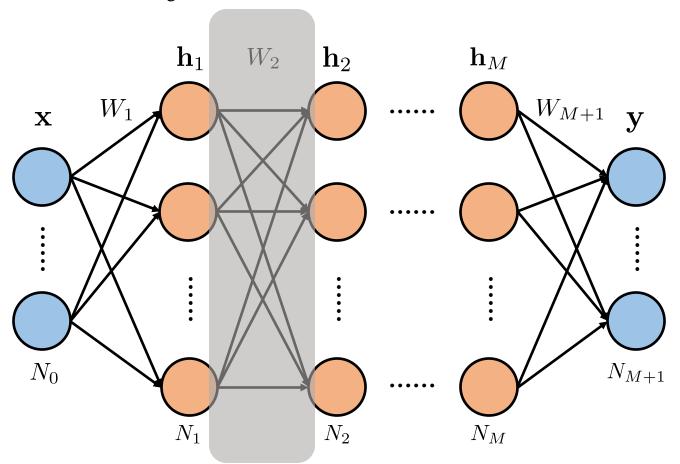
we can simply set:

$$\mathbb{V}\left[W_k[i,j]\right] = \frac{1}{N_{k-1}}$$

Assuming Tanh activation
$$\sigma(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$$
 and we are in the linear regime $\mathbf{h}_2[i] = \sigma(\sum_{j=1}^{N_1} W_2[i,j]\mathbf{h}_1[j]) \approx \sum_{j=1}^{N_1} W_2[i,j]\mathbf{h}_1[j]$

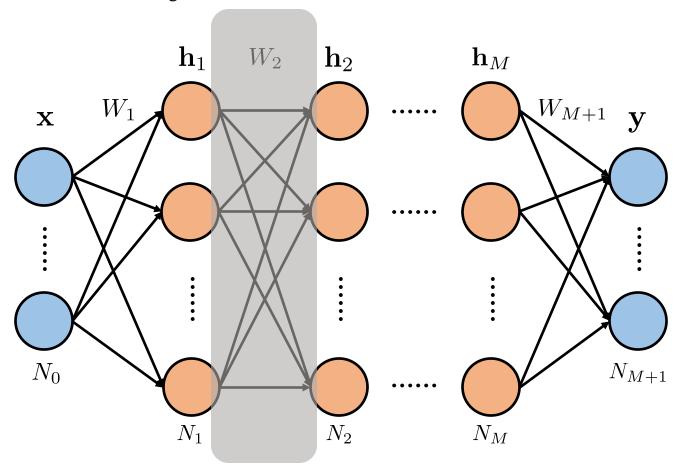
$$\mathbf{h}_{2}[i] = \sigma(\sum_{j=1}^{N_{1}} W_{2}[i,j]\mathbf{h}_{1}[j]) \approx \sum_{j=1}^{N_{1}} W_{2}[i,j]\mathbf{h}_{1}[j]$$

Let us look at the gradient w.r.t. activations



Assuming Tanh activation $\sigma(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$ and we are in the linear regime

Let us look at the gradient w.r.t. activations

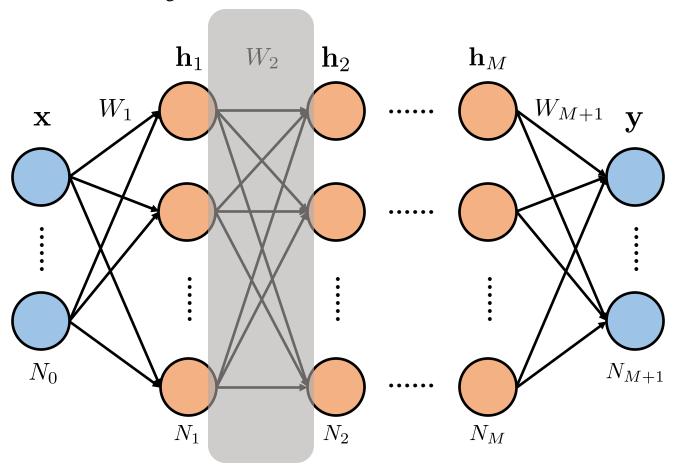


$$\mathbf{h}_2[i] = \sigma(\sum_{j=1}^{N_1} W_2[i,j]\mathbf{h}_1[j]) \approx \sum_{j=1}^{N_1} W_2[i,j]\mathbf{h}_1[j]$$

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Let us again assume i.i.d. and zero mean with

same variance for all $\frac{\partial L}{\partial \mathbf{h}_2[i]}$, $W_2[i,j]$, and $\mathbf{h}_2[i]$ at all layers, then

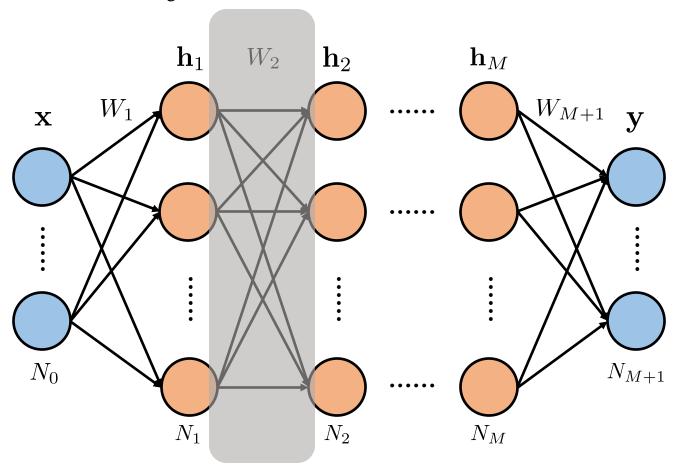
$$\mathbb{V}\left[\frac{\partial L}{\partial \mathbf{h}_{1}[j]}\right] \approx \sum_{i=1}^{N_{2}} \mathbb{V}\left[\frac{\partial L}{\partial \mathbf{h}_{2}[i]}\right] \mathbb{V}\left[W_{2}[i,j]\right]$$

$$= N_{2} \mathbb{V}\left[\frac{\partial L}{\partial \mathbf{h}_{2}[i]}\right] \mathbb{V}\left[W_{2}[i,j]\right]$$

$$= \mathbb{V}\left[\frac{\partial L}{\partial \mathbf{y}[i]}\right] \prod_{k=2}^{M+1} N_{k} \mathbb{V}\left[W_{k}[i,j]\right]$$

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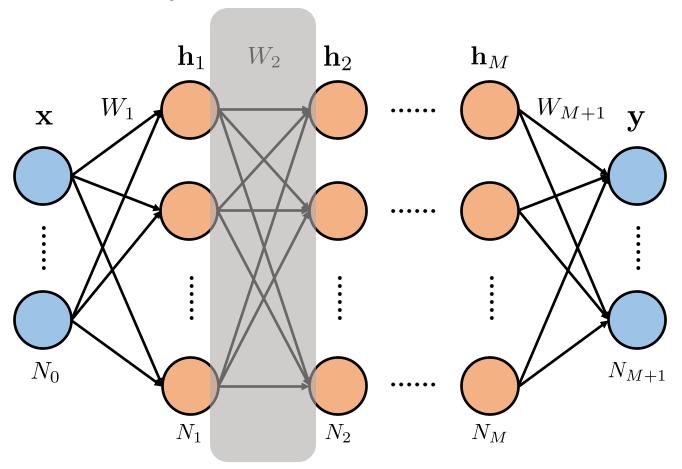
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Setting $\mathbb{V}\left[W_k[i,j]\right] = \frac{1}{N_k}$ preserves the

variance of gradients w.r.t. activations!

Assuming Tanh activation $\sigma(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$ and we are in the linear regime

Let us look at the gradient w.r.t. activations



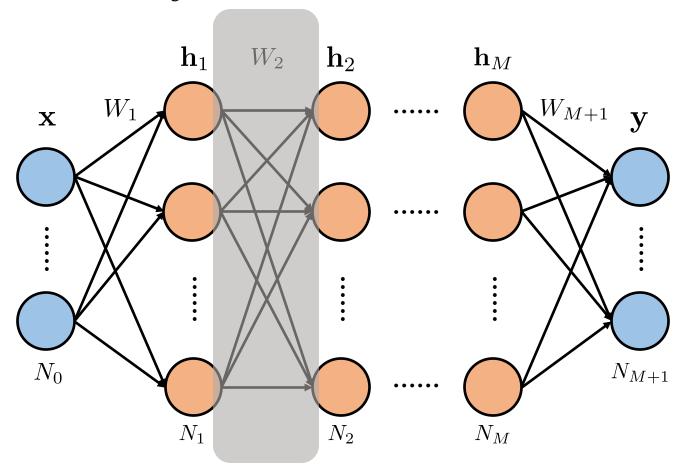
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What about the gradients w.r.t. weights?

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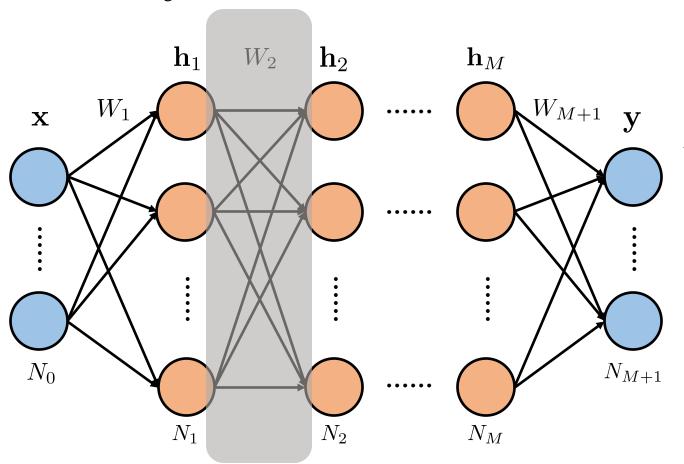
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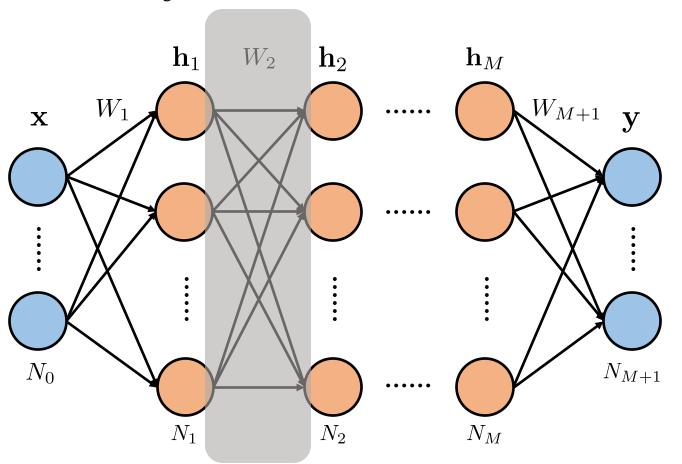
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$$\begin{split} \mathbb{V}\left[\frac{\partial L}{\partial W_{2}[i,j]}\right] &\approx \mathbb{V}\left[\frac{\partial L}{\partial \mathbf{h}_{2}[i]}\right] \mathbb{V}\left[\mathbf{h}_{1}[j]\right] \\ &= \left(\mathbb{V}\left[\frac{\partial L}{\partial \mathbf{y}[i]}\right] \prod_{k=3}^{M+1} N_{k} \mathbb{V}\left[W_{k}[i,j]\right]\right) \\ & \left(\mathbb{V}\left[\mathbf{x}[j]\right] \prod_{k=1}^{1} N_{k-1} \mathbb{V}\left[W_{k}[i,j]\right]\right) \\ &= \frac{N_{0}}{N_{1}} \left(\prod_{k=1}^{1} N_{k} \mathbb{V}\left[W_{k}[i,j]\right]\right) \left(\prod_{k=3}^{M+1} N_{k} \mathbb{V}\left[W_{k}[i,j]\right]\right) \mathbb{V}\left[\frac{\partial L}{\partial \mathbf{y}[i]}\right] \mathbb{V}\left[\mathbf{x}[j]\right] \\ &= \frac{N_{0}}{N_{1}} \mathbb{V}\left[\frac{\partial L}{\partial \mathbf{y}[i]}\right] \mathbb{V}\left[\mathbf{x}[j]\right] \end{split}$$

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Let us look at the gradient w.r.t. activations



$$\mathbf{h}_{2}[i] = \sigma(\sum_{j=1}^{N_{1}} W_{2}[i,j]\mathbf{h}_{1}[j]) \approx \sum_{j=1}^{N_{1}} W_{2}[i,j]\mathbf{h}_{1}[j]$$

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$$\begin{split} \mathbb{V}\left[\frac{\partial L}{\partial W_{2}[i,j]}\right] &\approx \mathbb{V}\left[\frac{\partial L}{\partial \mathbf{h}_{2}[i]}\right] \mathbb{V}\left[\mathbf{h}_{1}[j]\right] \\ &= \left(\mathbb{V}\left[\frac{\partial L}{\partial \mathbf{y}[i]}\right] \prod_{k=3}^{M+1} N_{k} \mathbb{V}\left[W_{k}[i,j]\right]\right) \\ & \left(\mathbb{V}\left[\mathbf{x}[j]\right] \prod_{k=1}^{1} N_{k-1} \mathbb{V}\left[W_{k}[i,j]\right]\right) \\ &= \frac{N_{0}}{N_{1}} \left(\prod_{k=1}^{1} N_{k} \mathbb{V}\left[W_{k}[i,j]\right]\right) \left(\prod_{k=3}^{M+1} N_{k} \mathbb{V}\left[W_{k}[i,j]\right]\right) \mathbb{V}\left[\frac{\partial L}{\partial \mathbf{y}[i]}\right] \mathbb{V}\left[\mathbf{x}[j]\right] \\ &= \frac{N_{0}}{N_{1}} \mathbb{V}\left[\frac{\partial L}{\partial \mathbf{y}[i]}\right] \mathbb{V}\left[\mathbf{x}[j]\right] \end{split}$$

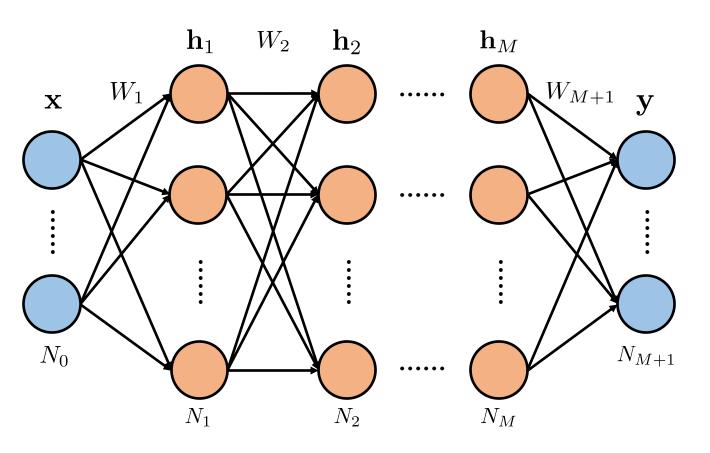
Setting $\mathbb{V}[W_k[i,j]] = \frac{1}{N_k}$ makes the variance of gradients w.r.t. weights behave reasonably (e.g., no exploding or vanishing)!

In summary, to preserve the variance of activations, we set

$$\mathbb{V}\left[W_k[i,j]\right] = \frac{1}{N_{k-1}}$$

to preserve the variance of gradients w.r.t. activations, we set

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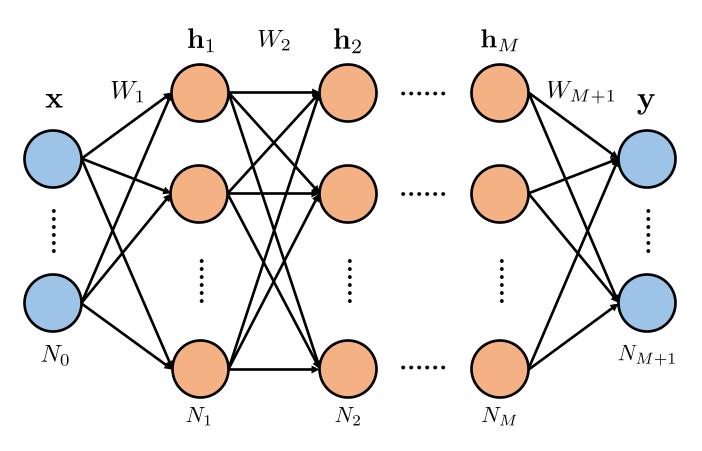


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To compromise between two goals, we can take the mean of the denominators:

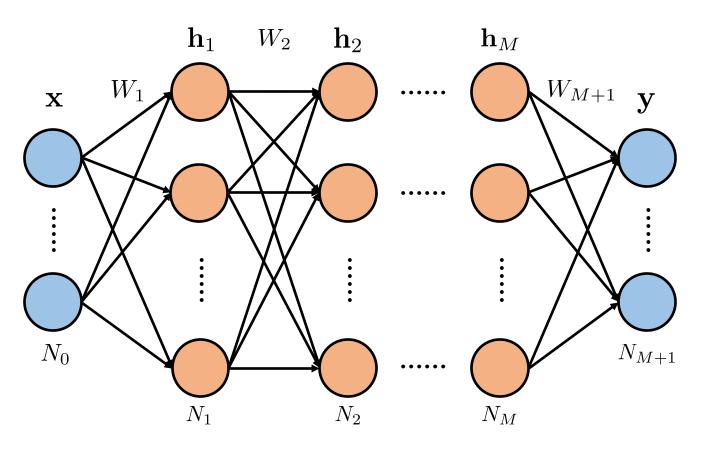
$$\mathbb{V}[W_k[i,j]] = \frac{1}{\frac{N_k + N_{k-1}}{2}} = \frac{2}{N_k + N_{k-1}}$$

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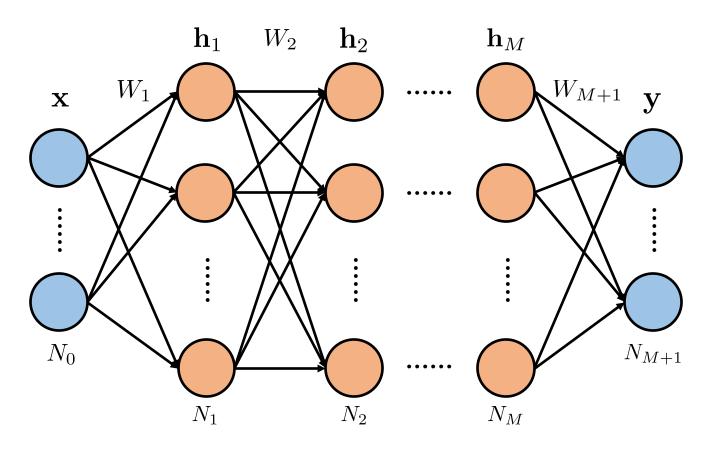
This is the so-called "Xavier Initialization" [3]!

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This is the so-called "Xavier Initialization" [3]!

By considering the effect of ReLU, we can similarly derive "Kaiming Initialization" [4]!

References

- [1] Robbins, H., & Monro, S. (1951). A stochastic approximation method. The annals of mathematical statistics, 400-407.
- [2] Rumelhart, D. E., Hinton, G. E., & Williams, R. J. (1986). Learning representations by back-propagating errors. nature, 323(6088), 533-536.
- [3] Glorot, X., & Bengio, Y. (2010). Understanding the difficulty of training deep feedforward neural networks. In Proceedings of the thirteenth international conference on artificial intelligence and statistics (pp. 249-256).
- [4] He, K., Zhang, X., Ren, S., & Sun, J. (2015). Delving deep into rectifiers: Surpassing human-level performance on imagenet classification. In Proceedings of the IEEE international conference on computer vision (pp. 1026-1034).

Questions?