CPEN 400D: Deep Learning

Lecture 2 (II): Backpropagation

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Winter, Term 2, 2022

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**!

Adjust parameters based on loss ⇔ Assign credits based on contribution

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- The most successful learning algorithm in machine learning so far is **gradient based learning**!

  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

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

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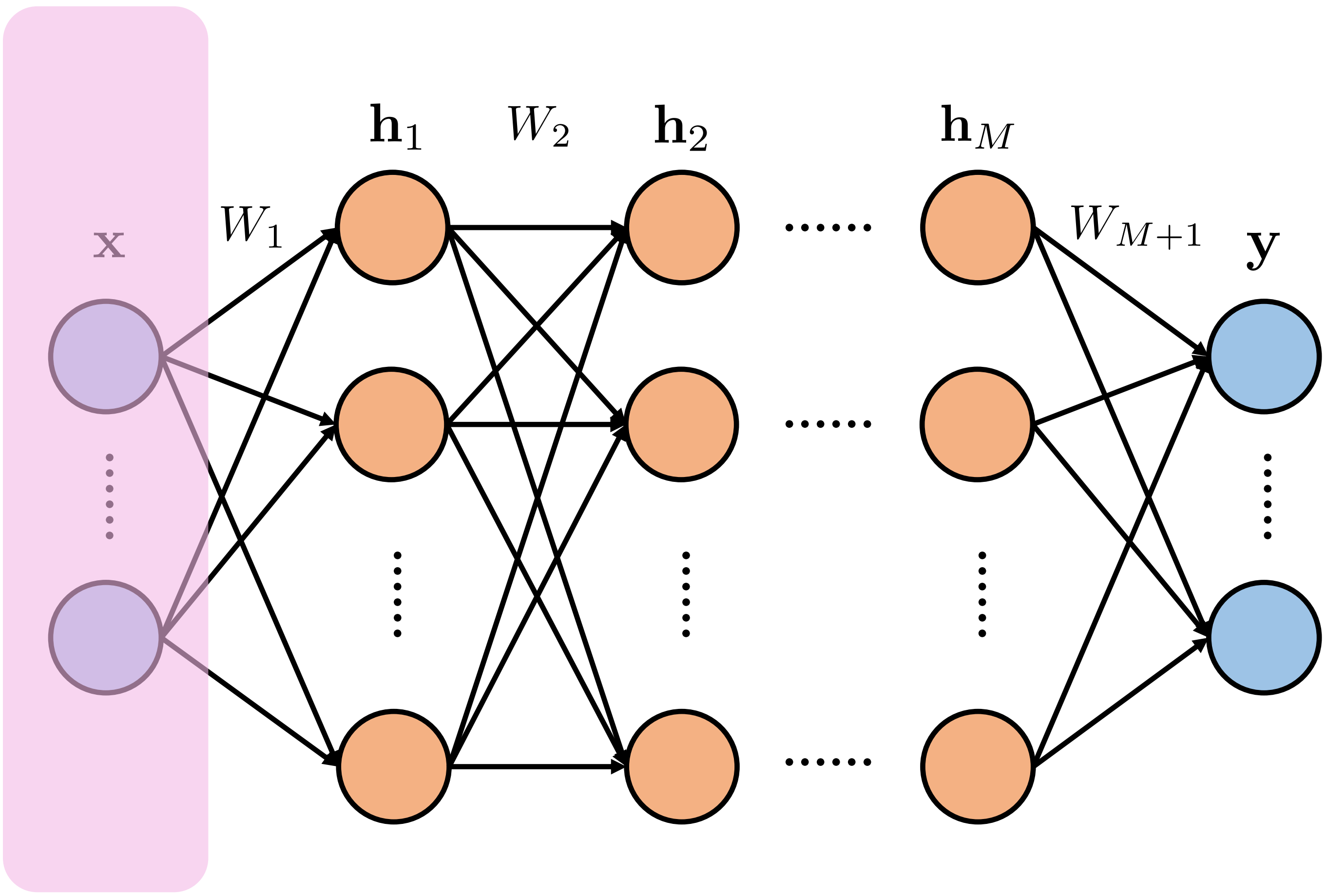
- Learning Algorithm for Feedforward Neural Networks:
    - **Backpropagation**
    - Weight Initialization
    - Learning Rate & Momentum & Adam
    - Weight Decay & Early Stopping

Feedforward Neural Networks

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

Input Sample



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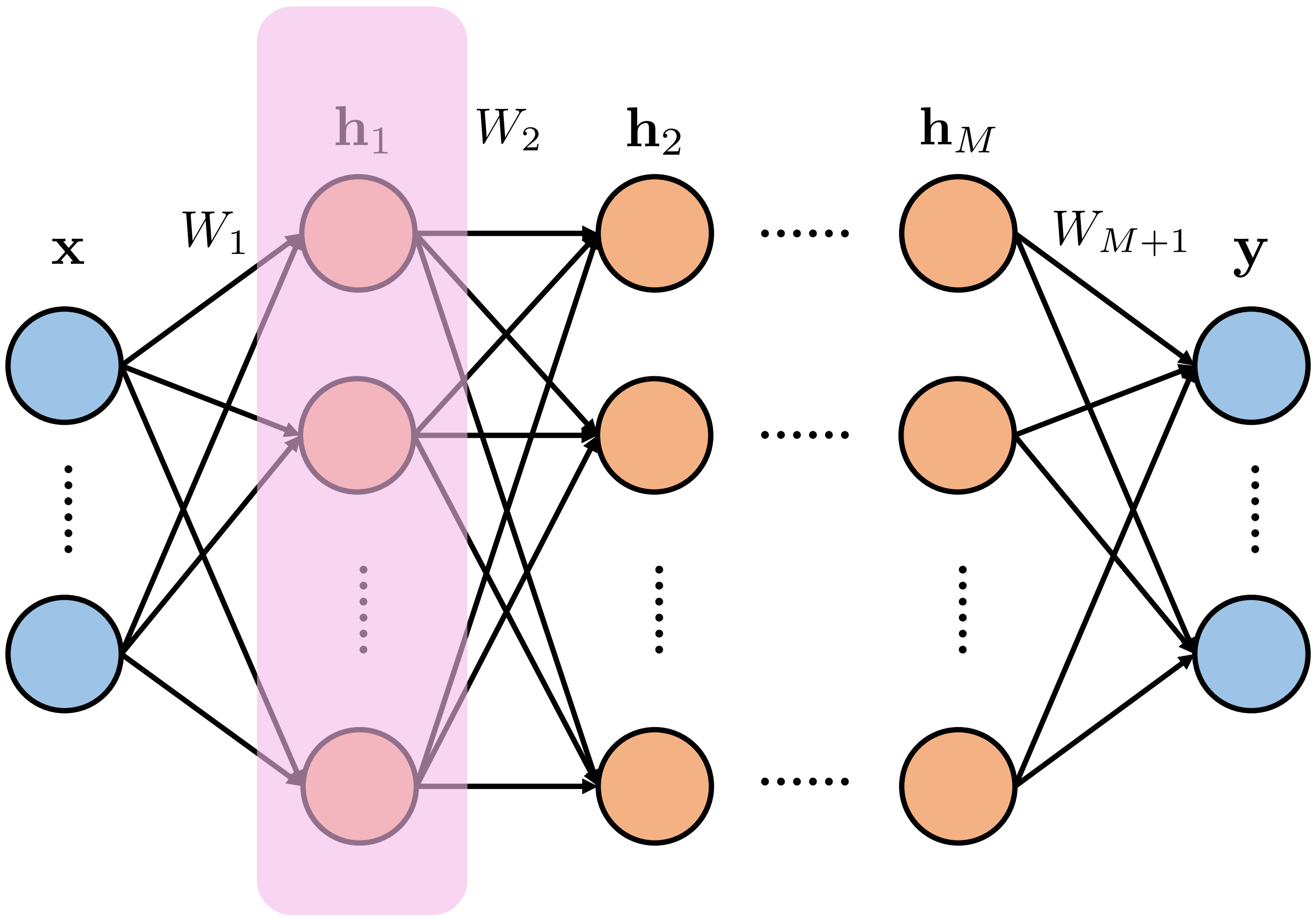

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$$\mathbf{h}_1 = \sigma\left(W_1 \mathbf{x}\right)$$

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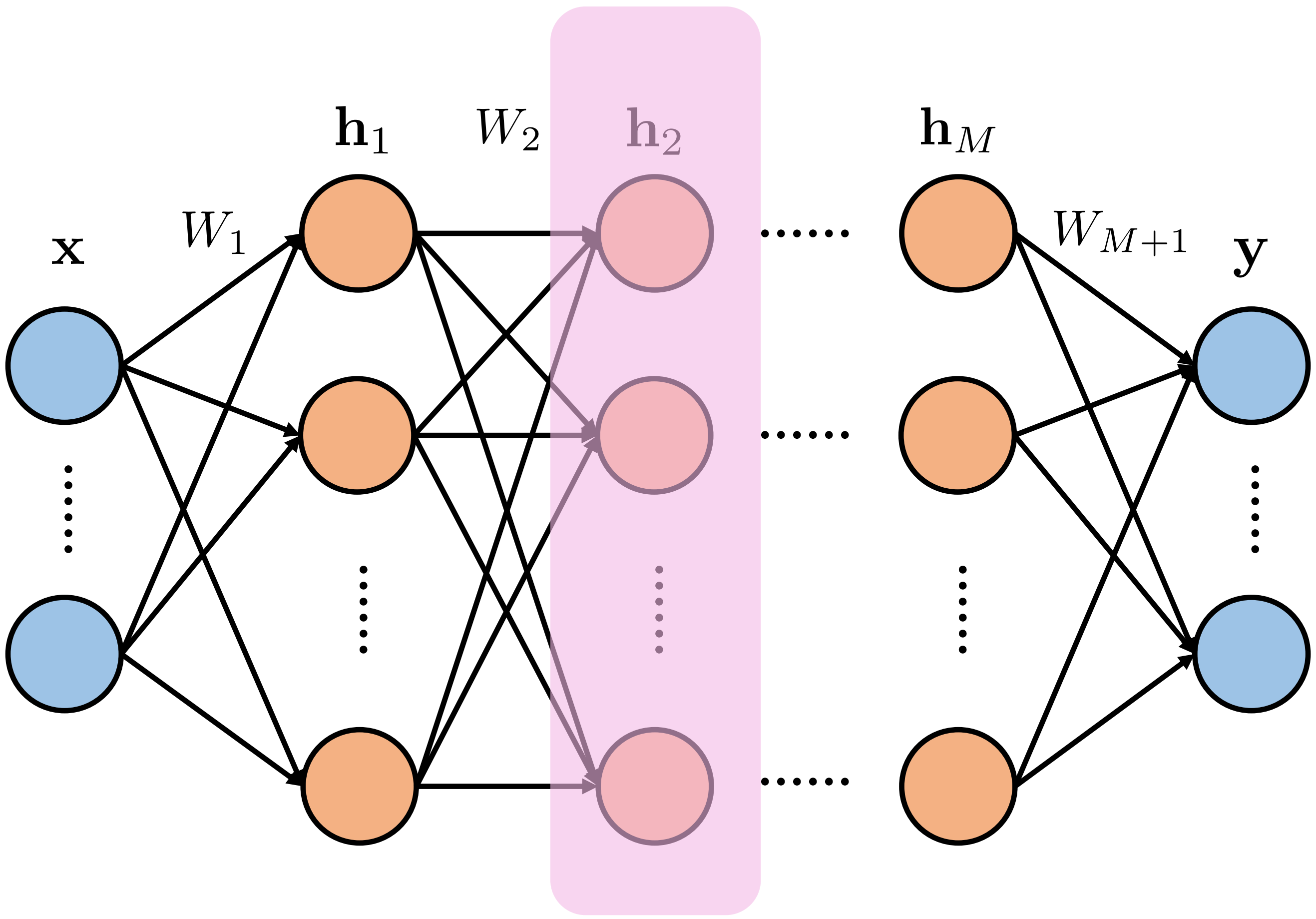

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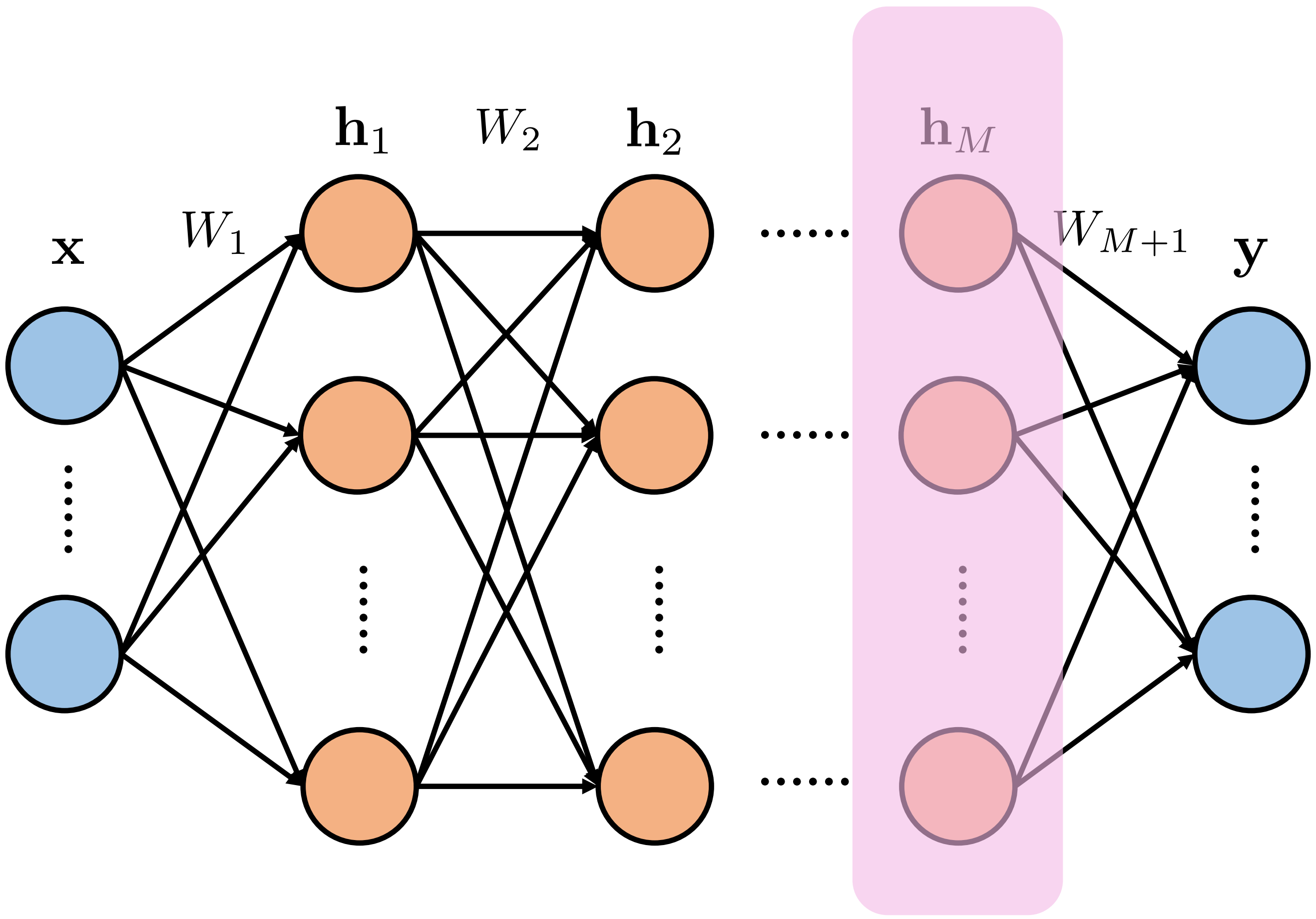

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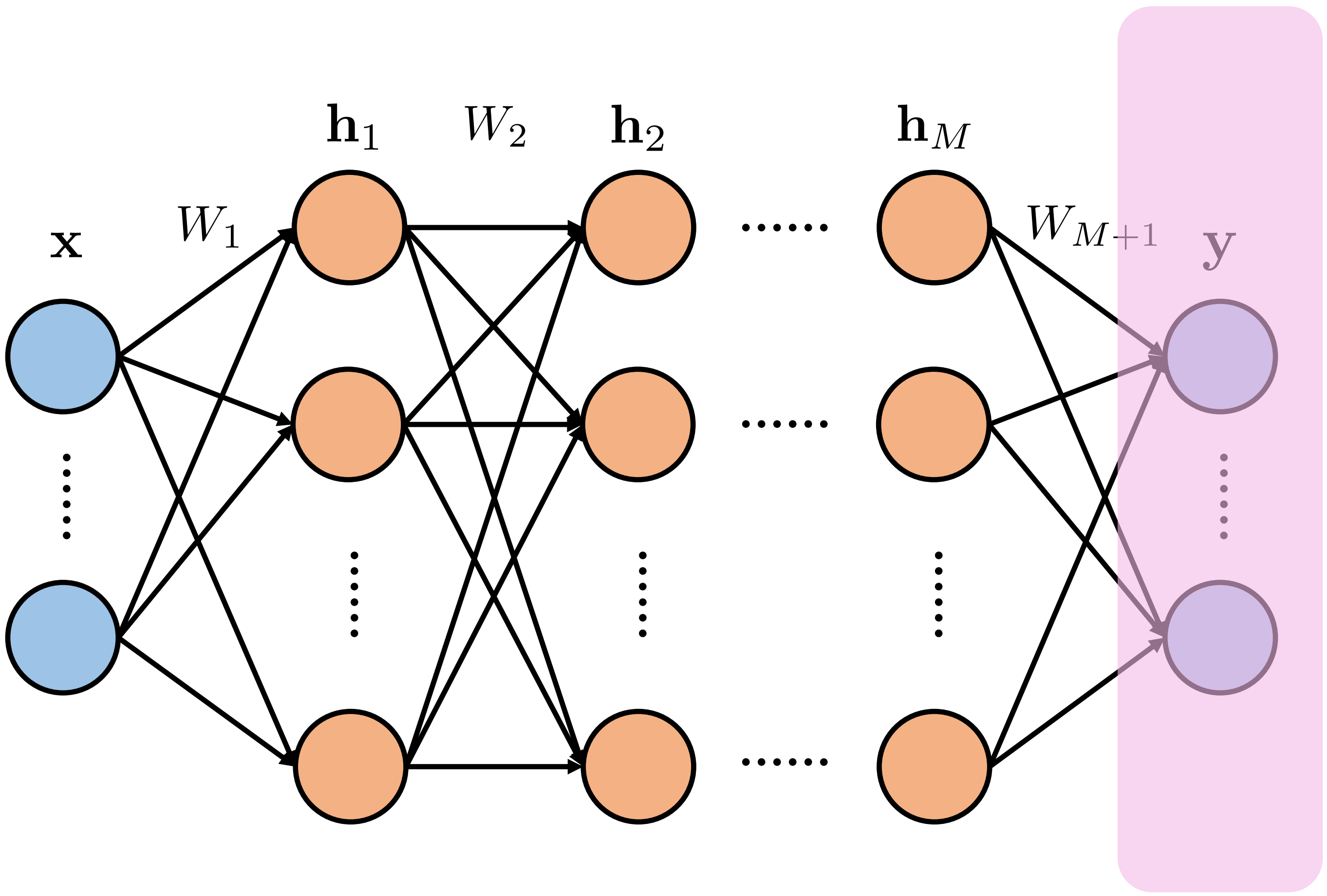

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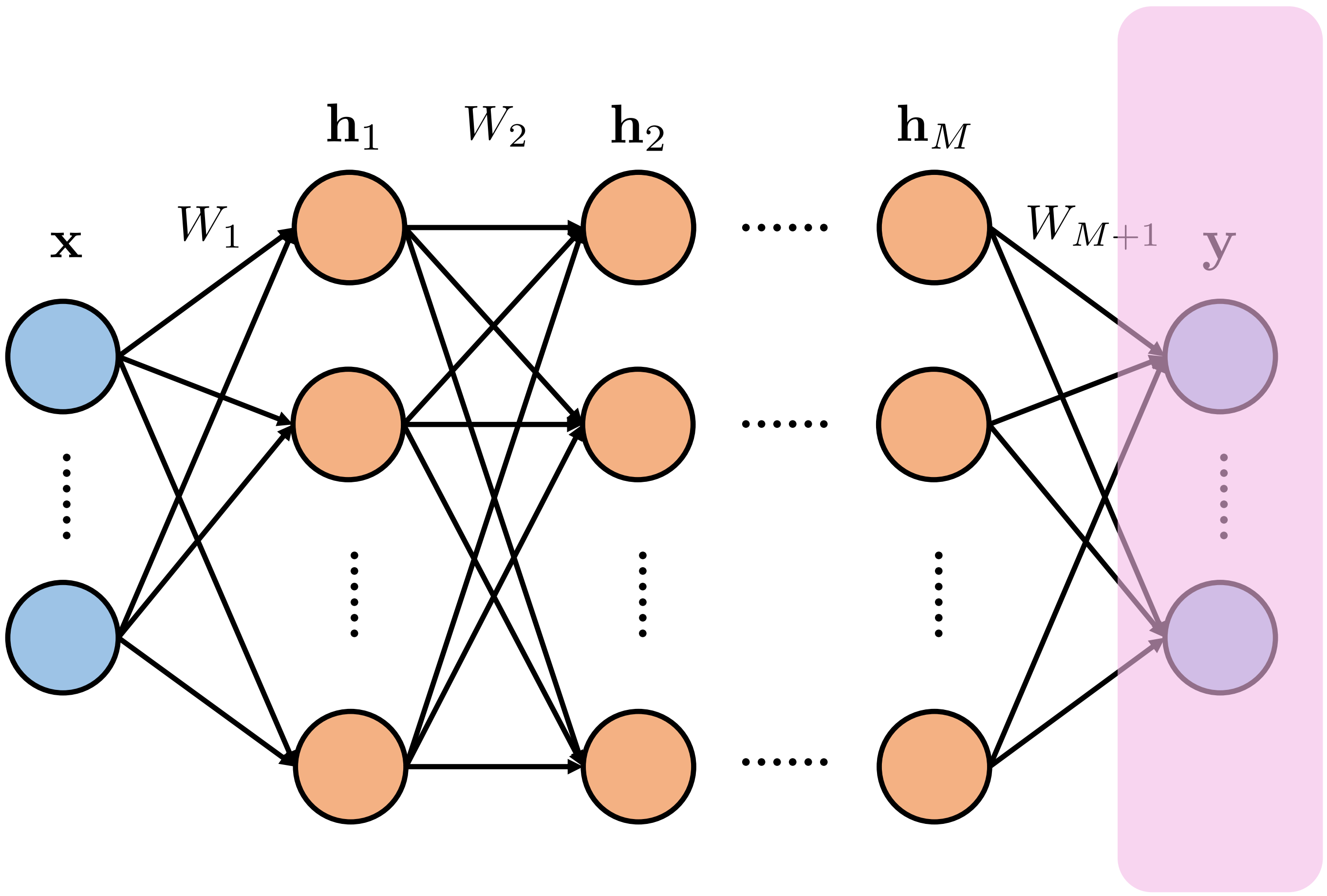

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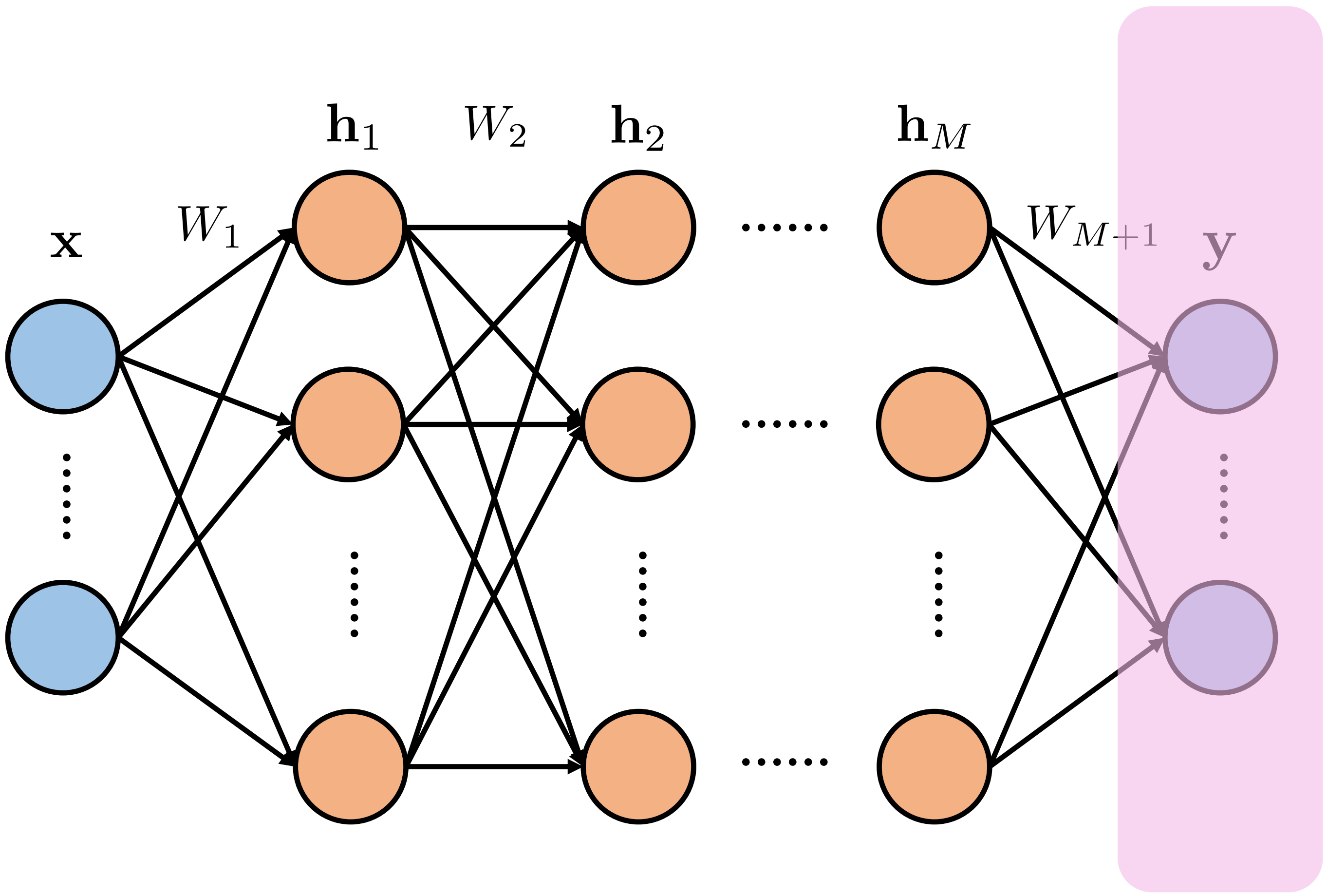

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Loss: $L = \ell(\mathbf{y}, \bar{\mathbf{y}})$

Mini-batch version:

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

Backpropagation

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 $\mathbf{p} = [\mathbf{p}_1, \mathbf{p}_2, \ldots, \mathbf{p}_n]^\top$ 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 $\mathbf{p} = [\mathbf{p}_1, \mathbf{p}_2, \ldots, \mathbf{p}_n]^\top$ is

$$\mathbf{J}_f(\mathbf{p}) = \begin{bmatrix} \nabla^{\mathrm{T}} f_1(\mathbf{p}) \\ \vdots \\ \nabla^{\mathrm{T}} f_m(\mathbf{p}) \end{bmatrix} = \begin{bmatrix} \dfrac{\partial f_1}{\partial x_1}(\mathbf{p}) & \cdots & \dfrac{\partial f_1}{\partial x_n}(\mathbf{p}) \\ \vdots & \ddots & \vdots \\ \dfrac{\partial f_m}{\partial x_1}(\mathbf{p}) & \cdots & \dfrac{\partial f_m}{\partial x_n}(\mathbf{p}) \end{bmatrix}$$

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

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- Scalar-valued & multiple variables $f : \mathbb{R}^m \to \mathbb{R}$ $g : \mathbb{R}^n \to \mathbb{R}^m$

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We can derive it from the single variable case!

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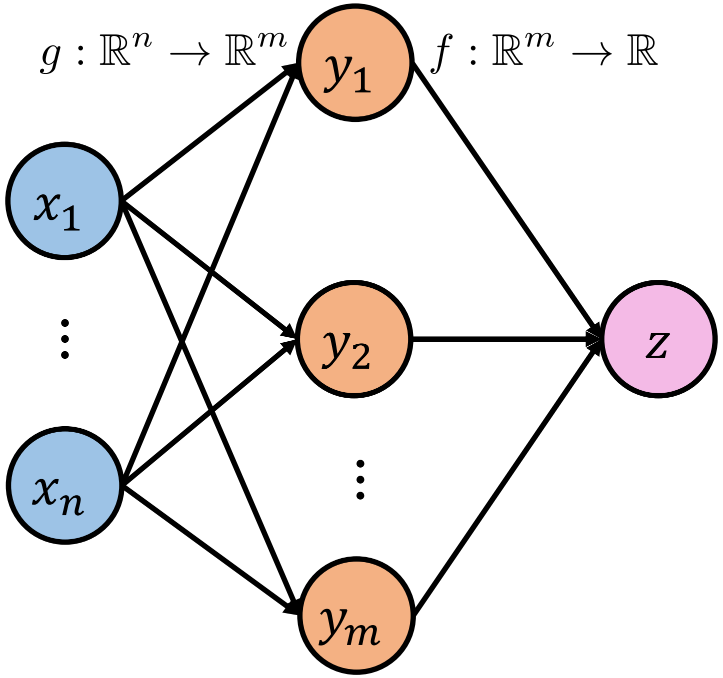

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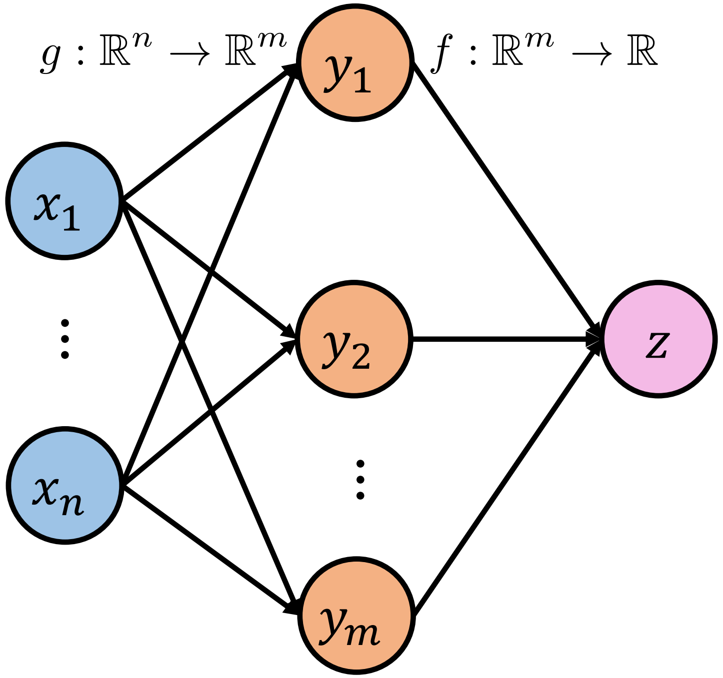

$$\frac{\partial z}{\partial x_1} = \sum_{i=1}^{m} \frac{\partial z}{\partial y_i} \frac{\partial y_i}{\partial x_1} = \begin{bmatrix} \frac{\partial z}{\partial y_1} & \cdots & \frac{\partial z}{\partial y_m} \end{bmatrix} \begin{bmatrix} \frac{\partial y_1}{\partial x_1} \\ \vdots \\ \frac{\partial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

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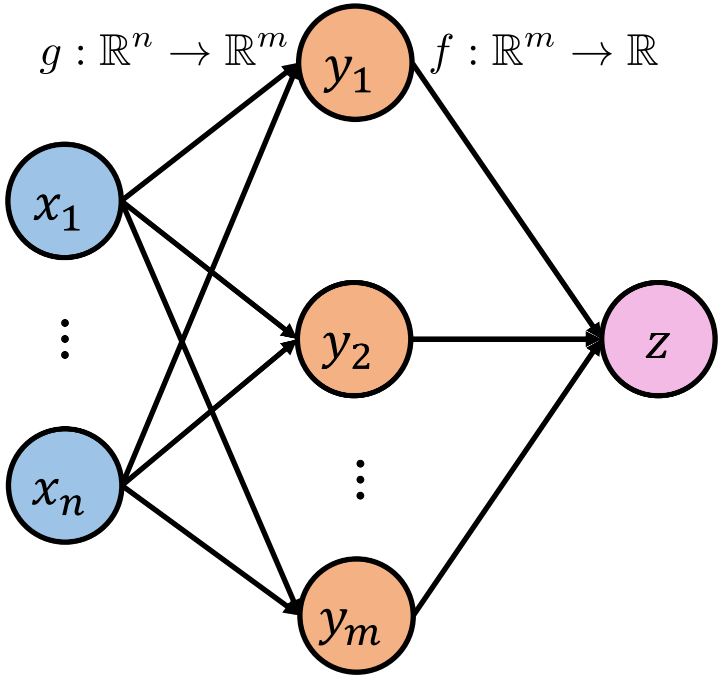

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Consider all possible paths from x_1 to z!

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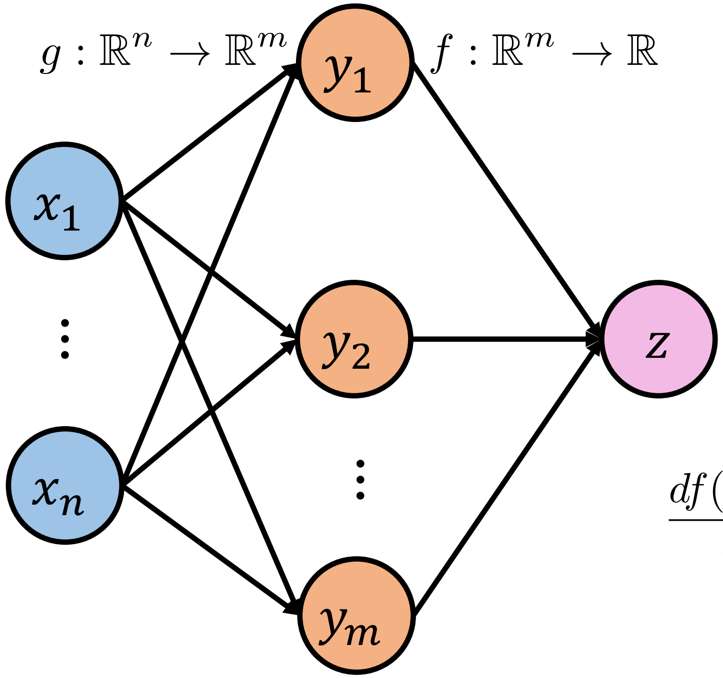

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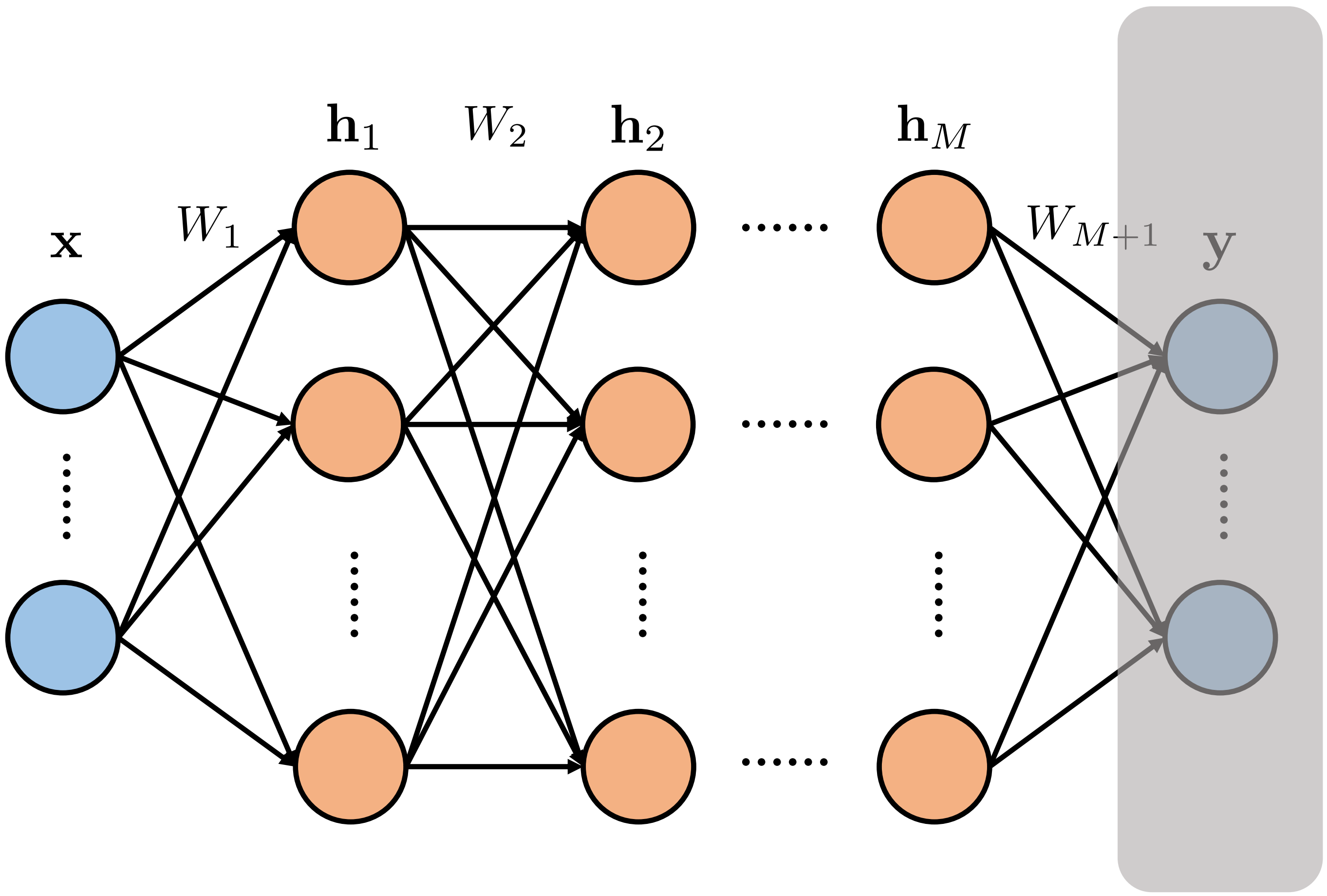
$$\frac{df(g(x))}{dx} = \frac{dz}{dx} = \begin{bmatrix} \frac{\partial z}{\partial x_1} \\ \vdots \\ \frac{\partial z}{\partial x_n} \end{bmatrix} = \left(\begin{bmatrix} \frac{\partial z}{\partial y_1} & \cdots & \frac{\partial z}{\partial y_m} \end{bmatrix} \begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_1}{\partial x_2} & \cdots & \frac{\partial y_1}{\partial x_n} \\ \vdots & \vdots & \vdots & \vdots \\ \frac{\partial y_m}{\partial x_1} & \frac{\partial y_m}{\partial x_2} & \cdots & \frac{\partial y_m}{\partial x_n} \end{bmatrix} \right)^\top = \mathbf{J}_g(x)^\top \nabla f(g(x))$$

Backpropagation

During the backward pass:

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



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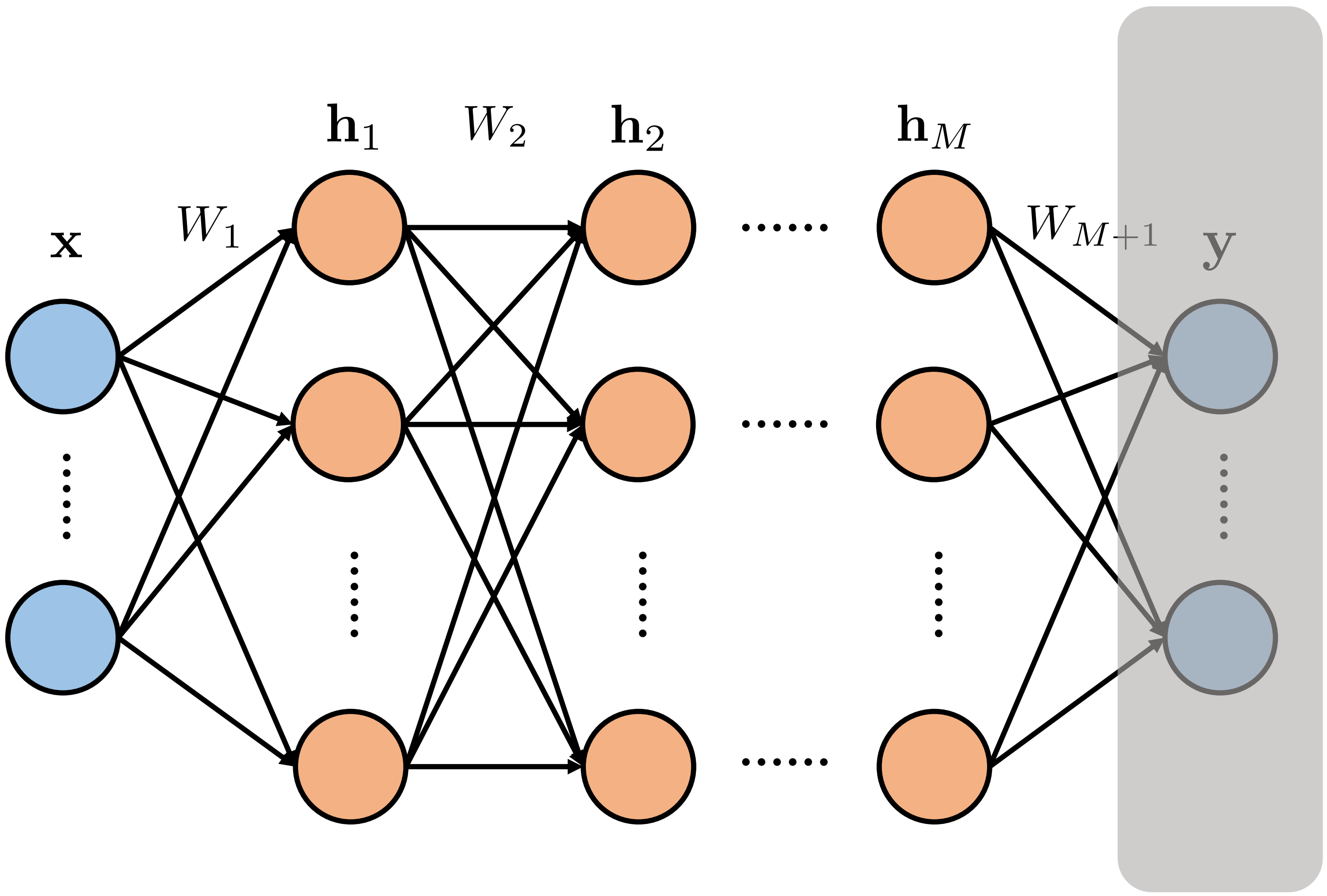
Gradient of loss w.r.t. $\mathbf{y}$: $\dfrac{\partial L}{\partial \mathbf{y}}$



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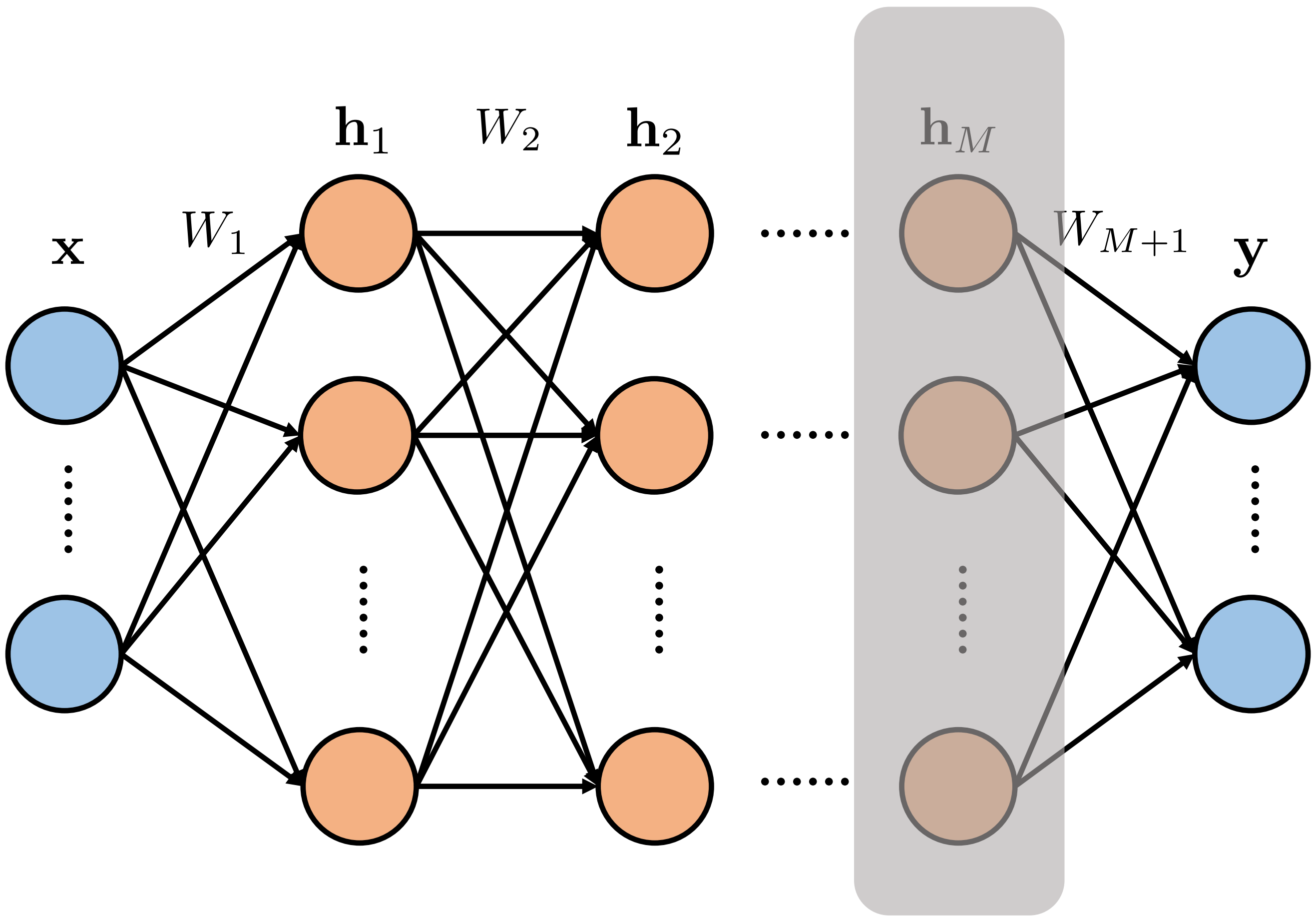

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Gradient of loss w.r.t. $\mathbf{h}_M$:

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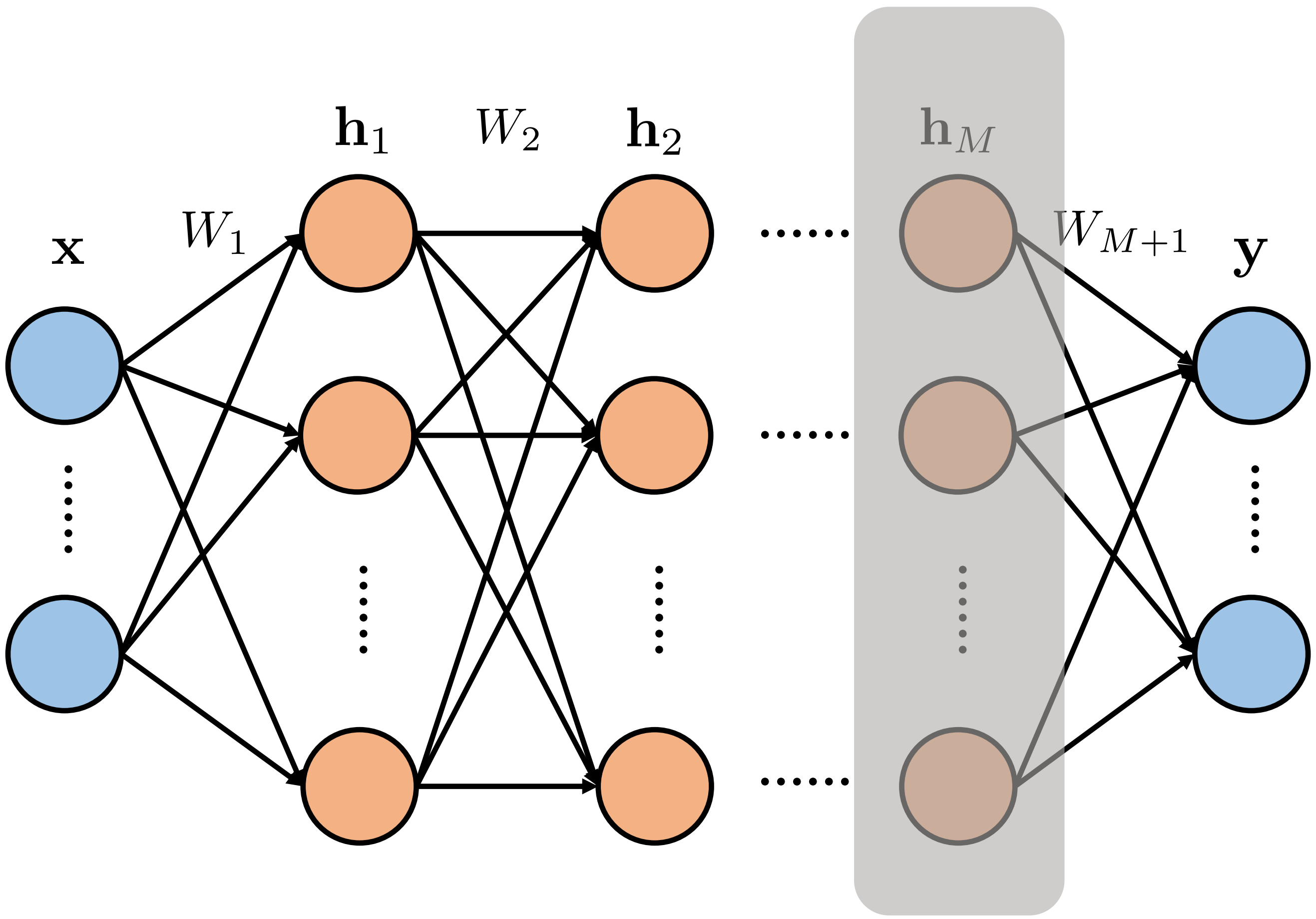

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Gradient of loss w.r.t. $\mathbf{h}_M$:

Apply the chain rule we learned before:

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

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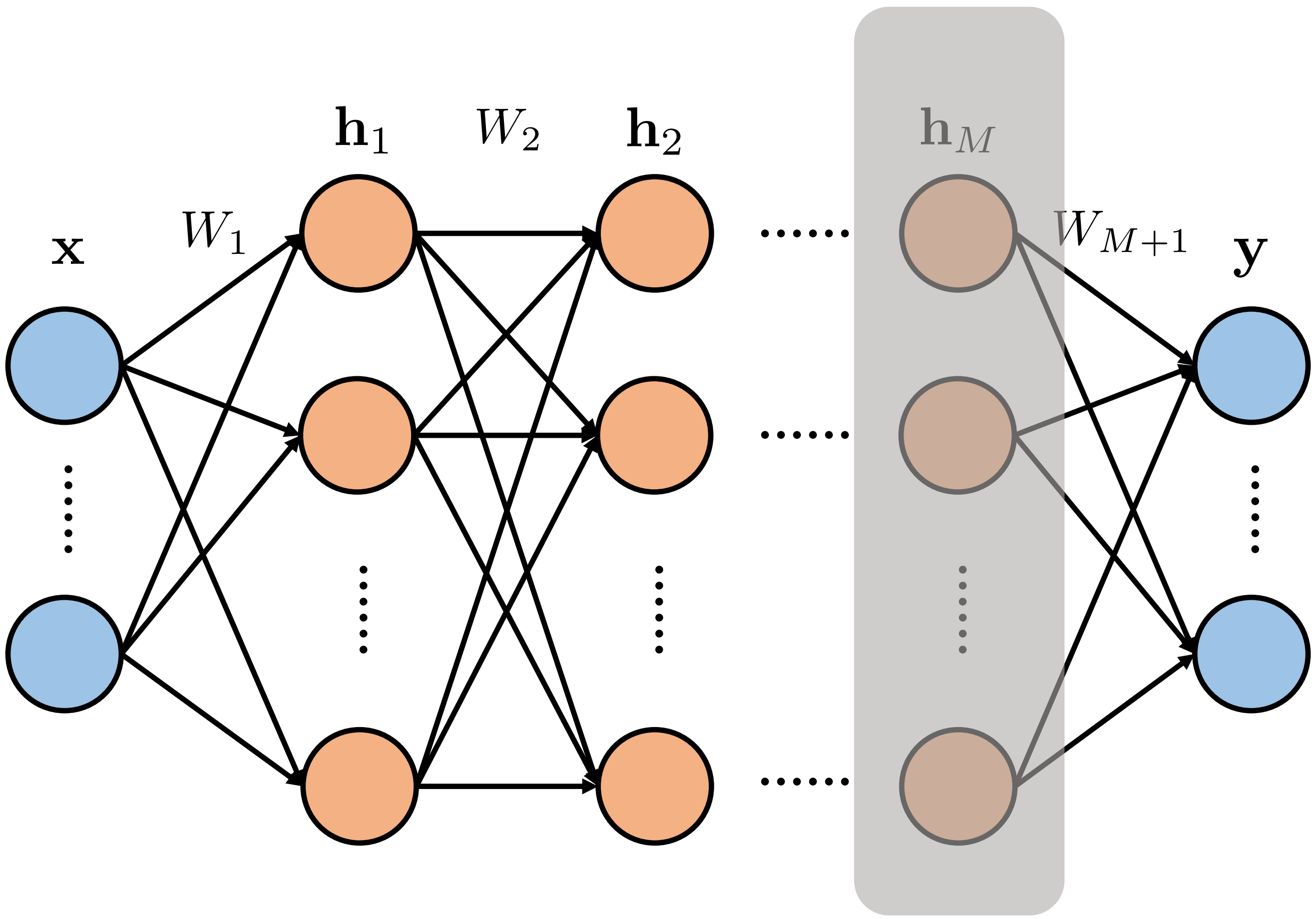

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Recall $\mathbf{y} = W_{M+1}\mathbf{h}_M$

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

Backpropagation

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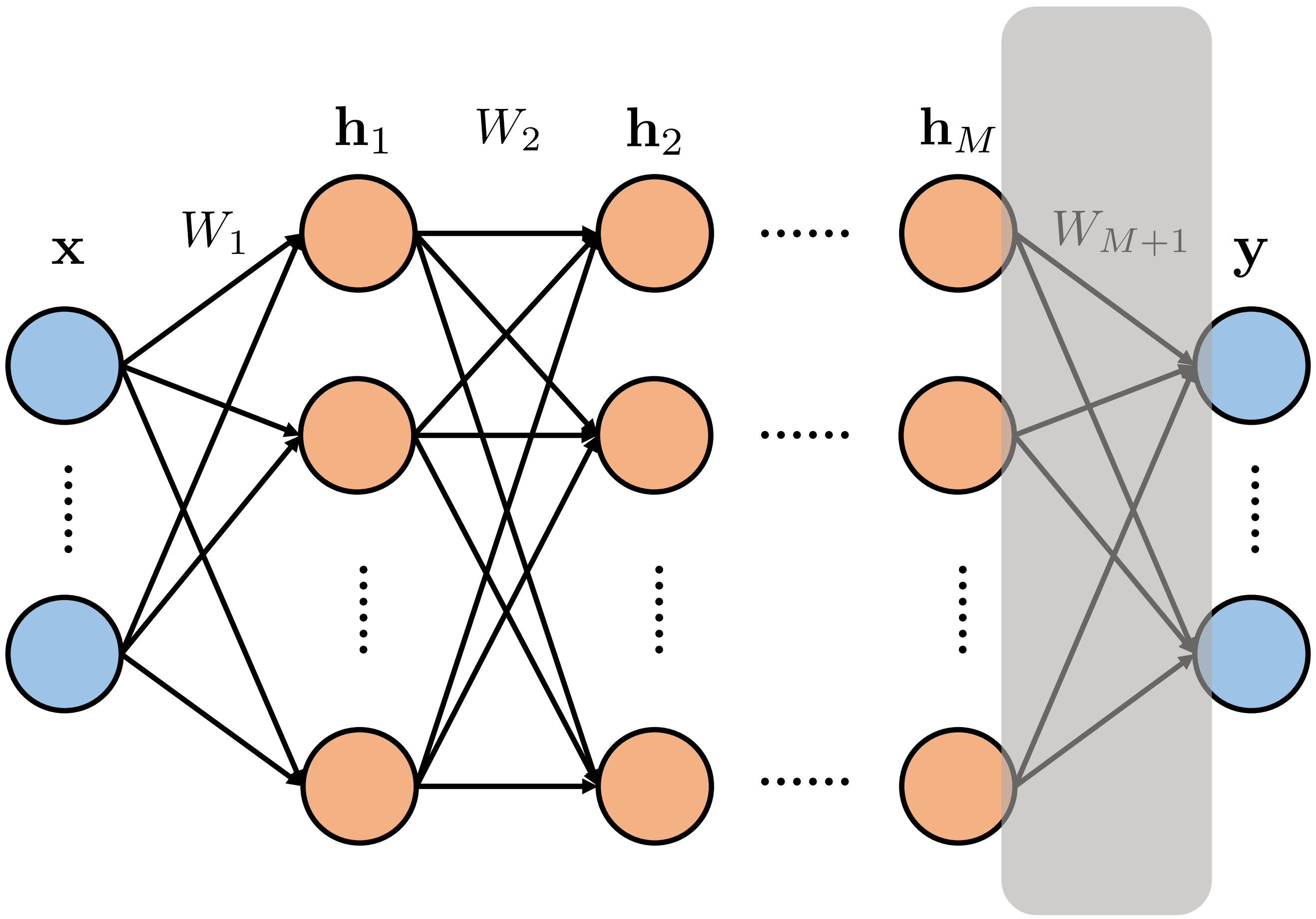

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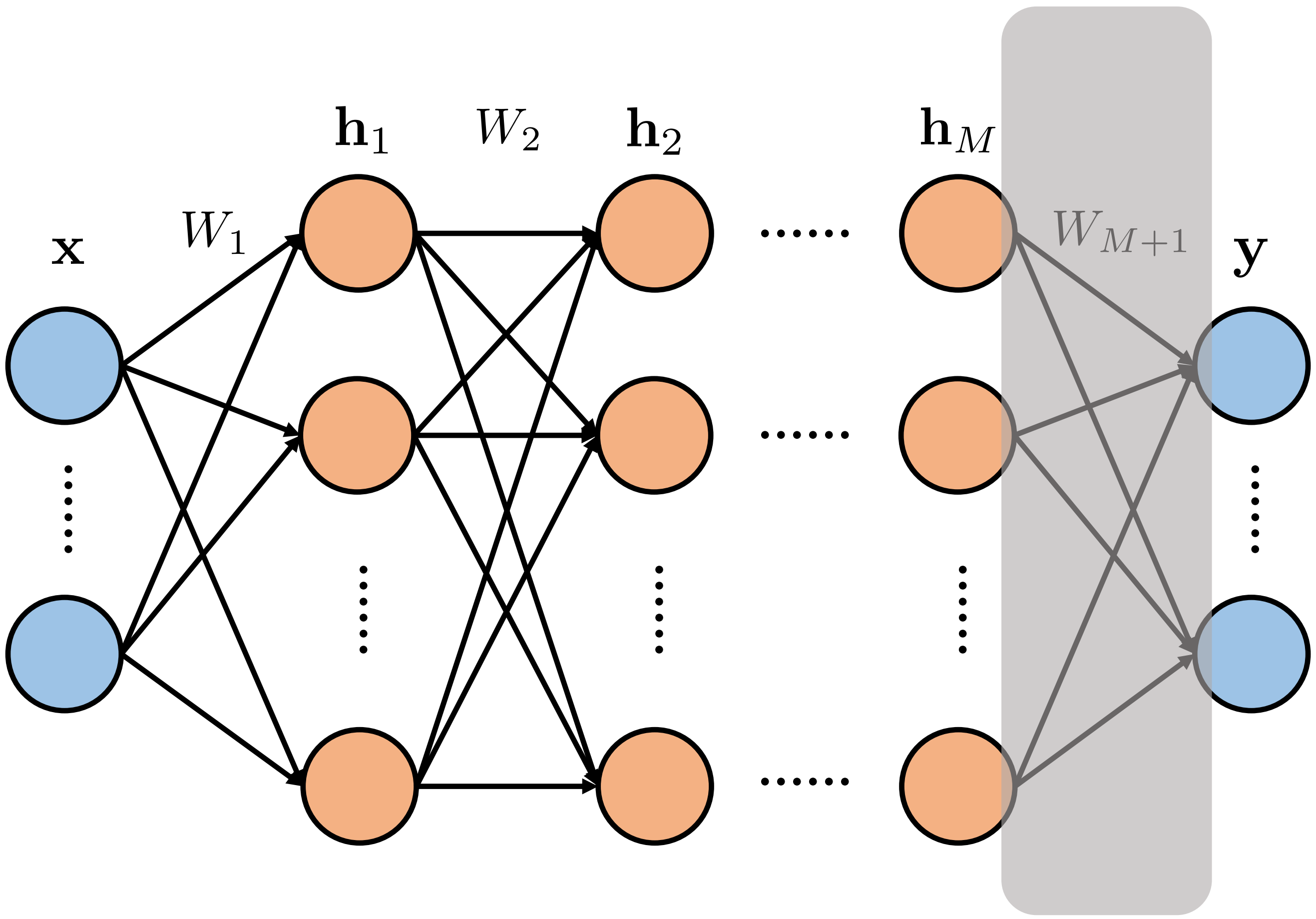

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Ideally, chain rule should be something like

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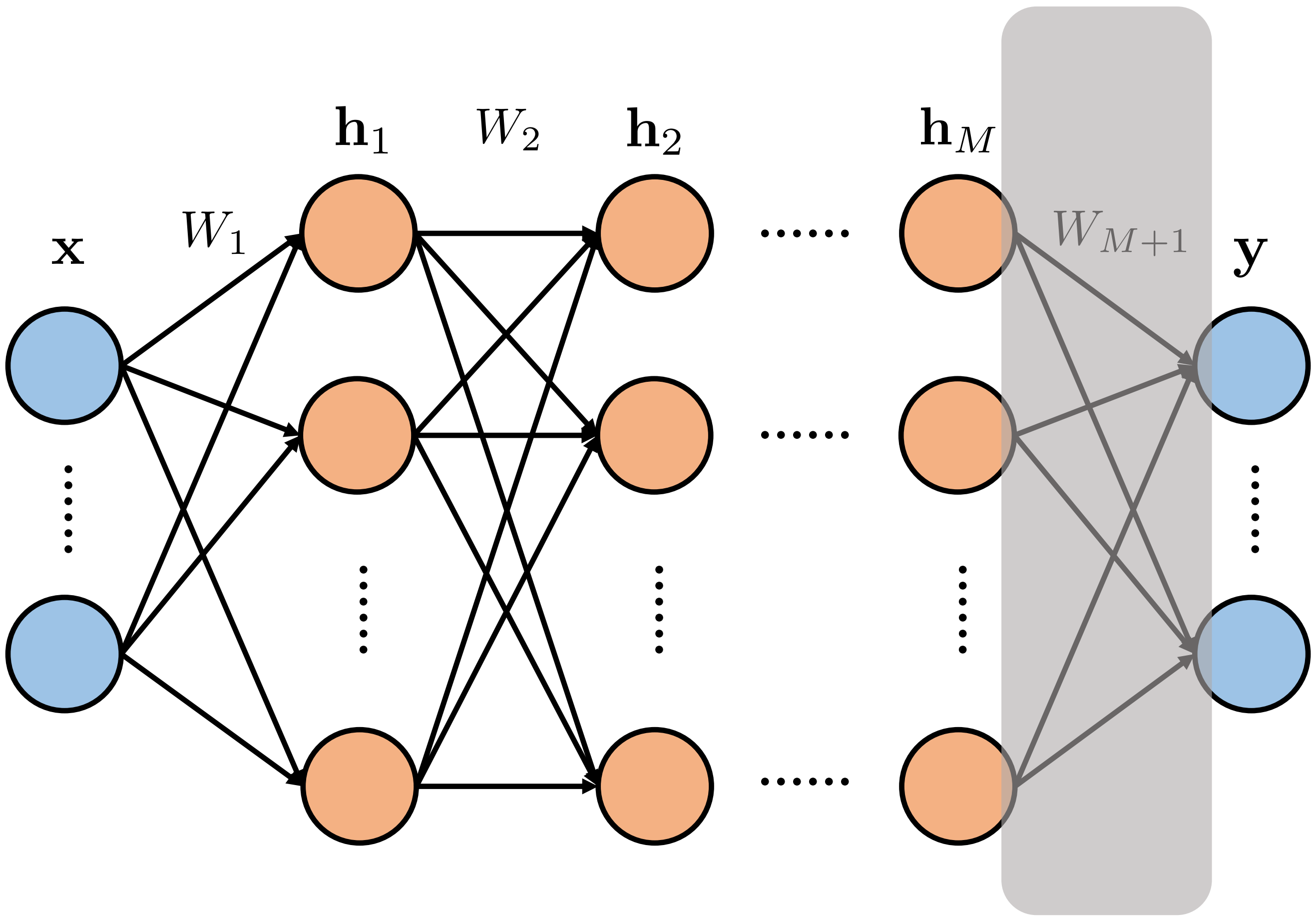

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But this is wrong, since $\dfrac{\partial \mathbf{y}}{\partial W_{M+1}}$ is the derivative of a vector w.r.t. a matrix, shapes do not work out!

Backpropagation

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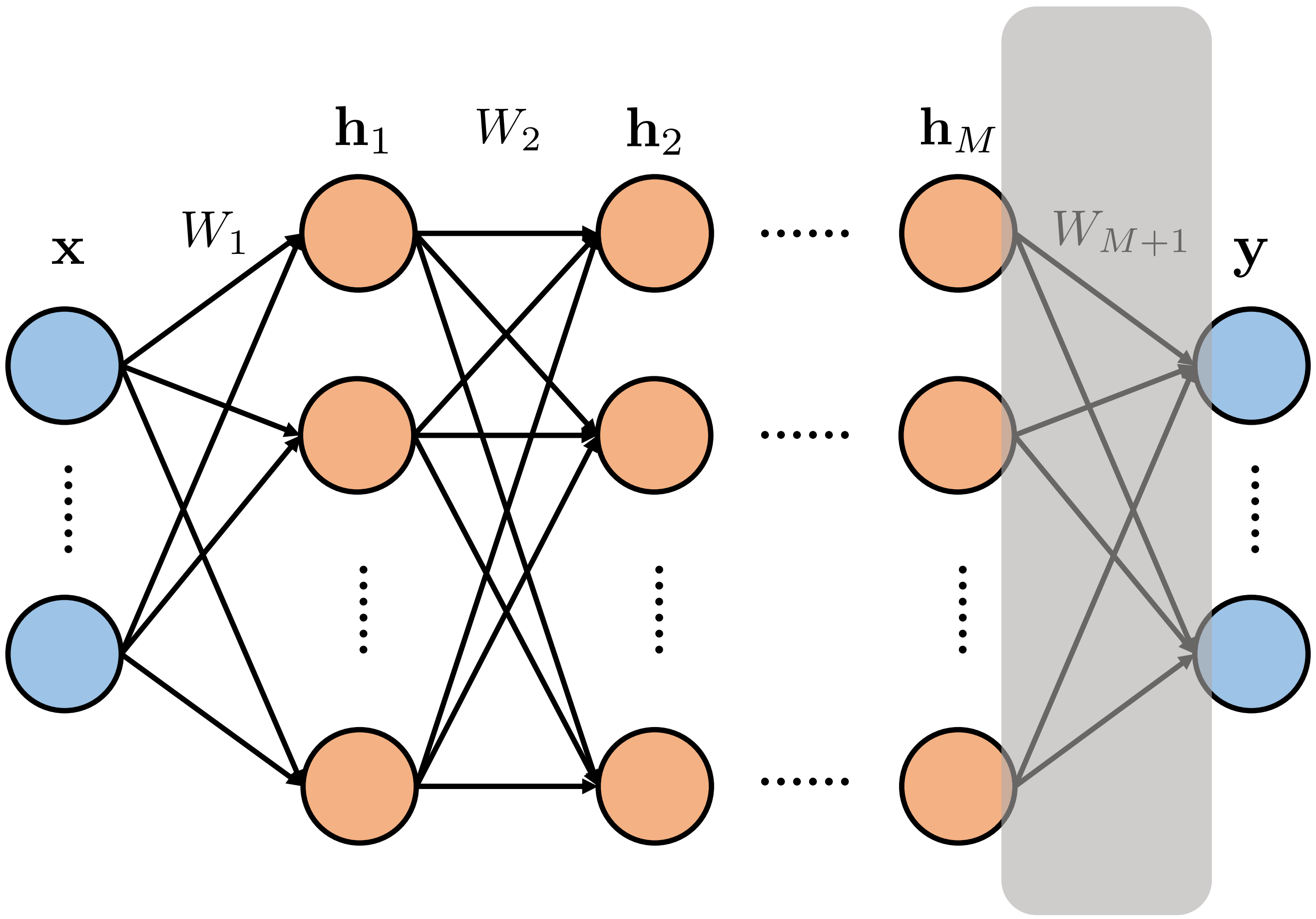

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Gradient of loss w.r.t. W_{M+1} :

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

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

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

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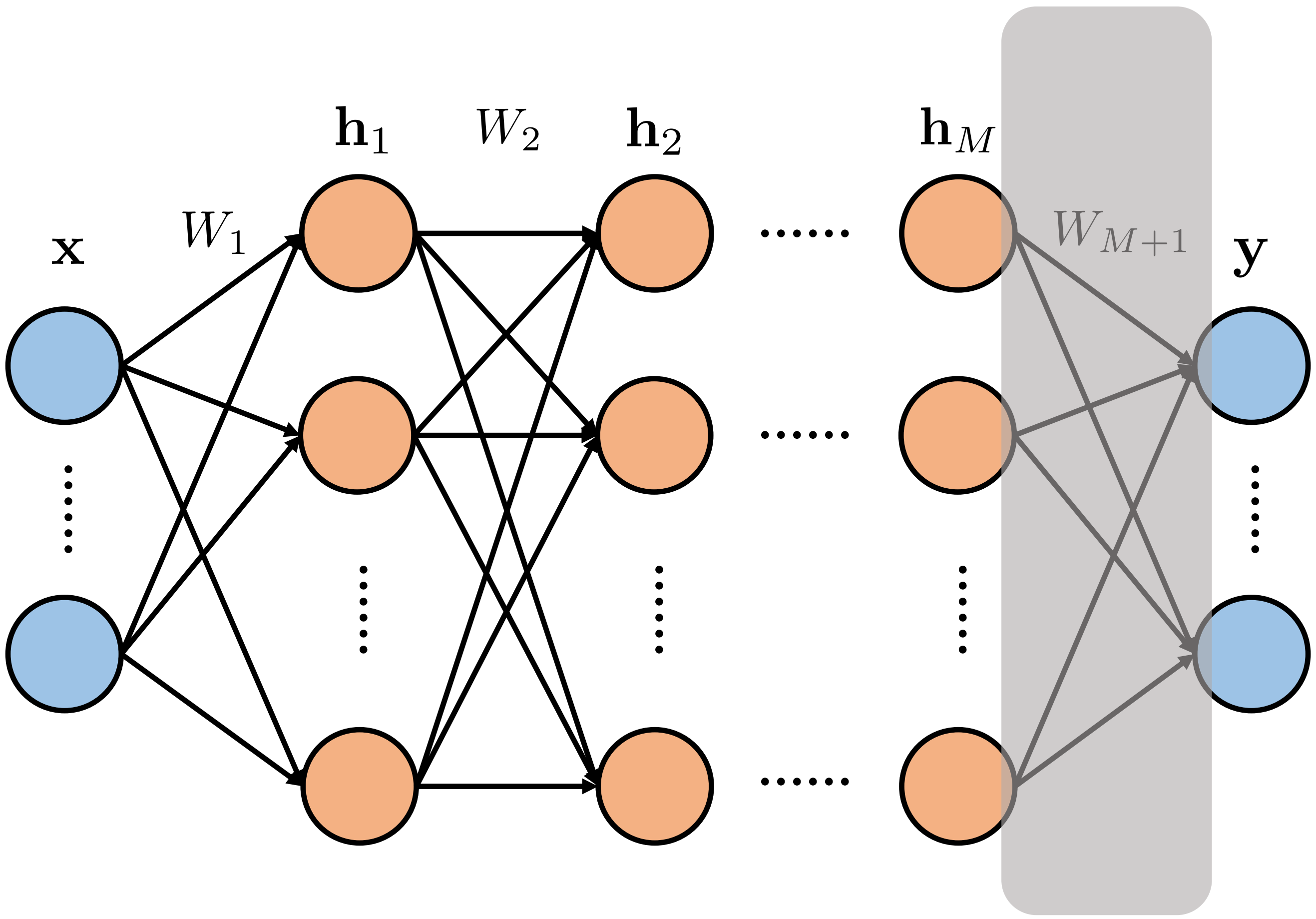

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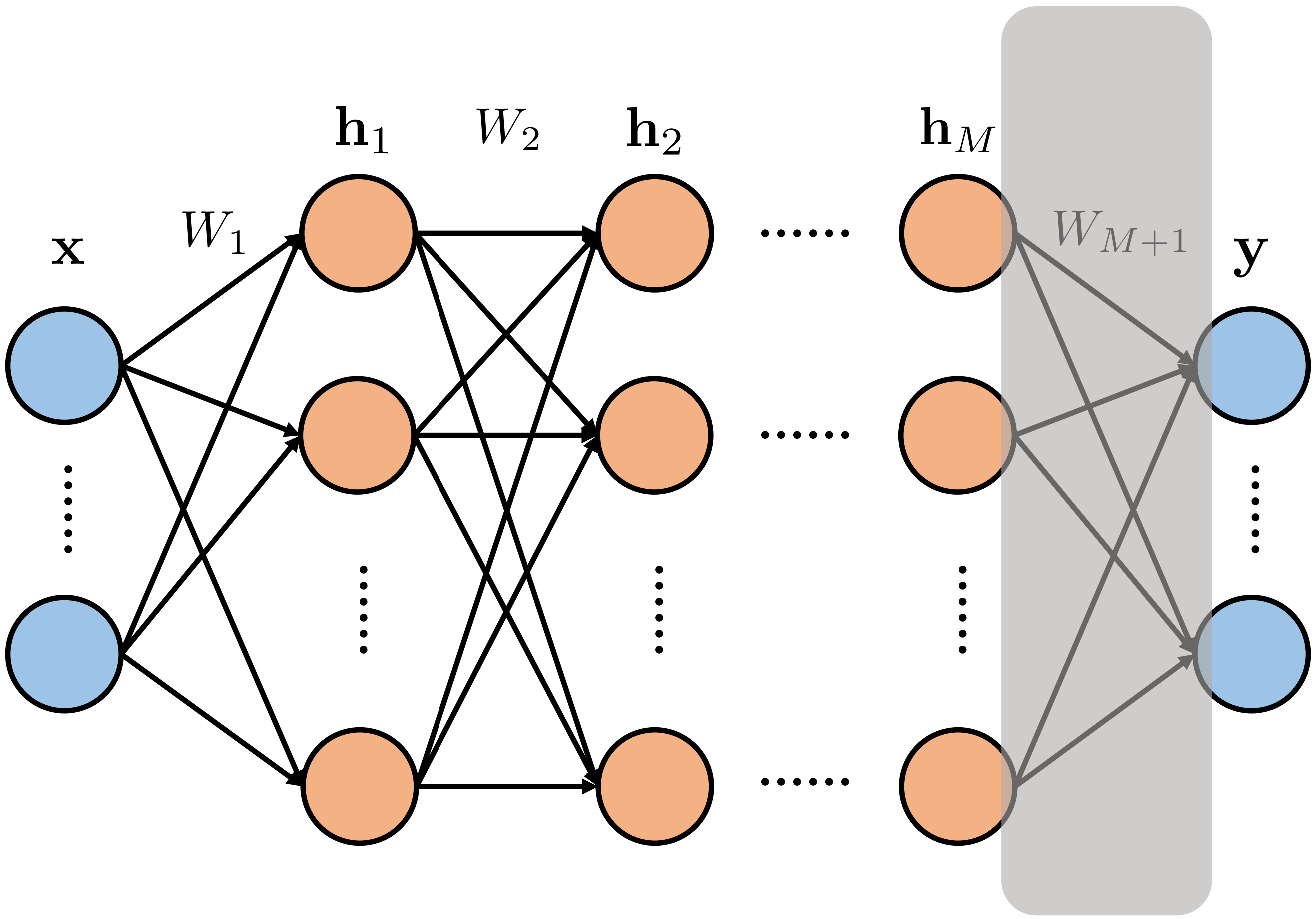

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We have

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

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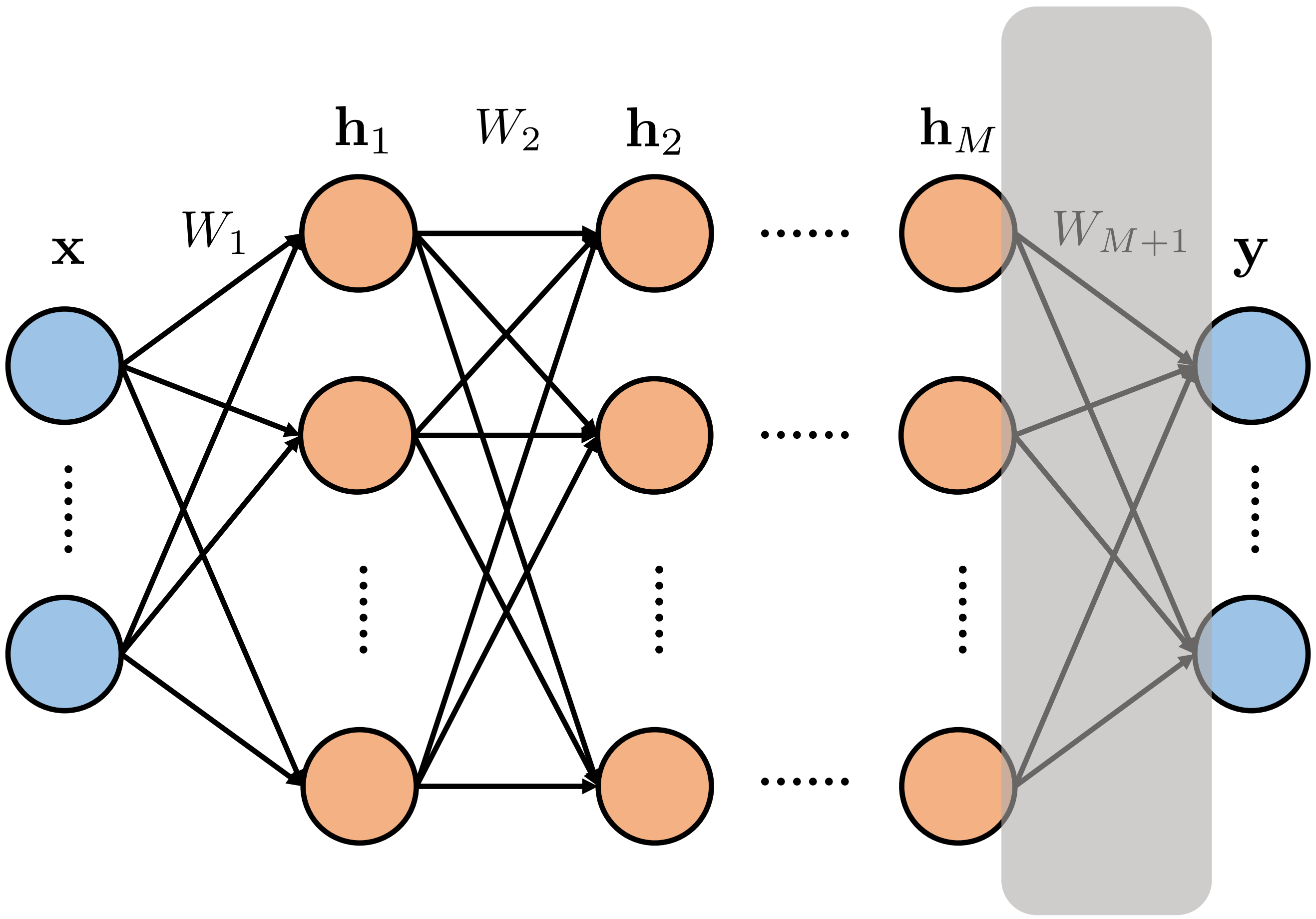

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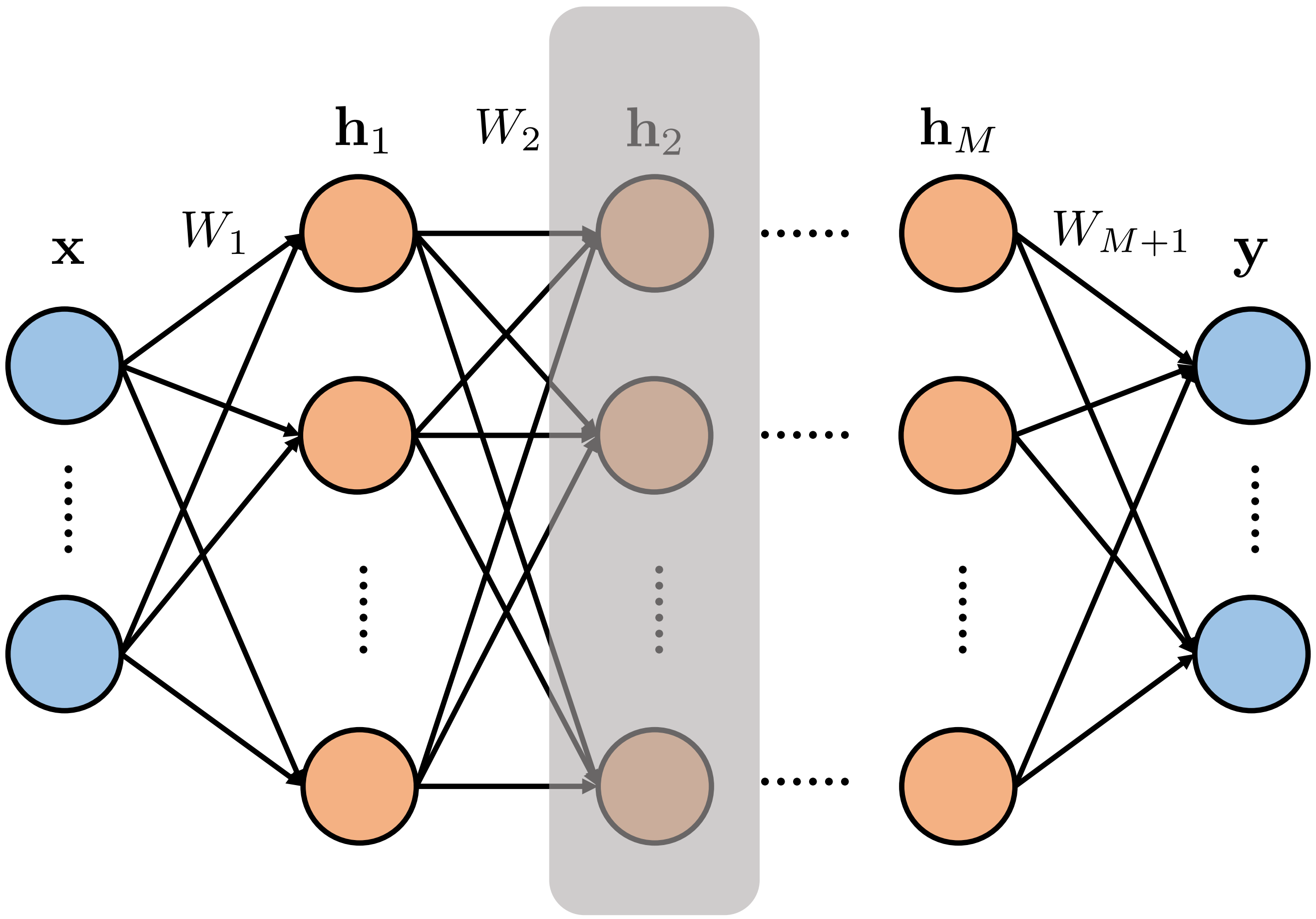

Loss: $L = \ell(\mathbf{y}, \bar{\mathbf{y}})$

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

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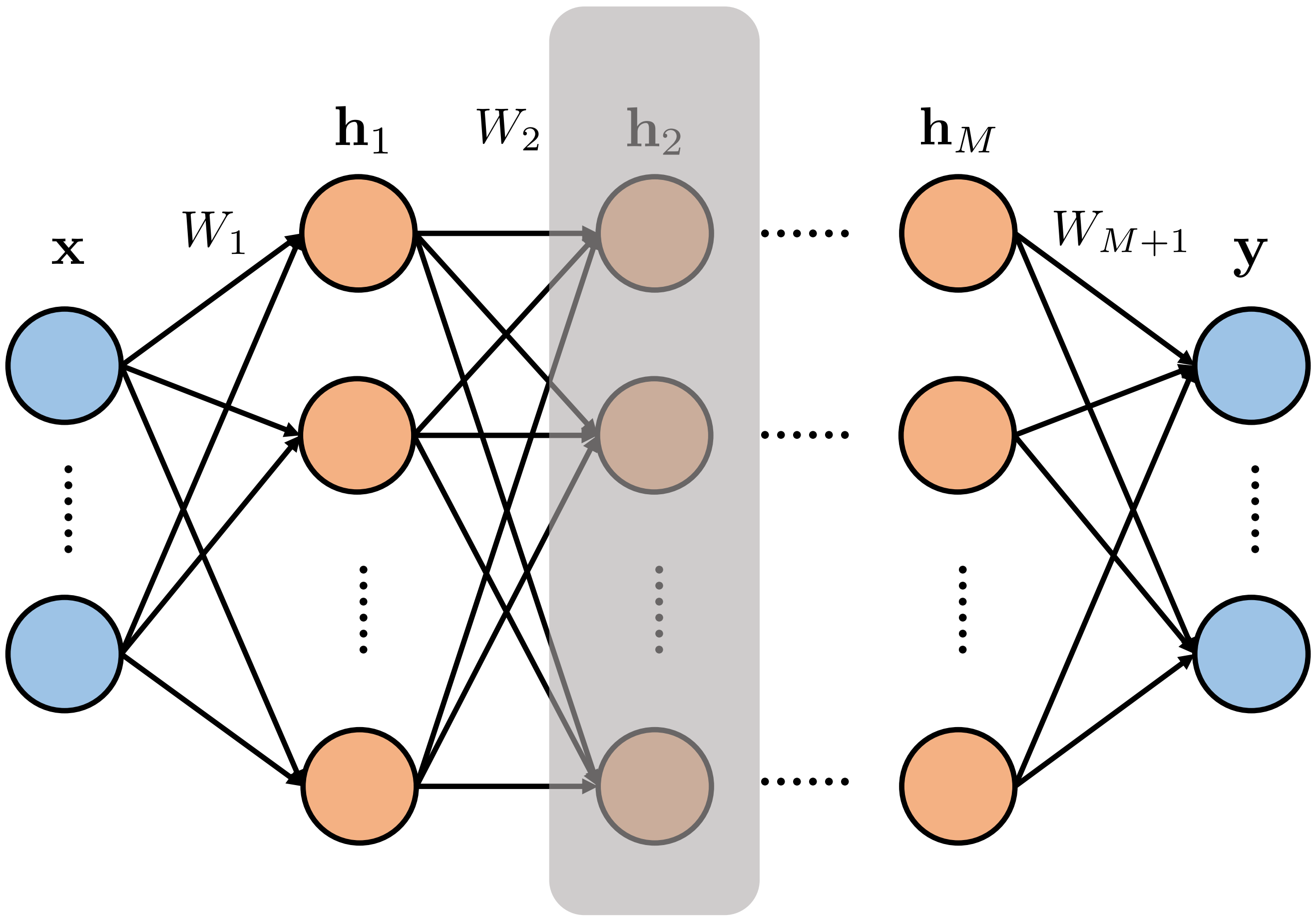

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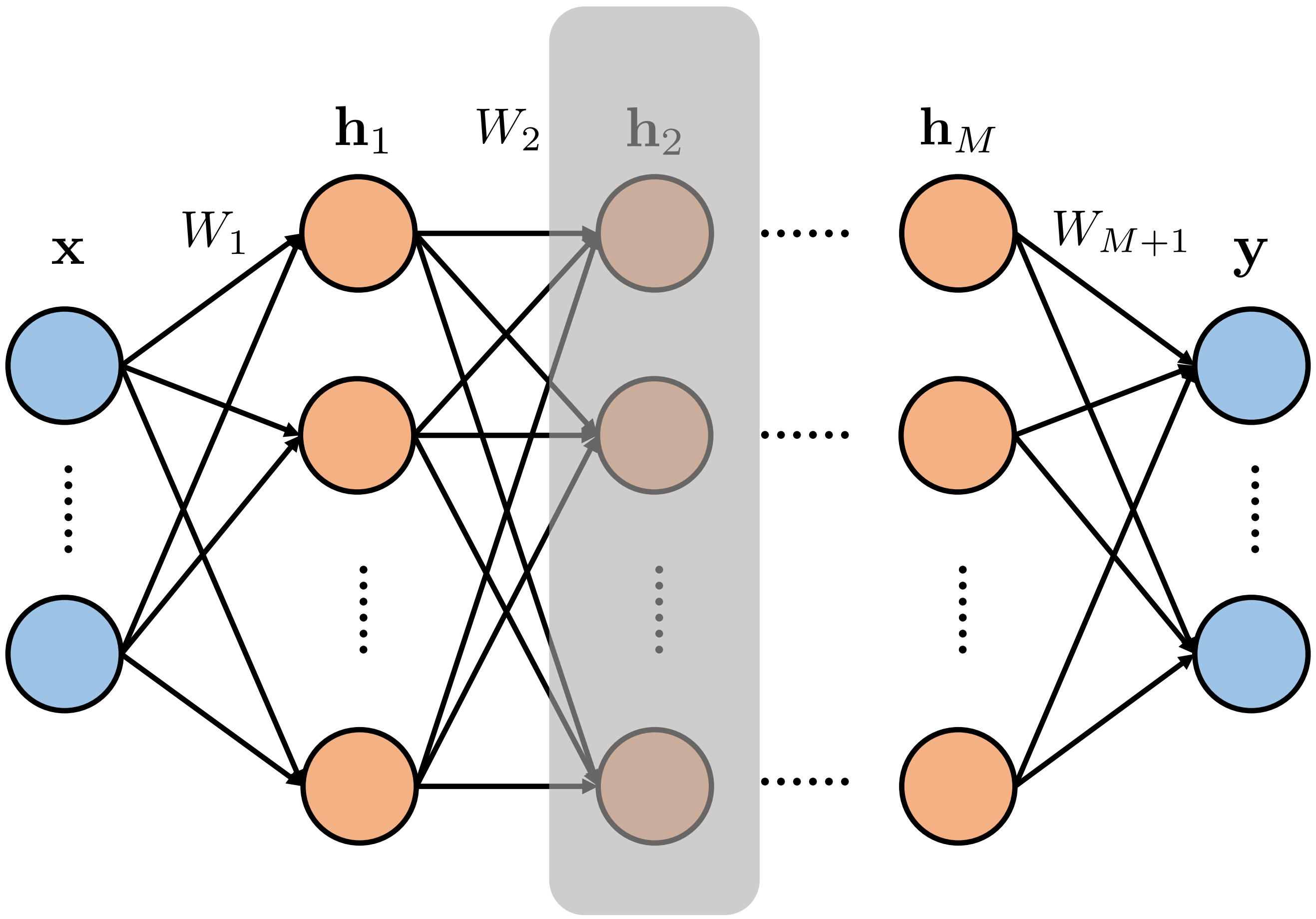

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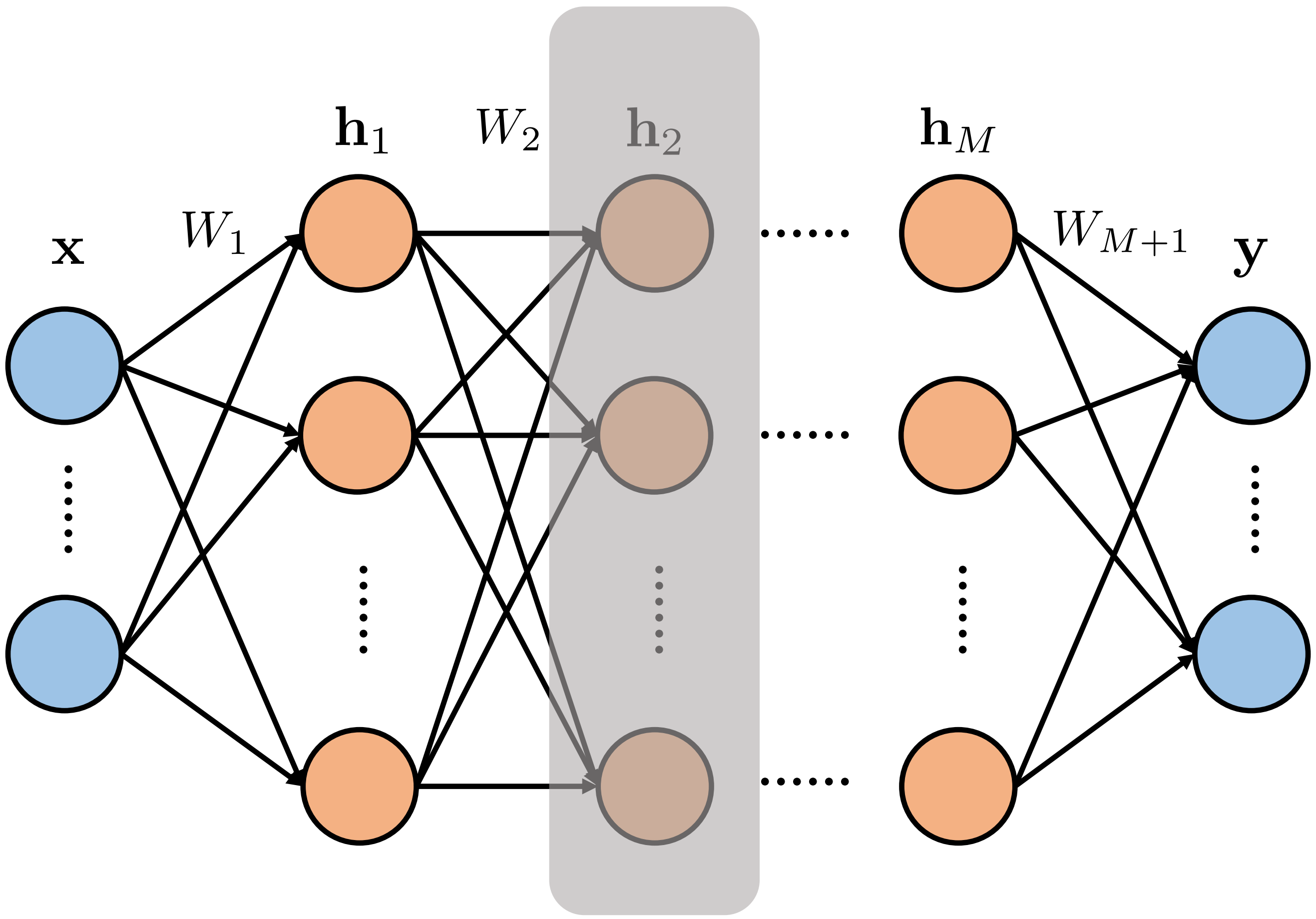

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$$\vdots$$

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

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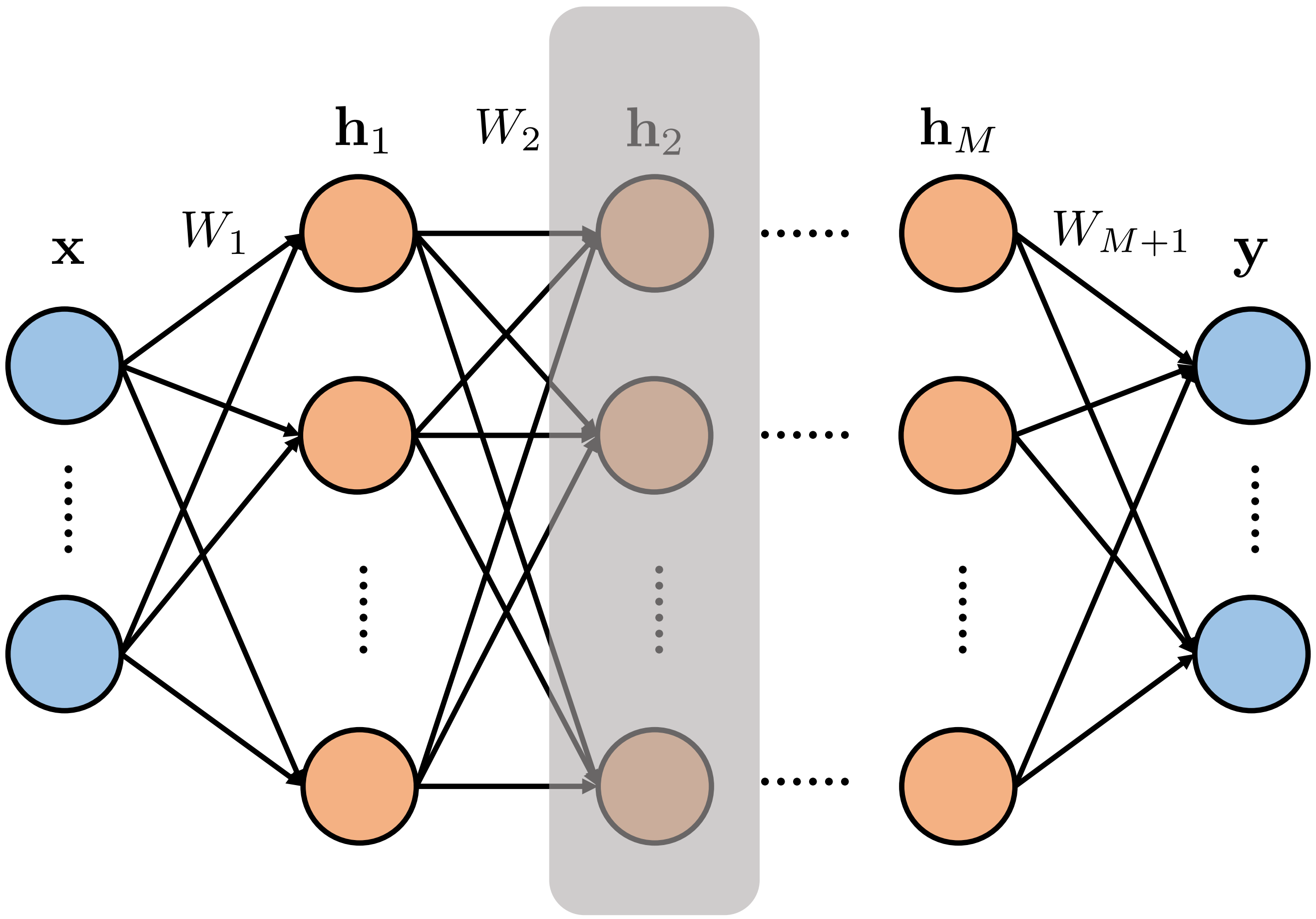

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General form:

$$\frac{\partial L}{\partial \mathbf{h}_i} = \mathbf{J}_{i+1}^\top \cdots \mathbf{J}_M^\top \frac{\partial L}{\partial \mathbf{y}} \quad \text{where} \quad \mathbf{J}_{i+1} \equiv \frac{\partial \mathbf{h}_{i+1}}{\partial \mathbf{h}_i}, \quad \mathbf{h}_{M+1} \equiv \mathbf{y}$$

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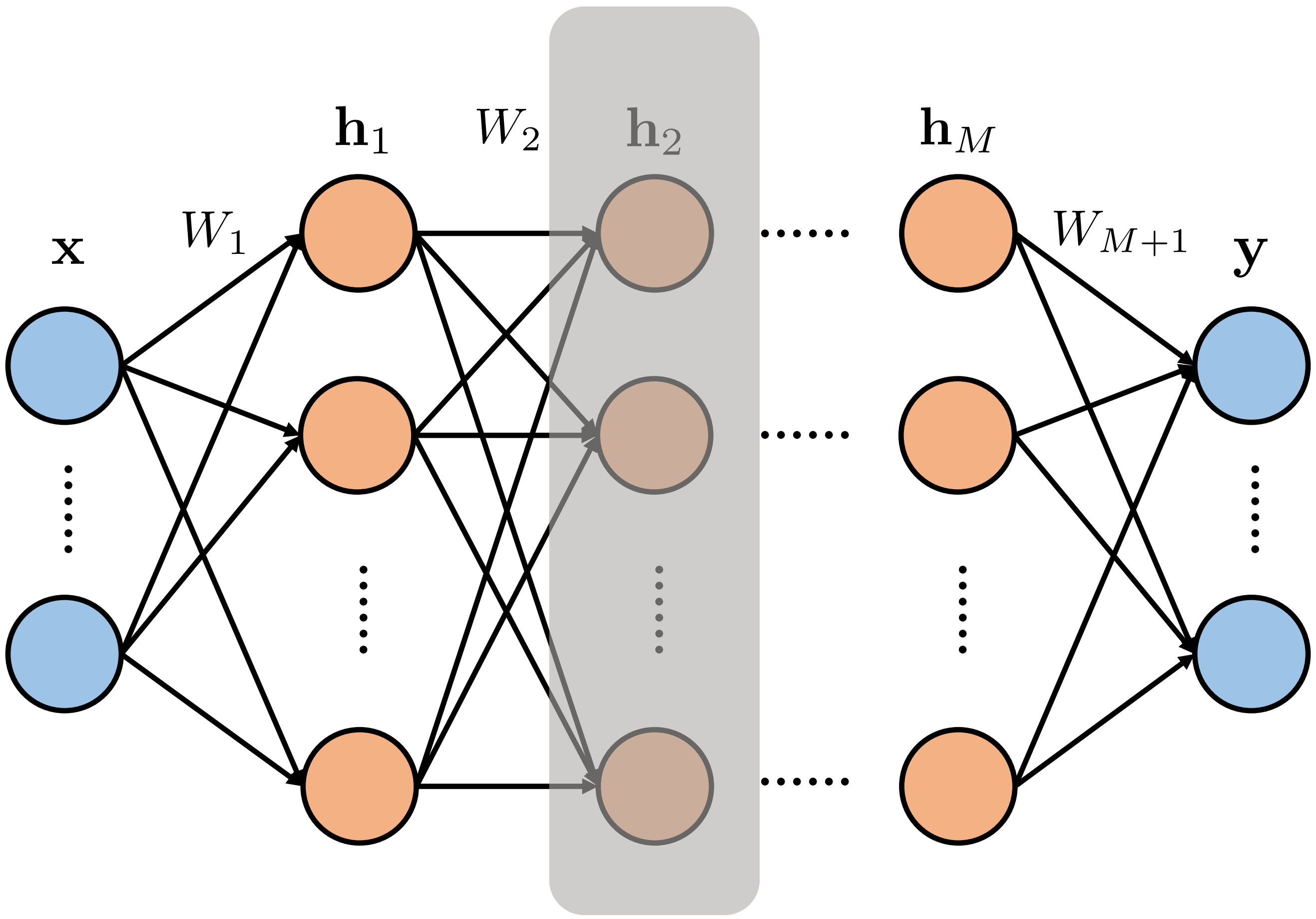

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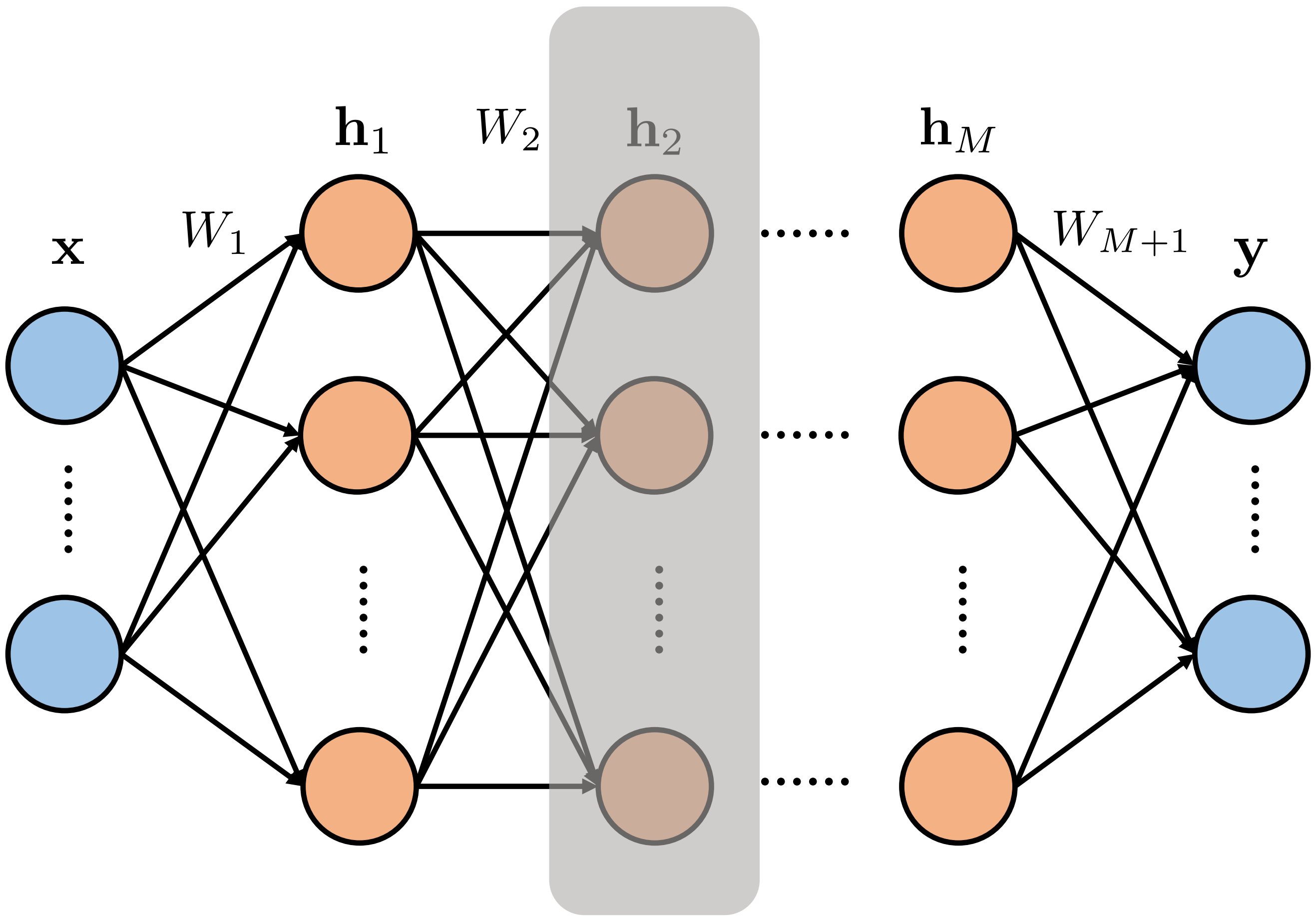

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Recall $\mathbf{h}_2 = \sigma\left(W_2 \mathbf{h}_1\right)$

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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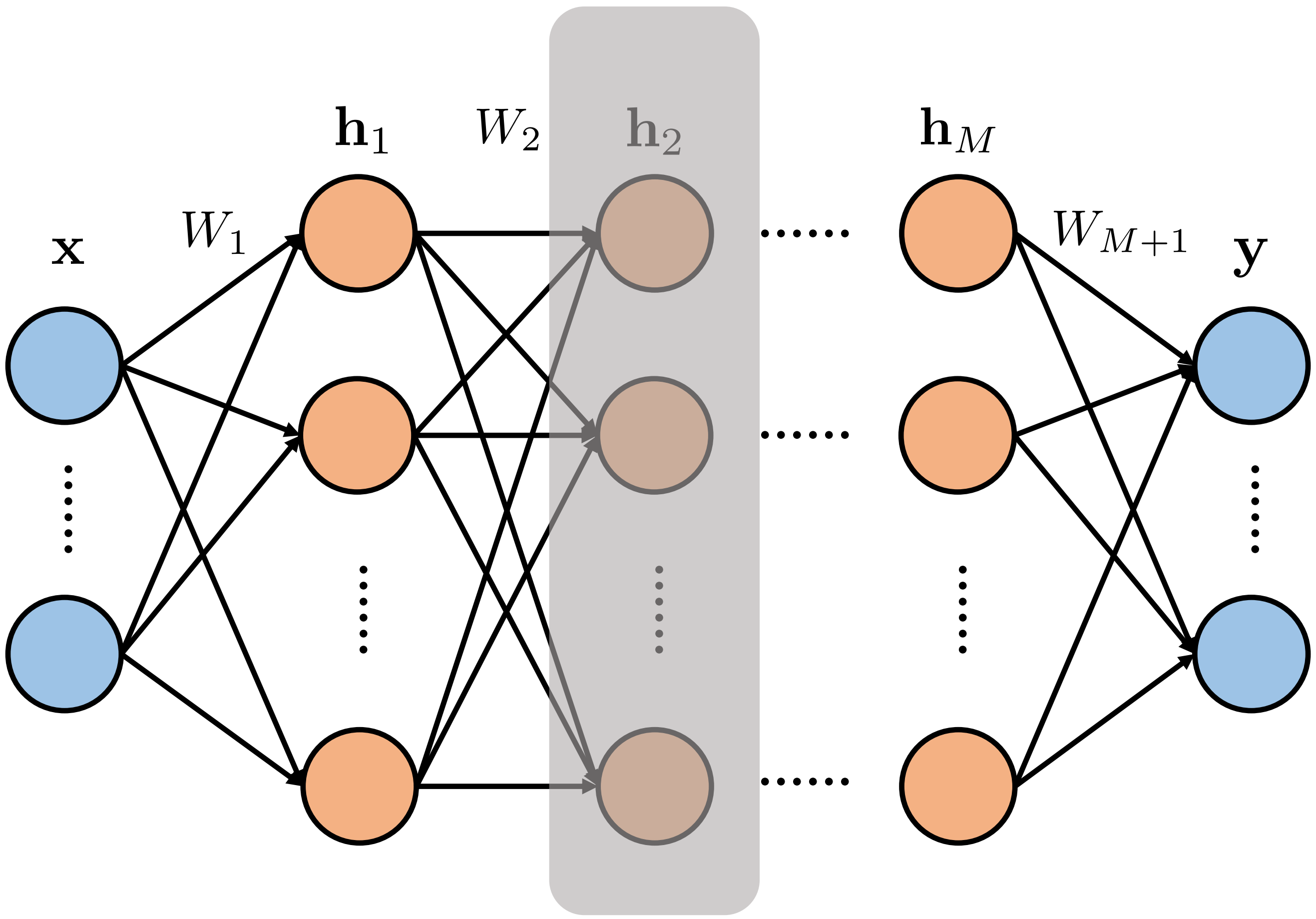

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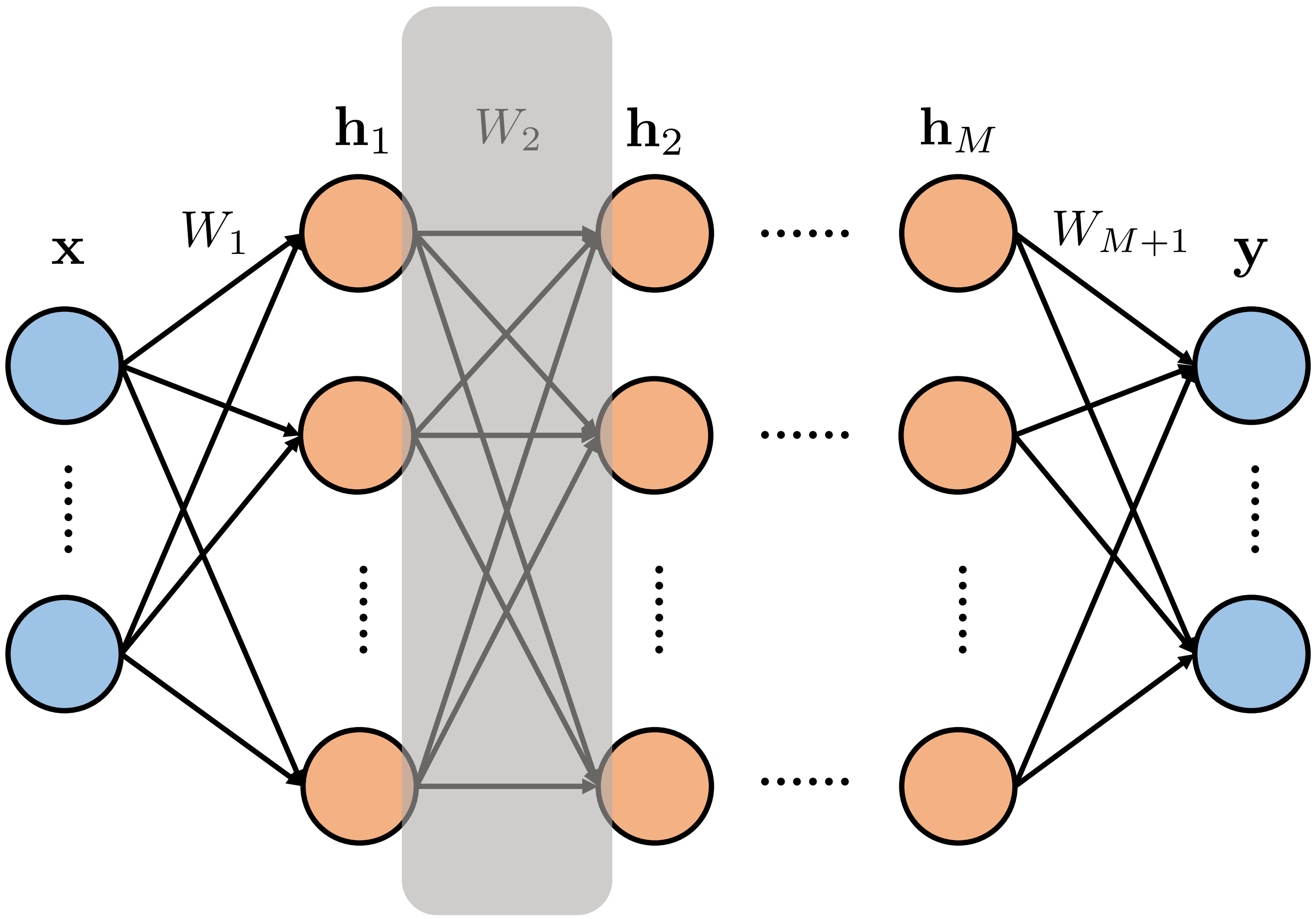
The Jacobian of element-wise nonlinearity is a diagonal matrix!

Backpropagation

During the backward pass:



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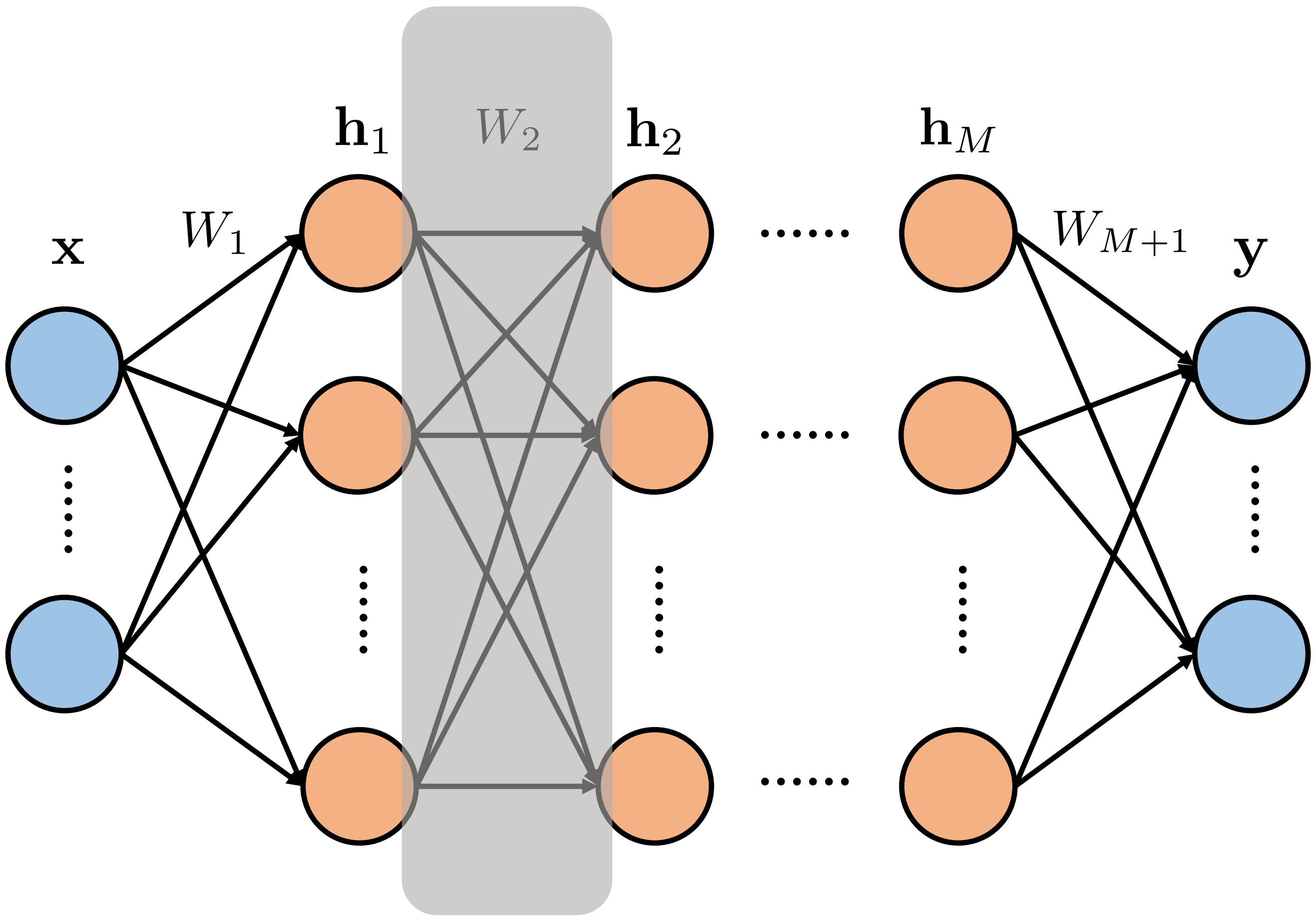

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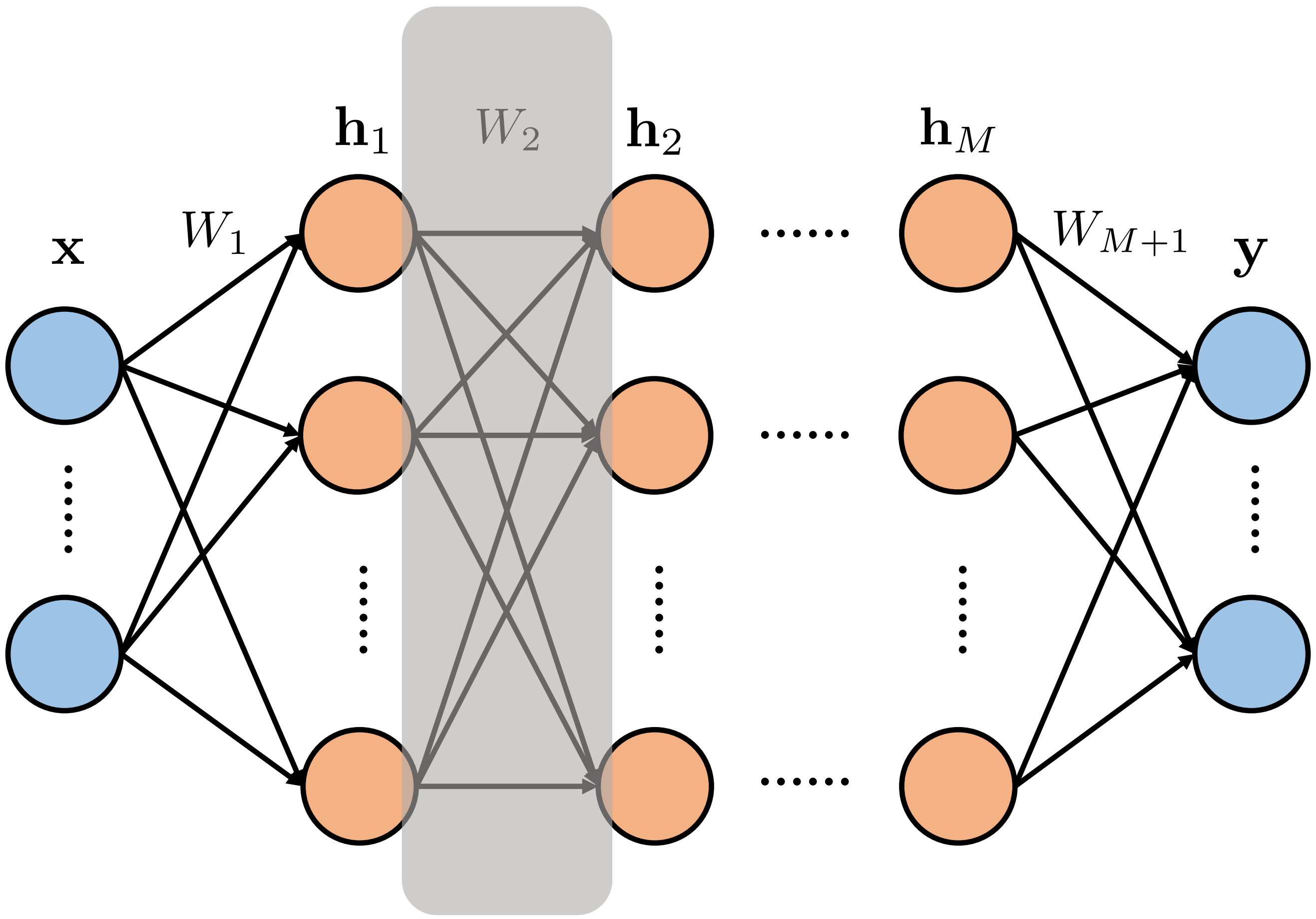

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Why?

Backpropagation

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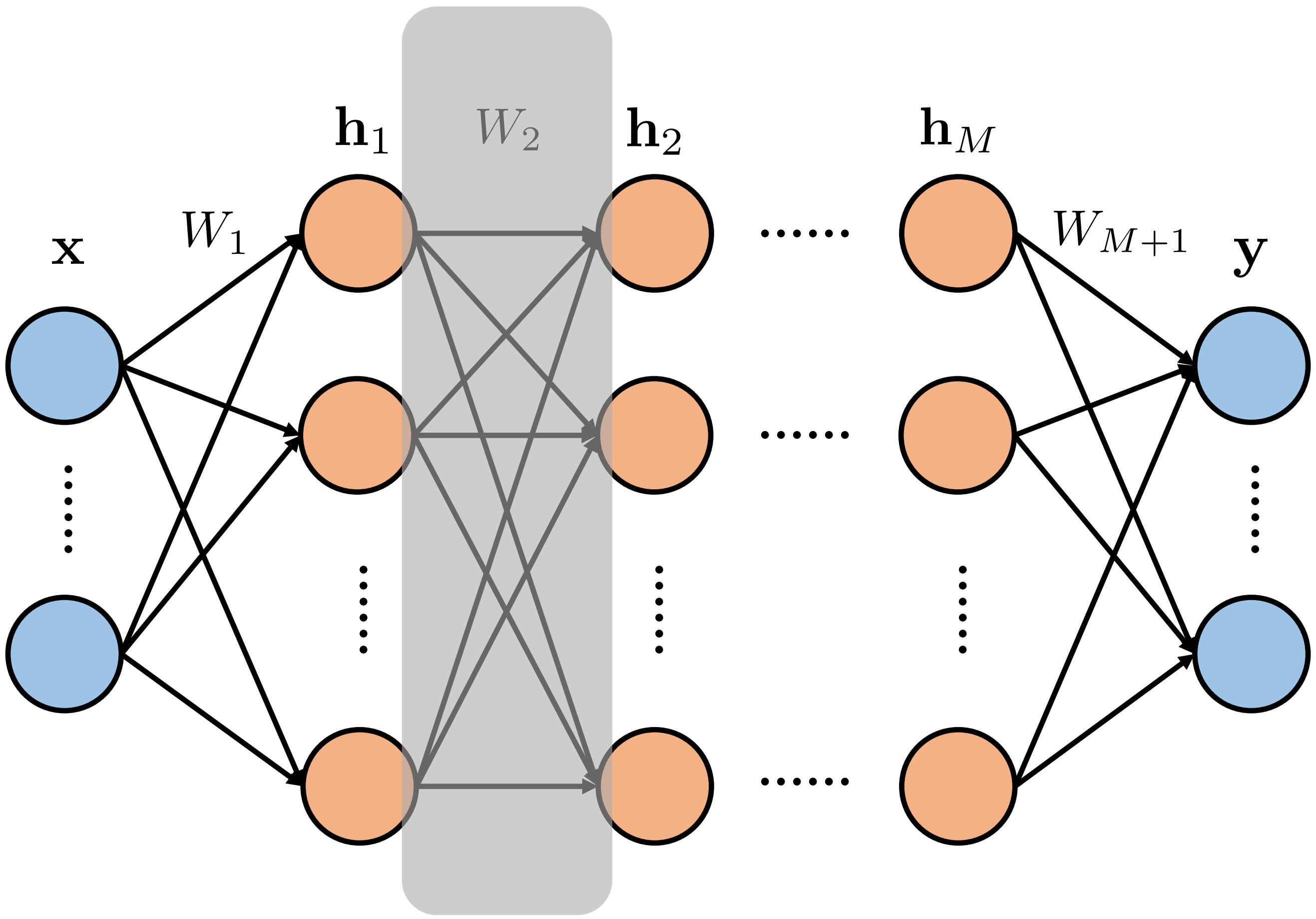

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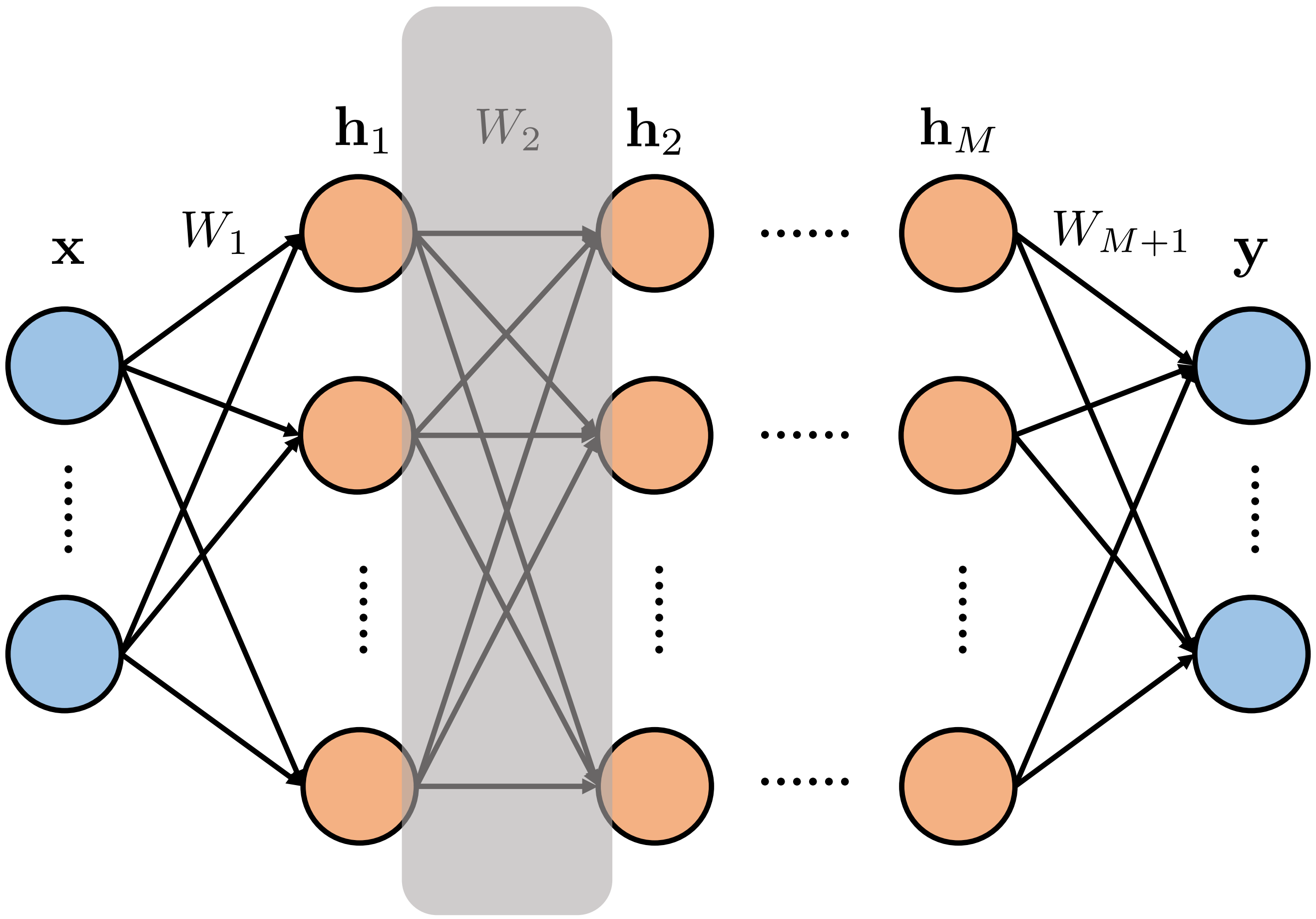

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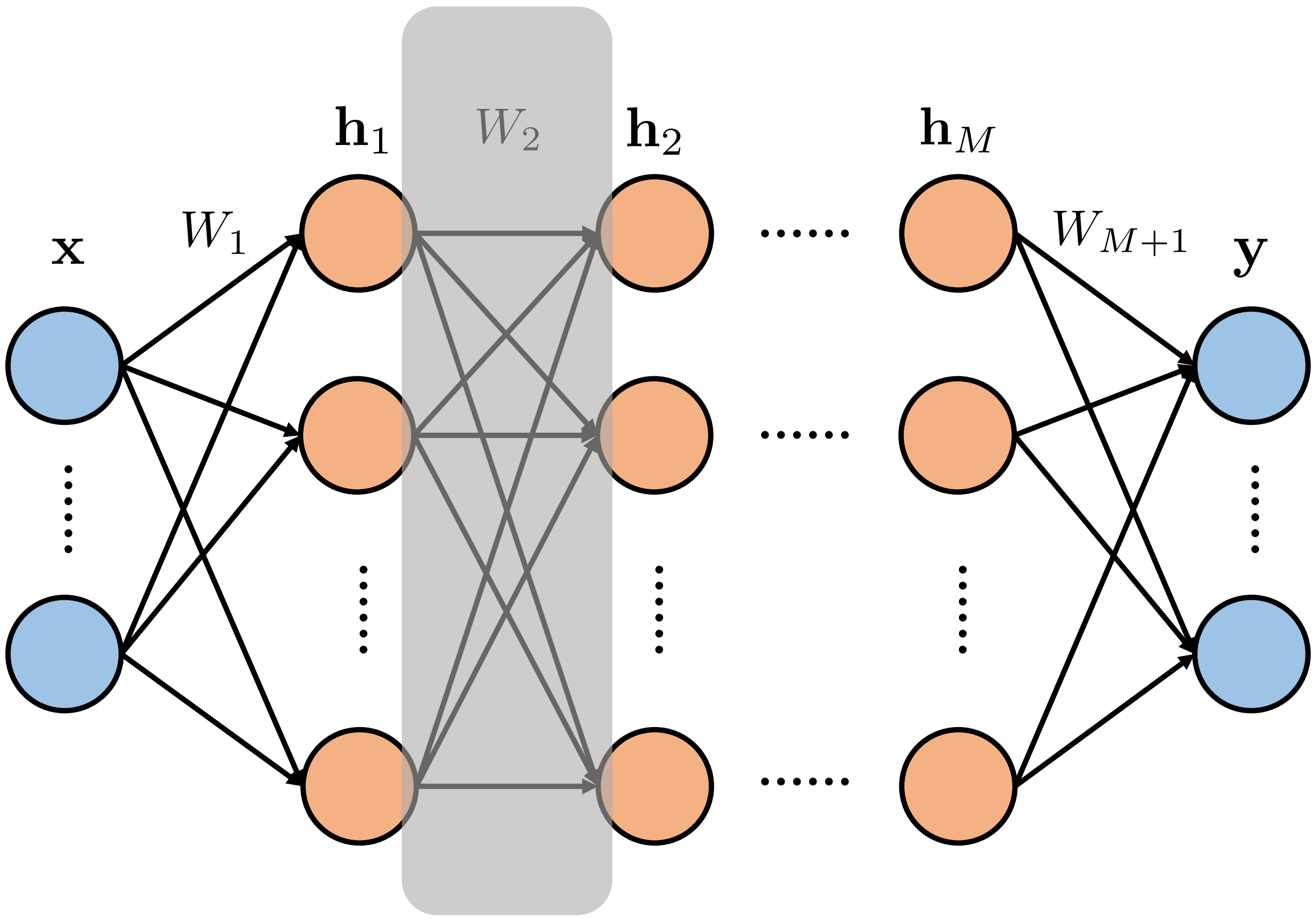

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Note $\mathbf{z}_2[i] = \sum_j W_2[i,j]\mathbf{h}_1[j]$

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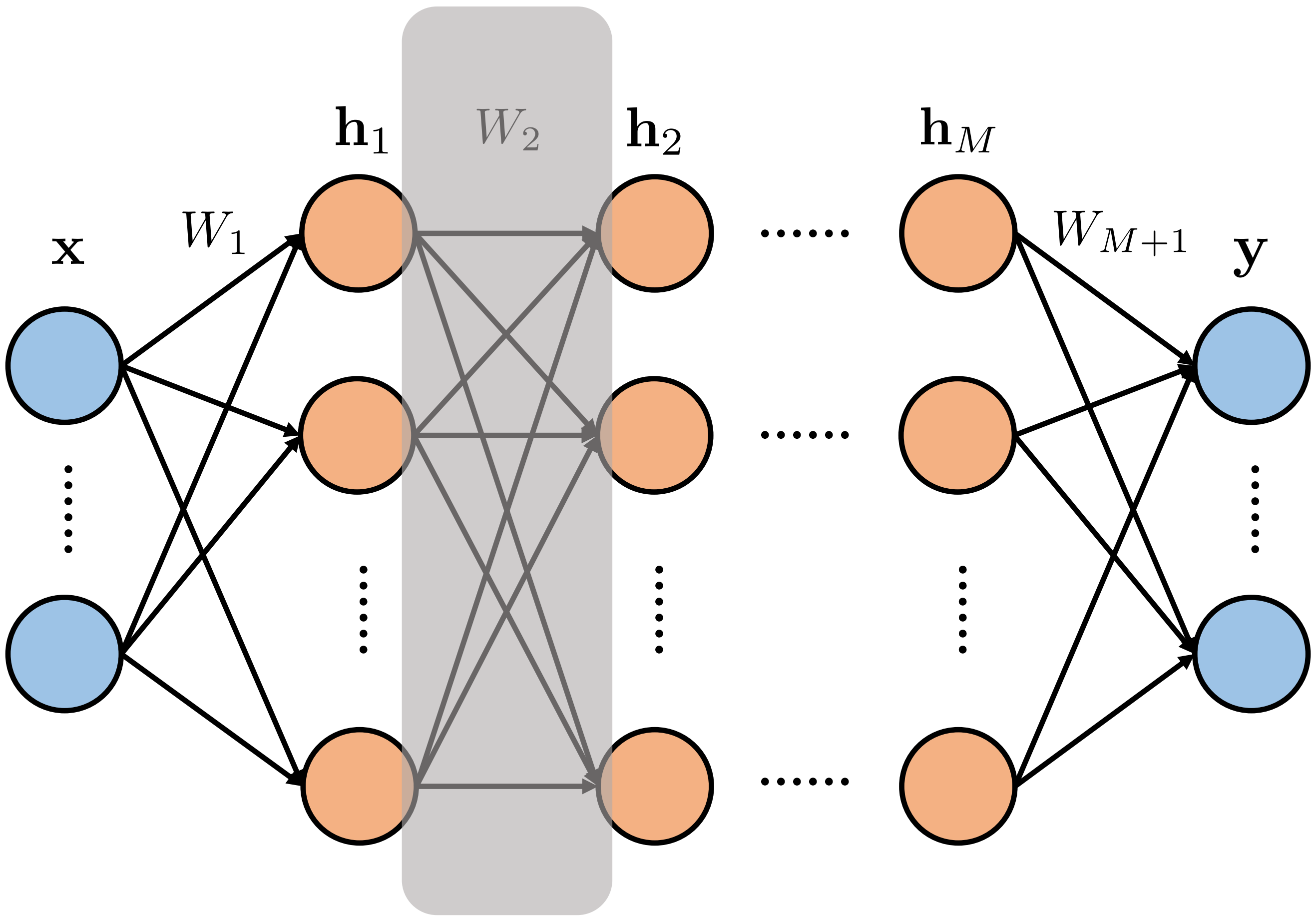

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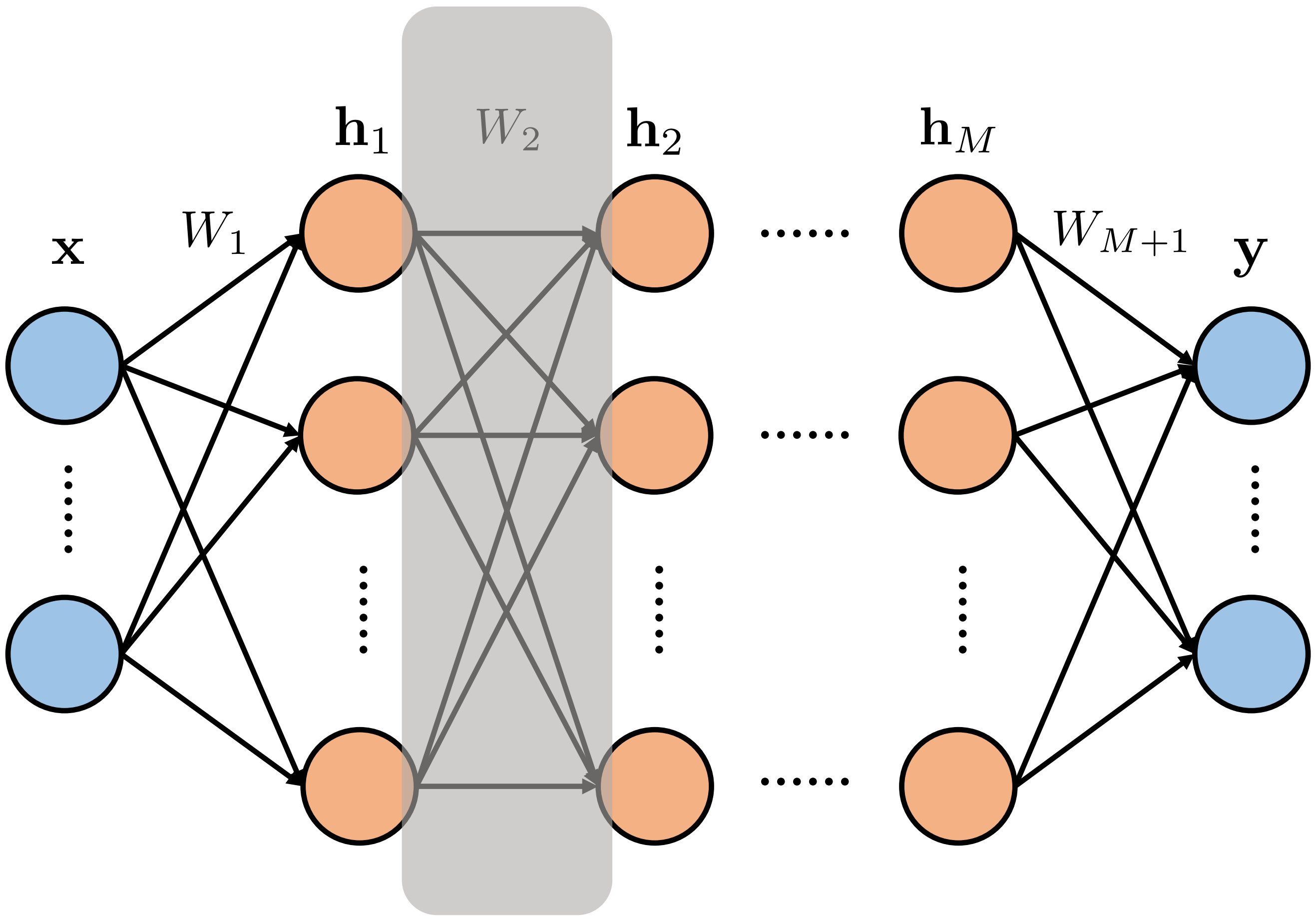

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Backpropagation

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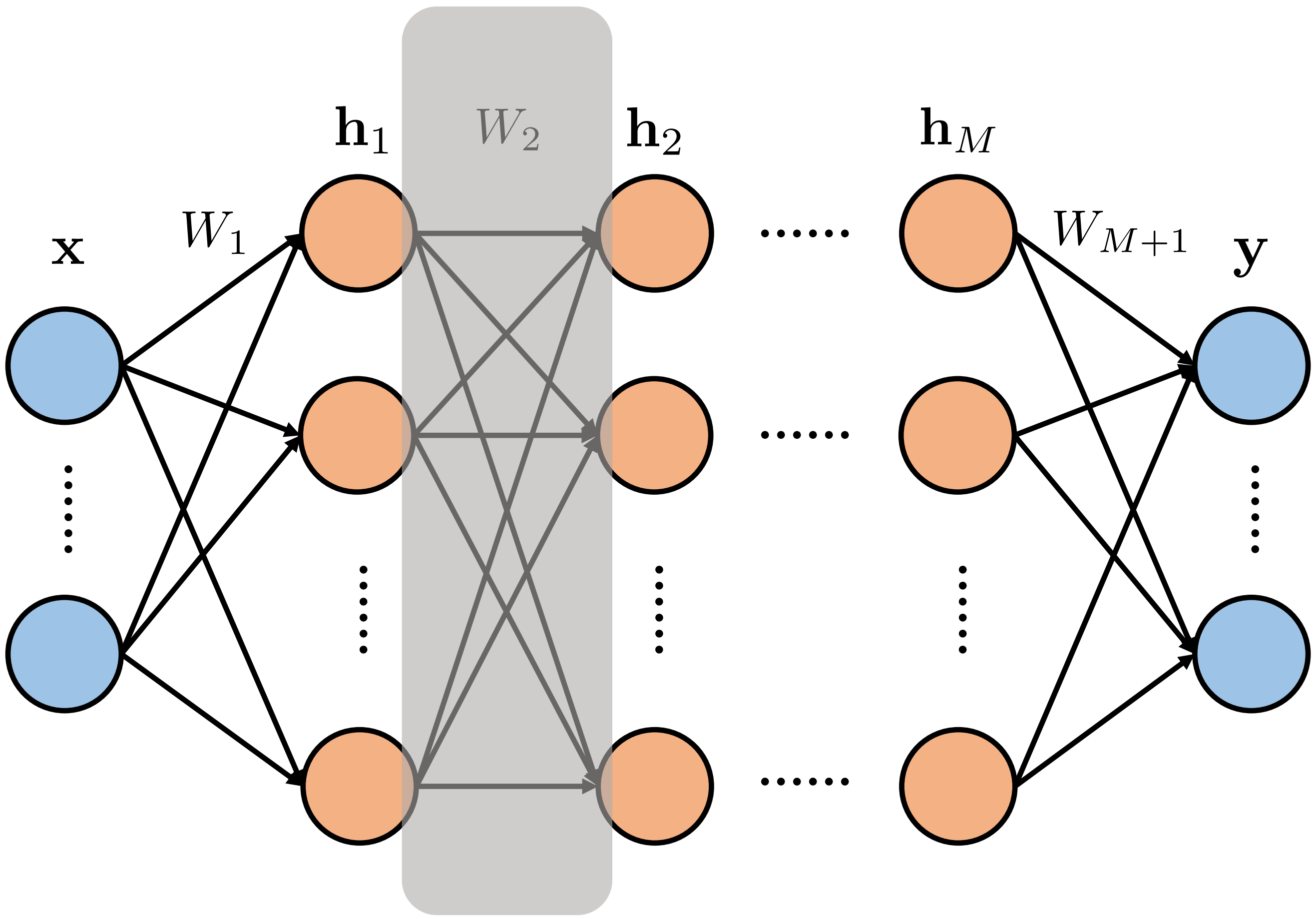

In summary:

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

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

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

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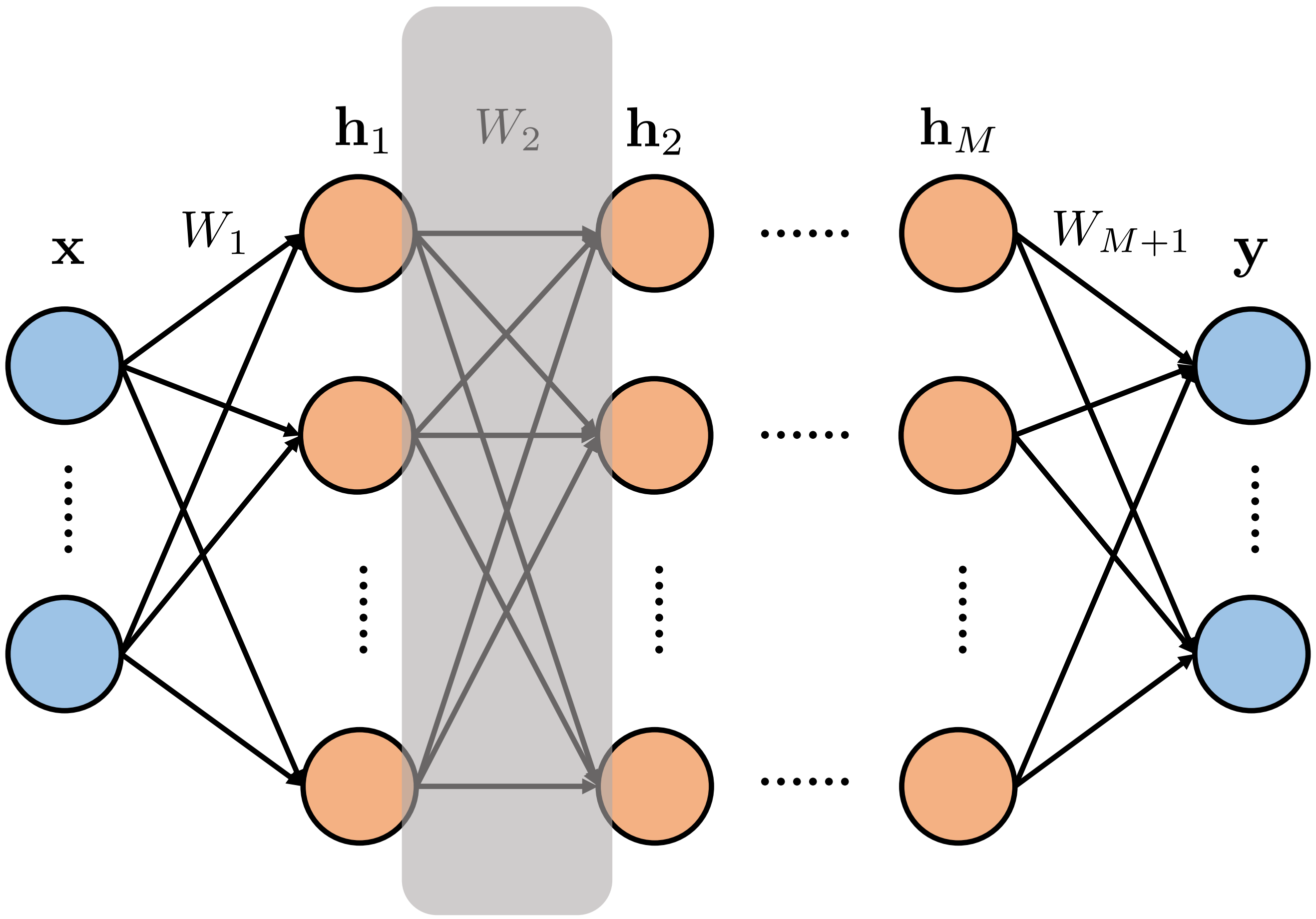

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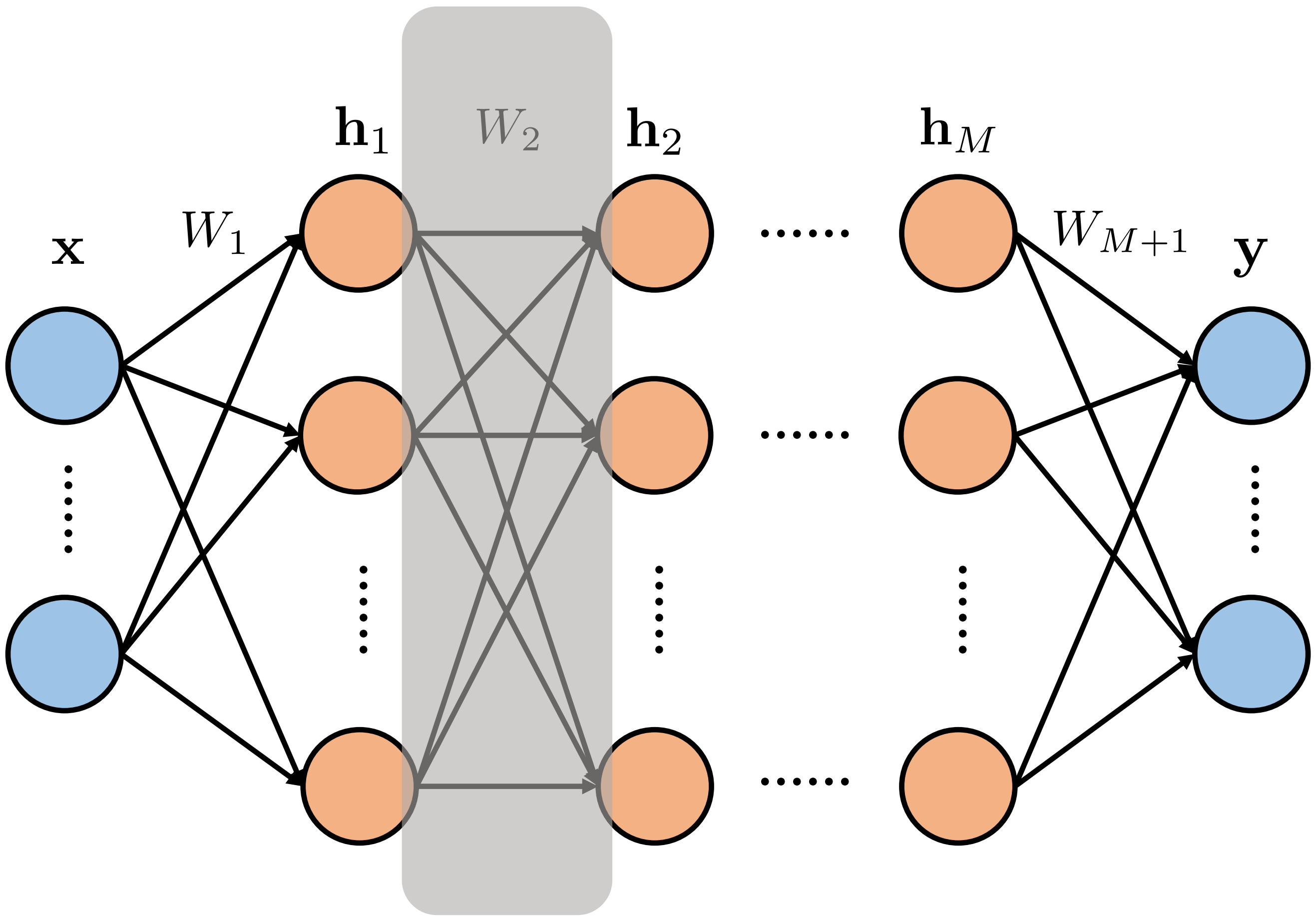
We can cache these tensors in the forward pass to avoid duplicated computation in the backward pass!

Forward vs. Backward



Computation in Forward Pass:

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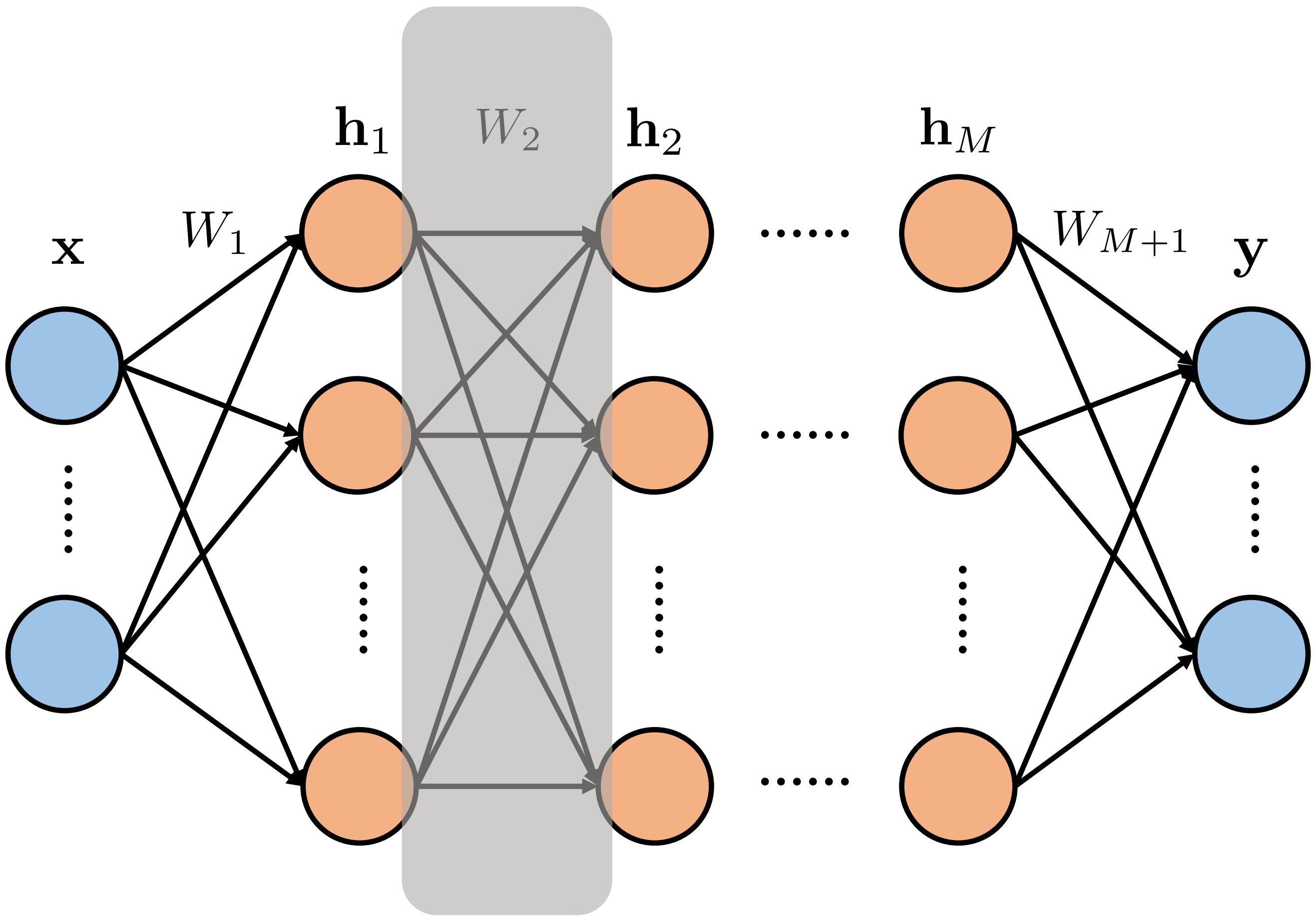

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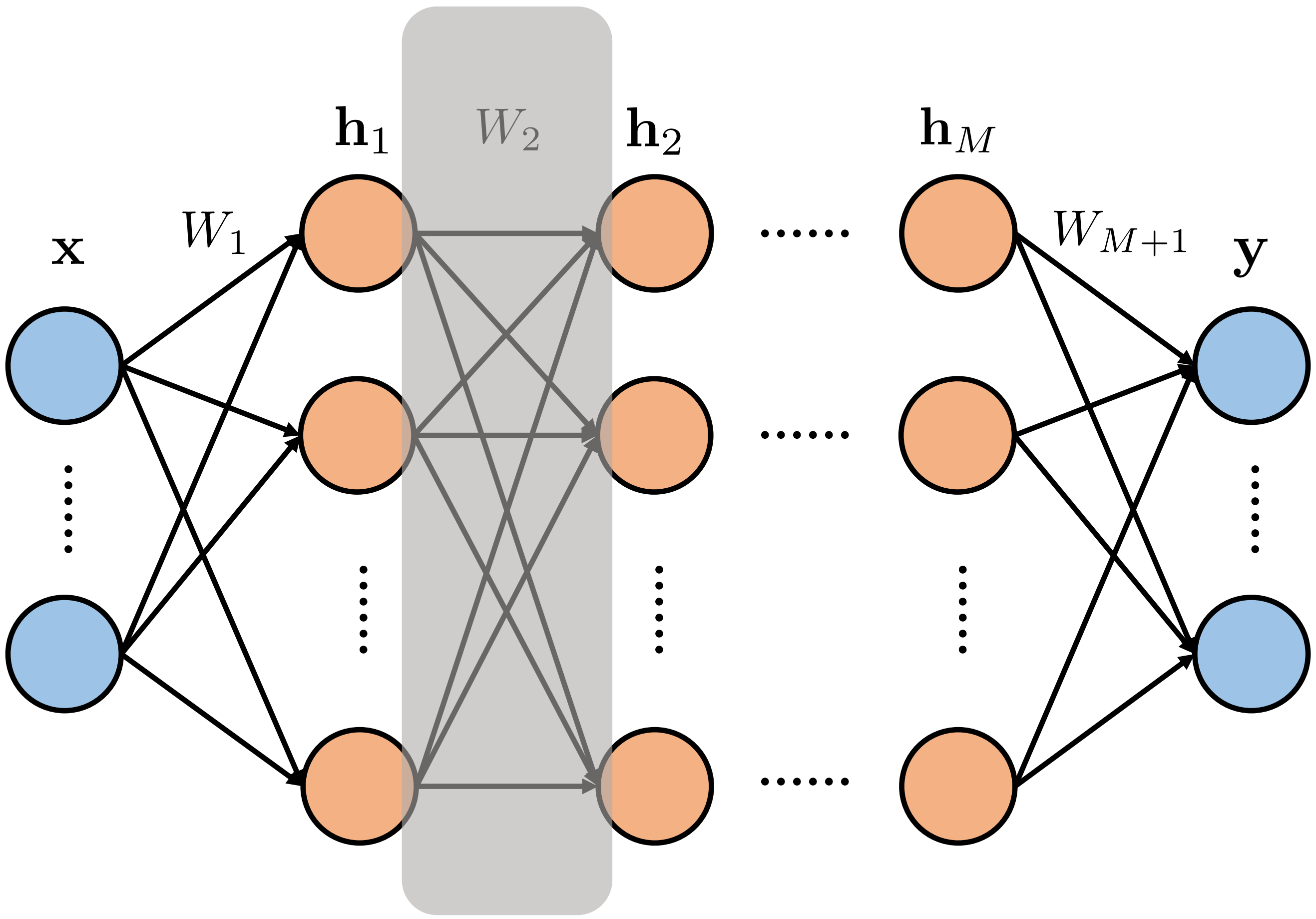

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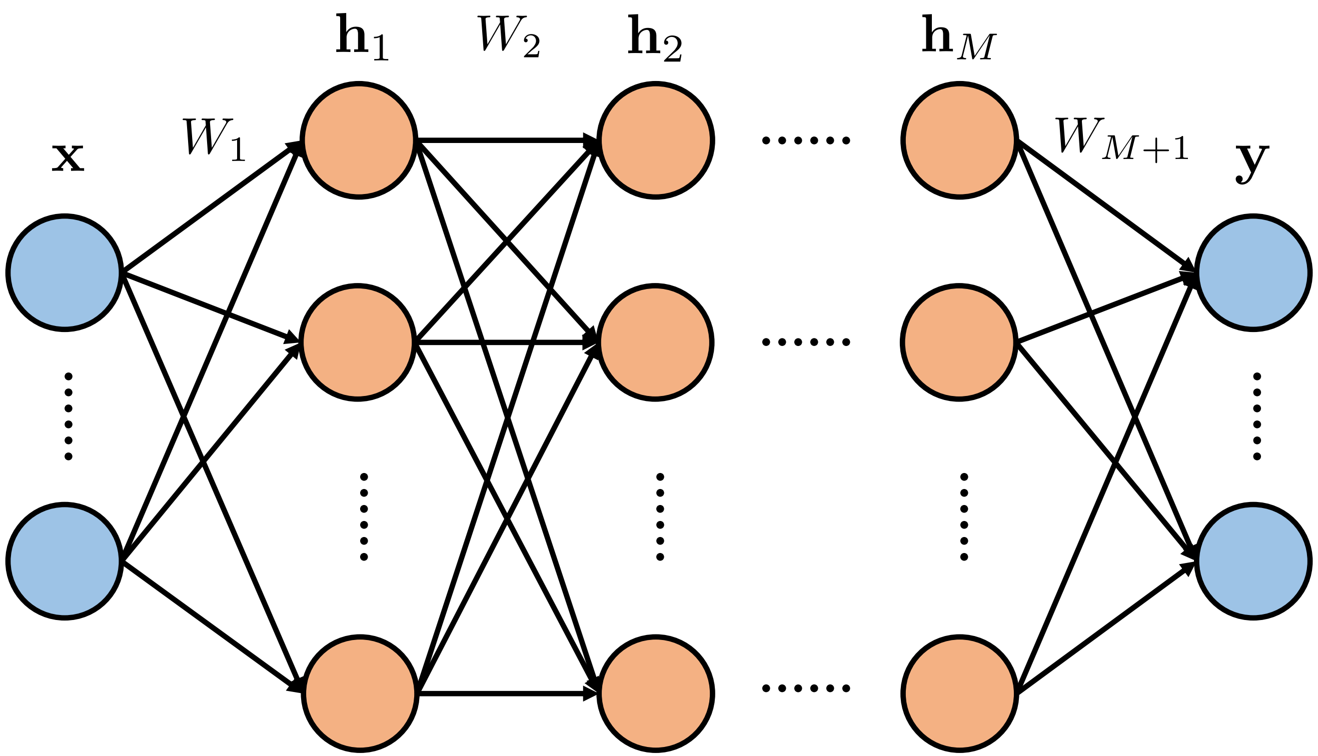
Backward pass is roughly twice as computationally expensive as Forward pass!

Outline

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

Initialization

How should we initialize the neural network?



Initialization

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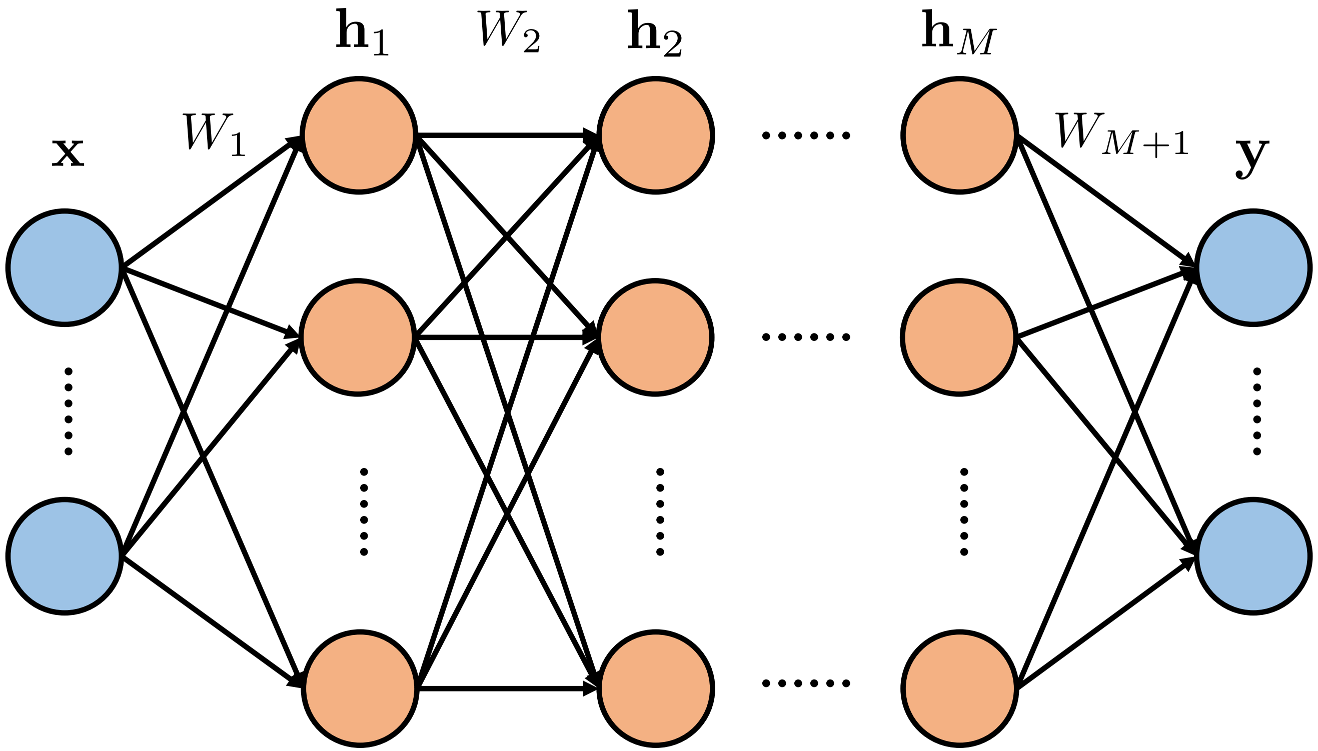
A lot of criterions for good initialization exist, e.g., *be close to some local optima*, *have a higher chance to reach a global optima*.



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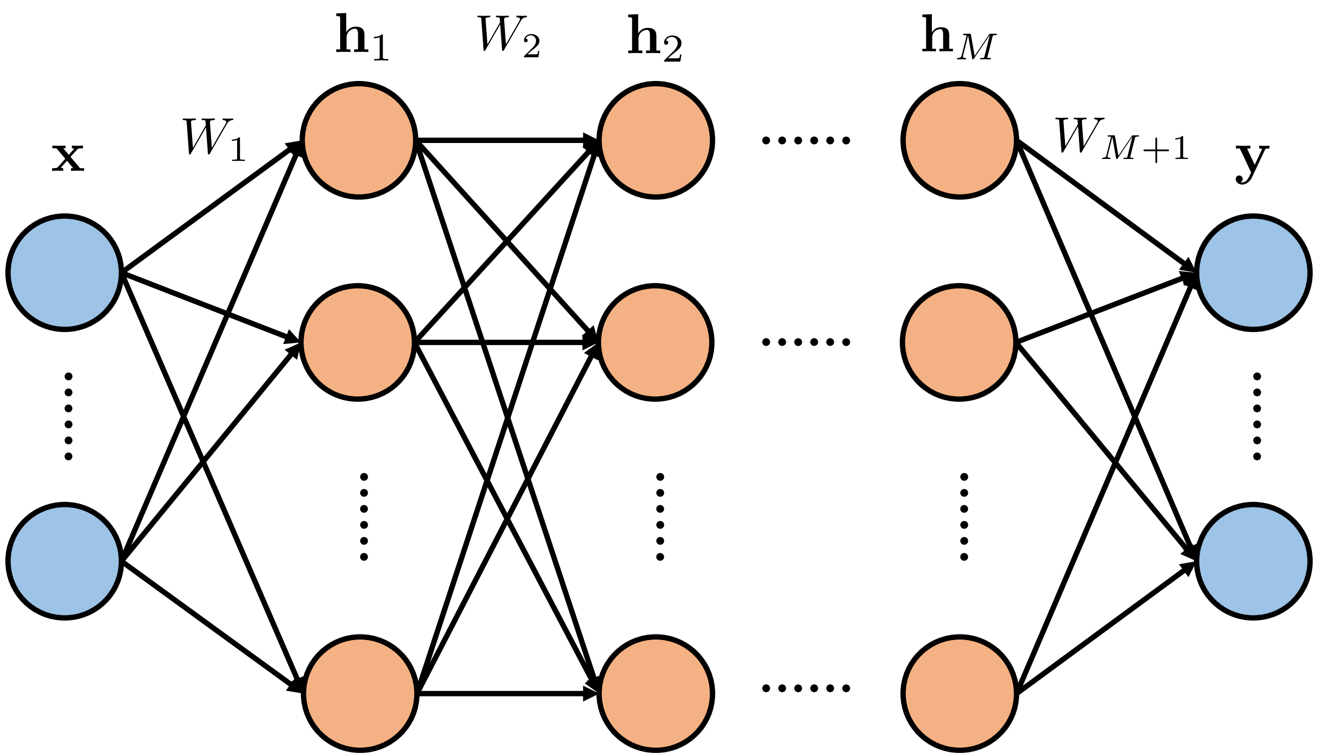

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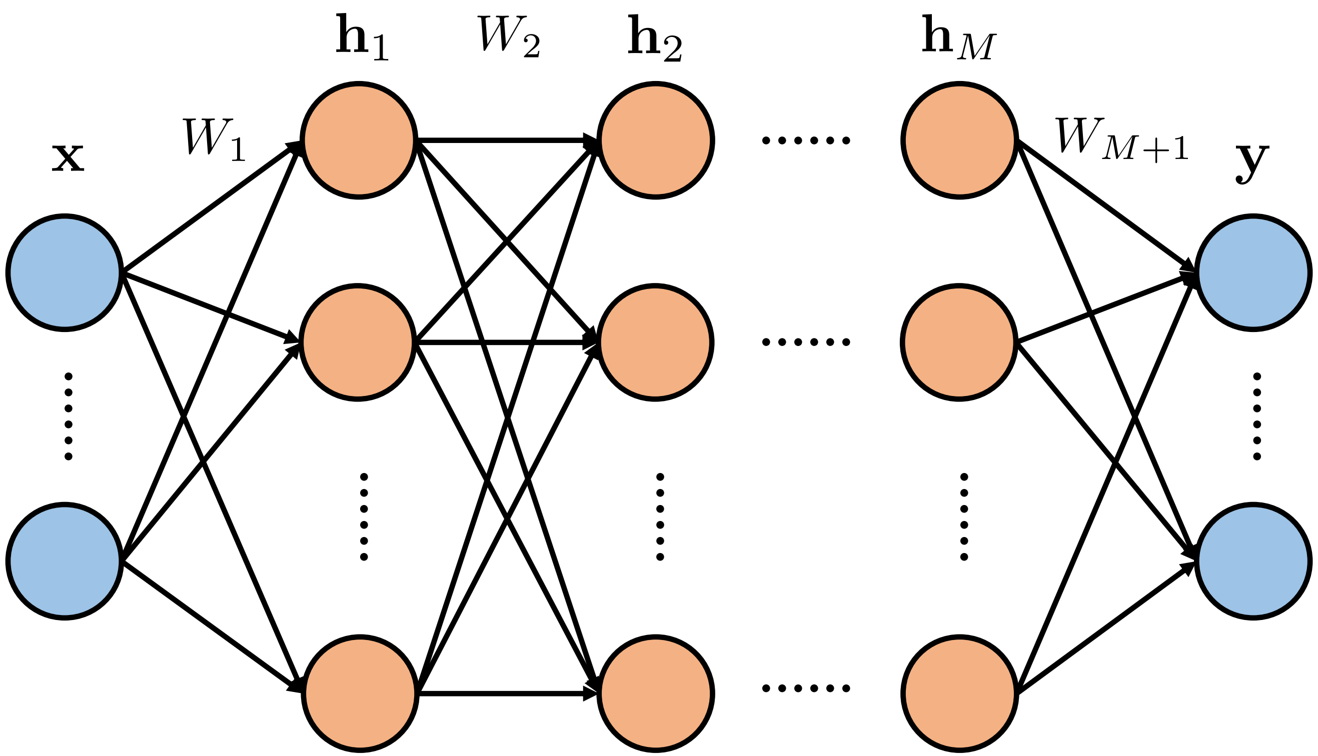

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We want to start with some **stable** initial neural network!

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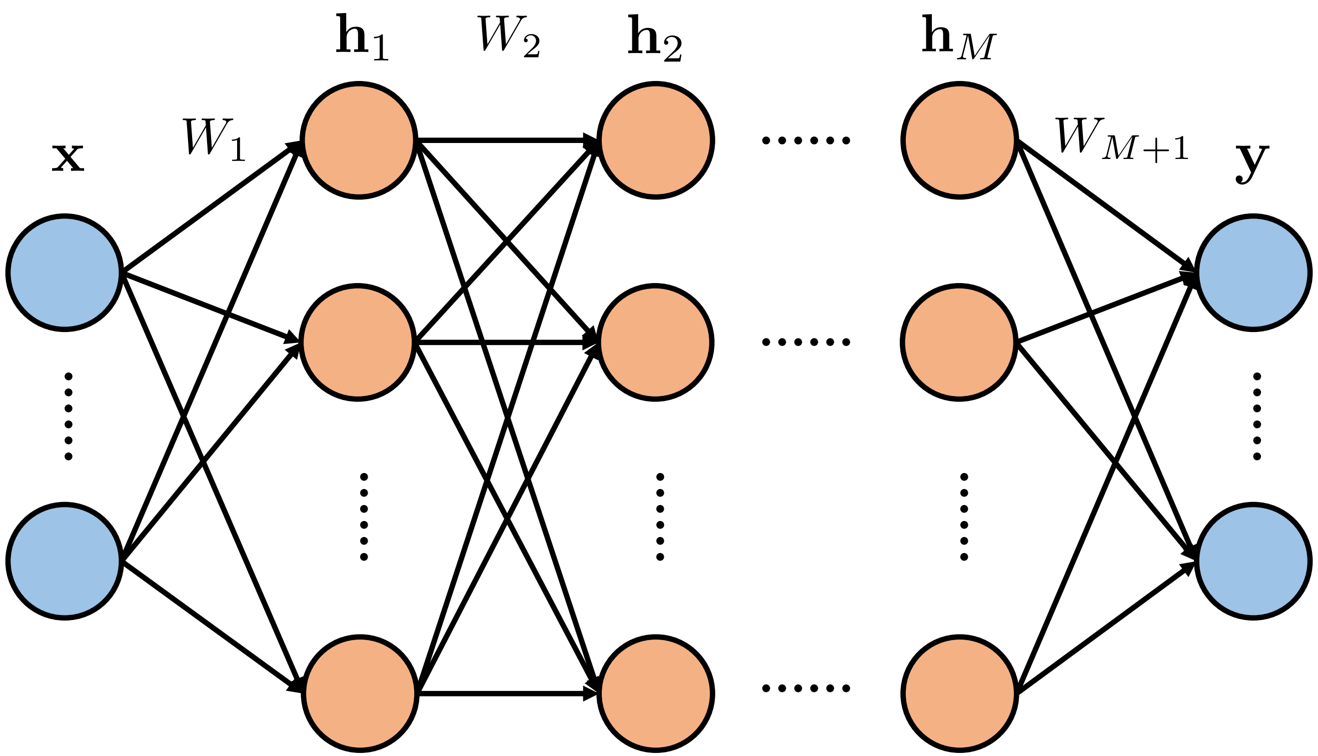

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There are also many stability notions. Let us look at the variance of the activations and gradients.

Initialization

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

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

Initialization

Let us recap some basic facts about variance

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

Initialization

Let us recap some basic facts about variance

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For two independent random variables, we have

$$\begin{aligned}
\mathbb{V}[x+y] &= \mathbb{E}[(x+y)^2] - \mathbb{E}[x+y]^2 \\
&= \mathbb{E}[x^2 + y^2 + 2xy] - (\mathbb{E}[x] + \mathbb{E}[y])^2 \\
&= \mathbb{E}[x^2] + \mathbb{E}[y^2] + 2\mathbb{E}[xy] - \mathbb{E}[x]^2 - \mathbb{E}[y]^2 - 2\mathbb{E}[x]\mathbb{E}[y] \\
&= \mathbb{V}[x] + \mathbb{V}[y] + 2(\mathbb{E}[xy] - \mathbb{E}[x]\mathbb{E}[y]) \\
&= \mathbb{V}[x] + \mathbb{V}[y] + 2\mathrm{Cov}(x, y)
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&= \mathbb{V}[x] + \mathbb{V}[y] + 2(\mathbb{E}[xy] - \mathbb{E}[x]\mathbb{E}[y]) \\
&= \mathbb{V}[x] + \mathbb{V}[y] + 2\mathrm{Cov}(x, y) \qquad \mathbb{E}[xy] = \mathbb{E}[x]\mathbb{E}[y]
\end{aligned}$$

Initialization

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

$$\begin{aligned}
\mathbb{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] \\
&= \mathbb{V}[x] + \mathbb{V}[y] + 2(\mathbb{E}[xy] - \mathbb{E}[x]\mathbb{E}[y]) \\
&= \mathbb{V}[x] + \mathbb{V}[y] + 2\mathrm{Cov}(x, y) \qquad\qquad \mathbb{E}[xy] = \mathbb{E}[x]\mathbb{E}[y] \\
&= \mathbb{V}[x] + \mathbb{V}[y]
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For two independent random variables, we have

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

$$\begin{aligned}
\mathbb{E}[xy] &= \mathbb{E}[x]\mathbb{E}[y] \\
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$$\mathbb{V}[x] = \mathbb{E}\left[(x - \mathbb{E}[x])^2\right] = \mathbb{E}[x^2] - (\mathbb{E}[x])^2$$

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

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

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

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

Initialization

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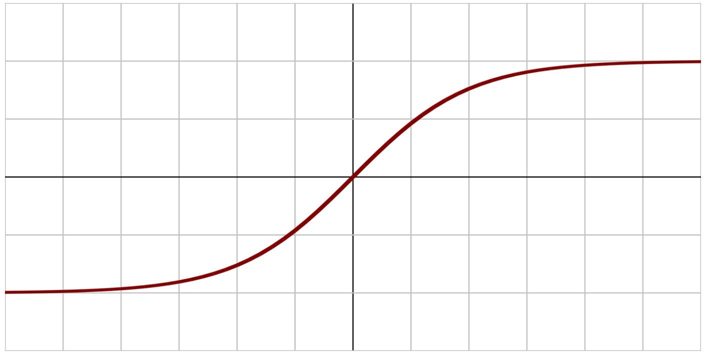
$$\mathbb{V}[x] = \mathbb{E}\left[(x - \mathbb{E}[x])^2\right] = \mathbb{E}[x^2] - (\mathbb{E}[x])^2$$

In summary, for two independent random variables, we have

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

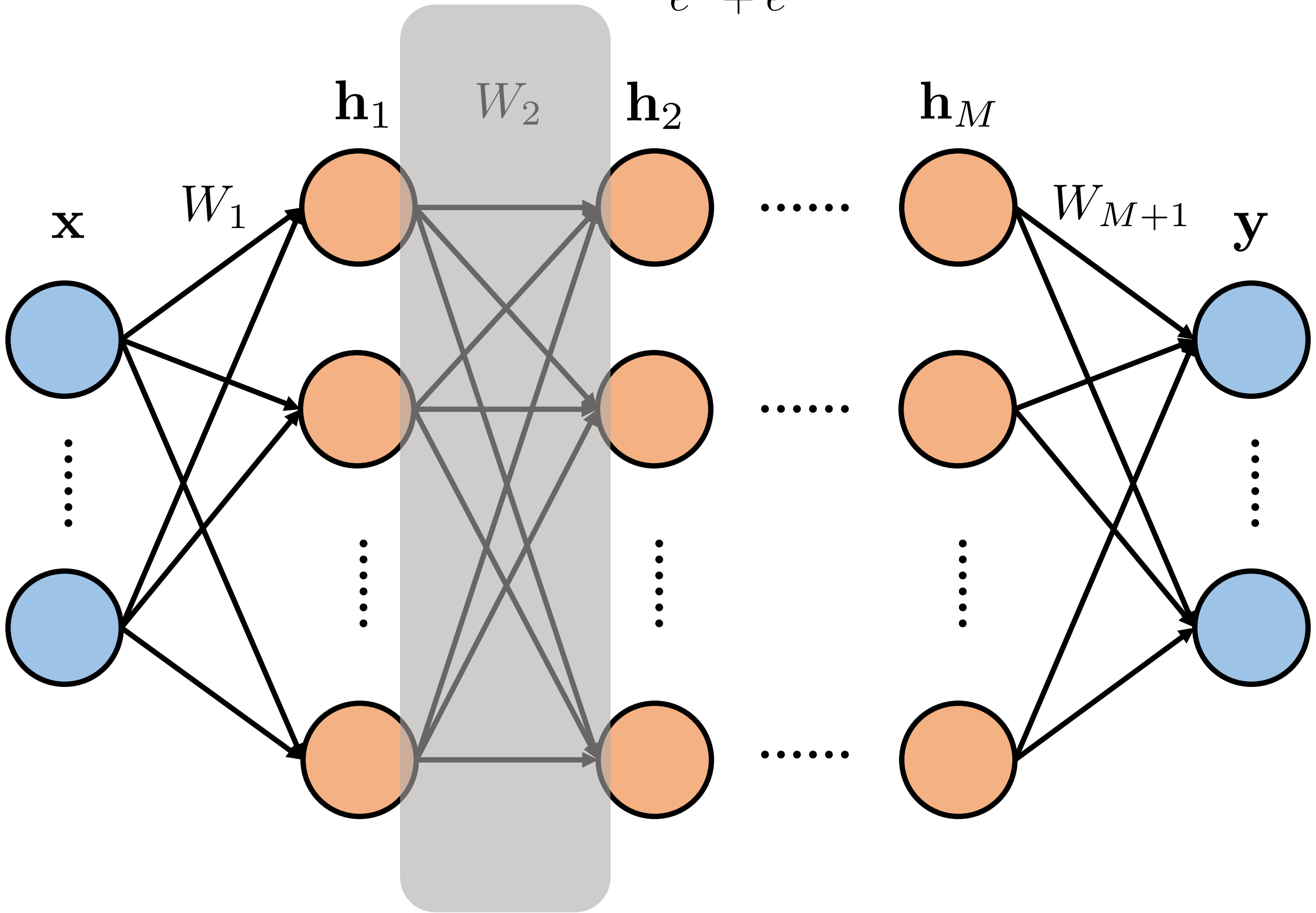
If $\mathbb{E}[x] = \mathbb{E}[y] = 0$, then $\mathbb{V}[xy] = \mathbb{V}[x]\mathbb{V}[y]$

Initialization: Forward Analysis



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

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



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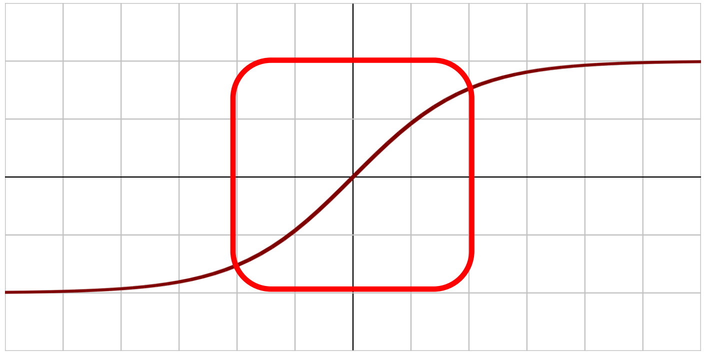

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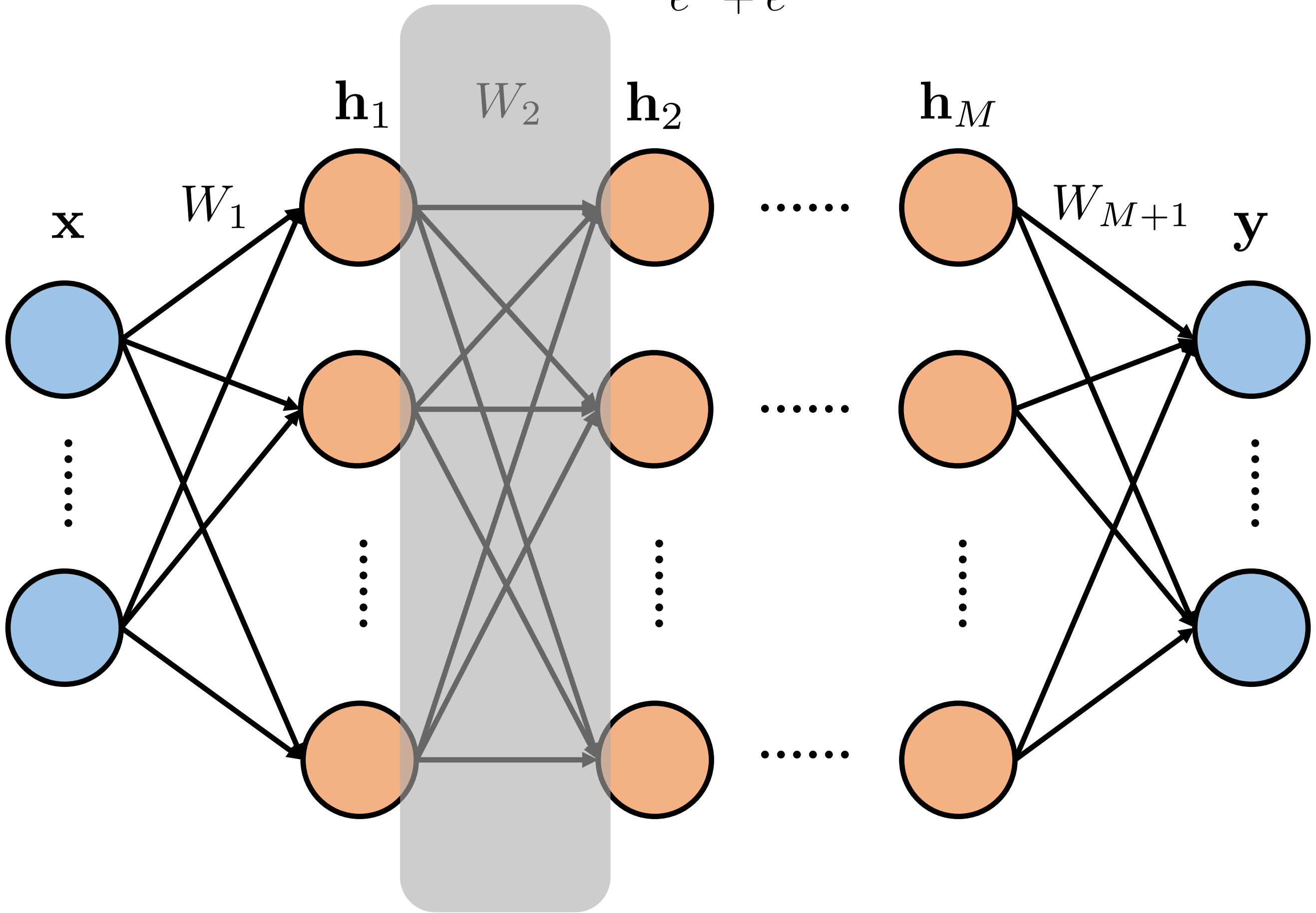

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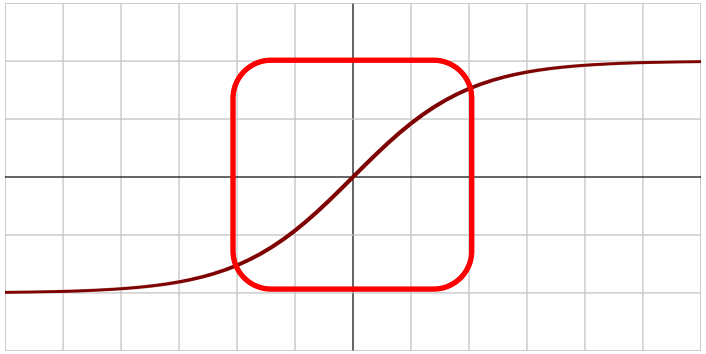
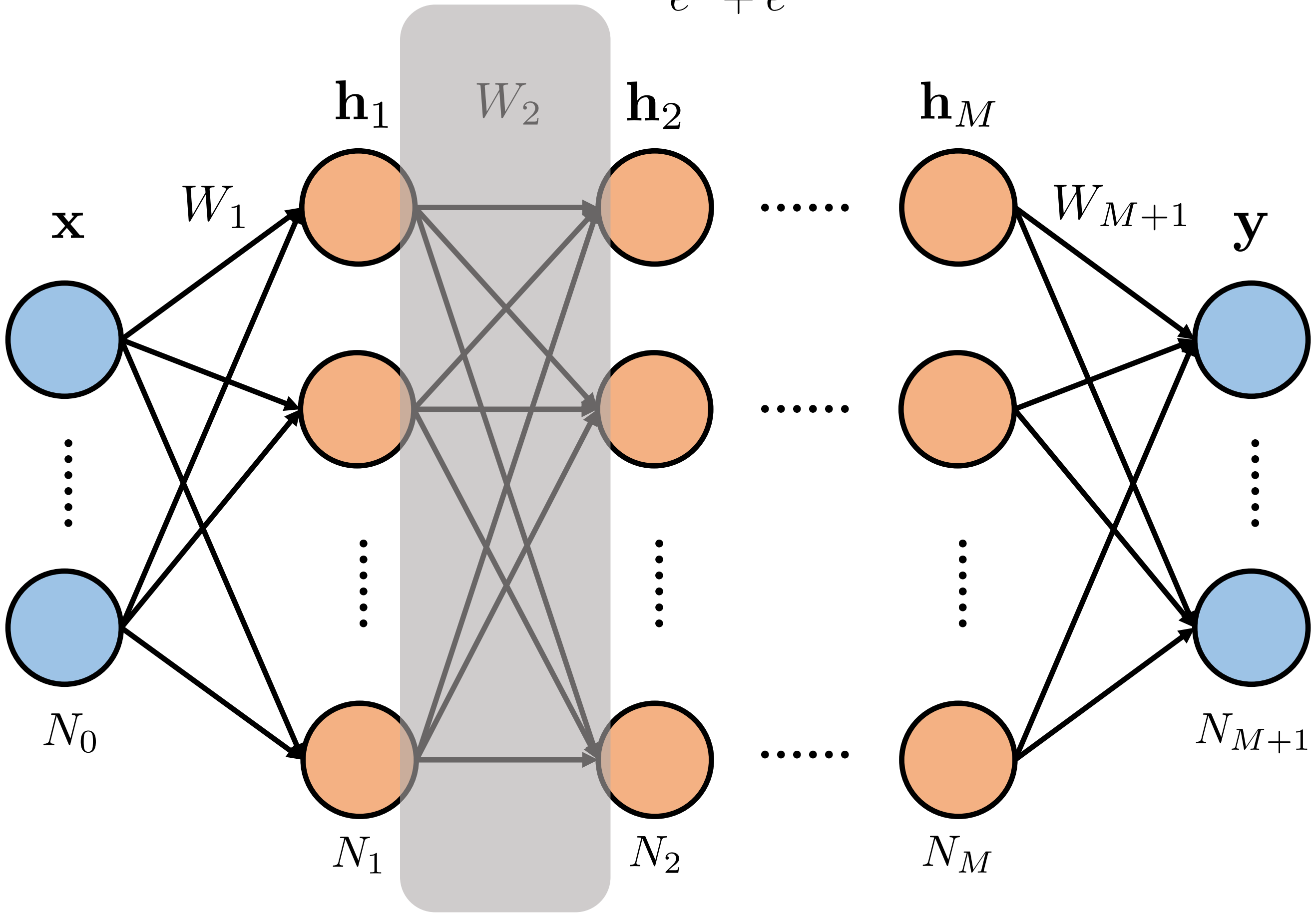


Then we have

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



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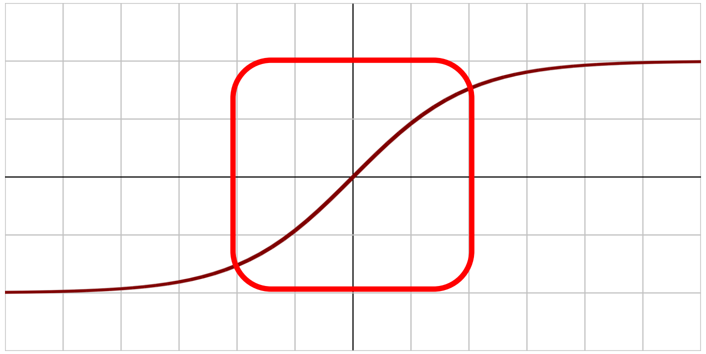

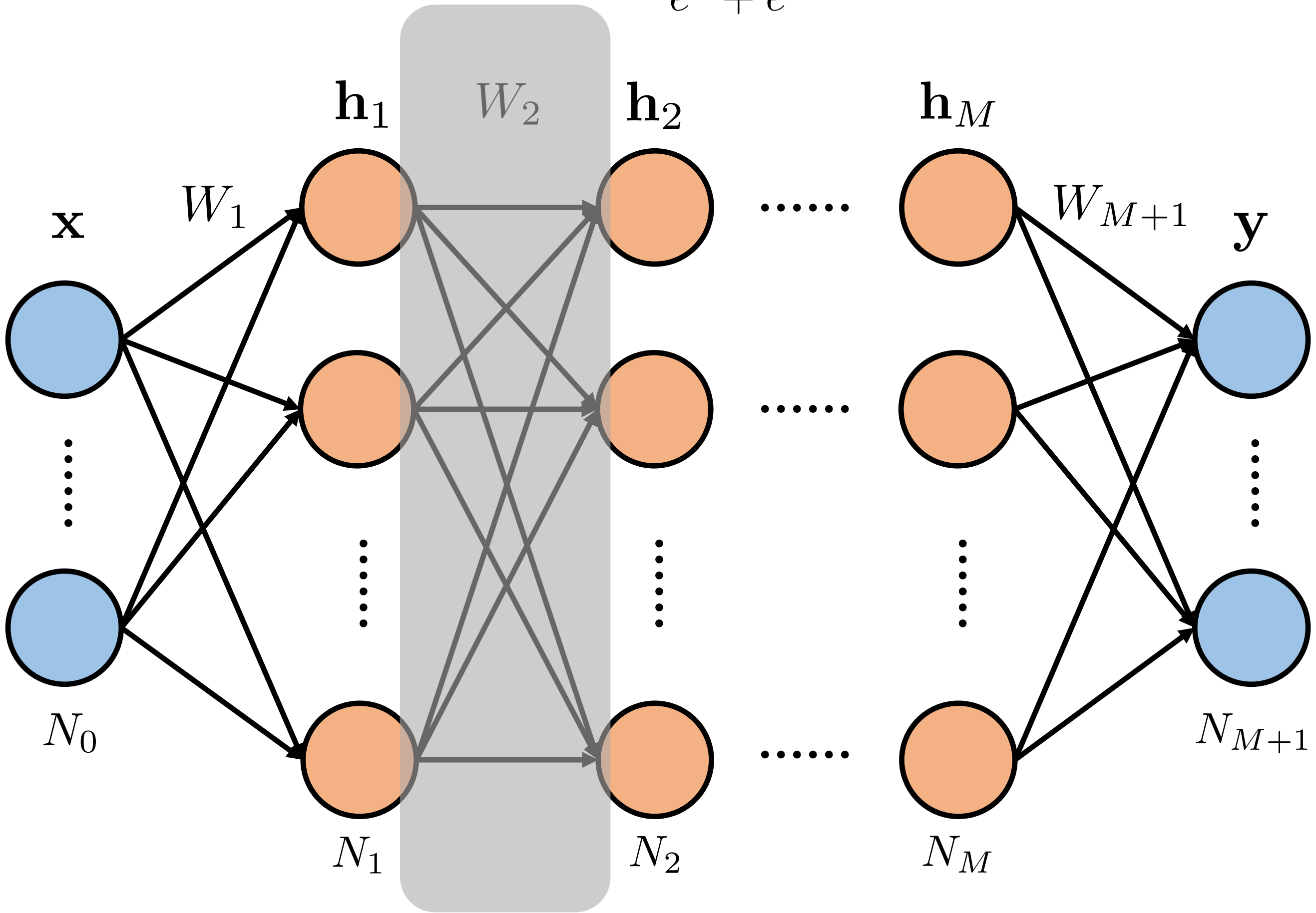

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We further assume i.i.d. and zero mean with same variance for all activations $\mathbf{h}_1[j]$ and all weights $W_2[i,j]$ at all layers, then

$$\begin{aligned}
\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] \\
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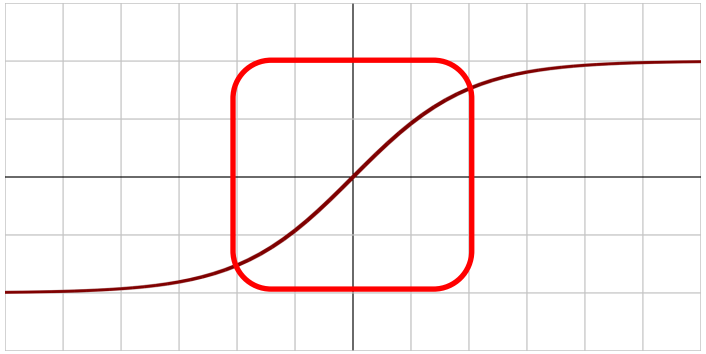

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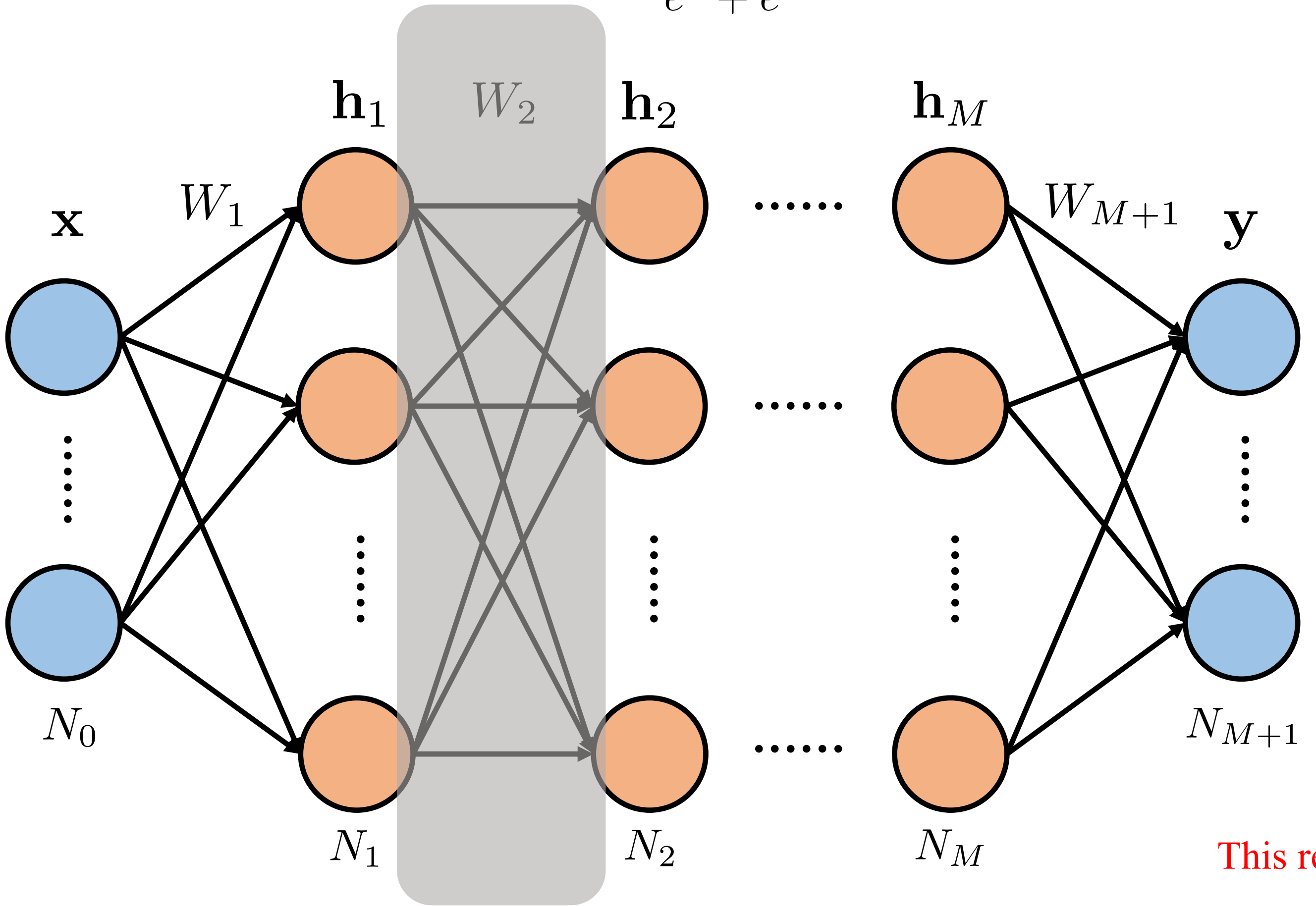

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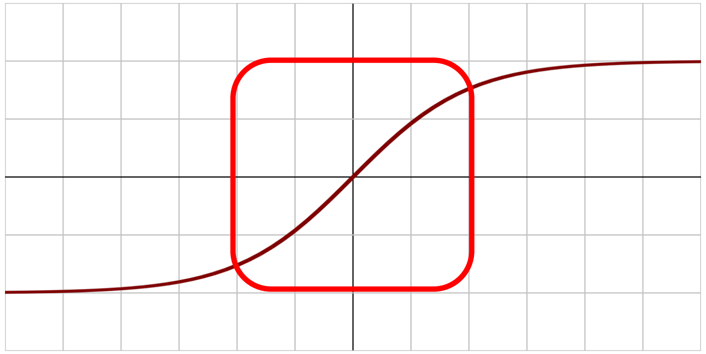
\end{aligned}$$

This relation holds for all layers given the assumptions!

Initialization: Forward Analysis



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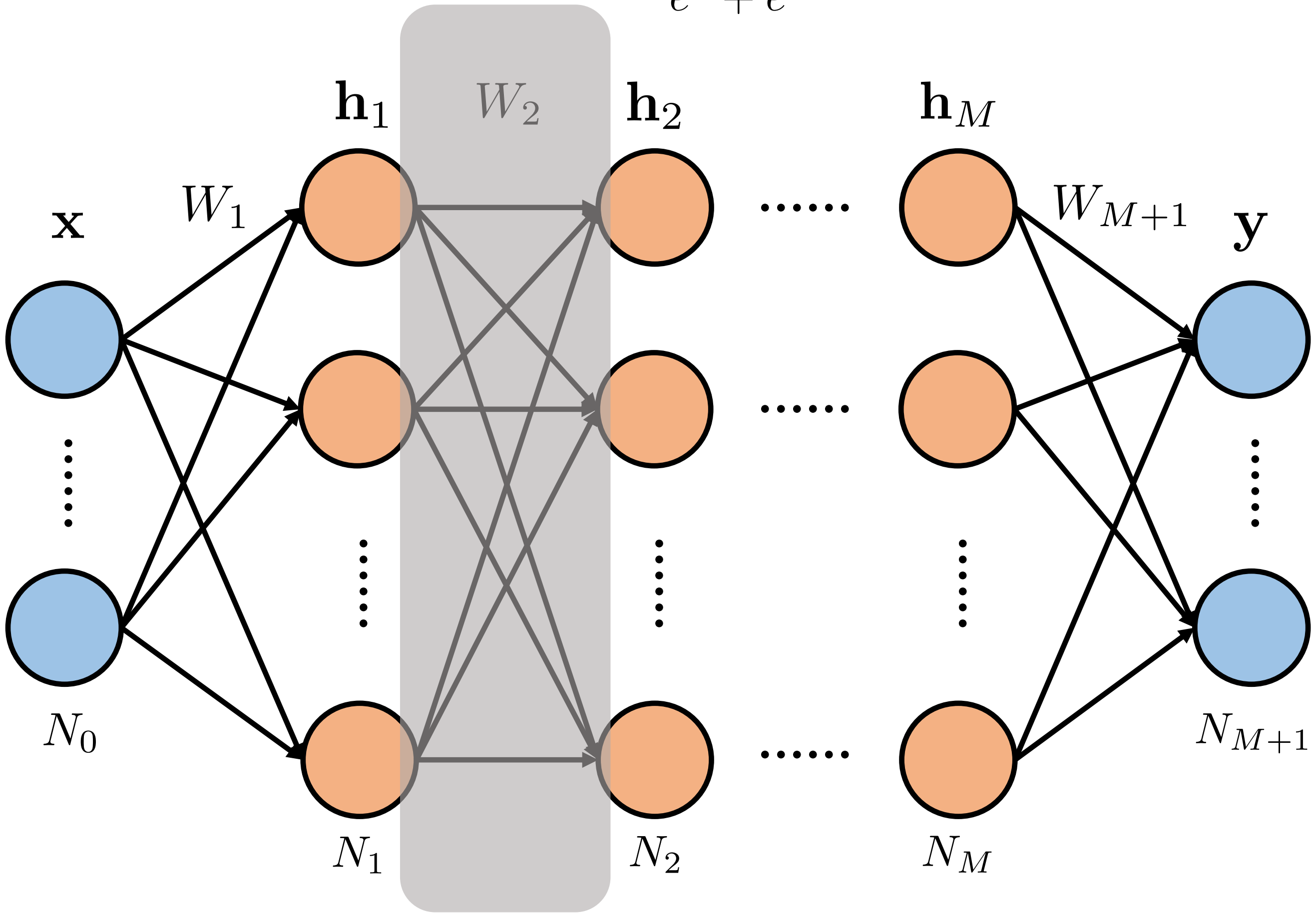
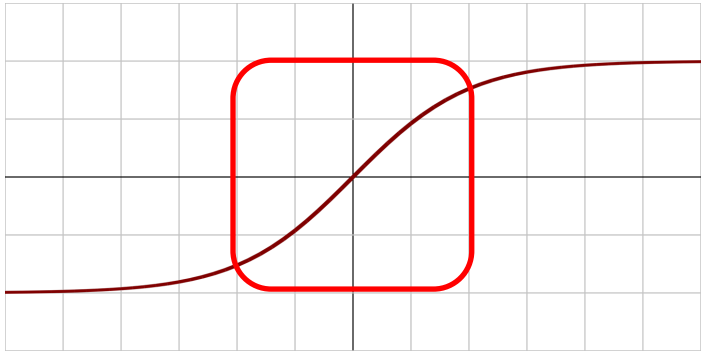


Then unroll the recursion, we have

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

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!

Initialization: Forward Analysis



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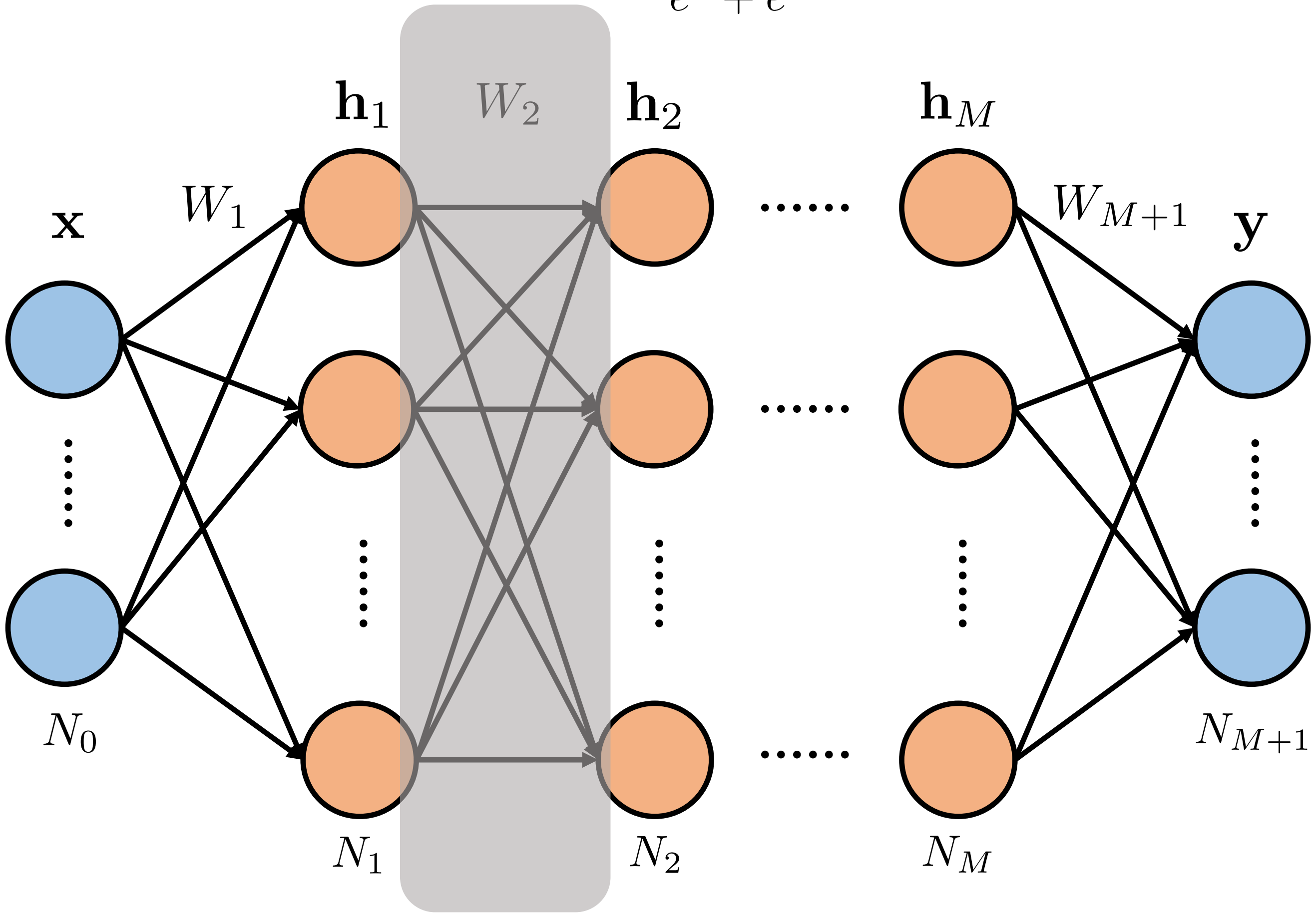

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To preserve the variance of activations through forward pass, i.e.,

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

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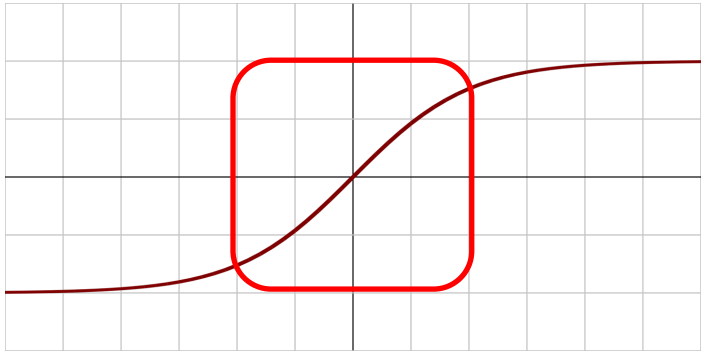

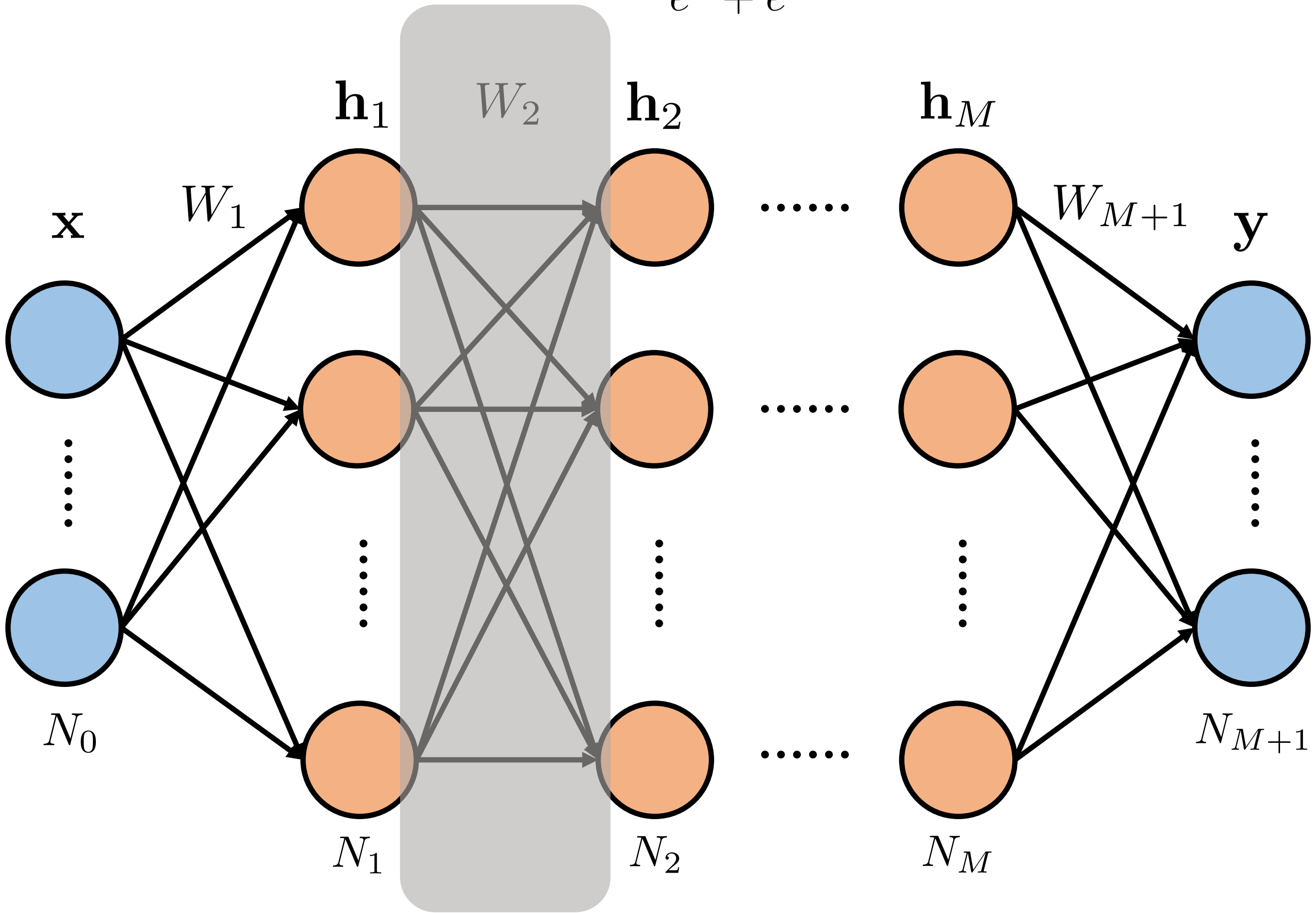

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$$\mathbb{V}\left[\mathbf{h}_l[i]\right] \approx \mathbb{V}\left[\mathbf{x}[j]\right]$$

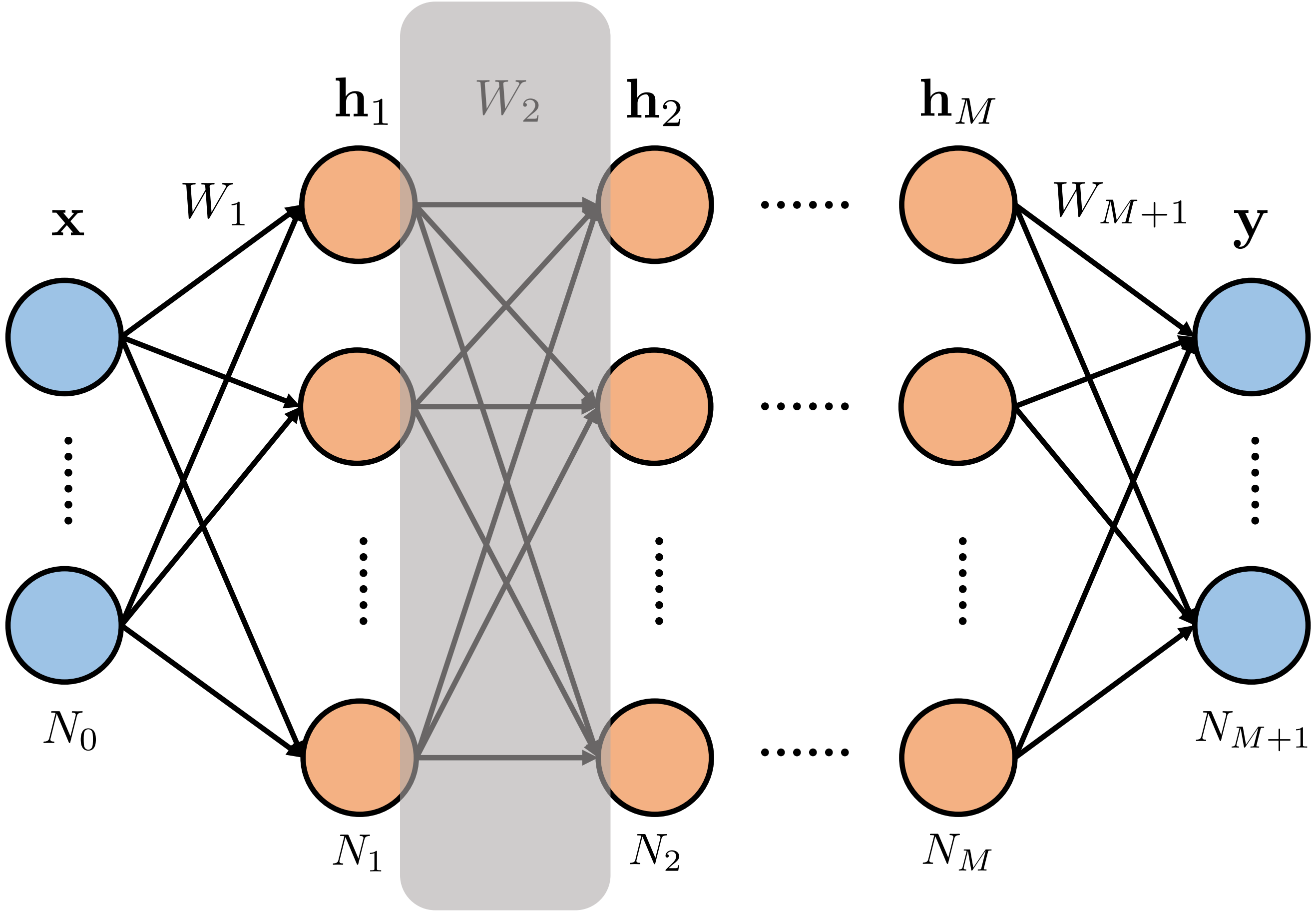
we can simply set:

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

Initialization: Backward Analysis

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

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



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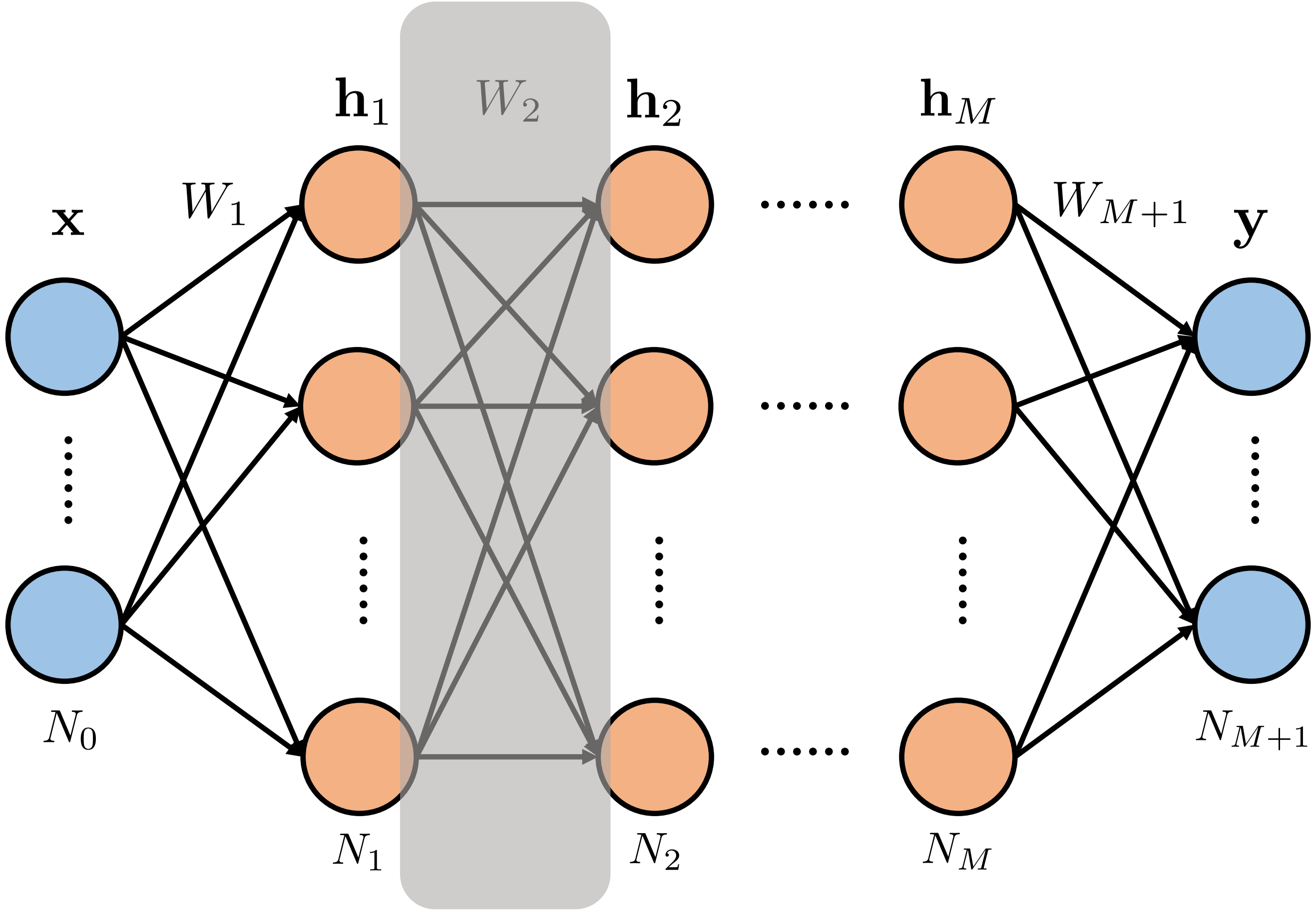
Let us look at the gradient w.r.t. activations

$$\frac{\partial L}{\partial \mathbf{h}_1[j]} = \sum_{i=1}^{N_2} \frac{\partial L}{\partial \mathbf{h}_2[i]} \frac{\partial \mathbf{h}_2[i]}{\partial \mathbf{h}_1[j]} \approx \sum_{i=1}^{N_2} \frac{\partial L}{\partial \mathbf{h}_2[i]} W_2[i,j]$$



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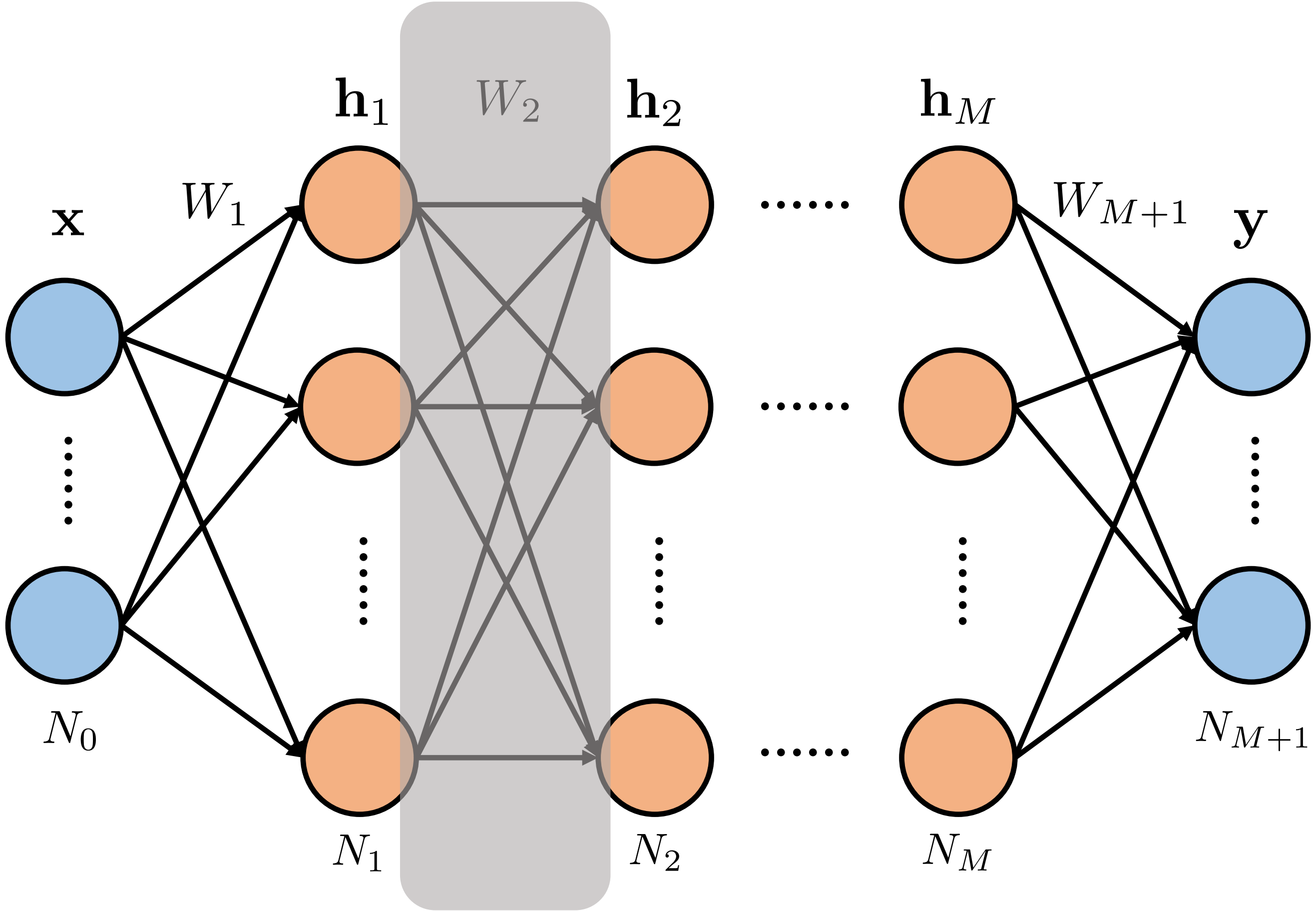

$$\mathbf{h}_2[i] = \sigma\left(\sum_j^{N_1} W_2[i,j]\mathbf{h}_1[j]\right) \approx \sum_{j=1}^{N_1} W_2[i,j]\mathbf{h}_1[j]$$

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

$$\begin{aligned}
\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] \\
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&= \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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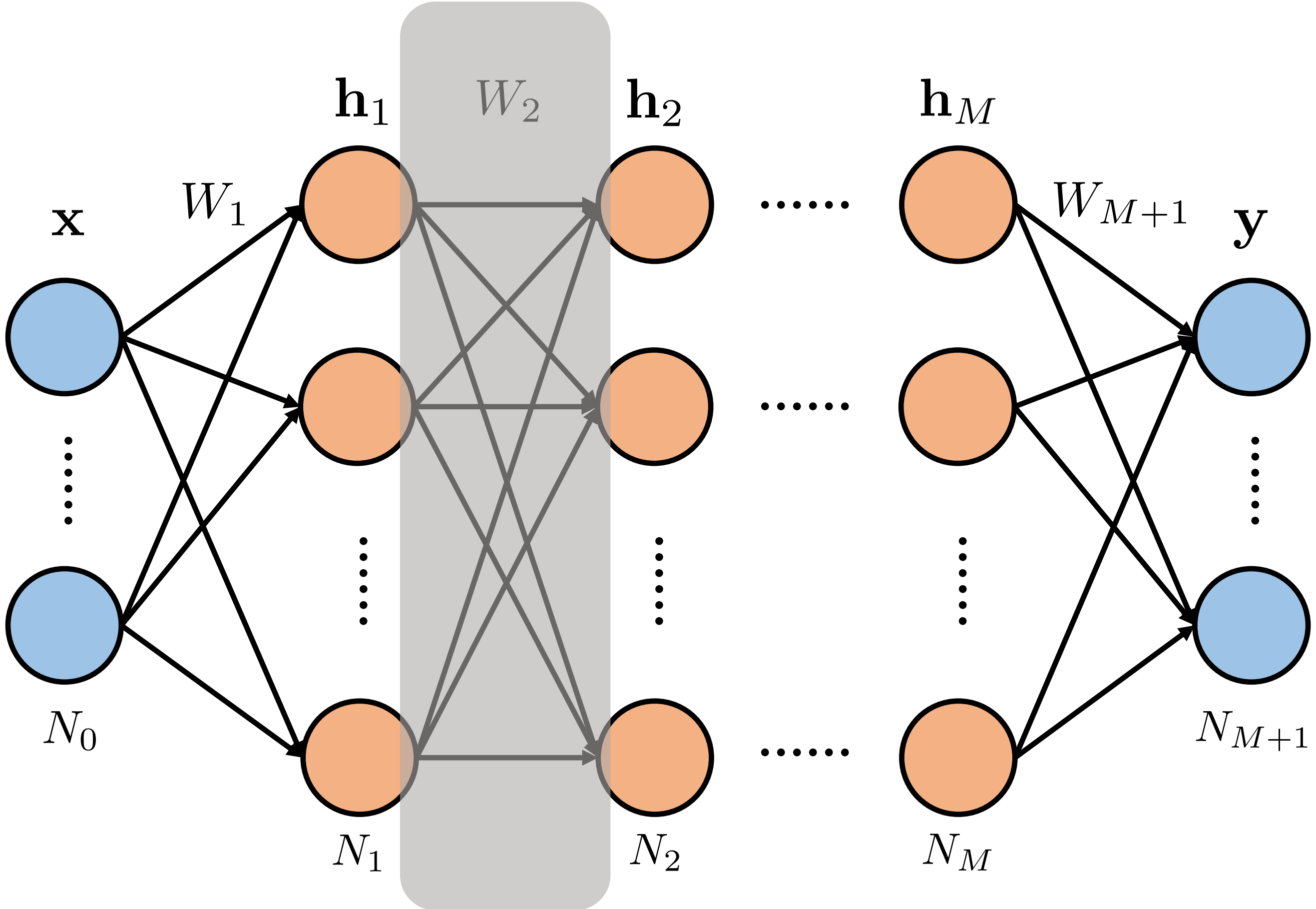

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\end{aligned}$$

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

variance of gradients w.r.t. activations!

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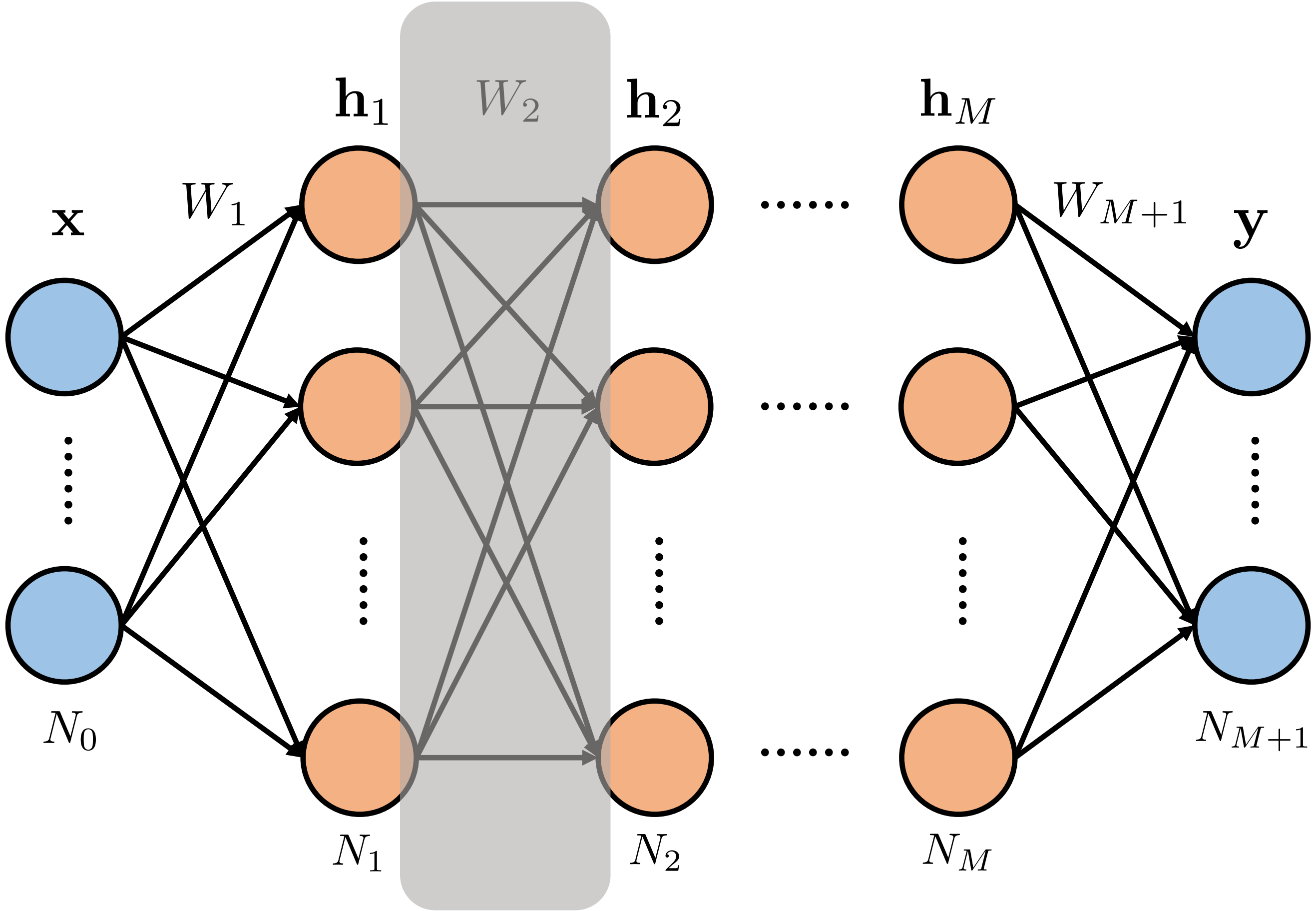
What about the gradients w.r.t. weights?



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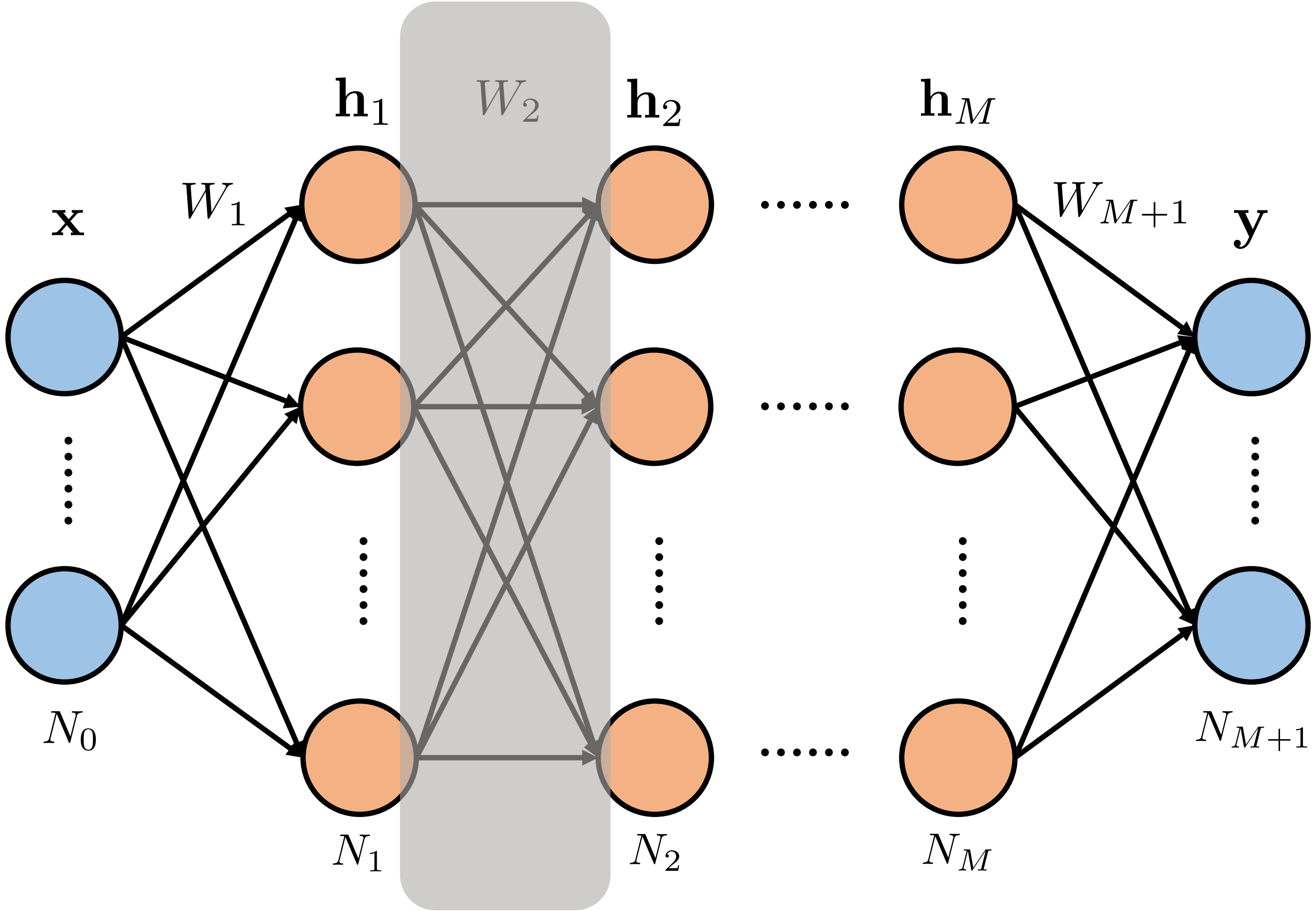

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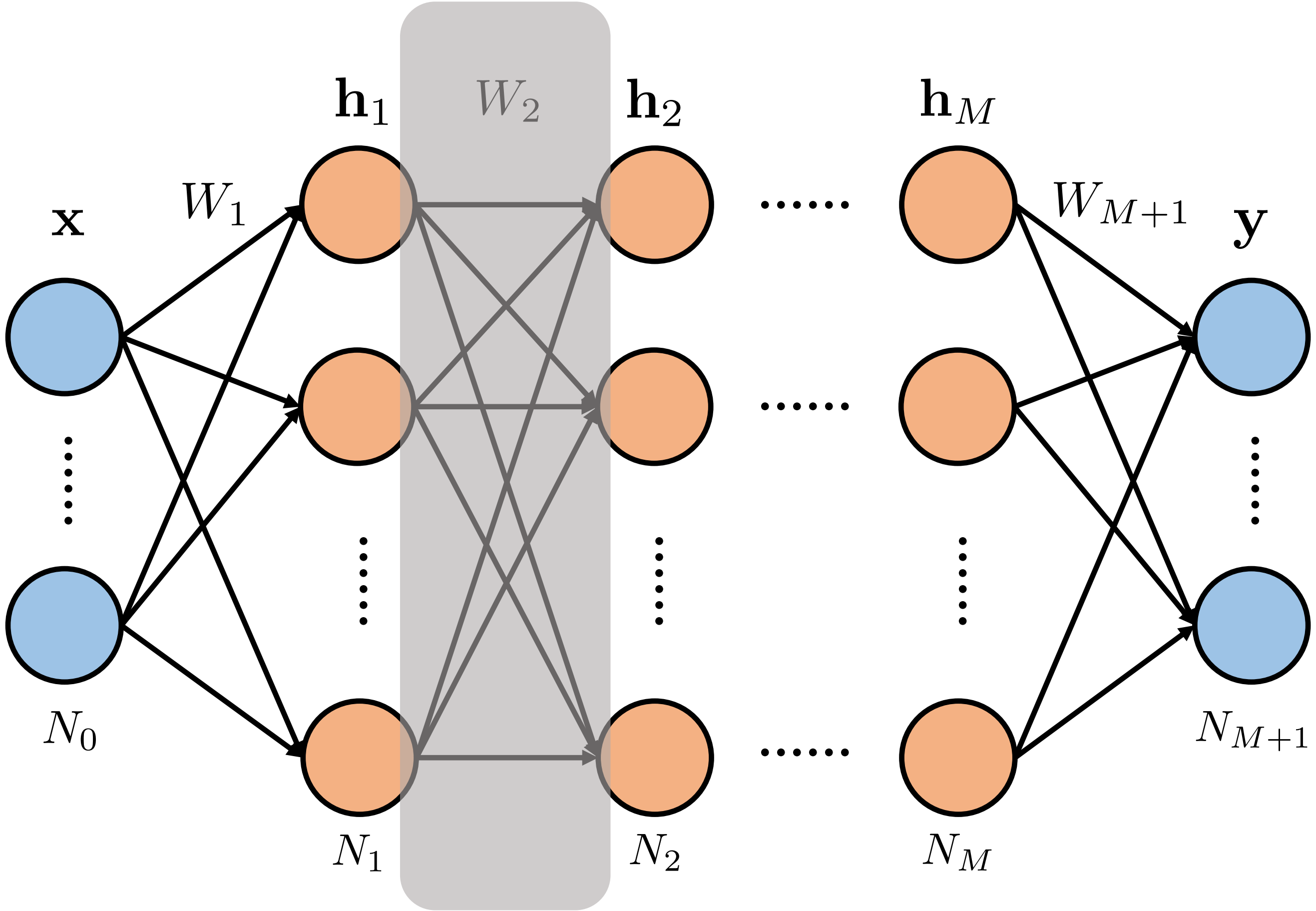

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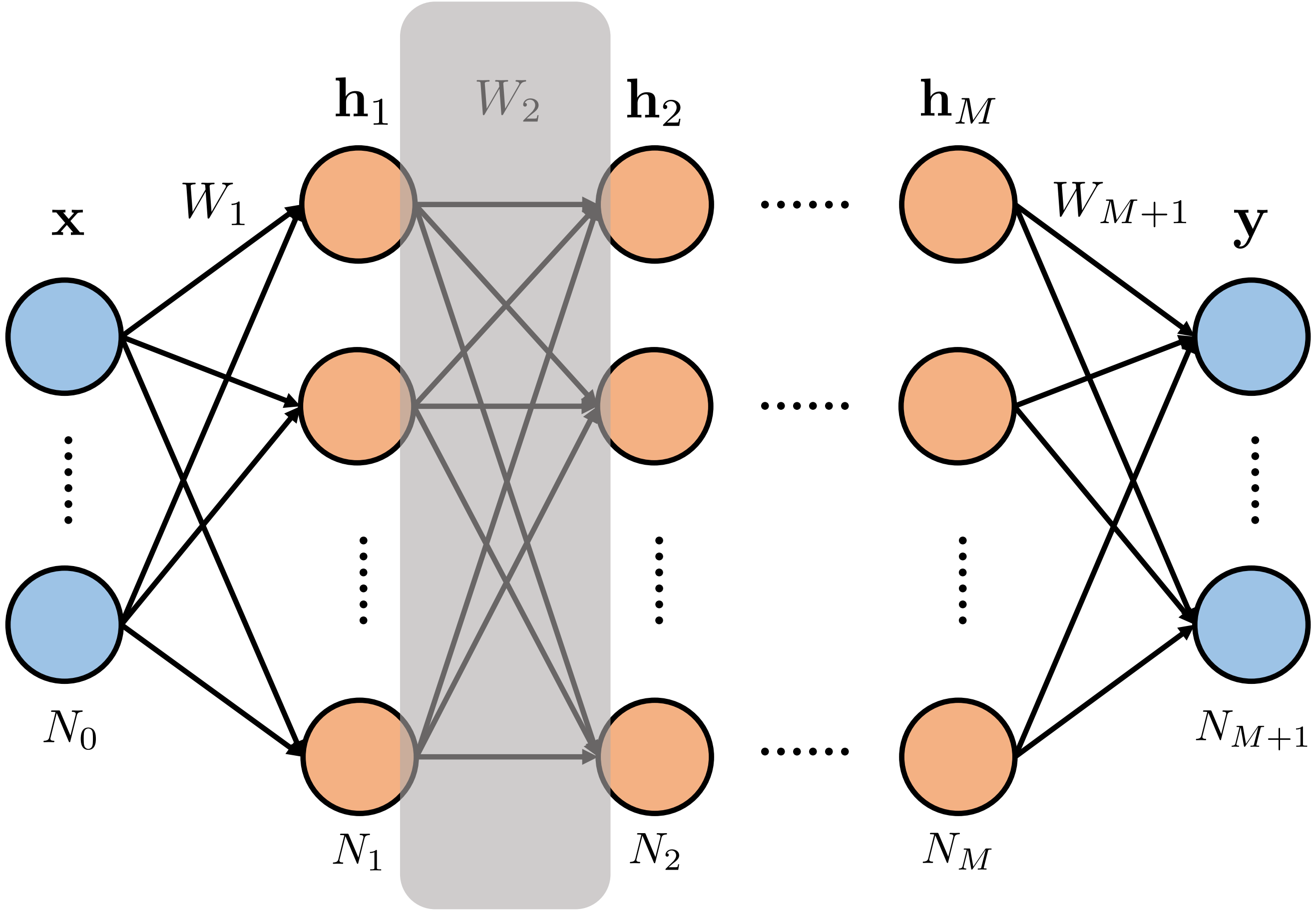
$$\frac{\partial L}{\partial W_2[i,j]} = \frac{\partial L}{\partial \mathbf{h}_2[i]} \frac{\partial \mathbf{h}_2[i]}{\partial W_2[i,j]} \approx \frac{\partial L}{\partial \mathbf{h}_2[i]} \mathbf{h}_1[j]$$

$$\begin{aligned}
\mathbb{V}\left[\frac{\partial L}{\partial W_2[i,j]}\right] &\approx \mathbb{V}\left[\frac{\partial L}{\partial \mathbf{h}_2[i]}\right] \mathbb{V}\left[\mathbf{h}_1[j]\right] \\
&= \left(\mathbb{V}\left[\frac{\partial L}{\partial \mathbf{y}[i]}\right] \prod_{k=3}^{M+1} N_k \mathbb{V}\left[W_k[i,j]\right]\right) \\
&\quad \left(\mathbb{V}\left[\mathbf{x}[j]\right] \prod_{k=1}^{1} N_{k-1} \mathbb{V}\left[W_k[i,j]\right]\right) \\
&= \frac{N_0}{N_1} \left(\prod_{k=1}^{1} N_k \mathbb{V}\left[W_k[i,j]\right]\right) \left(\prod_{k=3}^{M+1} N_k \mathbb{V}\left[W_k[i,j]\right]\right) \mathbb{V}\left[\frac{\partial L}{\partial \mathbf{y}[i]}\right] \mathbb{V}\left[\mathbf{x}[j]\right] \\
&= \frac{N_0}{N_1} \mathbb{V}\left[\frac{\partial L}{\partial \mathbf{y}[i]}\right] \mathbb{V}\left[\mathbf{x}[j]\right]
\end{aligned}$$

Initialization: Backward Analysis

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

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



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

$$\frac{\partial L}{\partial \mathbf{h}_1[j]} = \sum_{i=1}^{N_2} \frac{\partial L}{\partial \mathbf{h}_2[i]} \frac{\partial \mathbf{h}_2[i]}{\partial \mathbf{h}_1[j]} \approx \sum_{i=1}^{N_2} \frac{\partial L}{\partial \mathbf{h}_2[i]} W_2[i,j]$$

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

$$\frac{\partial L}{\partial W_2[i,j]} = \frac{\partial L}{\partial \mathbf{h}_2[i]} \frac{\partial \mathbf{h}_2[i]}{\partial W_2[i,j]} \approx \frac{\partial L}{\partial \mathbf{h}_2[i]}\mathbf{h}_1[j]$$

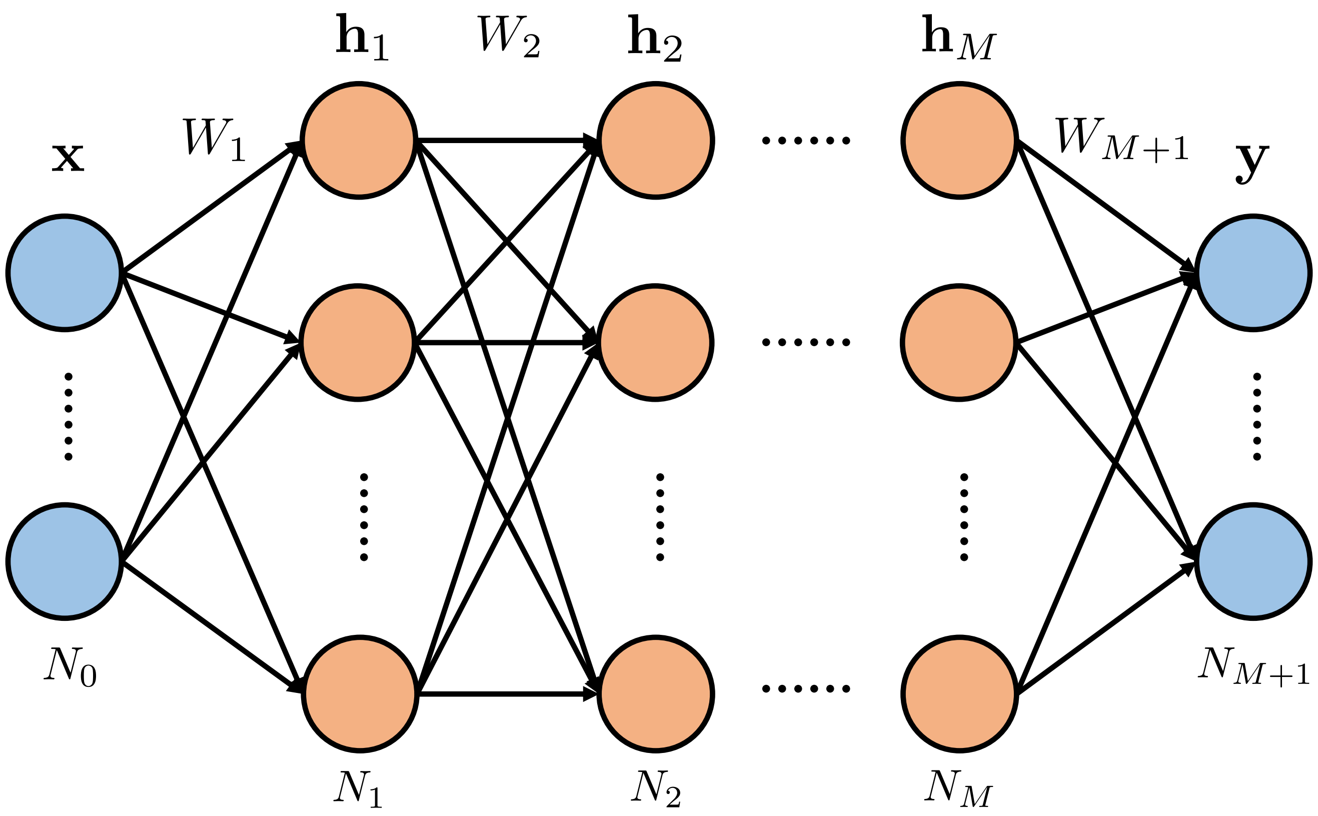
$$\begin{aligned}
\mathbb{V}\left[\frac{\partial L}{\partial W_2[i,j]}\right] &\approx \mathbb{V}\left[\frac{\partial L}{\partial \mathbf{h}_2[i]}\right]\mathbb{V}\left[\mathbf{h}_1[j]\right] \\
&= \left(\mathbb{V}\left[\frac{\partial L}{\partial \mathbf{y}[i]}\right]\prod_{k=3}^{M+1} N_k \mathbb{V}\left[W_k[i,j]\right]\right) \\
&\quad \left(\mathbb{V}\left[\mathbf{x}[j]\right]\prod_{k=1}^{1} N_{k-1} \mathbb{V}\left[W_k[i,j]\right]\right) \\
&= \frac{N_0}{N_1}\left(\prod_{k=1}^{1} N_k \mathbb{V}\left[W_k[i,j]\right]\right)\left(\prod_{k=3}^{M+1} N_k \mathbb{V}\left[W_k[i,j]\right]\right)\mathbb{V}\left[\frac{\partial L}{\partial \mathbf{y}[i]}\right]\mathbb{V}\left[\mathbf{x}[j]\right] \\
&= \frac{N_0}{N_1}\mathbb{V}\left[\frac{\partial L}{\partial \mathbf{y}[i]}\right]\mathbb{V}\left[\mathbf{x}[j]\right]
\end{aligned}$$

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

Initialization

In summary, to preserve the variance of activations, we set $\mathbb{V}\left[W_k[i,j]\right] = \dfrac{1}{N_{k-1}}$

to preserve the variance of gradients w.r.t. activations, we set $\mathbb{V}\left[W_k[i,j]\right] = \dfrac{1}{N_k}$



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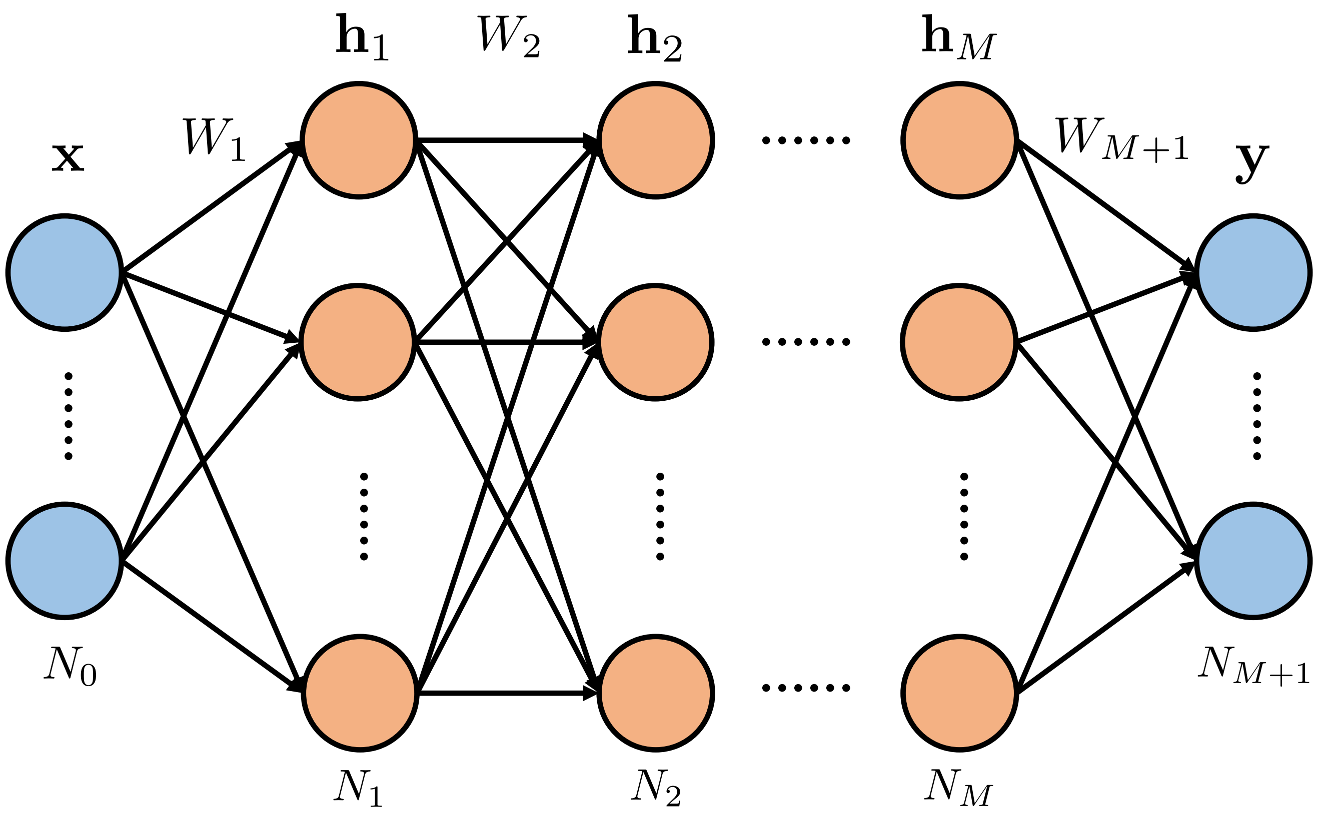

To compromise between two goals, we can take the mean of the denominators:

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

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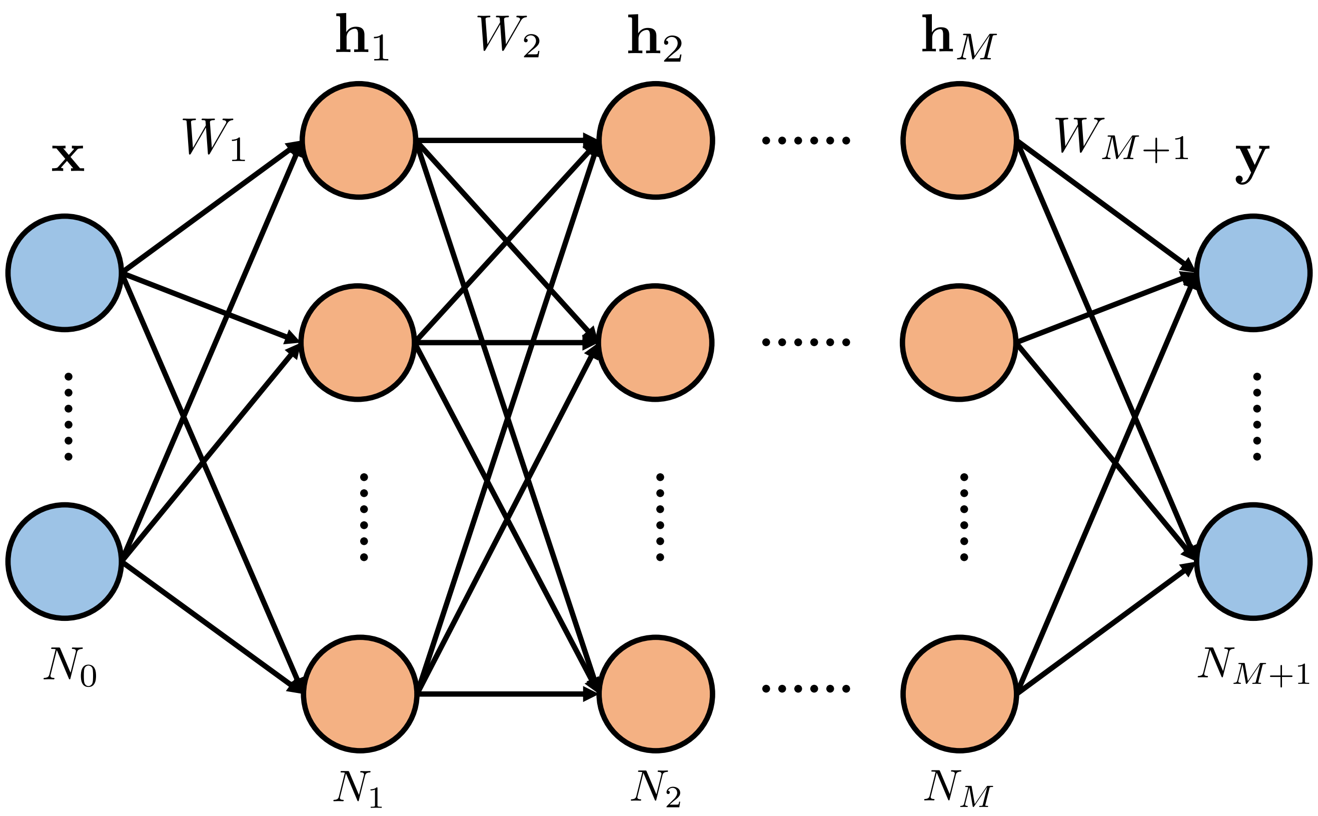

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This is the so-called “Xavier Initialization” [3]!

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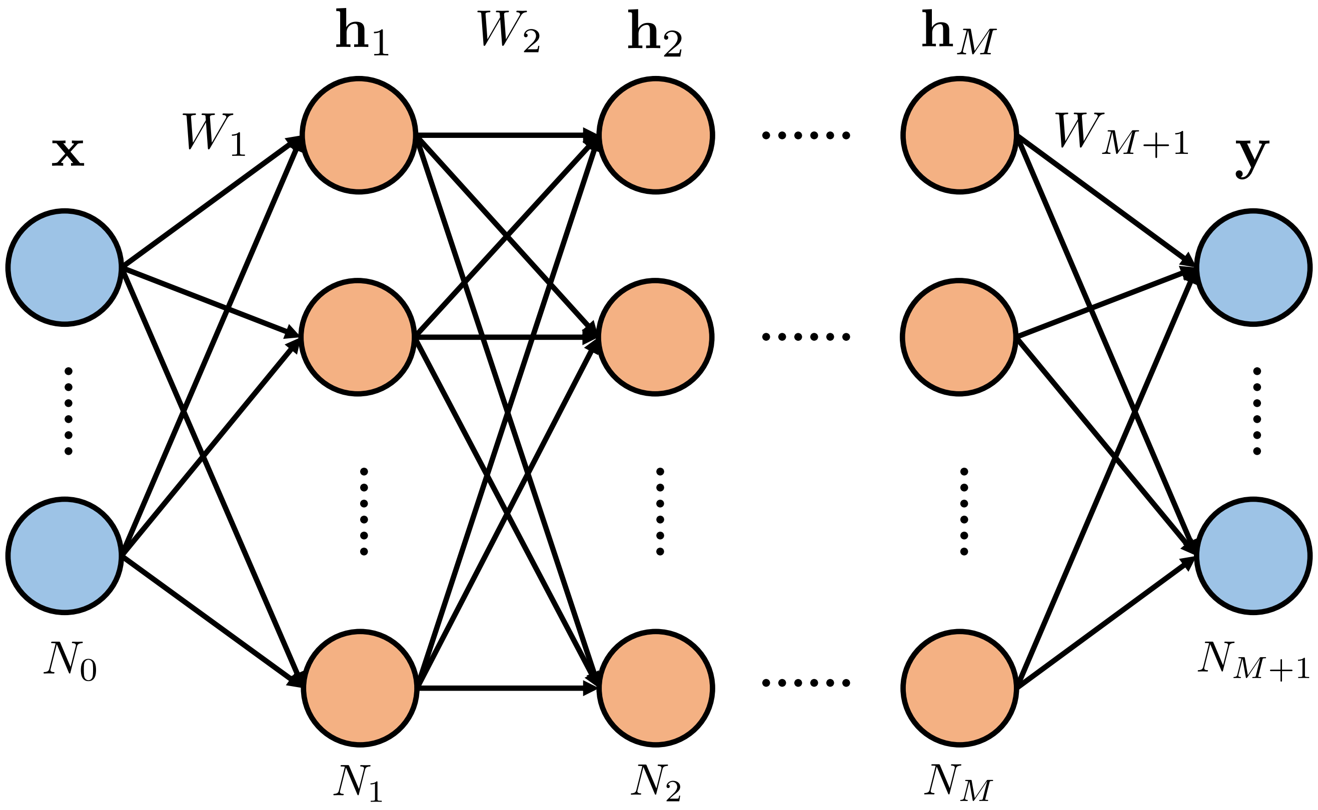

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By considering the effect of ReLU, we can similarly derive "Kaiming Initialization" [4]!

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?