Foundations of Machine Learning (ECE 5984)

- Neural Networks -

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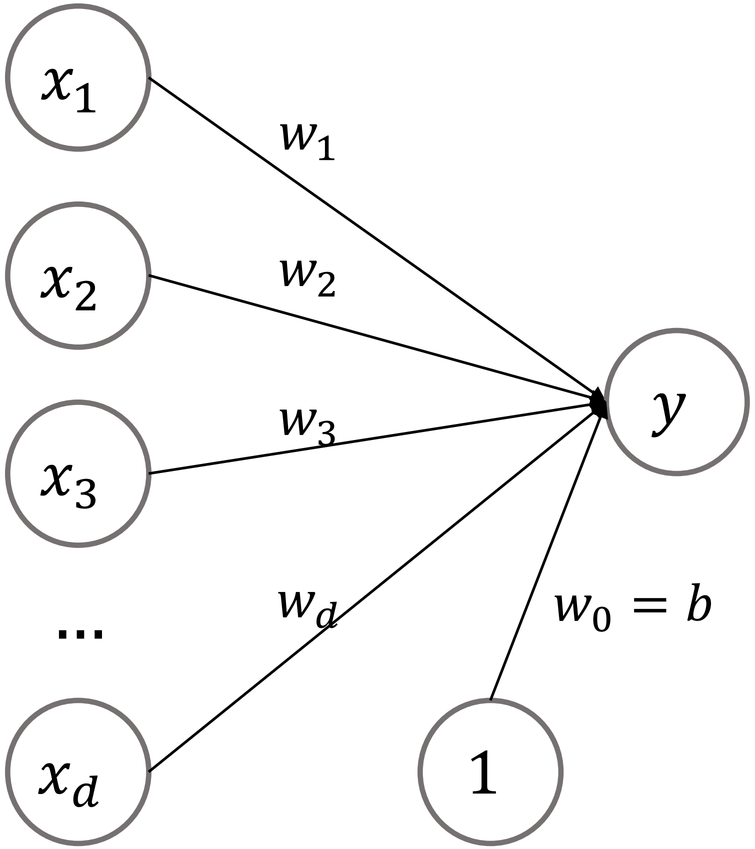
Multi-Layer Perceptron

Linear Models as Shallow Neural Networks

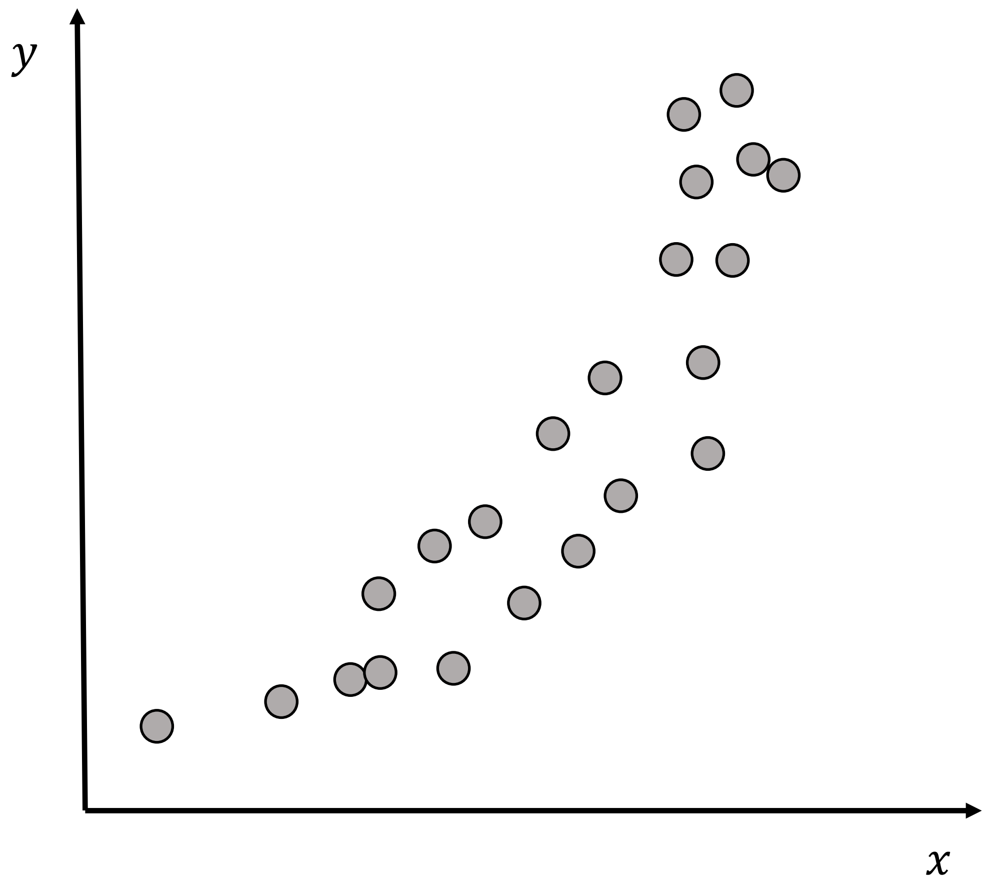
- It is a single layer neural network

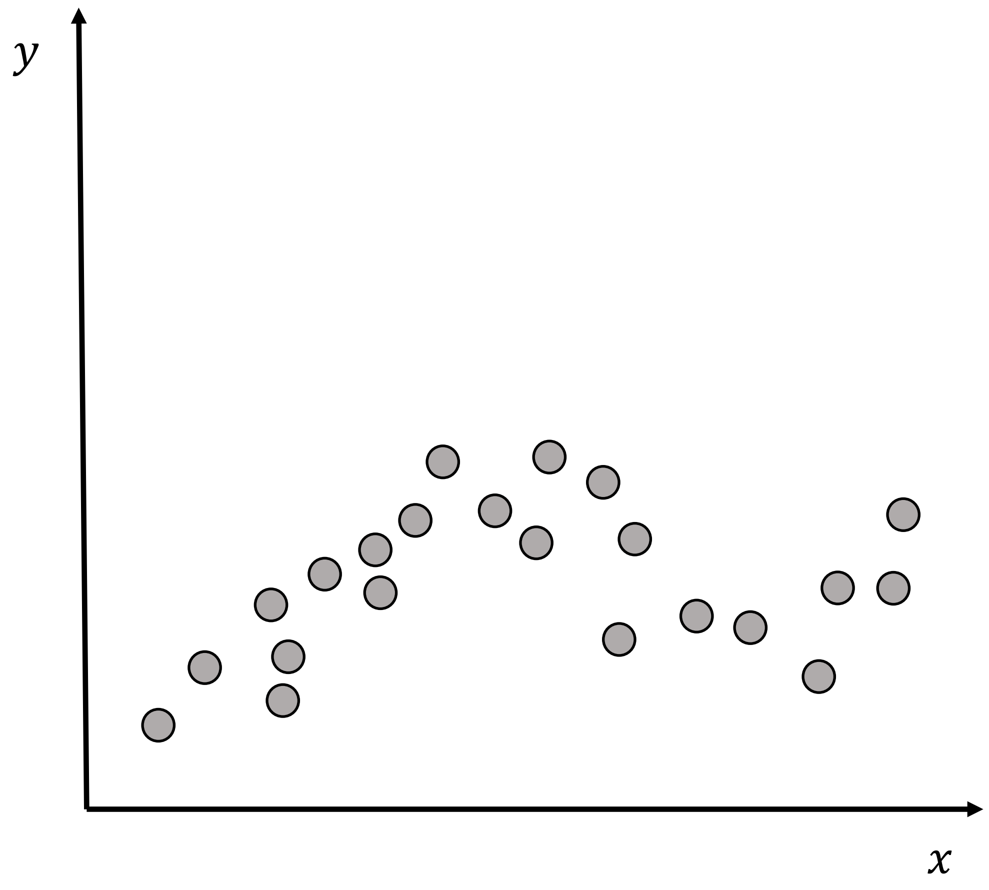


$$y = w^\top x$$

Linear Models

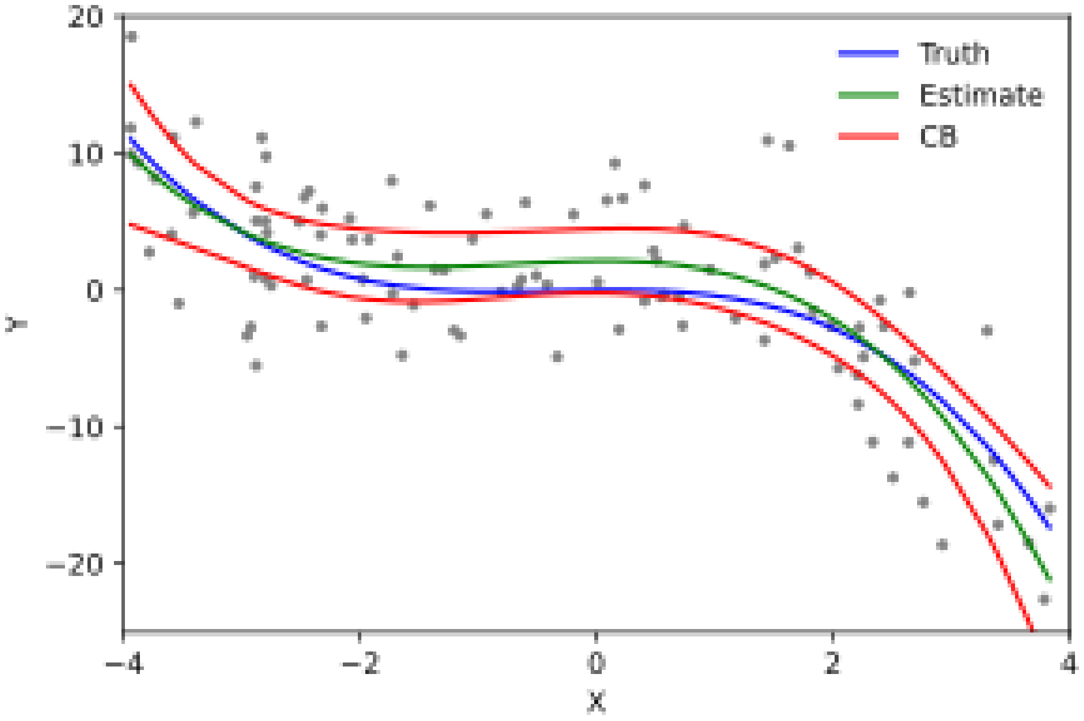
- Is linear model a good for all?





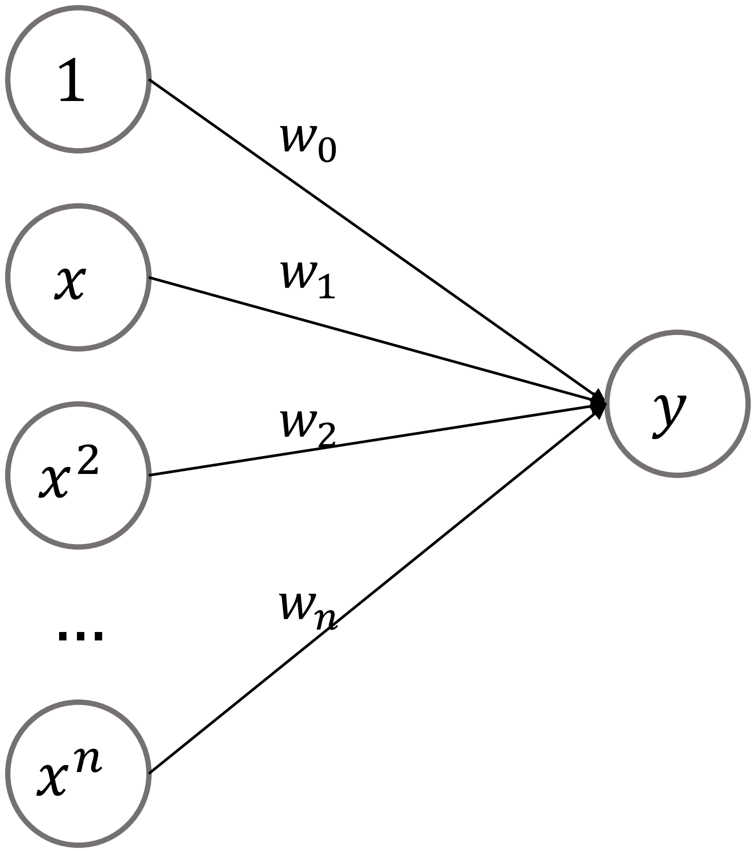
Nonlinear Models

- nth-degree Polynomial regression



$$f(x) = w_0 + w_1 x + w_2 x^2 + w_3 x^3 + \cdots + w_n x^n$$

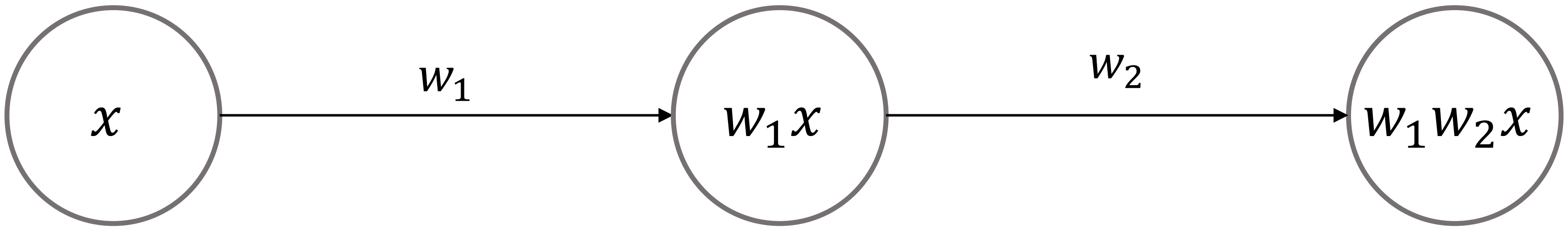
Polynomals as Neural Network



$$f(x) = w_0 + w_1 x + w_2 x^2 + w_3 x^3 + \cdots + w_n x^n$$

- Feature engineering is hard
- Can we make it non-linear w/o feature engineering?

Feed-Forward Neural Network

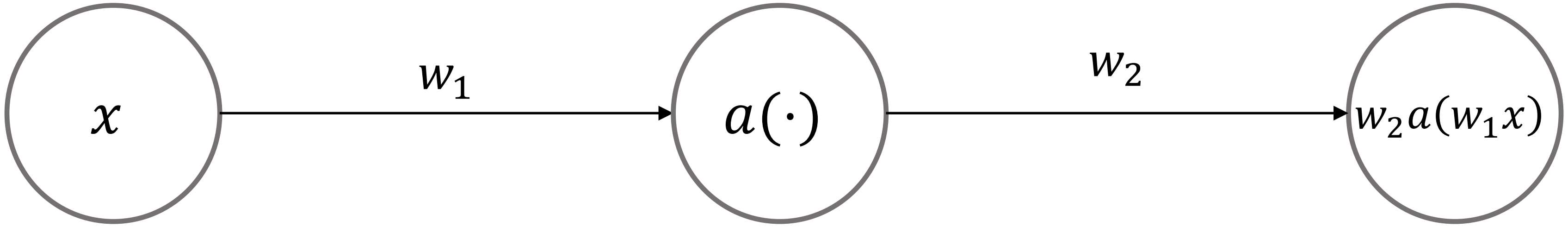


$$f(x) = w_1 w_2 x$$

Is it non-linear in x?

Feed-Forward Neural Network

- Using non-linear activation function



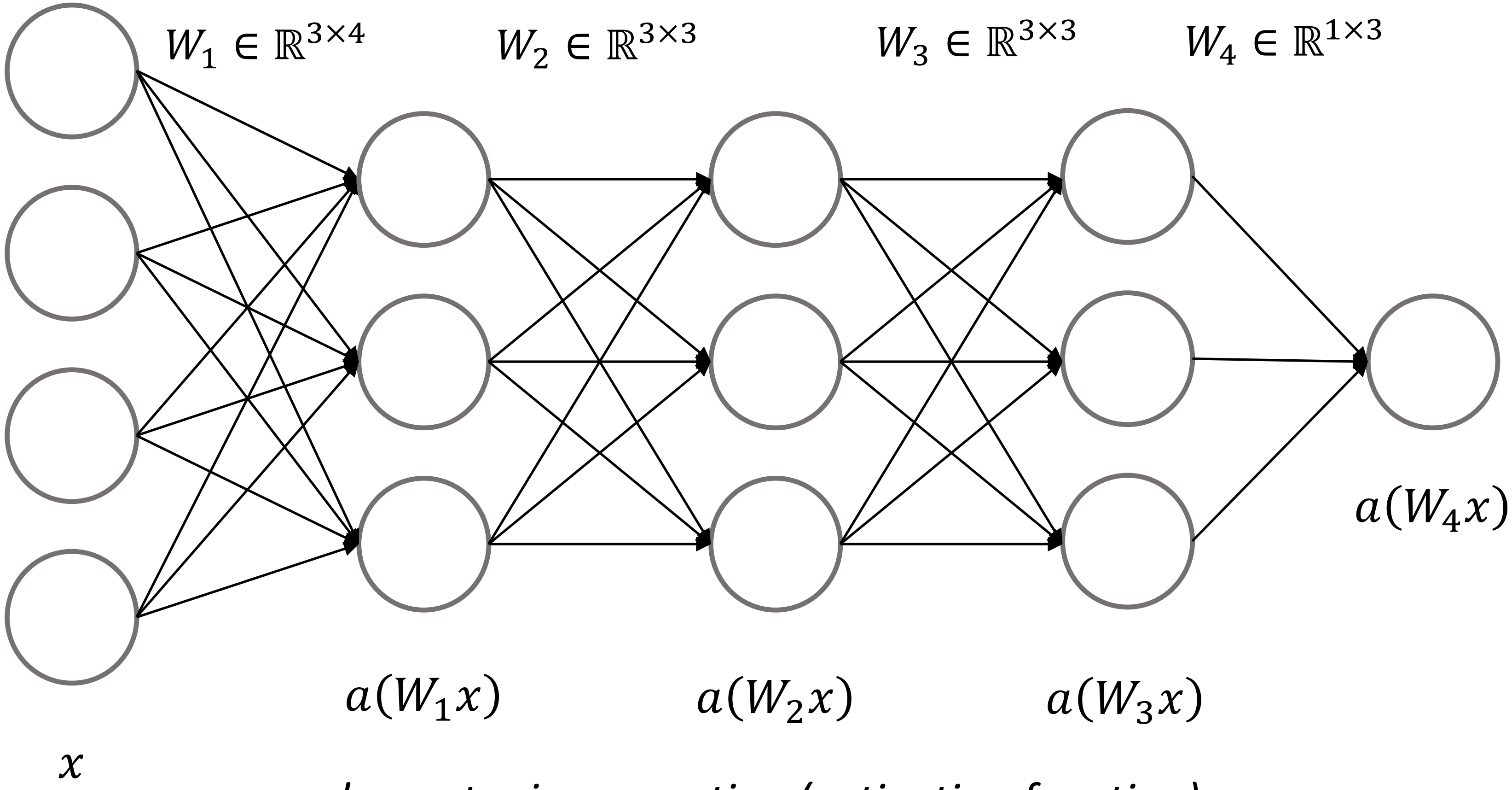
$$f(x) = w_2 a(w_1 x)$$

$$a(x) = \max(0, x)$$ (Rectifier Linear Unit)

$$a(x) = \frac{1}{1 + e^{-x}}$$ (Sigmoid)

Feed-Forward Neural Network

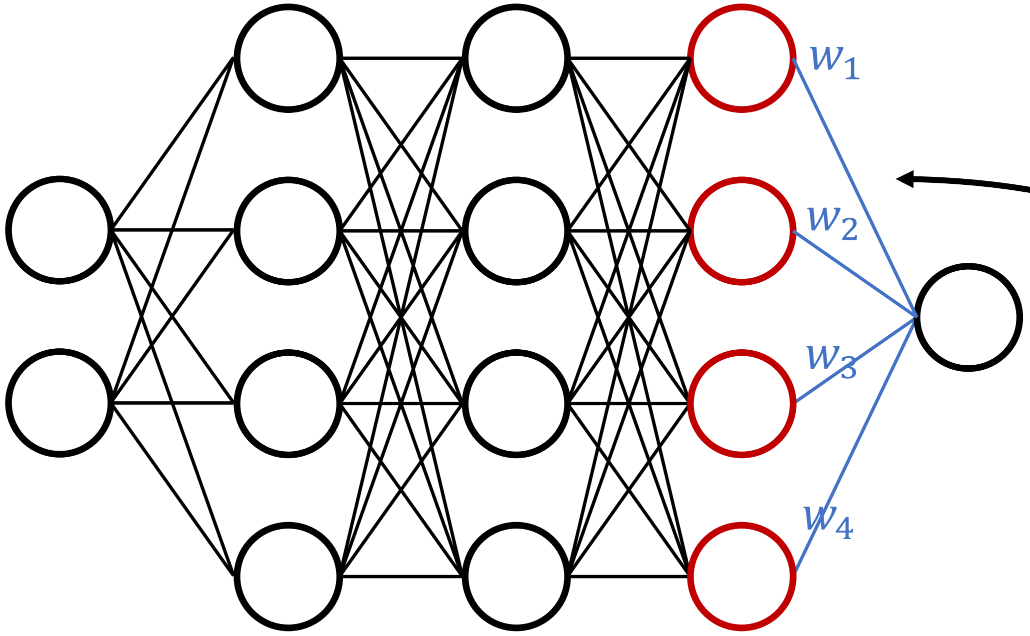
- AKA, Multi-Layer Perceptron



a: element-wise operation (activation function)

Feed-Forward Neural Network

- Connection to the Kernel Method

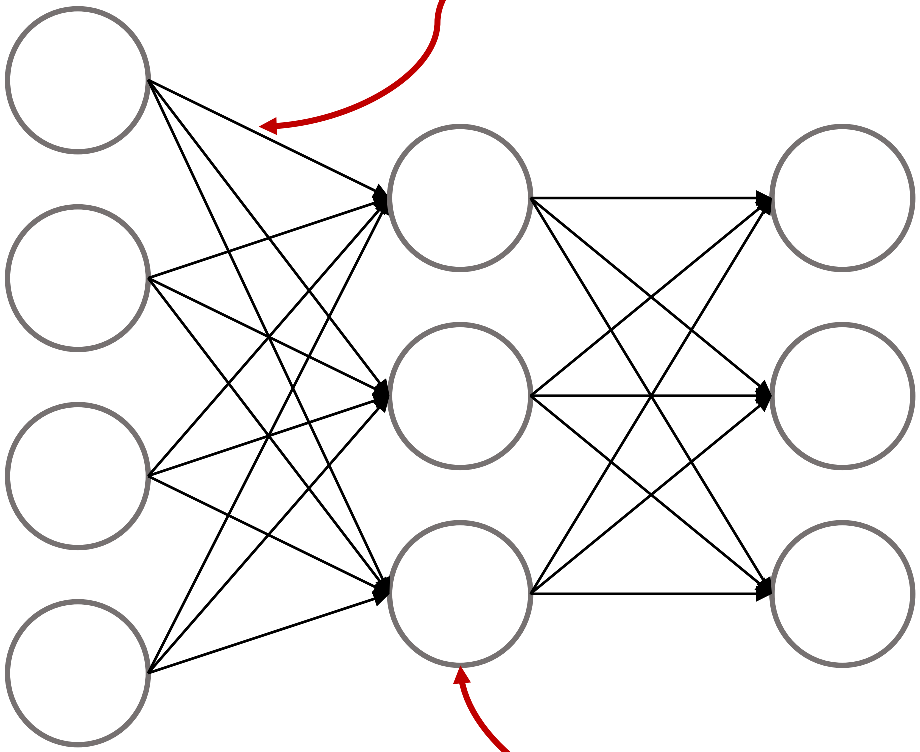


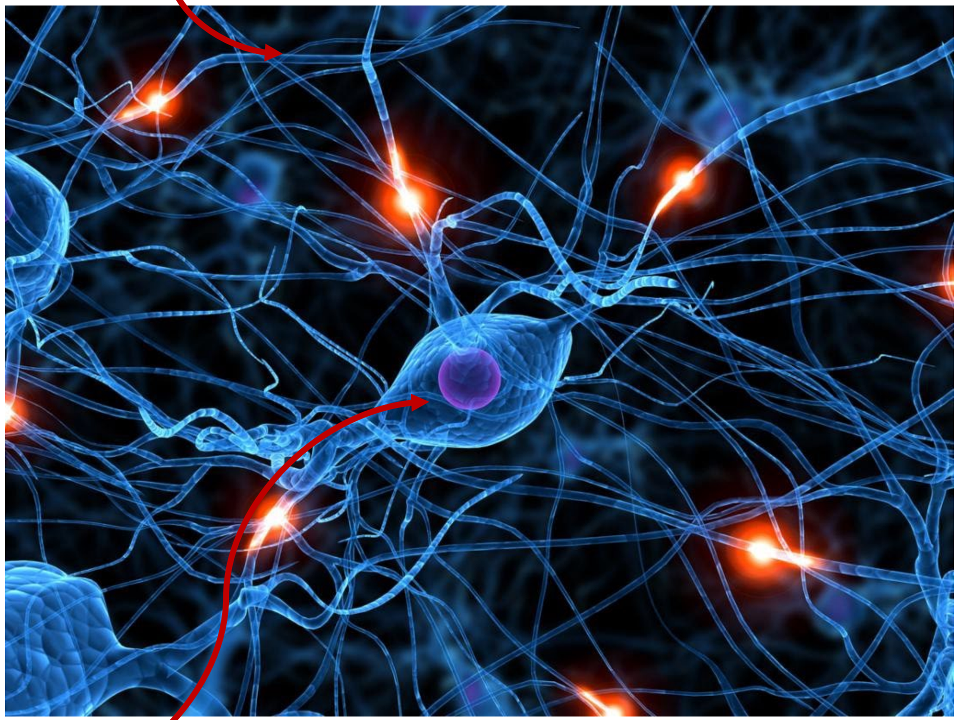
$$\sum_{j=1}^{d} w_j \phi_j(x)$$

Feed-Forward Neural Network

- Biology Inspired

Weights ≈ Synapses

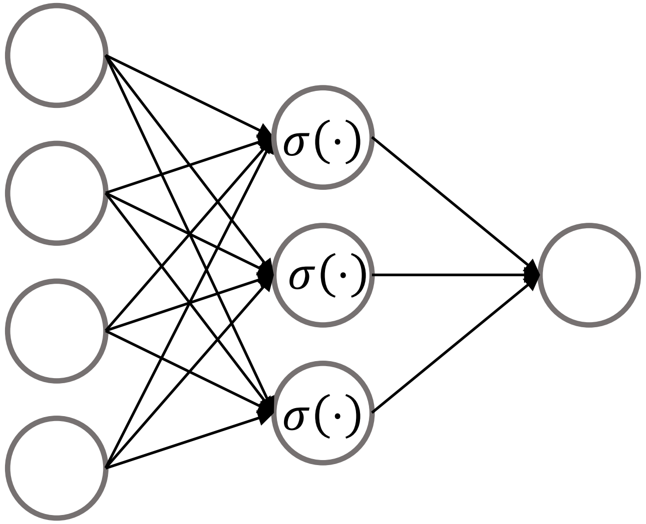




Units ≈ Neurons

Feed-Forward Neural Network

- Regression with two layers MLP



$D = \{(x^{(1)}, y^{(1)}), \dots, (x^{(N)}, y^{(N)})\}$

$x^{(i)} \in \mathbb{R}^d, y^{(i)} \in \mathbb{R}, X \in \mathbb{R}^{N \times d}, Y \in \mathbb{R}^N$

$\theta = \{W_1, W_2\}, W_1 \in \mathbb{R}^{h \times d}, W_2 \in \mathbb{R}^{1 \times h}$

$f_\theta(x) = W_2 \sigma(W_1 x)$

$f_\theta: \mathbb{R}^d \to \mathbb{R}$

$$L(\theta) = \frac{1}{2} \sum_{i=1}^{N} \left(y^{(i)} - f_\theta(x^{(i)})\right)^2 = \frac{1}{2} (Y - \sigma(W_1 X^\top)^\top W_2^\top)^\top (Y - \sigma(W_1 X^\top)^\top W_2^\top)$$

Feed-Forward Neural Network

- Regression with two layers MLP

$$D = \{(x^{(1)}, y^{(1)}), \dots, (x^{(N)}, y^{(N)})\}$$

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$$f_\theta : \mathbb{R}^d \to \mathbb{R}$$

1. Can you take the gradients w.r.t θ?
2. Does it have a closed form solution?
3. Is it a convex function?

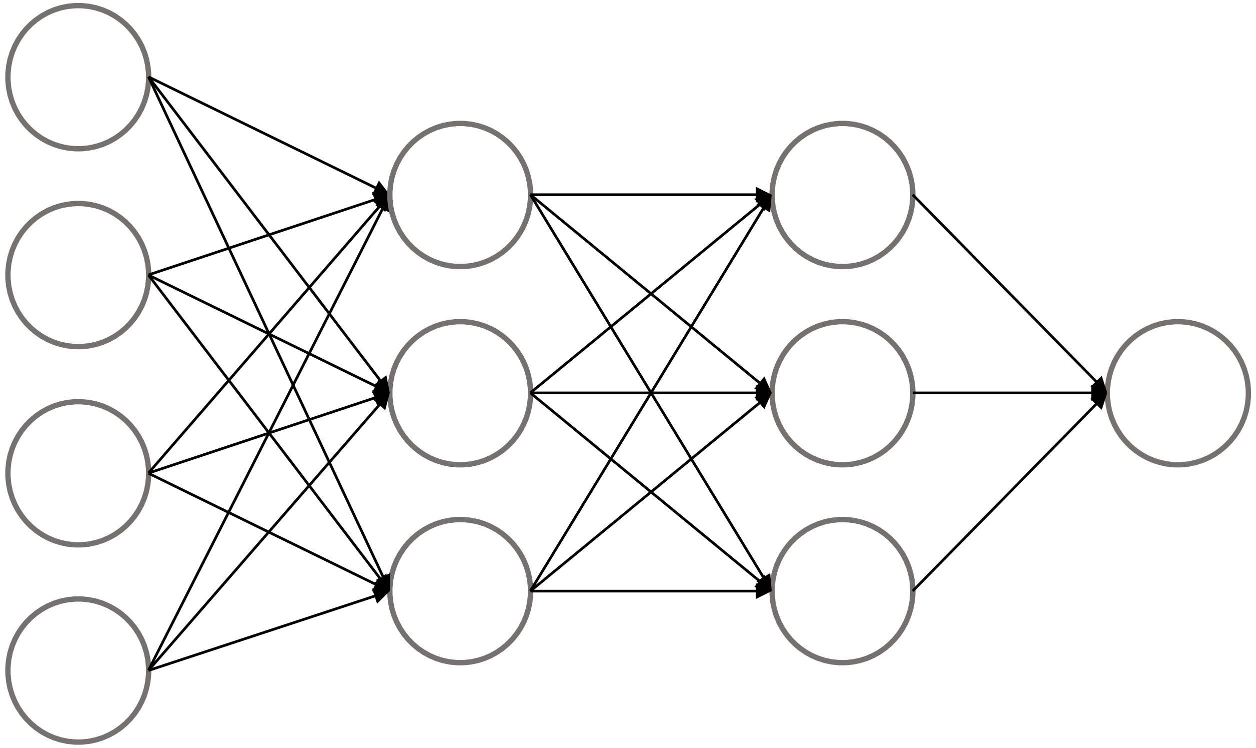
$$L(\theta) = \frac{1}{2}\sum_{i=1}^{N}\left(y^{(i)} - f_\theta(x^{(i)})\right)^2 = \frac{1}{2}(Y - \sigma(W_1 X^\top)^\top W_2^\top)^\top (Y - \sigma(W_1 X^\top)^\top W_2^\top)$$

Gradient Descent

- We are using *gradient descent* for training deep neural networks

$$W := W - \alpha \left(\frac{\partial L}{\partial W} \right)$$

(descent) (step-size) (gradient)



The Universal Approximator

The Universal Approximation Theorem

- A single hidden layer neural network can approximate any continuous function arbitrarily well, given enough hidden units.
- This holds for many different activation functions, e.g. sigmoid, tanh, ReLU, etc.

Cybenko Theorem

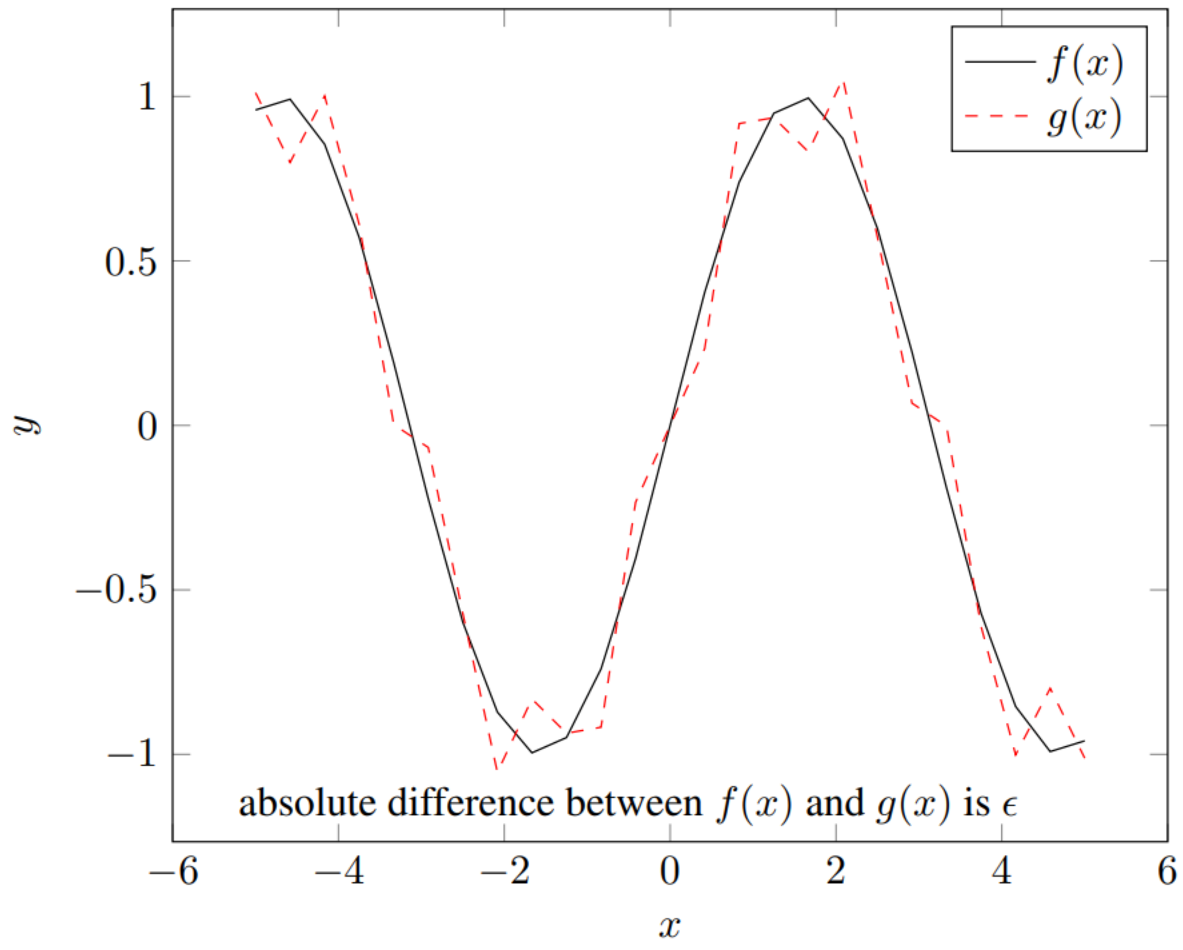
- Cybenko Approximation by Superposition of Sigmoidal Function

Let $C([0,1]^n)$ *denote the set of all continuous function* $[0,1]^n \to \mathbb{R}$, *let* σ *be any sigmoidal activation function then the finite sum of the form* $f(x) = \sum_{i=1}^{N} \alpha_i \, \sigma(w_i^\top x + b_i)$ *is dense in* $C([0,1]^n)$

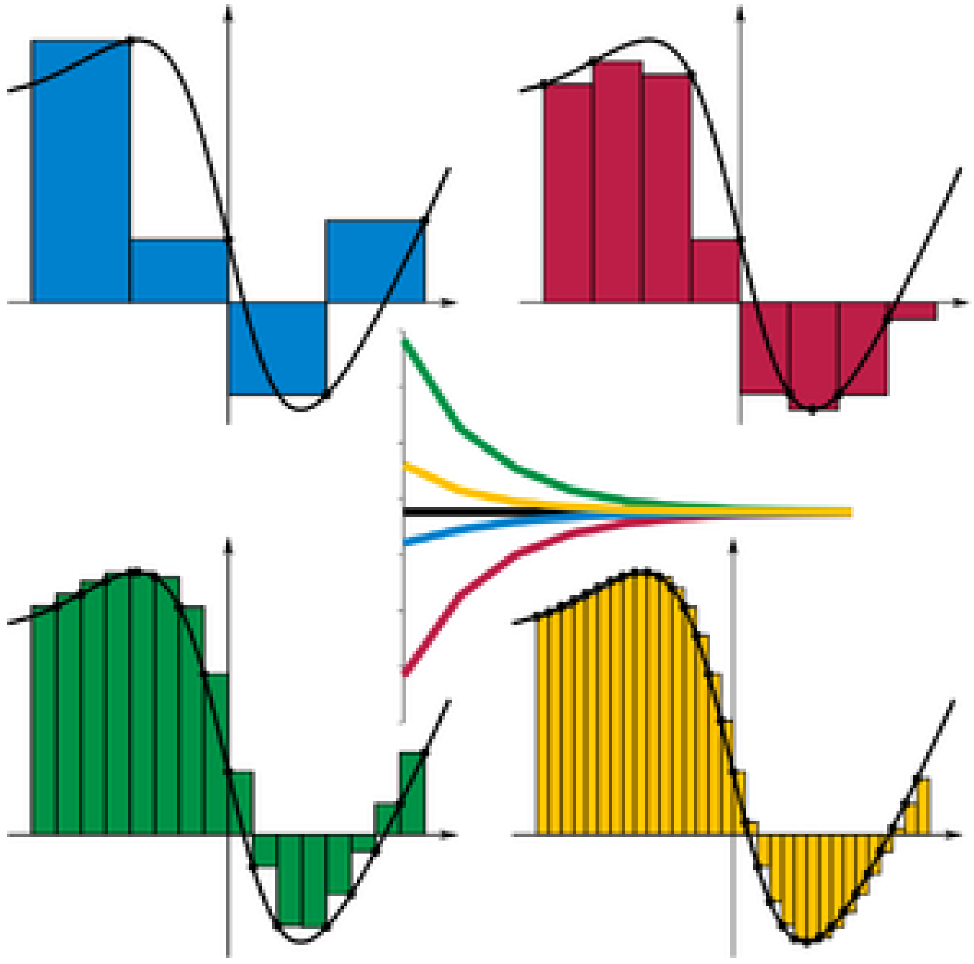
For any $g \subset C([0,1]^n)$ *and any* $\epsilon > 0$, *there exists* $f: x \to \sum_{i=1}^{N} \alpha_i \, \sigma\left(w_i^\top x + b_i\right)$, *such that* $|f(x) - g(x)| < \epsilon$ *for all* $x \subset [0,1]^n$.

Cybenko Theorem

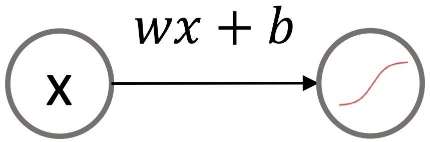
- Cybenko Approximation by Superposition of Sigmoidal Function



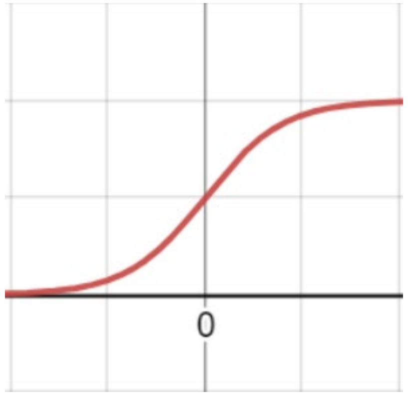
The Universal Approximation Theorem



The Universal Approximation Theorem



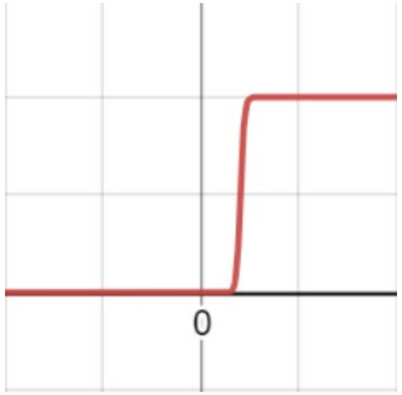
$w = 5, b = 0$



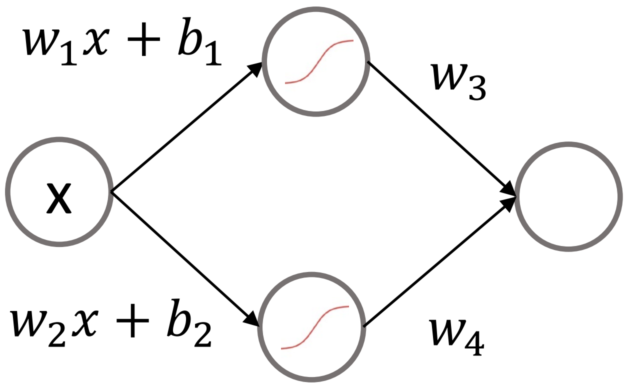
$w = 5, b = 3$

$w = 10, b = -7$

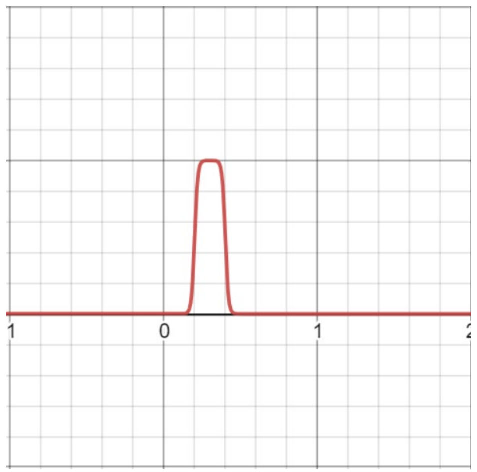
$w = 100, b = -20$



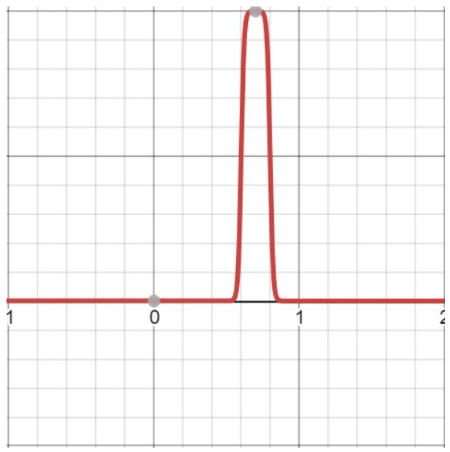
The Universal Approximation Theorem



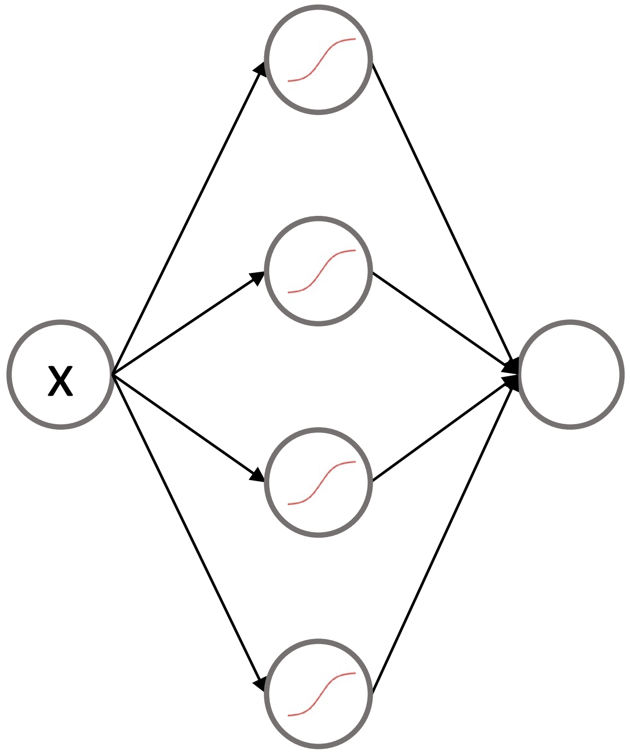
$w_1 = 100, b_1 = -20$
$w_2 = 100, b_2 = -40$
$w_3 = 1, w_4 = -1$

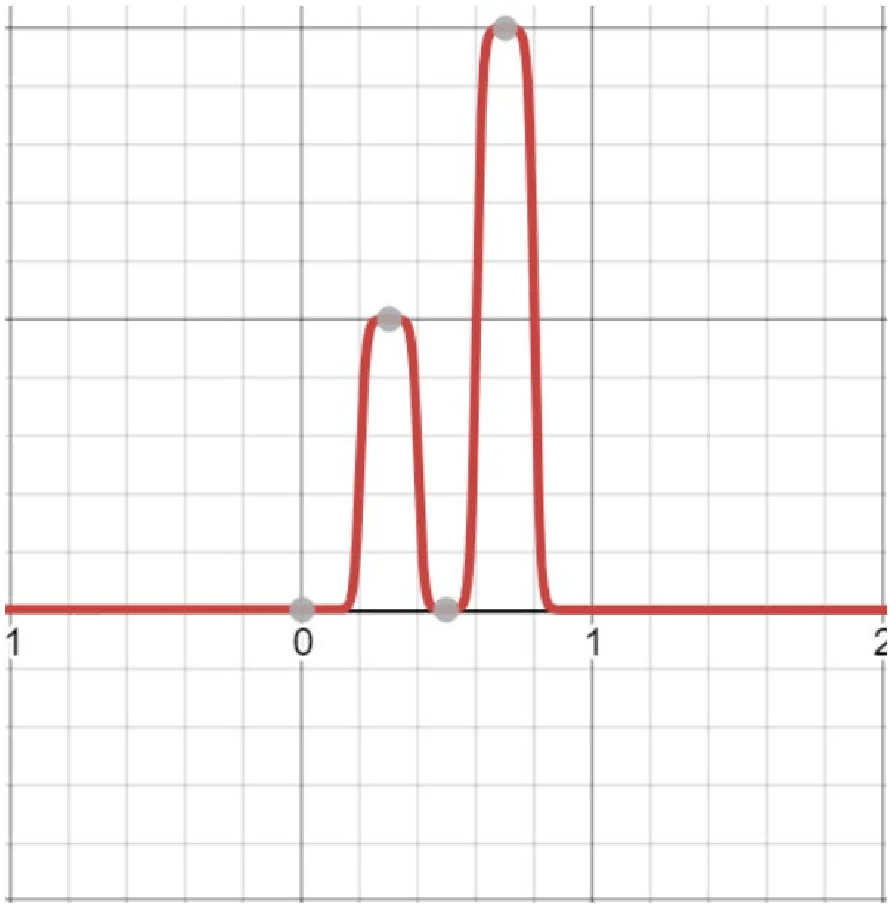


$w_1 = 100, b_1 = -60$
$w_2 = 100, b_2 = -80$
$w_3 = 2, w_4 = -2$

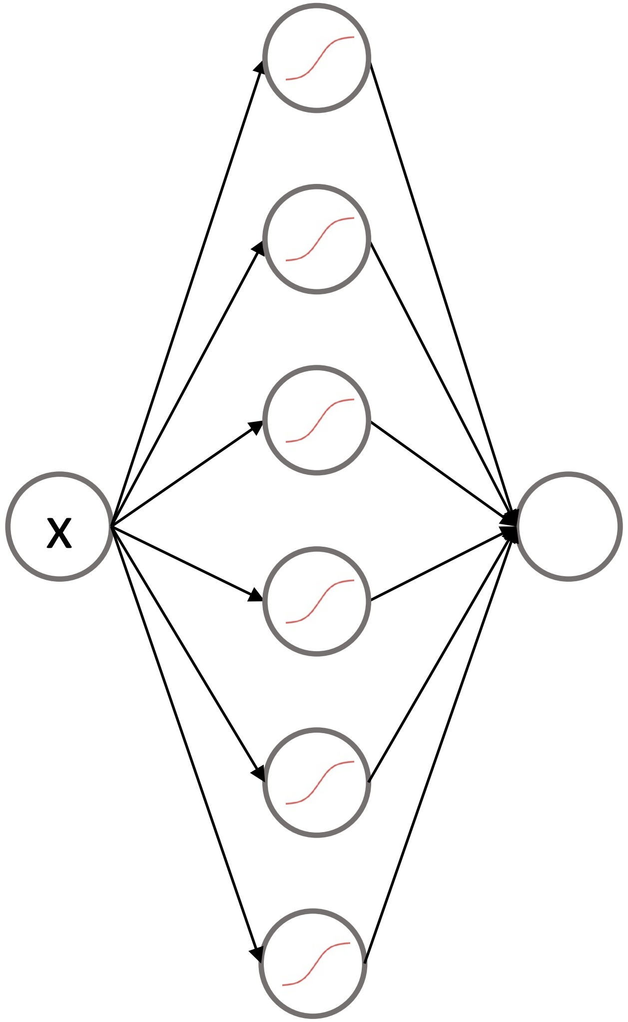


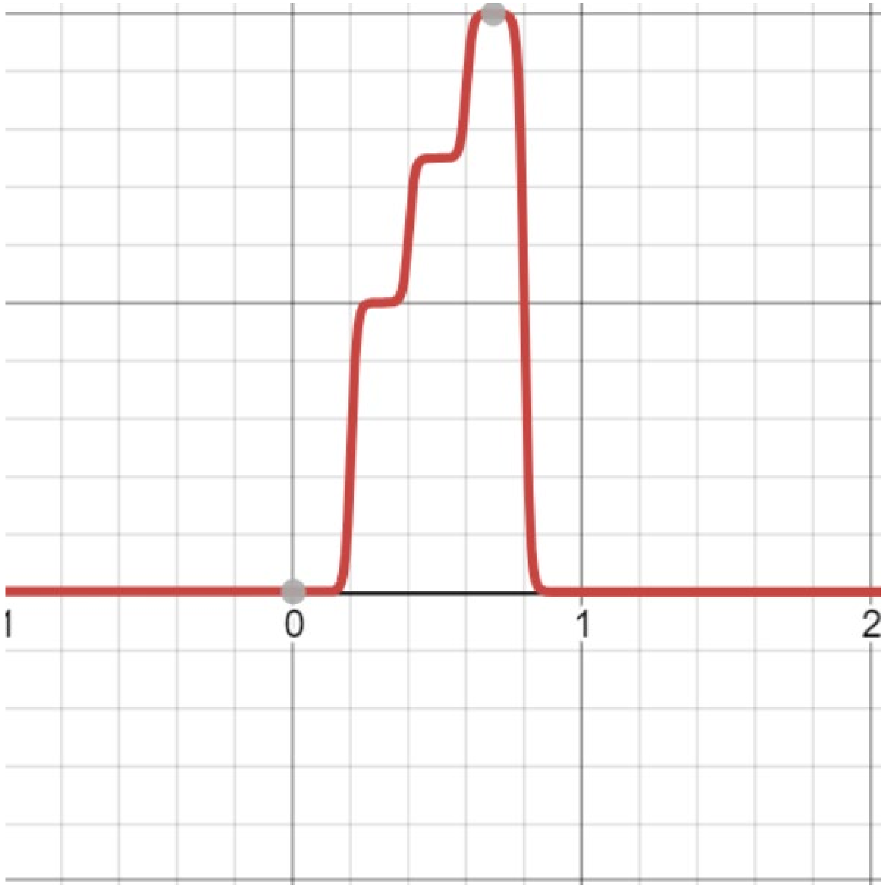
The Universal Approximation Theorem





The Universal Approximation Theorem





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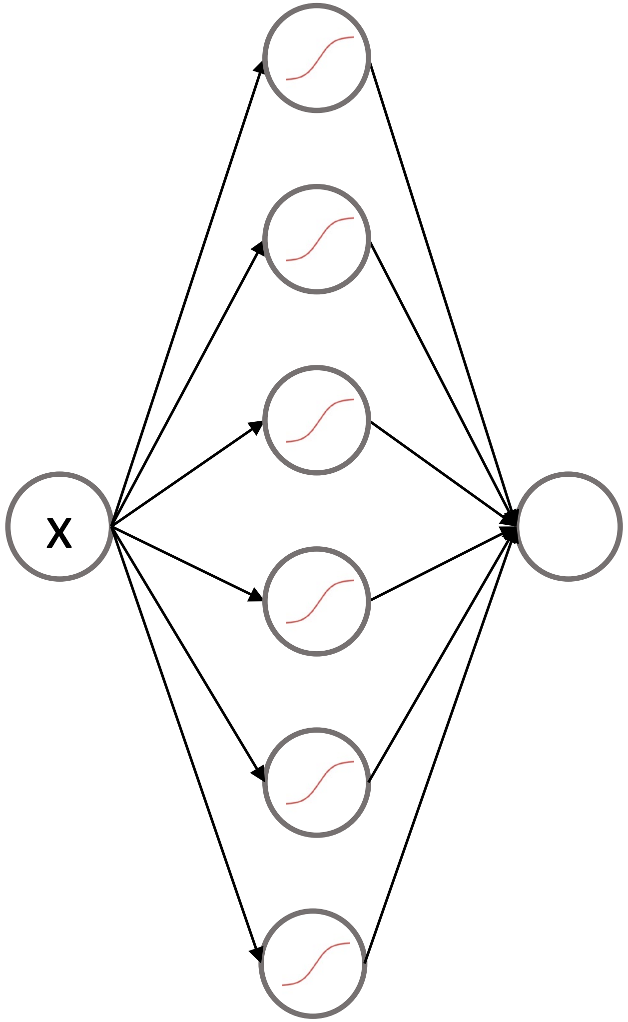
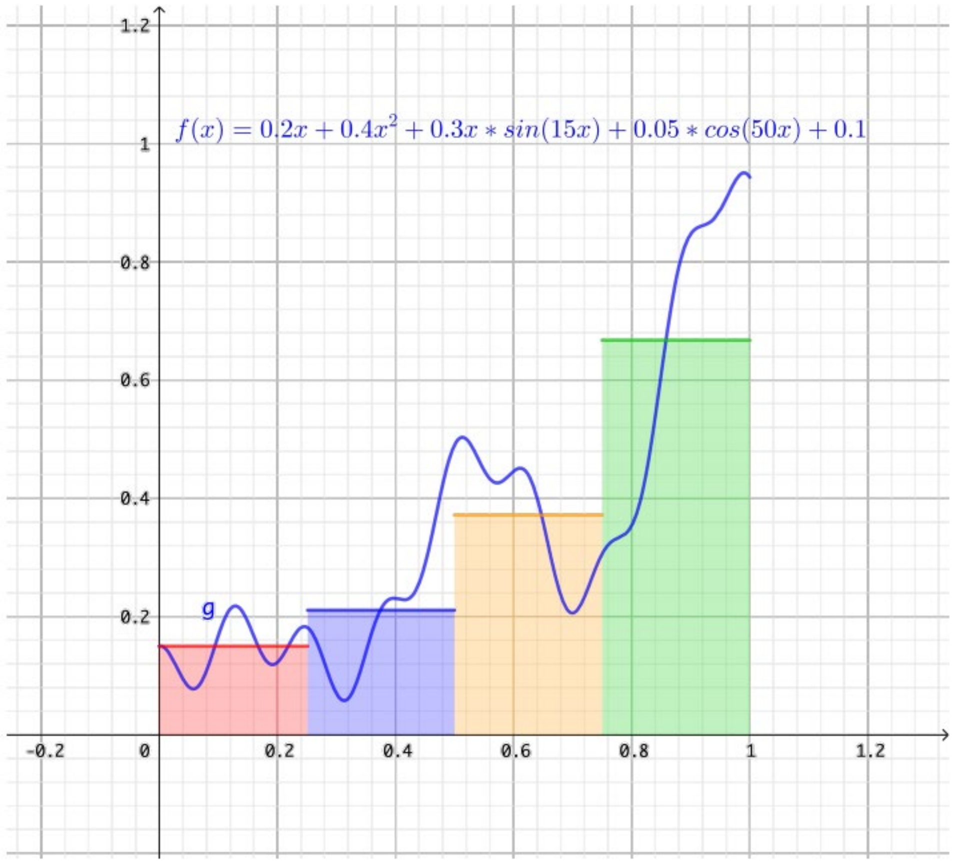
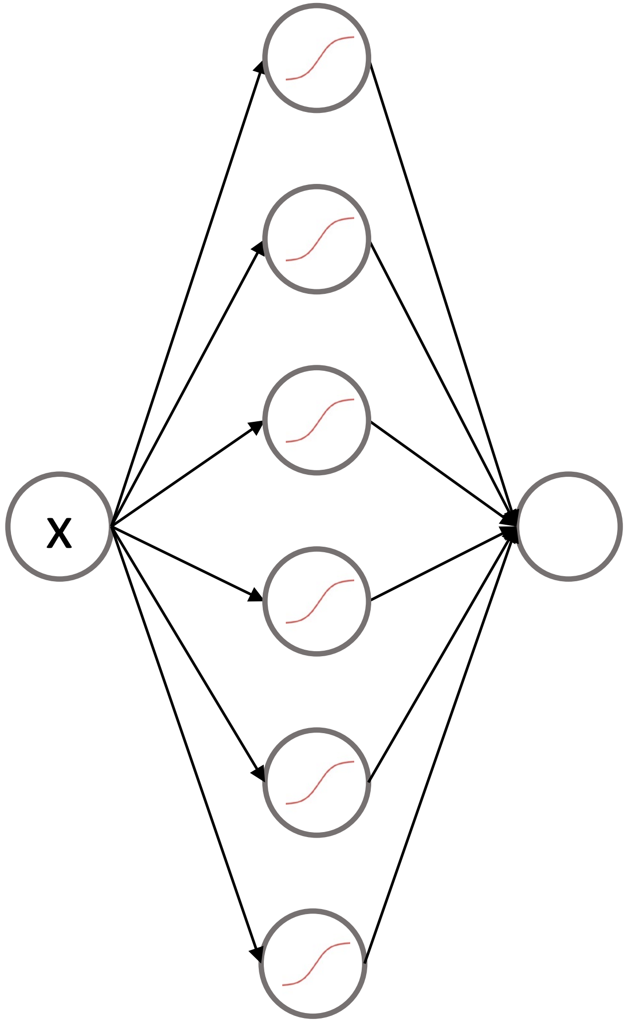
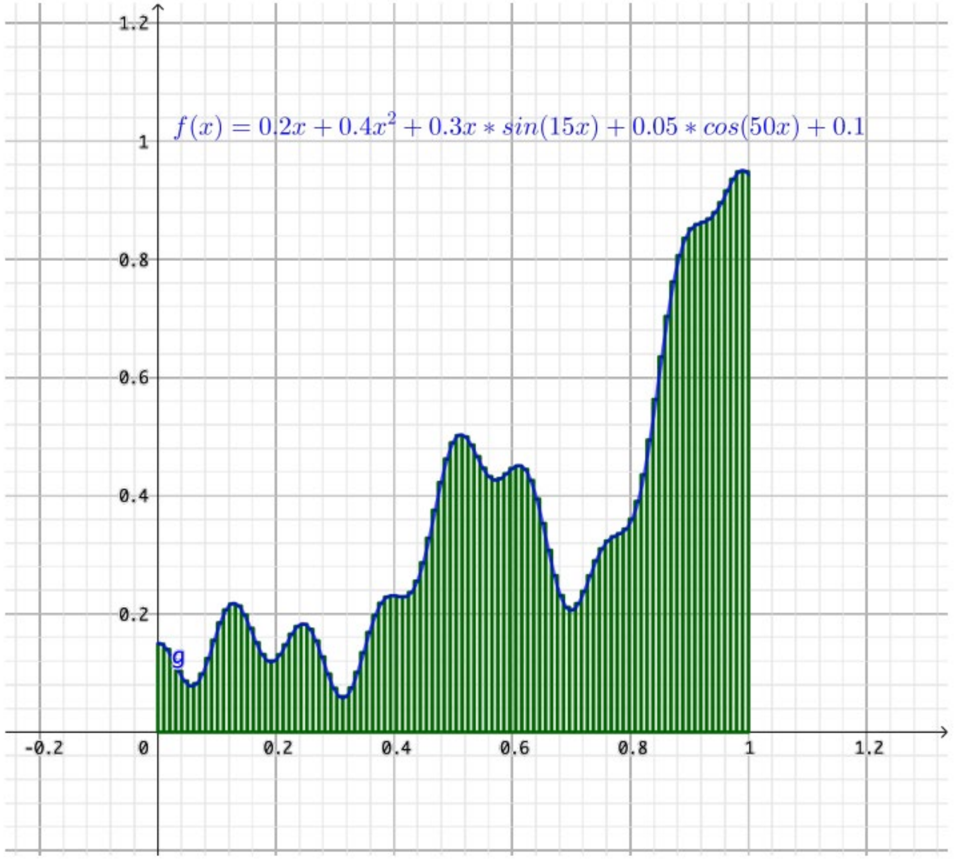


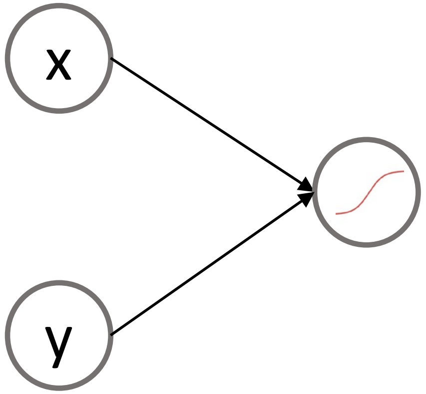


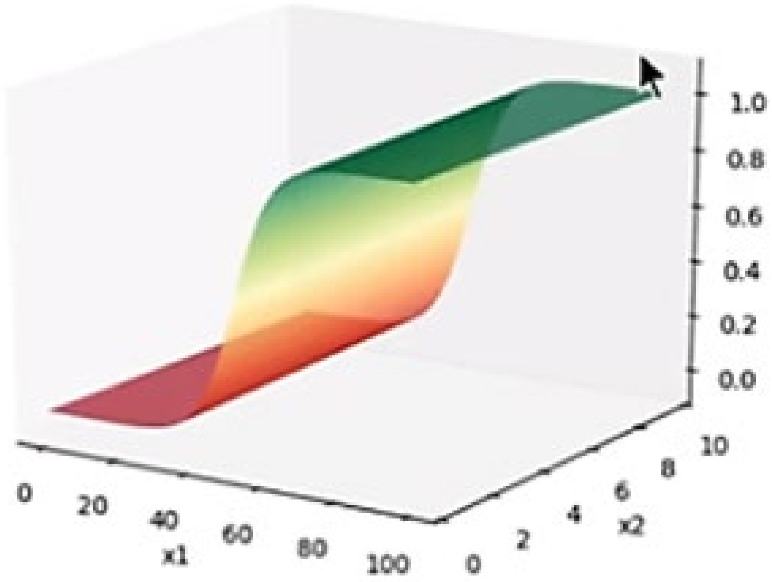
The Universal Approximation Theorem



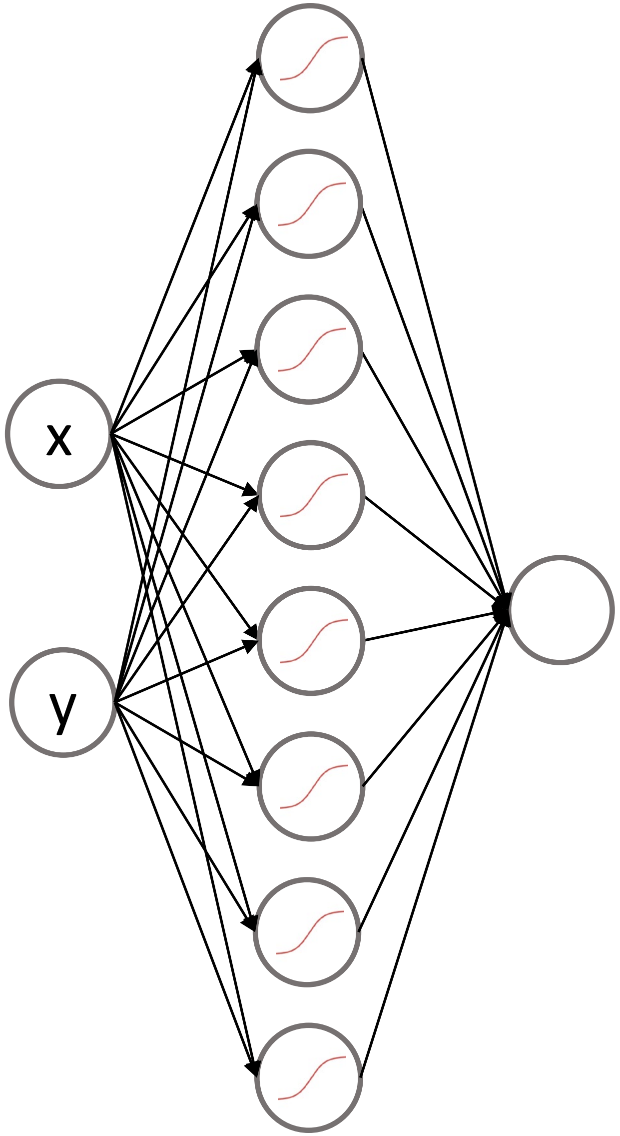


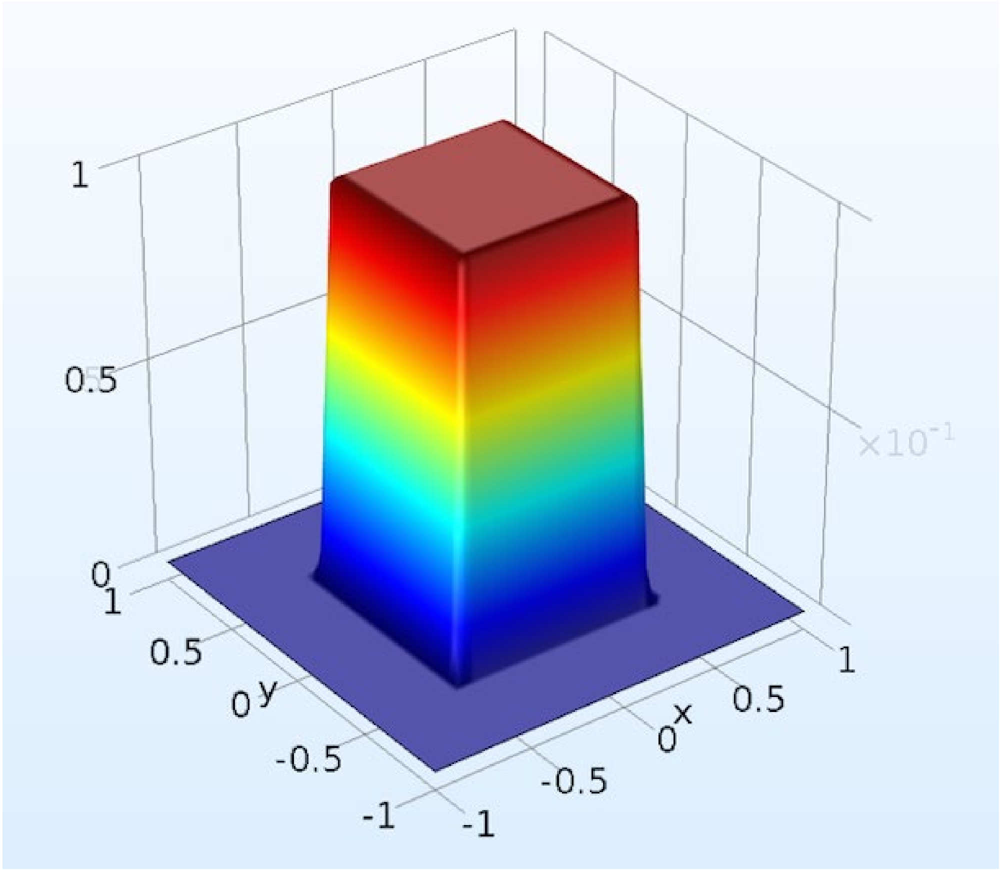
The Universal Approximator in 2D



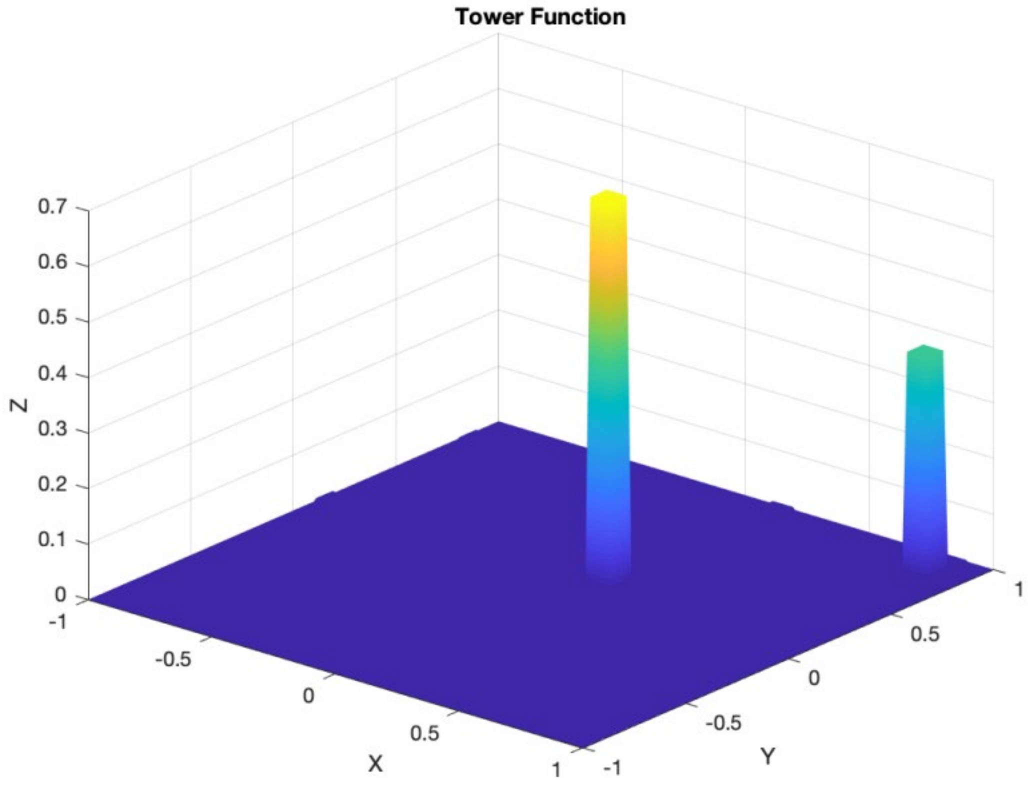


The Universal Approximator in 2D

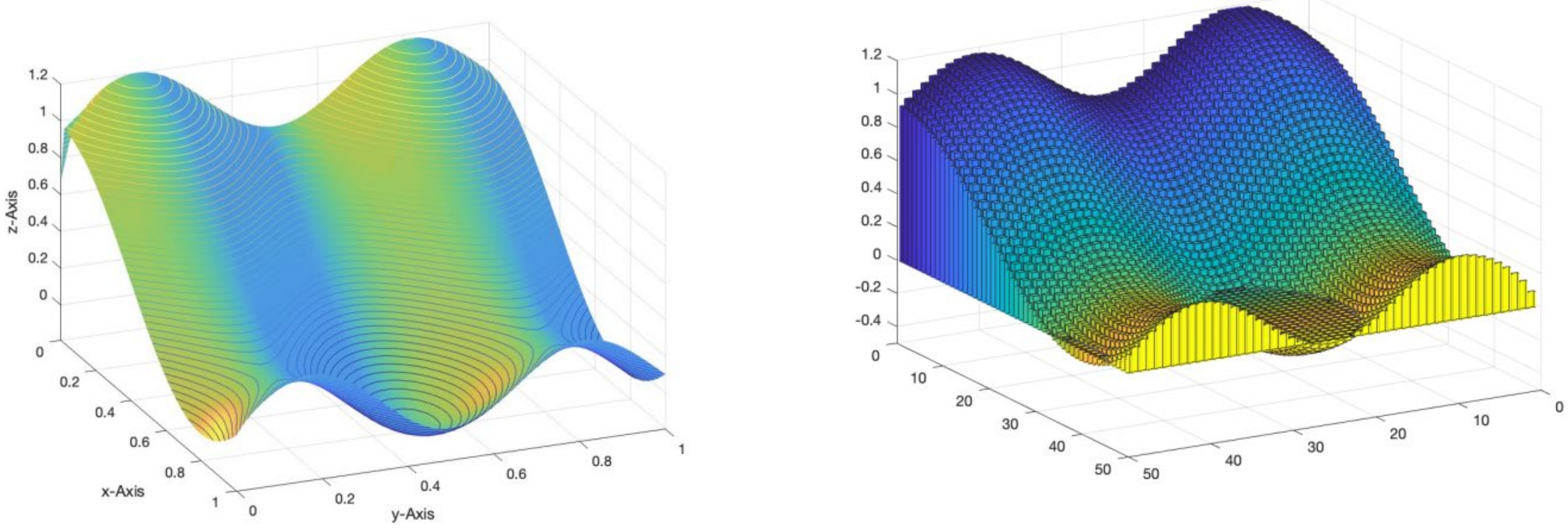




The Universal Approximator in 2D



The Universal Approximator in 2D



The Universal Approximation Theorem

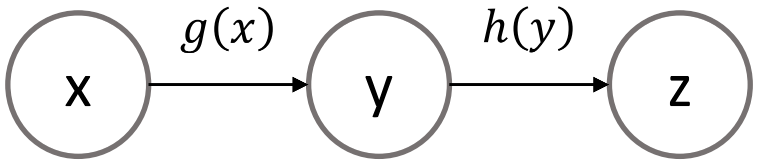
- Single layer might be enough, but it requires ‘enough’ neurons.
- Informally, ‘shallower and wider’ networks require exponentially more hidden units to compute ‘narrower and deeper’ neural networks
  - Lecture 2 | The Universal Approximation Theorem - YouTube

The Chain Rule

The Chain Rule

- A single variable chain rule

$$f, g, h: \mathbb{R} \to \mathbb{R}$$



$$f: h \circ g$$

$$f'(x) = h'\big(g(x)\big)g'(x)$$

$$\frac{dz}{dx} = \frac{dz}{dy}\frac{dy}{dx}$$

$$y = g(x), z = h(y)$$

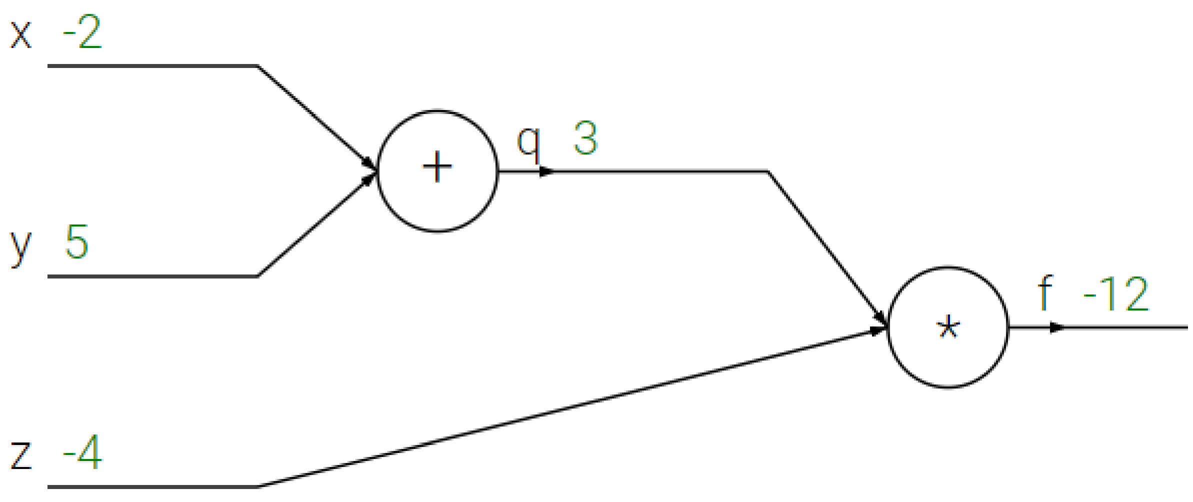
Simple Example

$$f(x, y, z) = (x + y)z$$

$$q = x + y, \qquad f = qz$$

$$\frac{\partial q}{\partial x} = 1, \qquad \frac{\partial q}{\partial y} = 1$$

$$\frac{\partial f}{\partial q} = z, \qquad \frac{\partial f}{\partial z} = q$$



Simple Example

$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial f}\frac{\partial f}{\partial q}\frac{\partial q}{\partial x}$$

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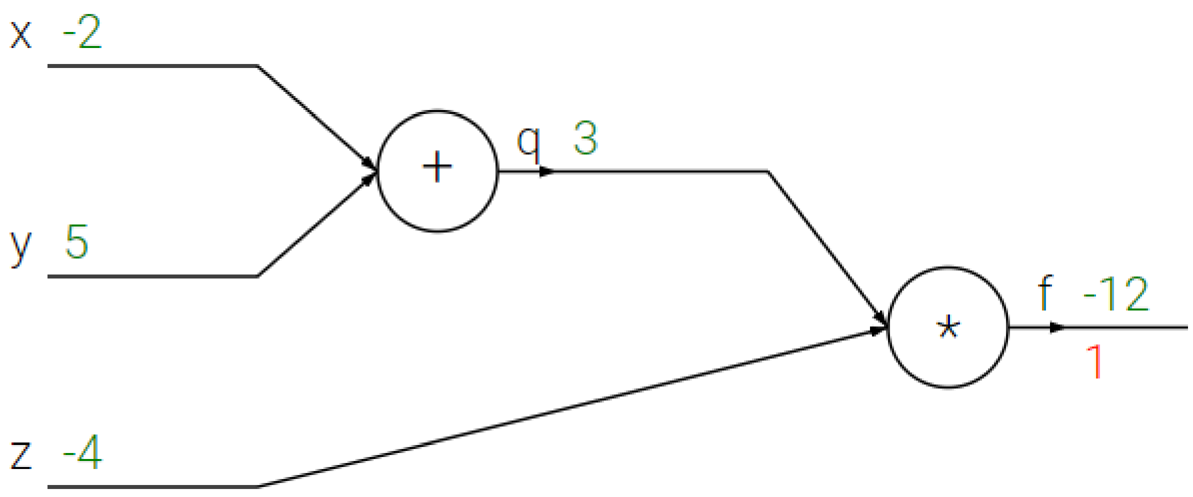

CS231n Convolutional Neural Networks for Visual Recognition

Simple Example

$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial f}\frac{\partial f}{\partial q}\frac{\partial q}{\partial x}$$

$$f(x, y, z) = (x + y)z$$

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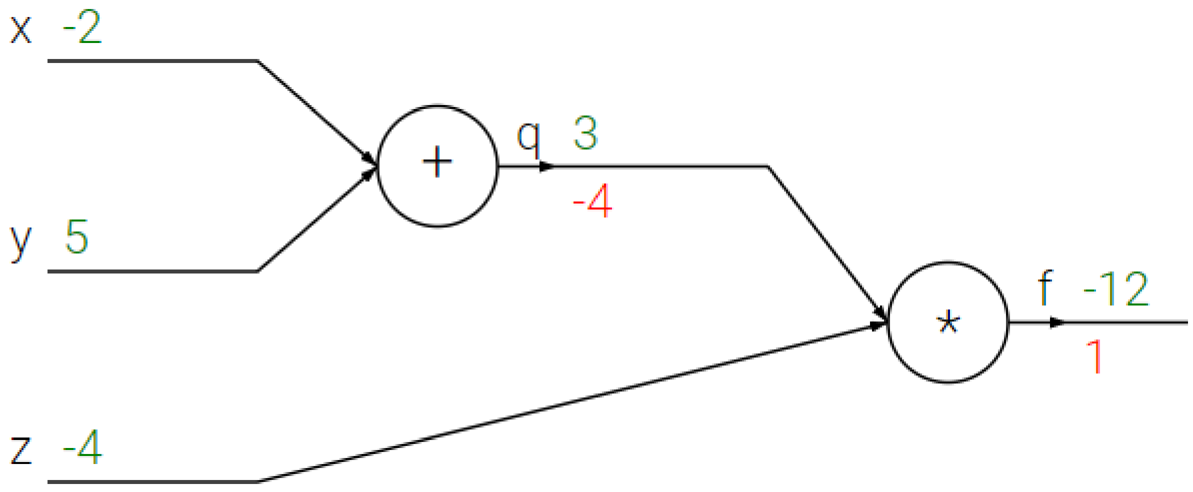

Simple Example

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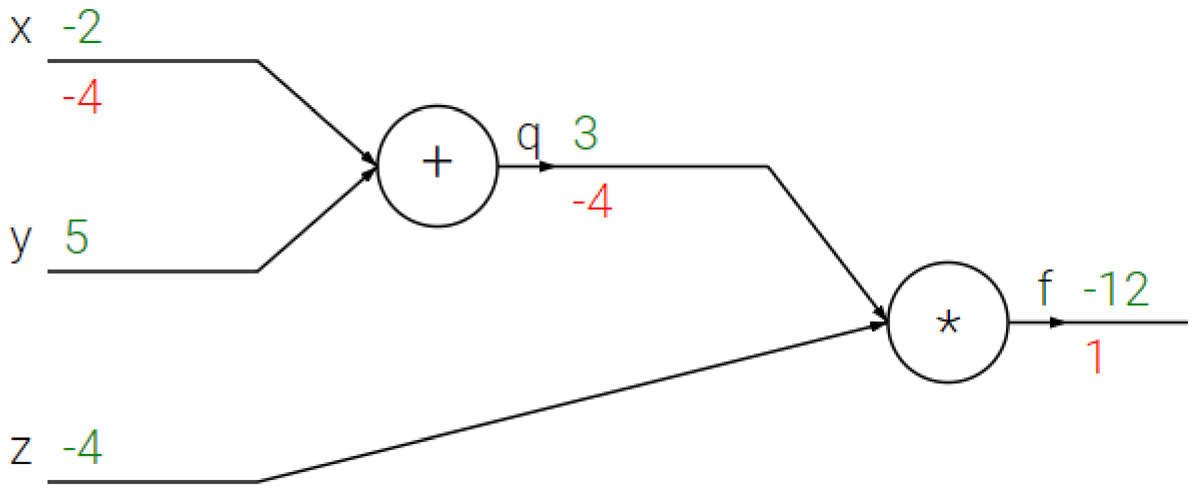

[CS231n Convolutional Neural Networks for Visual Recognition]

Simple Example

$$\frac{\partial f}{\partial y} = \frac{\partial f}{\partial f}\frac{\partial f}{\partial q}\frac{\partial q}{\partial y}$$

$$f(x, y, z) = (x + y)z$$

$$q = x + y, \qquad f = qz$$

$$\frac{\partial q}{\partial x} = 1, \qquad \frac{\partial q}{\partial y} = 1$$

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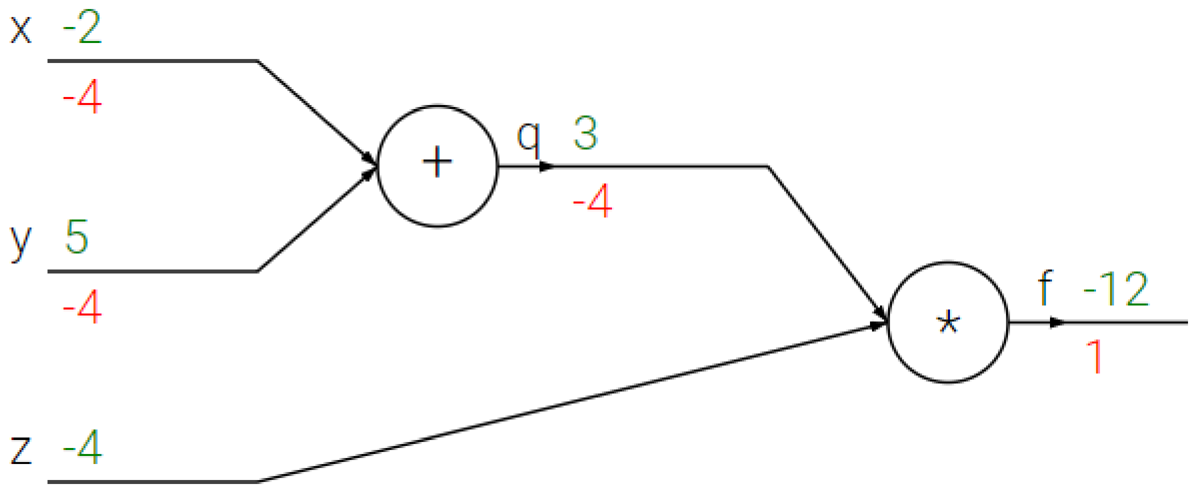

CS231n Convolutional Neural Networks for Visual Recognition

Simple Example

$$f(x, y, z) = (x + y)z$$

$$q = x + y, \qquad f = qz$$

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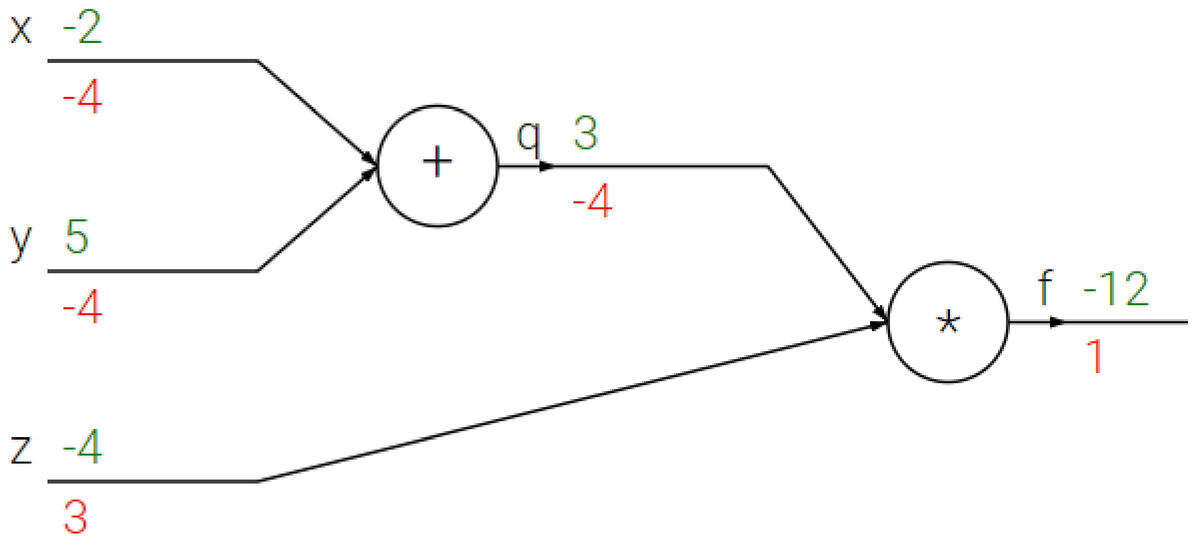
$$\frac{\partial f}{\partial q} = z, \qquad \frac{\partial f}{\partial z} = q$$

$$\frac{\partial f}{\partial z} = \frac{\partial f}{\partial f}\frac{\partial f}{\partial z}$$



CS231n Convolutional Neural Networks for Visual Recognition

Sigmoid Example

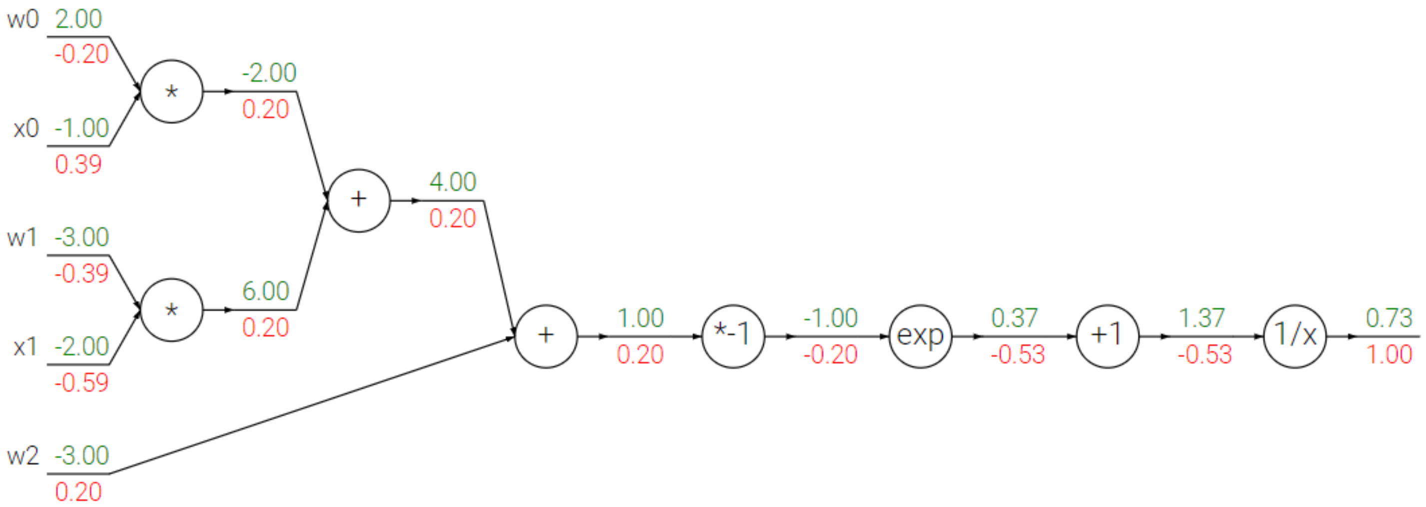
$$\sigma(x, w) = \frac{1}{1 + e^{-(w_0 x_0 + w_1 x_1 + w_2)}}$$

$$f(x) = \frac{1}{x}, \qquad g(x) = 1 + x, \qquad h(x) = e^{-x}, \qquad i(x) = w_0 x_0 + w_1 x_1 + w_2$$

Sigmoid Example

$$\sigma(x, w) = \frac{1}{1 + e^{-(w_0 x_0 + w_1 x_1 + w_2)}}$$

$$f(x) = \frac{1}{x}, \qquad g(x) = 1 + x, \qquad h(x) = e^{-x}, \qquad i(x) = w_0 x_0 + w_1 x_1 + w_2$$



[CS231n Convolutional Neural Networks for Visual Recognition]

Backpropagation Algorithm

Gradient

- In vector calculus, the *gradient* of a *scalar-valued* differentiable function $f: \mathbb{R}^n \to \mathbb{R}$ at the point x

$$\nabla f: \mathbb{R}^n \to \mathbb{R}^n \qquad \nabla f = \frac{\partial f}{\partial x} = \left[\frac{\partial f}{\partial x_1}, \cdots, \frac{\partial f}{\partial x_n}\right]$$

Jacobian

- In vector calculus, the *Jacobian* of a *vector-valued* differentiable function is the matrix of all its first-order partial derivatives.

$$f: \mathbb{R}^n \to \mathbb{R}^m$$

$$\mathbf{J}_{ij} = \frac{\partial f_i}{\partial x_j} \qquad \mathbf{J} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_m}{\partial x_1} & \cdots & \frac{\partial f_m}{\partial x_n} \end{bmatrix}$$

Matrix Calculus

$X \in \mathbb{R}^{n \times m}, y \in \mathbb{R}$

$f: \mathbb{R}^{n \times m} \to \mathbb{R}$

$y = f(x)$

$$\frac{\partial y}{\partial X} = \begin{bmatrix} \frac{\partial y}{\partial X_{11}} & \cdots & \frac{\partial y}{\partial X_{1m}} \\ \vdots & \ddots & \vdots \\ \frac{\partial y}{\partial X_{n1}} & \cdots & \frac{\partial y}{\partial X_{nm}} \end{bmatrix} \in \mathbb{R}^{n \times m}$$

Matrix Calculus

$X \in \mathbb{R}^{n \times m}, y \in \mathbb{R}^{l}$

$f: \mathbb{R}^{n \times m} \rightarrow \mathbb{R}^{l}$

$y = f(x)$

$$\frac{\partial y_1}{\partial X} = \begin{bmatrix} \frac{\partial y_1}{\partial X_{11}} & \cdots & \frac{\partial y_1}{\partial X_{1m}} \\ \vdots & \ddots & \vdots \\ \frac{\partial y_1}{\partial X_{n1}} & \cdots & \frac{\partial y_1}{\partial X_{nm}} \end{bmatrix} \in \mathbb{R}^{n \times m}$$

$\frac{\partial y}{\partial X} \in \mathbb{R}^{l \times n \times m}$ (3 dim tensor)

Finite Difference

- Numerical method to compute the gradients based on the definition of gradients

$$\frac{df}{dx} = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

$$\frac{df}{dx} \approx \frac{f(x+\Delta x) - f(x)}{\Delta x}$$

Forward difference

$$\frac{df}{dx} \approx \frac{f(x) - f(x-\Delta x)}{\Delta x}$$

Backward difference

$$\frac{df}{dx} \approx \frac{f(x+\Delta x) - f(x-\Delta x)}{2\Delta x}$$

Central difference

Finite Difference

- Numerical method to compute the gradients based on the definition of gradients

$$\frac{df}{dx} = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

$$\frac{df}{dx} \approx \frac{f(x+\Delta x) - f(x)}{\Delta x}$$

Forward difference

$$\frac{df}{dx} \approx \frac{f(x) - f(x-\Delta x)}{\Delta x}$$

Backward difference

$$\frac{df}{dx} \approx \frac{f(x+\Delta x) - f(x-\Delta x)}{2\Delta x}$$

Central difference

What's wrong with this approach?

The Chain Rule

- Multi-variable chain rule

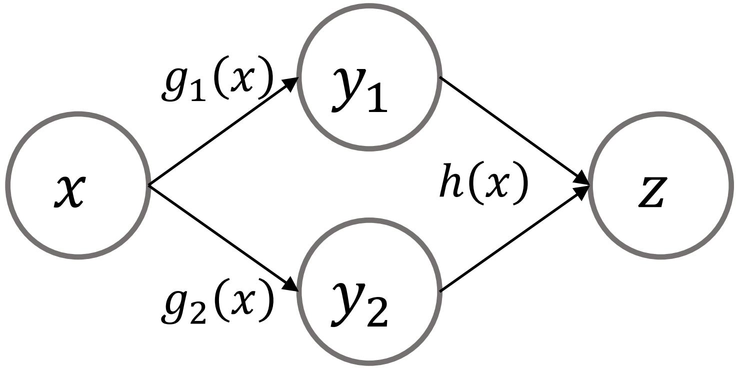
$$f, g_1, g_2 : \mathbb{R} \to \mathbb{R}, \qquad h : \mathbb{R}^2 \to \mathbb{R}$$

$$y_1 = g_1(x), \qquad y_2 = g_2(y)$$

$$z = h(y_1, y_2)$$

$$\frac{dz}{dx} = \frac{dz}{dy_1}\frac{dy_1}{dx} + \frac{dz}{dy_2}\frac{dy_2}{dx}$$

(Total derivative)



The Chain Rule

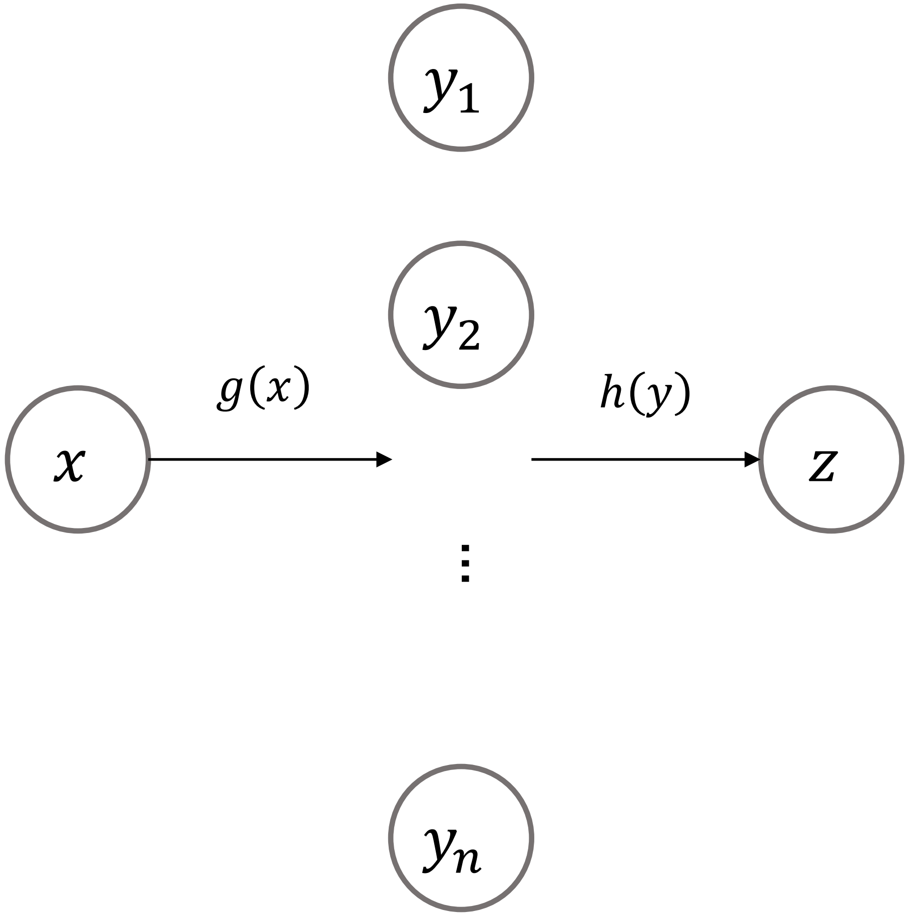
- Multi-variable chain rule

$$x \in \mathbb{R}, y \in \mathbb{R}^n, z \in \mathbb{R}$$

$$g: \mathbb{R} \to \mathbb{R}^n, \qquad y = g(x)$$

$$h: \mathbb{R}^n \to \mathbb{R}, \qquad z = h(y)$$

$$\frac{\partial z}{\partial x} = \sum_{i=1}^{n} \frac{\partial z}{\partial y_i}\frac{dy_i}{dx} = \underbrace{\frac{\partial z}{\partial y}}_{\in \mathbb{R}^{1\times n}} \overbrace{\frac{\partial y}{\partial x}}^{\in \mathbb{R}^{n\times 1}}$$



The Chain Rule

- Multi-variable chain rule

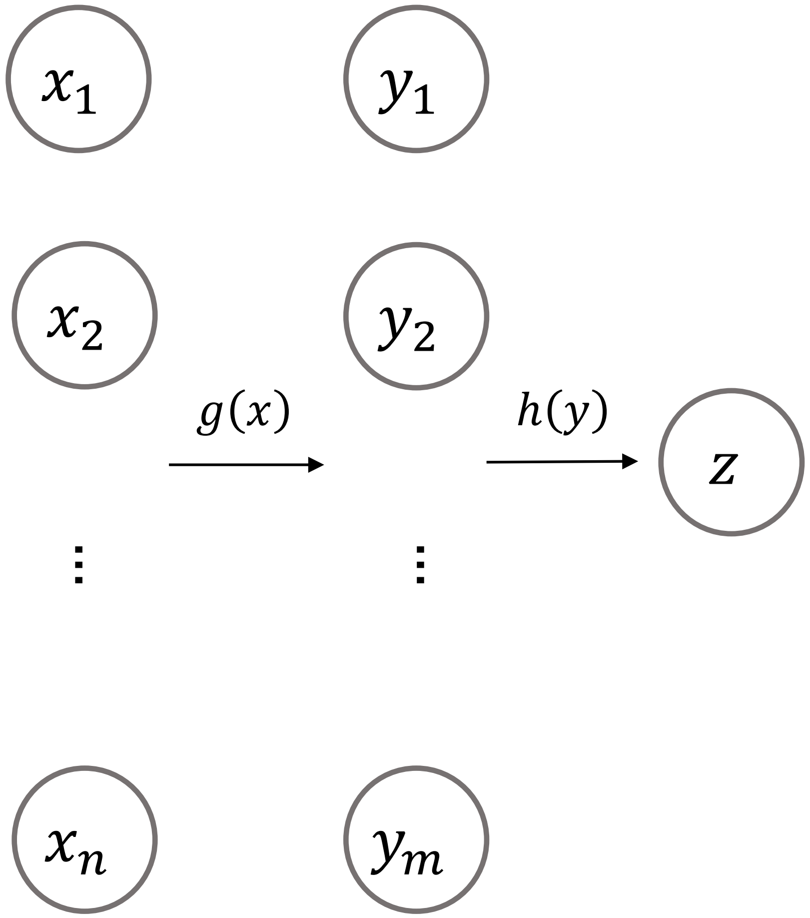
$$x \in \mathbb{R}^n, y \in \mathbb{R}^m, z \in \mathbb{R}$$

$$g: \mathbb{R}^n \to \mathbb{R}^m, \qquad y = g(x)$$

$$h: \mathbb{R}^m \to \mathbb{R}, \qquad z = h(y)$$

$$\frac{\partial z}{\partial x_j} = \sum_{i=1}^{m} \frac{\partial z}{\partial y_i} \frac{\partial y_i}{\partial x_j} = \underset{\in \mathbb{R}^{1\times m}}{\frac{\partial z}{\partial y}} \overset{\in \mathbb{R}^{m\times 1}}{\frac{\partial y}{\partial x_j}}$$

$$\frac{\partial z}{\partial x} = \left[\sum_{i=1}^{m} \frac{\partial z}{\partial y_i} \frac{\partial y_i}{\partial x_1}, \cdots, \sum_{i=1}^{m} \frac{\partial z}{\partial y_i} \frac{\partial y_i}{\partial x_n}\right] = \underset{\in \mathbb{R}^{1\times m}}{\frac{\partial z}{\partial y}} \overset{\in \mathbb{R}^{m\times n}}{\frac{\partial y}{\partial x}}$$



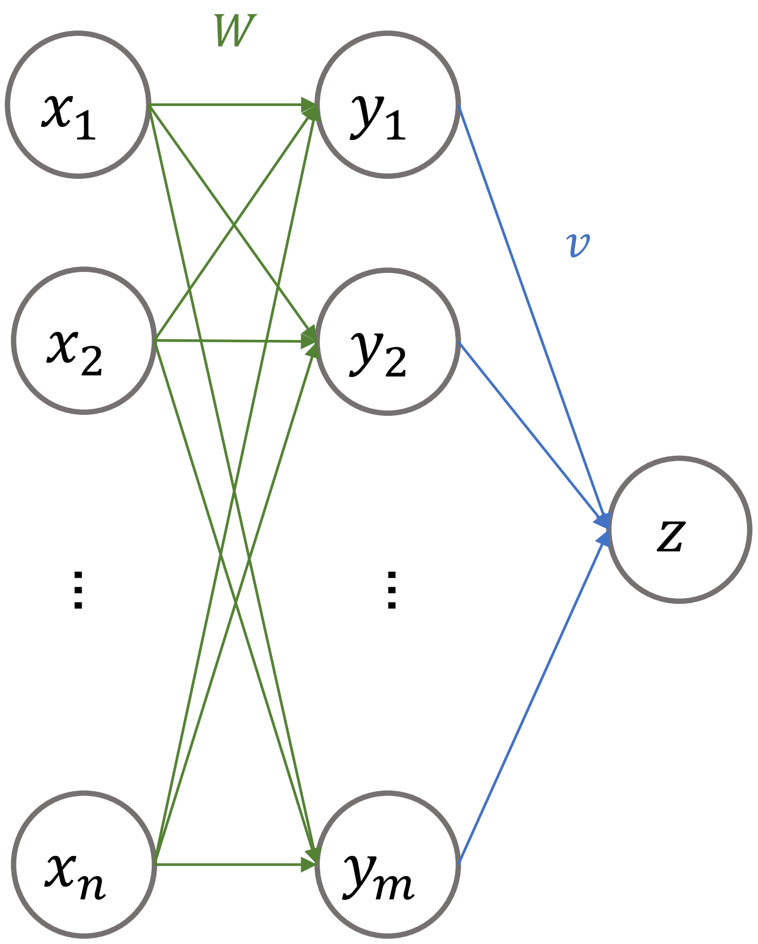
Two Layers MLP

$x \in \mathbb{R}^n, y \in \mathbb{R}^m, z \in \mathbb{R}, W \in \mathbb{R}^{m\times n}, v \in \mathbb{R}^m$

$$y = Wx \qquad z = \sum_{i=1}^{m} v_i y_i = v^\top y$$

$$\frac{\partial z}{\partial x_j} = \sum_{i=1}^{m} \frac{\partial z}{\partial y_i}\frac{\partial y_i}{\partial x_j} = \underbrace{\frac{\partial z}{\partial y}}_{\in \mathbb{R}^{1\times m}} \overbrace{\frac{\partial y}{\partial x_j}}^{\in \mathbb{R}^{m\times 1}}$$

$$\frac{\partial z}{\partial x} = \left[\sum_{i=1}^{m} \frac{\partial z}{\partial y_i}\frac{\partial y_i}{\partial x_1}, \cdots, \sum_{i=1}^{m} \frac{\partial z}{\partial y_i}\frac{\partial y_i}{\partial x_n}\right] = \underbrace{\frac{\partial z}{\partial y}}_{\in \mathbb{R}^{1\times m}} \overbrace{\frac{\partial y}{\partial x}}^{\in \mathbb{R}^{m\times n}} = v^\top W$$



Derivatives of Linear Layer

$$y = Wx \qquad z = \sum_{i=1}^{m} v_i y_i = v^\top y$$

$$\frac{\partial z}{\partial y} \qquad\qquad \frac{\partial y}{\partial x}$$

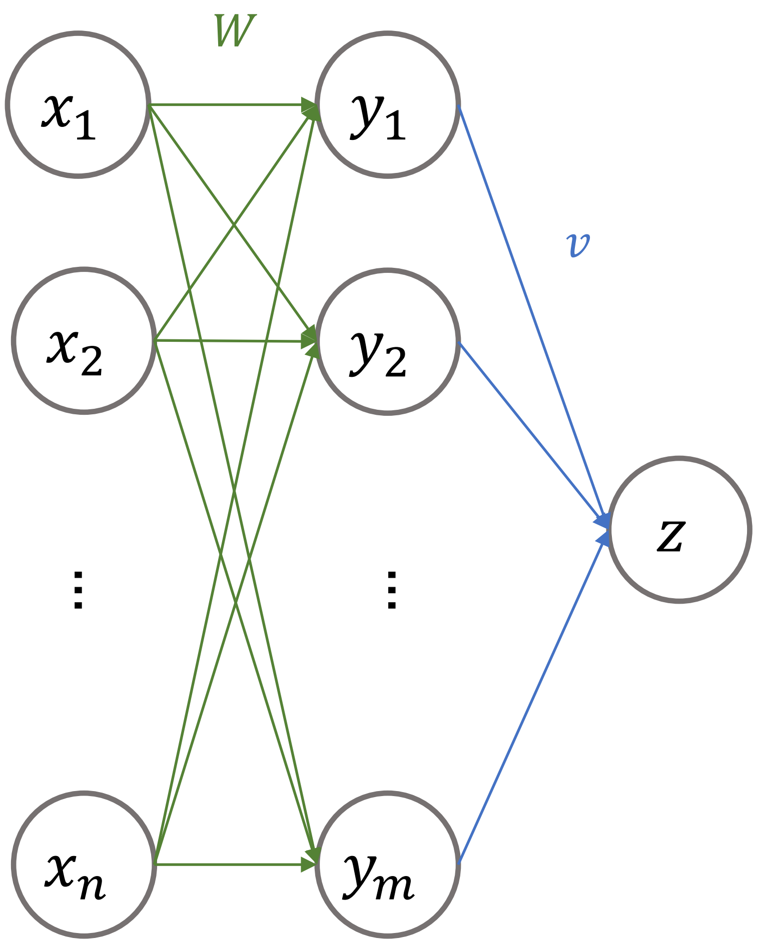
Two Layers MLP

$x \in \mathbb{R}^n, y \in \mathbb{R}^m, z \in \mathbb{R}, W \in \mathbb{R}^{m \times n}, v \in \mathbb{R}^m$

$$y = Wx \qquad z = \sum_{i=1}^{m} v_i y_i = v^\top y$$

$$\underbrace{\frac{\partial z}{\partial W}}_{\in \mathbb{R}^{m \times n}} = \underbrace{\frac{\partial z}{\partial y}}_{\in \mathbb{R}^{1 \times m}} \underbrace{\frac{\partial y}{\partial W}}_{\in \mathbb{R}^{m \times m \times n}}$$

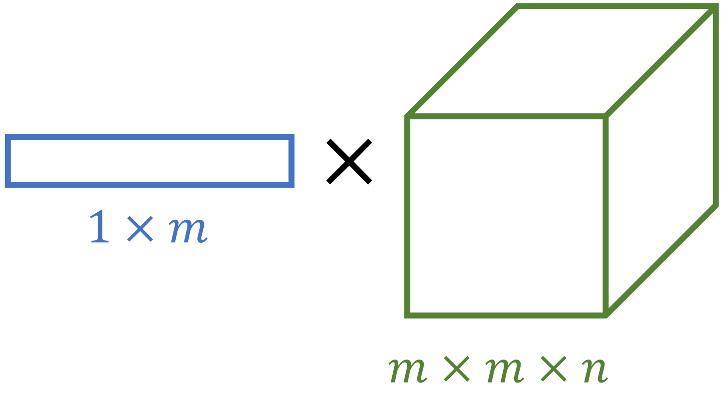
Tensor Product
(n-mode product)

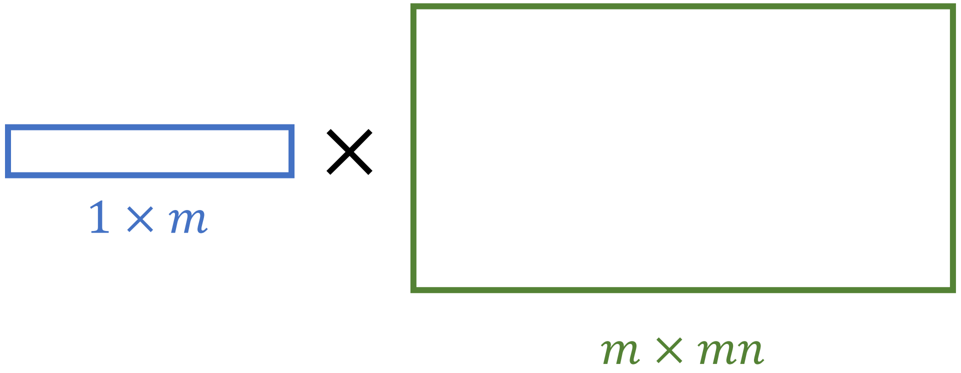


Tensor Product

- N-mode product
  - Matricization -> matrix multiplication

$$\underbrace{\frac{\partial z}{\partial W}}_{\in \mathbb{R}^{m\times n}} = \underbrace{\frac{\partial z}{\partial y}}_{\in \mathbb{R}^{1\times m}} \underbrace{\frac{\partial y}{\partial W}}_{\in \mathbb{R}^{m\times m\times n}}$$





Vector Jacobian Product (VJP)

- Jacobian is very sparse and explicit formation of it is too expensive

$x \in \mathbb{R}^n, y \in \mathbb{R}^m, z \in \mathbb{R}, W \in \mathbb{R}^{m \times n}, v \in \mathbb{R}^m$

$y = Wx$

$$\underset{\in \mathbb{R}^{m\times n}}{\frac{\partial y_1}{\partial W}} = \begin{bmatrix} \frac{\partial y_1}{\partial W_{11}} & \cdots & \frac{\partial y_1}{\partial W_{1n}} \\ \vdots & \ddots & \vdots \\ \frac{\partial y_1}{\partial W_{m1}} & \cdots & \frac{\partial y_1}{\partial W_{mn}} \end{bmatrix} = \begin{bmatrix} \frac{\partial y_1}{\partial W_{11}} & \cdots & \frac{\partial y_1}{\partial W_{1n}} \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$\underset{\in \mathbb{R}^{m\times n}}{\frac{\partial y_2}{\partial W}} = \begin{bmatrix} \frac{\partial y_2}{\partial W_{11}} & \cdots & \frac{\partial y_2}{\partial W_{1n}} \\ \vdots & \ddots & \vdots \\ \frac{\partial y_2}{\partial W_{m1}} & \cdots & \frac{\partial y_2}{\partial W_{mn}} \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 \\ \frac{\partial y_2}{\partial W_{21}} & \cdots & \frac{\partial y_2}{\partial W_{2n}} \\ 0 & 0 & 0 \end{bmatrix}$$

Vector Jacobian Product (VJP)

- Jacobian is very sparse and explicit formation of it is too expensive

$x \in \mathbb{R}^n, y \in \mathbb{R}^m, z \in \mathbb{R}, W \in \mathbb{R}^{m\times n}, v \in \mathbb{R}^m$

$y = Wx$

$$\underset{\in \mathbb{R}^{m\times mn}}{\mathrm{reshape}\left(\frac{\partial y}{\partial W}\right)} = \begin{bmatrix} \frac{\partial y_1}{\partial W_{11}} & \cdots & \frac{\partial y_1}{\partial W_{1n}} & 0 & 0 & 0 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & \frac{\partial y_2}{\partial W_{21}} & \cdots & \frac{\partial y_2}{\partial W_{2n}} & 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\partial y_3}{\partial W_{31}} & \cdots & \frac{\partial y_3}{\partial W_{3n}} & \cdots \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots \end{bmatrix}$$

Vector Jacobian Product (VJP)

- Jacobian is very sparse and explicit formation of it is too expensive

$$\frac{\partial z}{\partial y}\mathrm{reshape}\left(\frac{\partial y}{\partial W}\right) =$$

$$\begin{bmatrix} \frac{\partial z}{\partial y_1} & \frac{\partial z}{\partial y_2} & \cdots & \frac{\partial z}{\partial y_m} \end{bmatrix} \begin{bmatrix} \frac{\partial y_1}{\partial W_{11}} & \cdots & \frac{\partial y_1}{\partial W_{1n}} & 0 & 0 & 0 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & \frac{\partial y_2}{\partial W_{21}} & \cdots & \frac{\partial y_2}{\partial W_{2n}} & 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\partial y_3}{\partial W_{31}} & \cdots & \frac{\partial y_3}{\partial W_{3n}} & \cdots \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots \end{bmatrix}$$

$$= \begin{bmatrix} \frac{\partial z}{\partial y_1}\frac{\partial y_1}{\partial W_{11}} & \cdots & \frac{\partial z}{\partial y_1}\frac{\partial y_1}{\partial W_{1n}} & \frac{\partial z}{\partial y_2}\frac{\partial y_2}{\partial W_{21}} & \cdots & \frac{\partial z}{\partial y_2}\frac{\partial y_2}{\partial W_{2n}} & \cdots \end{bmatrix}$$

Vector Jacobian Product (VJP)

- Jacobian is very sparse and explicit formation of it is too expensive

$$\frac{\partial z}{\partial W} = \frac{\partial z}{\partial y}\frac{\partial y}{\partial W} = \mathrm{reshape}\left(\frac{\partial z}{\partial y}\,\mathrm{reshape}\left(\frac{\partial y}{\partial W}\right)\right)$$

$$= \mathrm{reshape}\left(\left[\frac{\partial z}{\partial y_1}\frac{\partial y_1}{\partial W_{11}} \quad \cdots \quad \frac{\partial z}{\partial y_1}\frac{\partial y_1}{\partial W_{1n}} \quad \frac{\partial z}{\partial y_2}\frac{\partial y_2}{\partial W_{21}} \quad \cdots \quad \frac{\partial z}{\partial y_2}\frac{\partial y_2}{\partial W_{2n}} \quad \cdots\right]\right)$$

$$= \begin{bmatrix} \frac{\partial z}{\partial y_1}\frac{\partial y_1}{\partial W_{11}} & \cdots & \frac{\partial z}{\partial y_1}\frac{\partial y_1}{\partial W_{1n}} \\ \vdots & \ddots & \vdots \\ \frac{\partial z}{\partial y_m}\frac{\partial y_m}{\partial W_{m1}} & \cdots & \frac{\partial z}{\partial y_m}\frac{\partial y_m}{\partial W_{mn}} \end{bmatrix} = \begin{bmatrix} \frac{\partial z}{\partial y_1}x_1 & \cdots & \frac{\partial z}{\partial y_1}x_n \\ \vdots & \ddots & \vdots \\ \frac{\partial z}{\partial y_m}x_1 & \cdots & \frac{\partial z}{\partial y_m}x_n \end{bmatrix} = \left(\frac{\partial z}{\partial y}\right)^\top x^\top$$

Vector Jacobian Product (VJP)

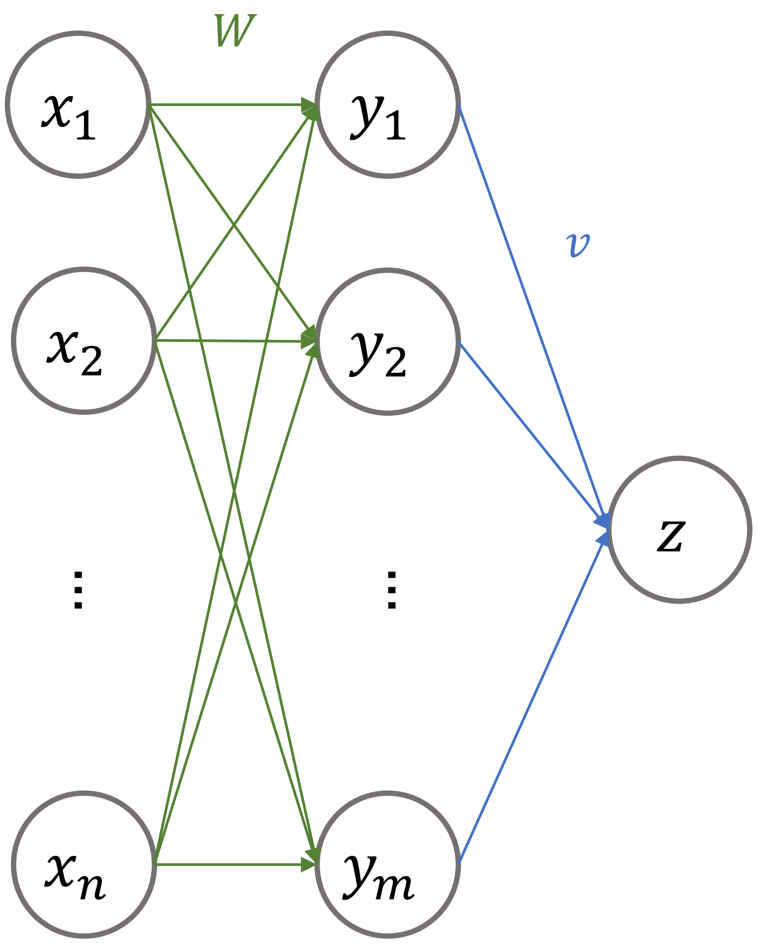
- Explicit formation of Jacobian is too expensive

$$x \in \mathbb{R}^n, y \in \mathbb{R}^m, z \in \mathbb{R}, W \in \mathbb{R}^{m\times n}, v \in \mathbb{R}^m$$

$$y = Wx \qquad z = \sum_{i=1}^{m} v_i y_i = v^\top y$$

$$\underbrace{\frac{\partial z}{\partial W}}_{\in \mathbb{R}^{m\times n}} = \underbrace{\frac{\partial z}{\partial y}}_{\in \mathbb{R}^{1\times m}} \underbrace{\frac{\partial y}{\partial W}}_{\in \mathbb{R}^{m\times m\times n}}$$

$$\underbrace{\frac{\partial z}{\partial W}}_{\in \mathbb{R}^{m\times n}} = \underbrace{\left(\frac{\partial z}{\partial y}\right)^\top}_{\in \mathbb{R}^{m\times 1}} \underbrace{x^\top}_{\in \mathbb{R}^{1\times n}}$$



We almost never explicitly construct Jacobians ($\frac{\partial y}{\partial W}$). We instead directly compute vector-Jacobian product (VJP, $\frac{\partial z}{\partial y}\frac{\partial y}{\partial W}$) in more efficient way ($\left(\frac{\partial z}{\partial y}\right)^\top x^\top$)

Vector Jacobian Product (VJP)

- Elementwise activation functions

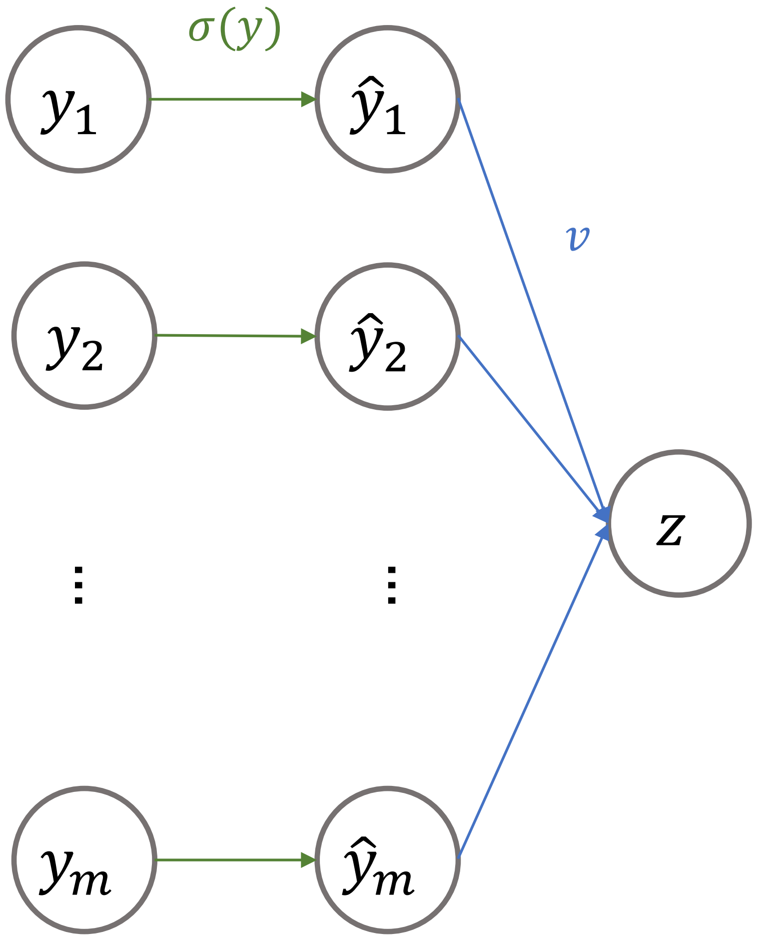
$$y \in \mathbb{R}^m, \hat{y} \in \mathbb{R}^m$$

$$\hat{y} = \sigma(y) \qquad z = \sum_{i=1}^{m} v_i \hat{y}_i = v^\top \hat{y}$$

$$\underbrace{\frac{\partial z}{\partial y}}_{\in \mathbb{R}^{1\times m}} = \underbrace{\frac{\partial z}{\partial \hat{y}}}_{\in \mathbb{R}^{1\times m}} \underbrace{\frac{\partial \hat{y}}{\partial y}}_{\in \mathbb{R}^{m\times m}}$$

$$\frac{\partial \hat{y}}{\partial y} = \begin{bmatrix} \frac{\partial \hat{y}_1}{\partial y_1} & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \frac{\partial \hat{y}_m}{\partial y_m} \end{bmatrix}$$

$$= \begin{bmatrix} \sigma(y_1)(1-\sigma(y_1)) & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \sigma(y_m)(1-\sigma(y_m)) \end{bmatrix}$$



Vector Jacobian Product (VJP)

- Elementwise activation functions

$$\underbrace{\frac{\partial z}{\partial y}}_{\in \mathbb{R}^{1\times m}} = \underbrace{\frac{\partial z}{\partial \hat{y}}}_{\in \mathbb{R}^{1\times m}} \underbrace{\frac{\partial \hat{y}}{\partial y}}_{\in \mathbb{R}^{m\times m}}$$

$$\frac{\partial \hat{y}}{\partial y} = \begin{bmatrix} \frac{\partial \hat{y}_1}{\partial y_1} & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \frac{\partial \hat{y}_m}{\partial y_m} \end{bmatrix} = \begin{bmatrix} \sigma(y_1)(1-\sigma(y_1)) & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \sigma(y_m)(1-\sigma(y_m)) \end{bmatrix}$$

Element-wise product

$$\frac{\partial z}{\partial y} = \underbrace{\frac{\partial z}{\partial \hat{y}}}_{\in \mathbb{R}^{1\times m}} \odot \overbrace{\Big(\sigma(y)\big(1-\sigma(y)\big)\Big)^{\top}}^{\in \mathbb{R}^{1\times m}}$$

Automatic Differentiation

Automatic Differentiation (AD)

- A procedure for automatic evaluation of derivatives of arbitrary algebraic functions
- Backpropagation == reverse-mode AD

Reverse-Mode AD (a.k.a Backpropagation)

$f: \mathbb{R}^{n_1} \to \mathbb{R}^{n_2}$

$g: \mathbb{R}^{n_2} \to \mathbb{R}^{n_3}$

$h: \mathbb{R}^{n_3} \to \mathbb{R}^{n_4}$

$i: \mathbb{R}^{n_4} \to \mathbb{R}$

Loss function:
scalar function

$$
\begin{aligned}
b &= f(a) \\
c &= g(b) \\
d &= h(c) \\
e &= i(d)
\end{aligned}
$$

$$\frac{\partial e}{\partial a}?$$

Reverse-Mode AD (a.k.a Backpropagation)

$f: \mathbb{R}^{n_1} \to \mathbb{R}^{n_2}$

$g: \mathbb{R}^{n_2} \to \mathbb{R}^{n_3}$

$h: \mathbb{R}^{n_3} \to \mathbb{R}^{n_4}$

$i: \mathbb{R}^{n_4} \to \mathbb{R}$

Loss function:
scalar function

$$b = f(a)$$
$$c = g(b)$$
$$d = h(c)$$
$$e = i(d)$$

$$\frac{\partial e}{\partial d} = \underbrace{\frac{\partial e}{\partial e}}_{\in \mathbb{R}^{1\times 1}} \underbrace{\frac{\partial e}{\partial d}}_{\in \mathbb{R}^{1\times n_4}} = 1 \frac{\partial e}{\partial d}$$

Reverse-Mode AD (a.k.a Backpropagation)

$f: \mathbb{R}^{n_1} \to \mathbb{R}^{n_2}$

$g: \mathbb{R}^{n_2} \to \mathbb{R}^{n_3}$

$h: \mathbb{R}^{n_3} \to \mathbb{R}^{n_4}$

$i: \mathbb{R}^{n_4} \to \mathbb{R}$

Loss function:
scalar function

$$b = f(a)$$
$$c = g(b)$$
$$d = h(c)$$
$$e = i(d)$$

$$\frac{\partial e}{\partial d} = \underbrace{\frac{\partial e}{\partial e}}_{\in \mathbb{R}^{1\times 1}} \underbrace{\frac{\partial e}{\partial d}}_{\in \mathbb{R}^{1\times n_4}} = 1 \frac{\partial e}{\partial d}$$

$$\frac{\partial e}{\partial c} = \frac{\partial e}{\partial e} \frac{\partial e}{\partial d} \frac{\partial d}{\partial c} = \underbrace{\frac{\partial e}{\partial d}}_{\in \mathbb{R}^{1\times n_4}} \underbrace{\frac{\partial d}{\partial c}}_{\in \mathbb{R}^{n_4\times n_3}}$$

Reverse-Mode AD (a.k.a Backpropagation)

$f: \mathbb{R}^{n_1} \to \mathbb{R}^{n_2}$

$g: \mathbb{R}^{n_2} \to \mathbb{R}^{n_3}$

$h: \mathbb{R}^{n_3} \to \mathbb{R}^{n_4}$

$i: \mathbb{R}^{n_4} \to \mathbb{R}$

Loss function:
scalar function

$$b = f(a)$$
$$c = g(b)$$
$$d = h(c)$$
$$e = i(d)$$

$$\frac{\partial e}{\partial d} = \underbrace{\frac{\partial e}{\partial e}}_{\in \mathbb{R}^{1\times 1}} \underbrace{\frac{\partial e}{\partial d}}_{\in \mathbb{R}^{1\times n_4}} = 1 \frac{\partial e}{\partial d}$$

$$\frac{\partial e}{\partial c} = \frac{\partial e}{\partial e}\frac{\partial e}{\partial d}\frac{\partial d}{\partial c} = \underbrace{\frac{\partial e}{\partial d}}_{\in \mathbb{R}^{1\times n_4}} \underbrace{\frac{\partial d}{\partial c}}_{\in \mathbb{R}^{n_4\times n_3}}$$

$$\frac{\partial e}{\partial b} = \frac{\partial e}{\partial e}\frac{\partial e}{\partial d}\frac{\partial d}{\partial c}\frac{\partial c}{\partial b} = \underbrace{\frac{\partial e}{\partial c}}_{\in \mathbb{R}^{1\times n_3}} \underbrace{\frac{\partial c}{\partial b}}_{\in \mathbb{R}^{n_3\times n_2}}$$

Reverse-Mode AD (a.k.a Backpropagation)

$f: \mathbb{R}^{n_1} \to \mathbb{R}^{n_2}$

$g: \mathbb{R}^{n_2} \to \mathbb{R}^{n_3}$

$h: \mathbb{R}^{n_3} \to \mathbb{R}^{n_4}$

$i: \mathbb{R}^{n_4} \to \mathbb{R}$

Loss function:
scalar function

$$b = f(a)$$
$$c = g(b)$$
$$d = h(c)$$
$$e = i(d)$$

$$\frac{\partial e}{\partial d} = \frac{\partial e}{\partial e}\frac{\partial e}{\partial d} = \underbrace{1}_{\in \mathbb{R}^{1\times 1}} \underbrace{\frac{\partial e}{\partial d}}_{\in \mathbb{R}^{1\times n_4}}$$

$$\frac{\partial e}{\partial c} = \frac{\partial e}{\partial e}\frac{\partial e}{\partial d}\frac{\partial d}{\partial c} = \underbrace{\frac{\partial e}{\partial d}}_{\in \mathbb{R}^{1\times n_4}} \underbrace{\frac{\partial d}{\partial c}}_{\in \mathbb{R}^{n_4\times n_3}}$$

$$\frac{\partial e}{\partial b} = \frac{\partial e}{\partial e}\frac{\partial e}{\partial d}\frac{\partial d}{\partial c}\frac{\partial c}{\partial b} = \underbrace{\frac{\partial e}{\partial c}}_{\in \mathbb{R}^{1\times n_3}} \underbrace{\frac{\partial c}{\partial b}}_{\in \mathbb{R}^{n_3\times n_2}}$$

$$\frac{\partial e}{\partial a} = \frac{\partial e}{\partial e}\frac{\partial e}{\partial d}\frac{\partial d}{\partial c}\frac{\partial c}{\partial b}\frac{\partial b}{\partial a} = \underbrace{\frac{\partial e}{\partial b}}_{\in \mathbb{R}^{1\times n_2}} \underbrace{\frac{\partial b}{\partial a}}_{\in \mathbb{R}^{n_2\times n_1}}$$

$\boxed{\text{Vector-Jacobian Product (VJP)}}$

Reverse-Mode AD (a.k.a Backpropagation)

$f: \mathbb{R}^{n_1} \to \mathbb{R}^{n_2}$

$g: \mathbb{R}^{n_2} \to \mathbb{R}^{n_3}$

$h: \mathbb{R}^{n_3} \to \mathbb{R}^{n_4}$

$i: \mathbb{R}^{n_4} \to \mathbb{R}^{3}$

$$b = f(a)$$
$$c = g(b)$$
$$d = h(c)$$
$$e = i(d)$$

What if i is vector-valued function?

$$\frac{\partial e}{\partial d} = \frac{\partial e}{\partial e}\frac{\partial e}{\partial d} = \underbrace{\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}}_{\in \mathbb{R}^{3\times 3}} \underbrace{\frac{\partial e}{\partial d}}_{\in \mathbb{R}^{3\times n_4}}$$

3 X Computation

$$\frac{\partial e}{\partial c} = \frac{\partial e}{\partial e}\frac{\partial e}{\partial d}\frac{\partial d}{\partial c} = \underbrace{\frac{\partial e}{\partial d}}_{\in \mathbb{R}^{3\times n_4}} \underbrace{\frac{\partial d}{\partial c}}_{\in \mathbb{R}^{n_4\times n_3}}$$

$$\frac{\partial e}{\partial b} = \frac{\partial e}{\partial e}\frac{\partial e}{\partial d}\frac{\partial d}{\partial c}\frac{\partial c}{\partial b} = \underbrace{\frac{\partial e}{\partial c}}_{\in \mathbb{R}^{3\times n_3}} \underbrace{\frac{\partial c}{\partial b}}_{\in \mathbb{R}^{n_3\times n_2}}$$

$$\frac{\partial e}{\partial a} = \frac{\partial e}{\partial e}\frac{\partial e}{\partial d}\frac{\partial d}{\partial c}\frac{\partial c}{\partial b}\frac{\partial b}{\partial a} = \underbrace{\frac{\partial e}{\partial b}}_{\in \mathbb{R}^{3\times n_2}} \underbrace{\frac{\partial b}{\partial a}}_{\in \mathbb{R}^{n_2\times n_1}}$$

Reverse-Mode AD (a.k.a Backpropagation)

$f: \mathbb{R}^{n_1} \to \mathbb{R}^{n_2}$

$g: \mathbb{R}^{n_2} \to \mathbb{R}^{n_3}$

$h: \mathbb{R}^{n_3} \to \mathbb{R}^{n_4}$

$i: \mathbb{R}^{n_4} \to \mathbb{R}^{3}$

$$b = f(a)$$
$$c = g(b)$$
$$d = h(c)$$
$$e = i(d)$$

$$\frac{\partial e}{\partial d} = \frac{\partial e}{\partial e}\frac{\partial e}{\partial d} = \underbrace{\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}}_{\in \mathbb{R}^{3\times 3}} \underbrace{\frac{\partial e}{\partial d}}_{\in \mathbb{R}^{3\times n_4}}$$

$$\frac{\partial e_1}{\partial d}$$

Forward-Mode AD

single variable

$f: \mathbb{R} \to \mathbb{R}^{n_1}$

$g: \mathbb{R}^{n_1} \to \mathbb{R}^{n_2}$

$h: \mathbb{R}^{n_2} \to \mathbb{R}^{n_3}$

$L: \mathbb{R}^{n_3} \to \mathbb{R}^{n_4}$

$$b = f(a)$$
$$c = g(b)$$
$$d = h(c)$$
$$e = L(d)$$

$$\frac{\partial b}{\partial a} = \underbrace{\frac{\partial b}{\partial a}}^{\in \mathbb{R}^{n_1 \times 1}} \overbrace{\frac{\partial a}{\partial a}}^{\in \mathbb{R}^{1\times 1}} = \frac{\partial b}{\partial a} 1$$

Forward-Mode AD

single variable

$f: \mathbb{R} \to \mathbb{R}^{n_1}$

$g: \mathbb{R}^{n_1} \to \mathbb{R}^{n_2}$

$h: \mathbb{R}^{n_2} \to \mathbb{R}^{n_3}$

$L: \mathbb{R}^{n_3} \to \mathbb{R}^{n_4}$

$$b = f(a)$$
$$c = g(b)$$
$$d = h(c)$$
$$e = L(d)$$

$$\frac{\partial b}{\partial a} = \underbrace{\frac{\partial b}{\partial a}}^{\in \mathbb{R}^{n_1 \times 1}} \overbrace{\frac{\partial a}{\partial a}}^{\in \mathbb{R}^{1 \times 1}} = \frac{\partial b}{\partial a} 1$$

$$\frac{\partial c}{\partial a} = \frac{\partial c}{\partial b} \frac{\partial b}{\partial a} \frac{\partial a}{\partial a} = \overbrace{\frac{\partial c}{\partial b}}^{\in \mathbb{R}^{n_2 \times n_1}} \overbrace{\frac{\partial b}{\partial a}}^{\in \mathbb{R}^{n_1 \times 1}}$$

Forward-Mode AD

single variable

$f: \mathbb{R} \to \mathbb{R}^{n_1}$

$g: \mathbb{R}^{n_1} \to \mathbb{R}^{n_2}$

$h: \mathbb{R}^{n_2} \to \mathbb{R}^{n_3}$

$L: \mathbb{R}^{n_3} \to \mathbb{R}^{n_4}$

$$b = f(a)$$
$$c = g(b)$$
$$d = h(c)$$
$$e = L(d)$$

$$\frac{\partial b}{\partial a} = \underbrace{\frac{\partial b}{\partial a}}_{\in \mathbb{R}^{n_1 \times 1}} \underbrace{\frac{\partial a}{\partial a}}_{\in \mathbb{R}^{1 \times 1}} = \frac{\partial b}{\partial a} 1$$

$$\frac{\partial c}{\partial a} = \frac{\partial c}{\partial b} \frac{\partial b}{\partial a} \frac{\partial a}{\partial a} = \underbrace{\frac{\partial c}{\partial b}}_{\in \mathbb{R}^{n_2 \times n_1}} \underbrace{\frac{\partial b}{\partial a}}_{\in \mathbb{R}^{n_1 \times 1}}$$

$$\frac{\partial d}{\partial a} = \frac{\partial d}{\partial c} \frac{\partial c}{\partial b} \frac{\partial b}{\partial a} \frac{\partial a}{\partial a} = \underbrace{\frac{\partial d}{\partial c}}_{\in \mathbb{R}^{n_3 \times n_2}} \underbrace{\frac{\partial c}{\partial a}}_{\in \mathbb{R}^{n_2 \times 1}}$$

Forward-Mode AD

single variable

$f: \mathbb{R} \to \mathbb{R}^{n_1}$

$g: \mathbb{R}^{n_1} \to \mathbb{R}^{n_2}$

$h: \mathbb{R}^{n_2} \to \mathbb{R}^{n_3}$

$L: \mathbb{R}^{n_3} \to \mathbb{R}^{n_4}$

$$b = f(a)$$
$$c = g(b)$$
$$d = h(c)$$
$$e = L(d)$$

$$\frac{\partial b}{\partial a} = \frac{\partial b}{\partial a}\frac{\partial a}{\partial a} = \underbrace{\frac{\partial b}{\partial a}}_{\in \mathbb{R}^{n_1 \times 1}} \underbrace{1}_{\in \mathbb{R}^{1 \times 1}}$$

$$\frac{\partial c}{\partial a} = \frac{\partial c}{\partial b}\frac{\partial b}{\partial a}\frac{\partial a}{\partial a} = \underbrace{\frac{\partial c}{\partial b}}_{\in \mathbb{R}^{n_2 \times n_1}} \underbrace{\frac{\partial b}{\partial a}}_{\in \mathbb{R}^{n_1 \times 1}}$$

$$\frac{\partial d}{\partial a} = \frac{\partial d}{\partial c}\frac{\partial c}{\partial b}\frac{\partial b}{\partial a}\frac{\partial a}{\partial a} = \underbrace{\frac{\partial d}{\partial c}}_{\in \mathbb{R}^{n_3 \times n_2}} \underbrace{\frac{\partial c}{\partial a}}_{\in \mathbb{R}^{n_2 \times 1}}$$

$$\frac{\partial e}{\partial a} = \frac{\partial e}{\partial d}\frac{\partial d}{\partial c}\frac{\partial c}{\partial b}\frac{\partial b}{\partial a}\frac{\partial a}{\partial a} = \underbrace{\frac{\partial e}{\partial d}}_{\in \mathbb{R}^{n_4 \times n_3}} \underbrace{\frac{\partial d}{\partial a}}_{\in \mathbb{R}^{n_3 \times 1}}$$

Jacobian-Vector Product (JVP)

Forward-Mode AD

$f: \mathbb{R}^3 \rightarrow \mathbb{R}^{n_1}$

$g: \mathbb{R}^{n_1} \rightarrow \mathbb{R}^{n_2}$

$h: \mathbb{R}^{n_2} \rightarrow \mathbb{R}^{n_3}$

$L: \mathbb{R}^{n_3} \rightarrow \mathbb{R}^{n_4}$

$$b = f(a)$$
$$c = g(b)$$
$$d = h(c)$$
$$e = L(d)$$

What if input is Multi-variables?

$$\frac{\partial b}{\partial a} = \frac{\partial b}{\partial a}\frac{\partial a}{\partial a} = \underbrace{\frac{\partial b}{\partial a}}_{\in \mathbb{R}^{n_1 \times 3}} \underbrace{\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}}_{\in \mathbb{R}^{3 \times 3}}$$

3 X Computation

$$\frac{\partial c}{\partial a} = \frac{\partial c}{\partial b}\frac{\partial b}{\partial a}\frac{\partial a}{\partial a} = \underbrace{\frac{\partial c}{\partial b}}_{\in \mathbb{R}^{n_2 \times n_1}}\underbrace{\frac{\partial b}{\partial a}}_{\in \mathbb{R}^{n_1 \times 3}}$$

$$\frac{\partial d}{\partial a} = \frac{\partial d}{\partial c}\frac{\partial c}{\partial b}\frac{\partial b}{\partial a}\frac{\partial a}{\partial a} = \underbrace{\frac{\partial d}{\partial c}}_{\in \mathbb{R}^{n_3 \times n_2}}\underbrace{\frac{\partial c}{\partial a}}_{\in \mathbb{R}^{n_2 \times 3}}$$

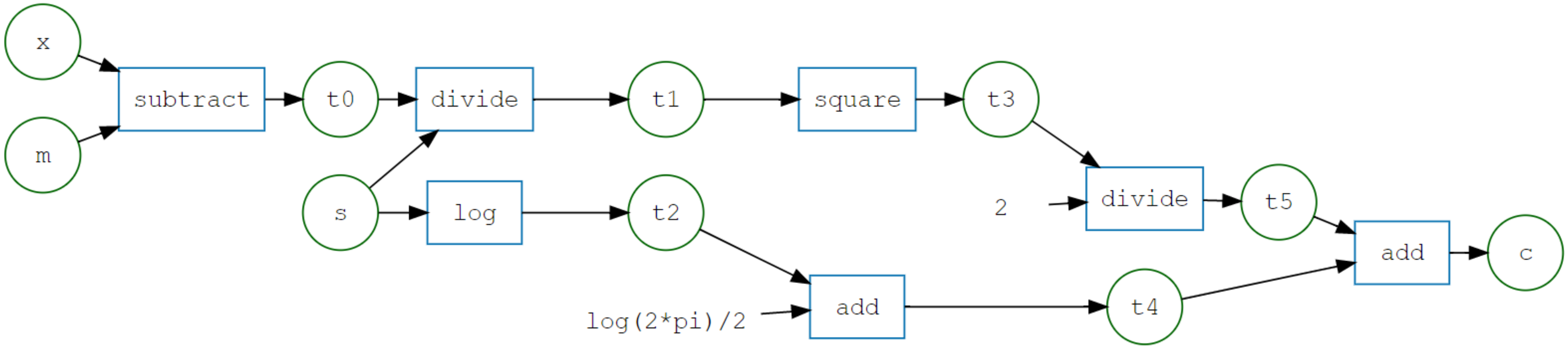
$$\frac{\partial e}{\partial a} = \frac{\partial e}{\partial d}\frac{\partial d}{\partial c}\frac{\partial c}{\partial b}\frac{\partial b}{\partial a}\frac{\partial a}{\partial a} = \underbrace{\frac{\partial e}{\partial d}}_{\in \mathbb{R}^{n_4 \times n_3}}\underbrace{\frac{\partial d}{\partial a}}_{\in \mathbb{R}^{n_3 \times 3}}$$

Automatic Differentiation (AD)

- For low dimensional outputs and high dimensional inputs
  - Objective function w/ deep neural networks
  - reverse-mode AD
- For high dimensional outputs and low dimensional inputs
  - Forward-mode AD

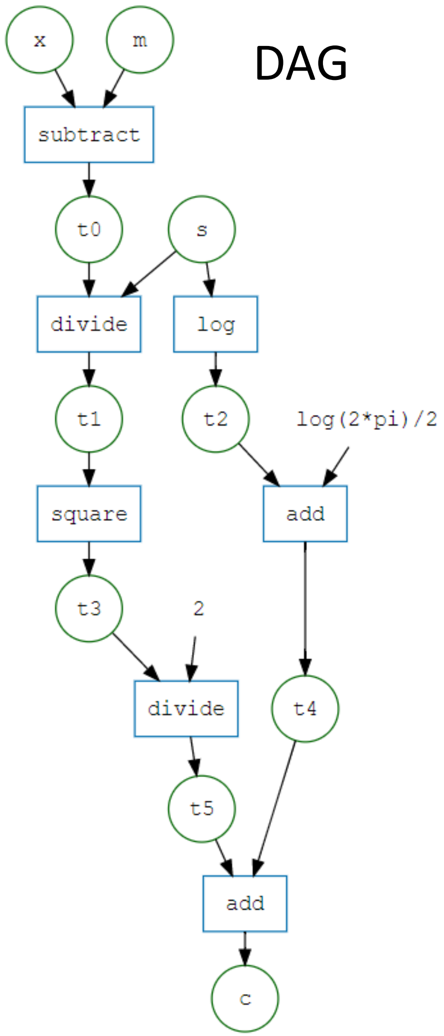
Computational Graph

```
t0 = x - m
t1 = t0 / s
t2 = np.log(s)
t3 = t1**2
t4 = t2 + np.log(2 * np.pi) / 2
t5 = t3 / 2
c = t4 + t5
```

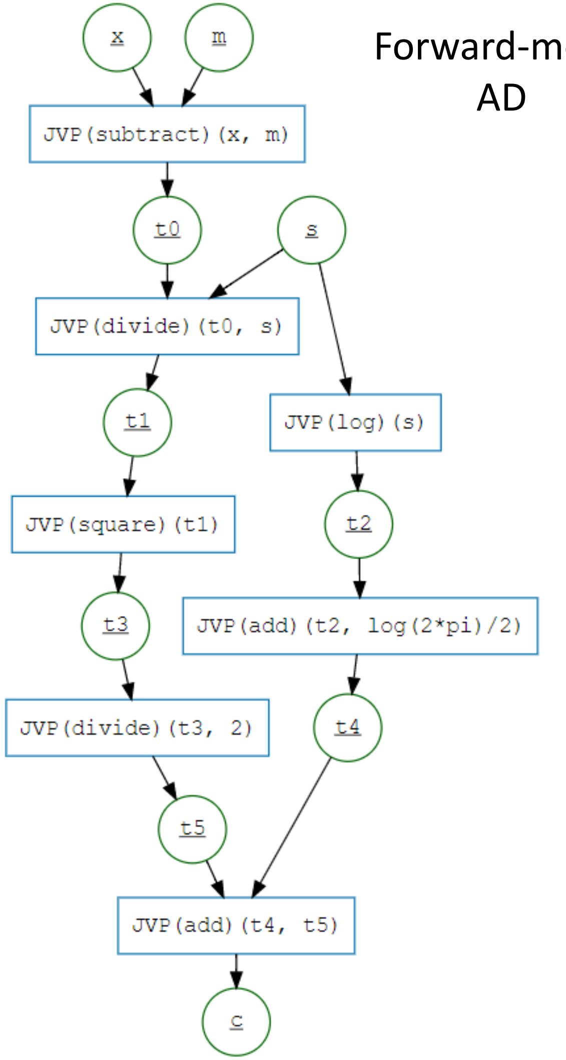


https://matt-graham.github.io/

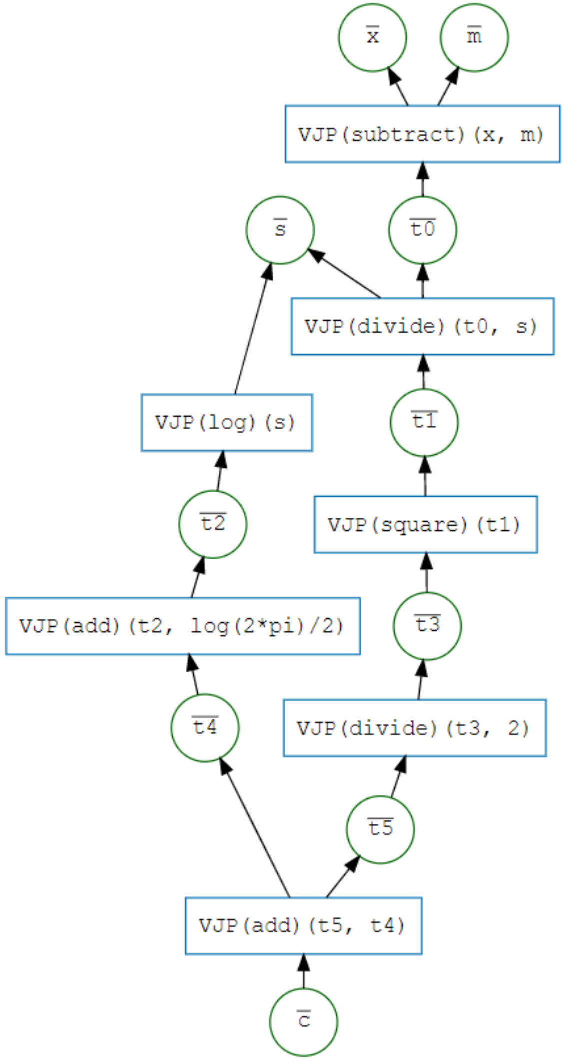
Automatic Differentiation



DAG



Forward-mode AD



Reverse-mode AD

https://matt-graham.github.io/

References

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