Lecture # 3
Introduction to Deep Learning

Deep Learning

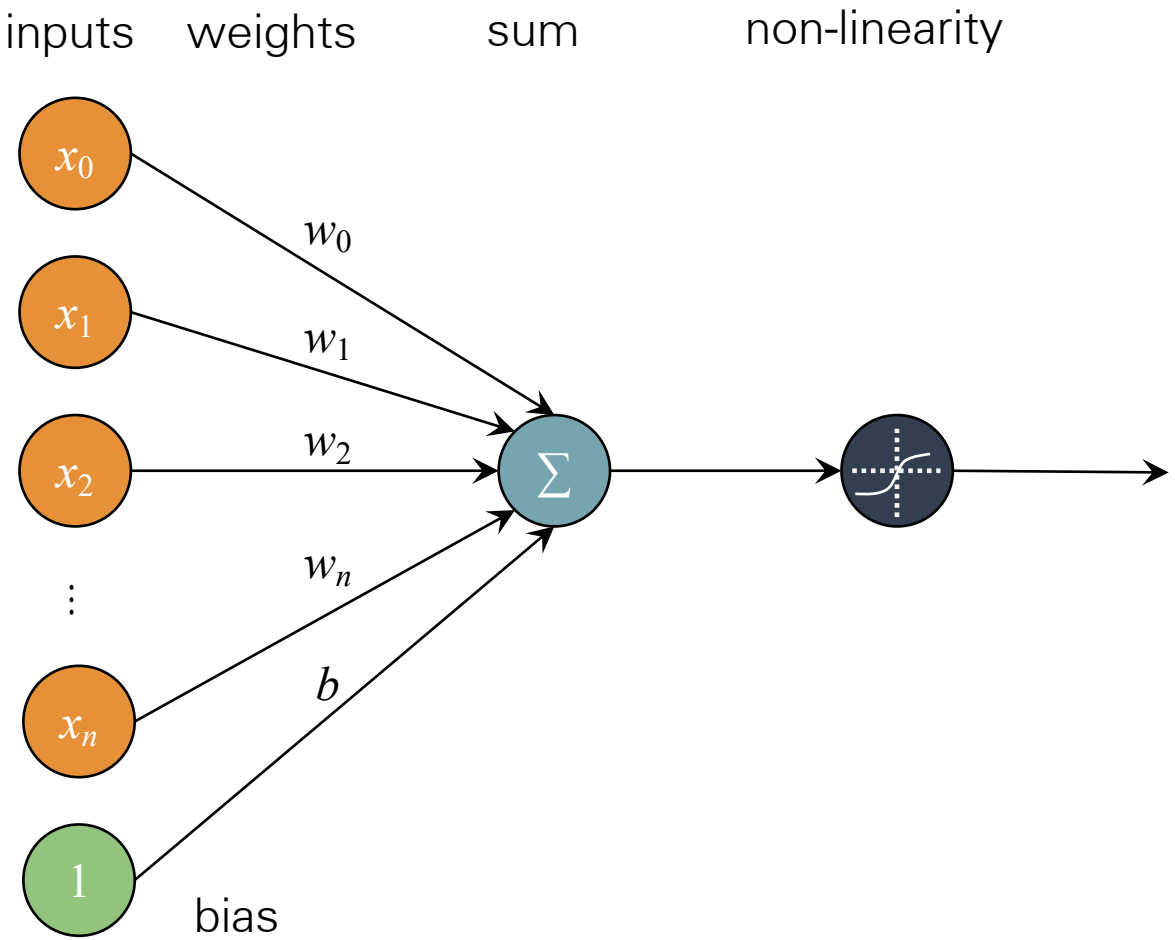
Lecture overview

- the perceptron
- the multi-layer perceptron
- stochastic gradient descent
- backpropagation
- shallow yet very powerful: `word2vec`

- **Disclaimer:** Much of the material and slides for this lecture were borrowed from
  - Hugo Larochelle's Neural networks slides
  - Nick Locascio's MIT 6.S191 slides
  - Efstratios Gavves and Max Willing's UvA deep learning class
  - Leonid Sigal's CPSC532L class
  - Richard Socher's CS224d class
  - Dan Jurafsky's CS124 class

The Perceptron

The Perceptron



Perceptron Forward Pass

- Neuron pre-activation (or input activation)

$$a(\mathbf{x}) = b + \sum_i w_i x_i = b + \mathbf{w}^\top \mathbf{x}$$

- Neuron output activation:

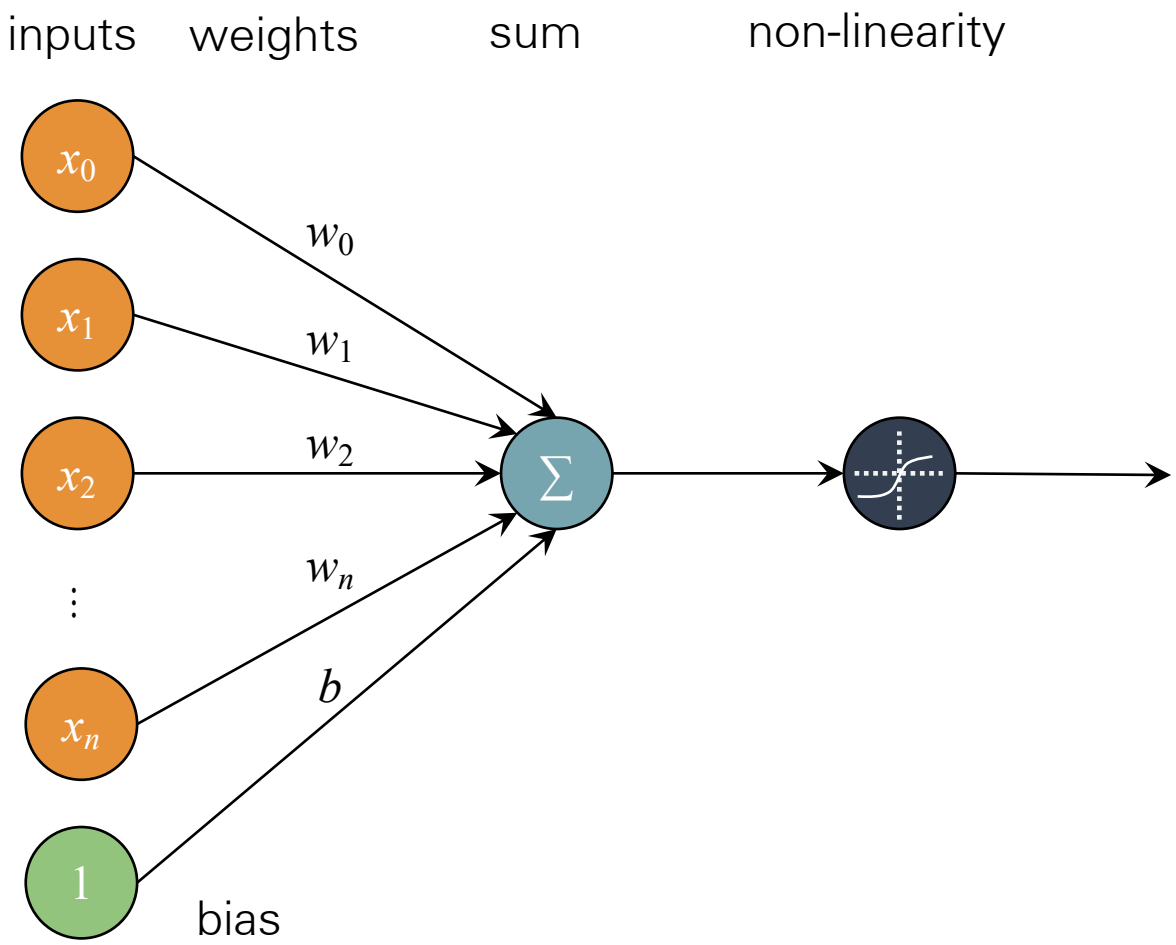
$$h(\mathbf{x}) = g(a(\mathbf{x})) = g(b + \sum_i w_i x_i)$$

where

$\mathbf{w}$ are the weights (parameters)

b is the bias term

$g(\cdot)$ is called the activation function



Output Activation of The Neuron

$$h(\mathbf{x}) = g(a(\mathbf{x})) = g(b + \sum_i w_i x_i)$$

Range is determined by $g(\cdot)$

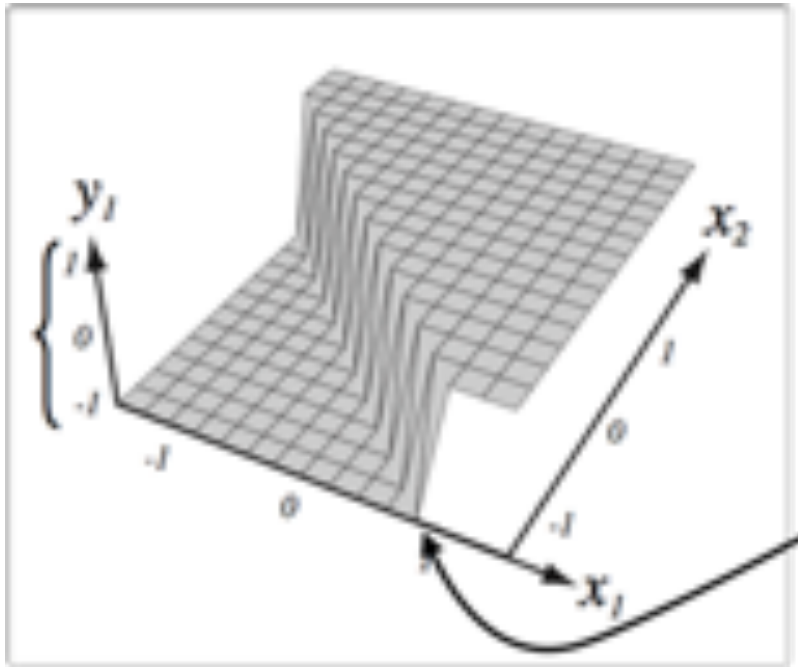
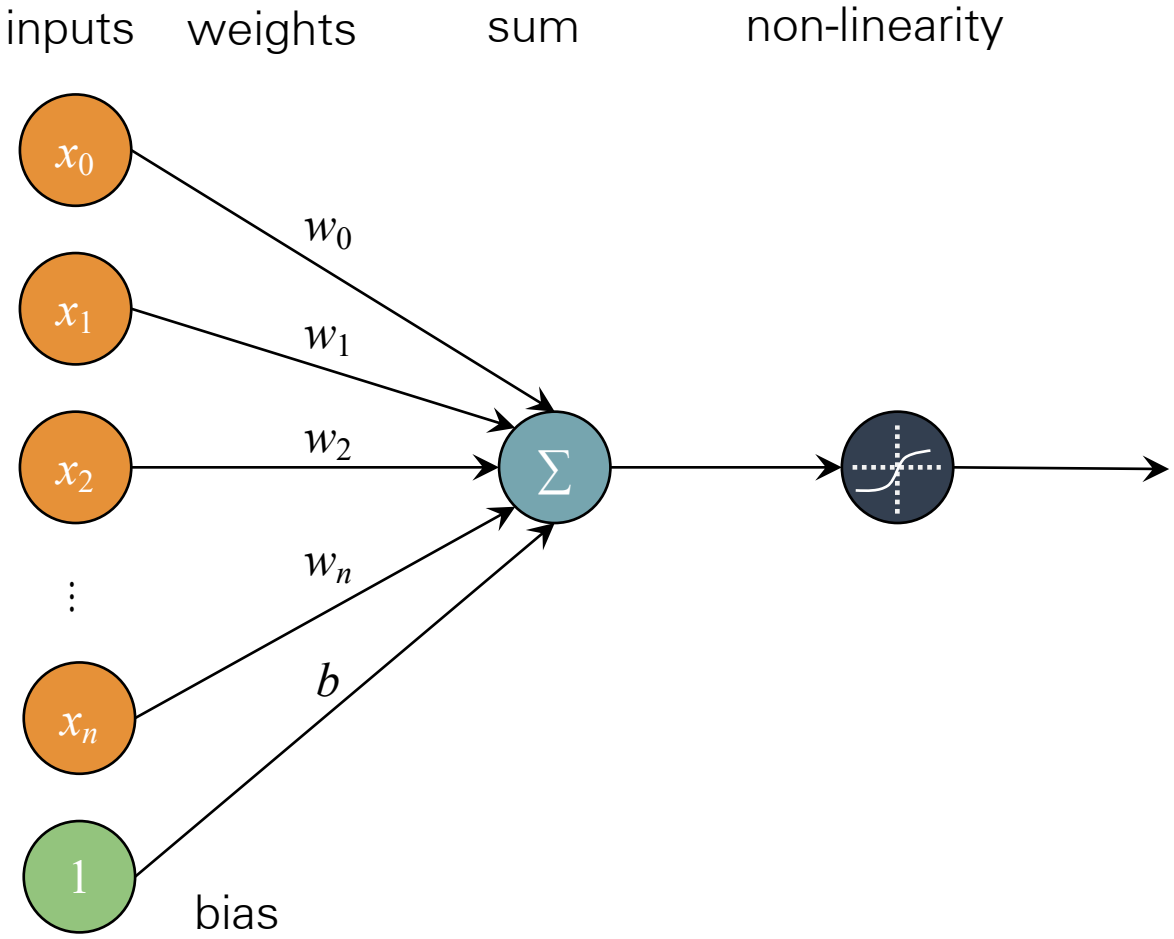


Image credit: Pascal Vincent

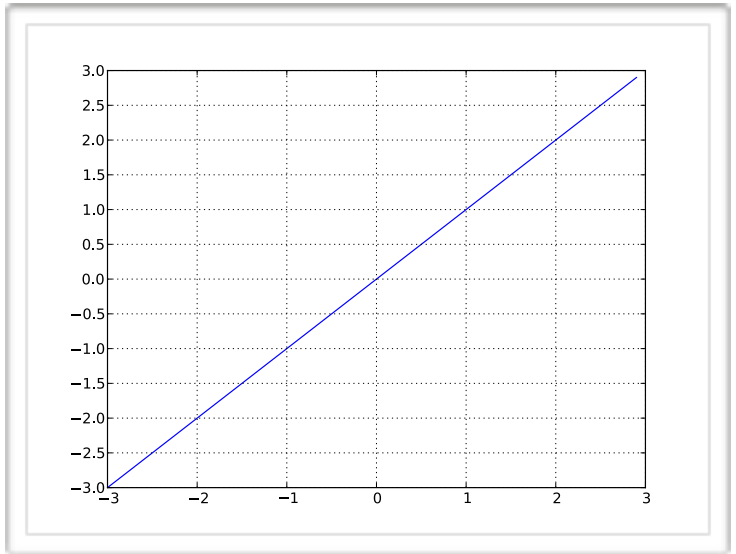
Bias only changes the position of the riff



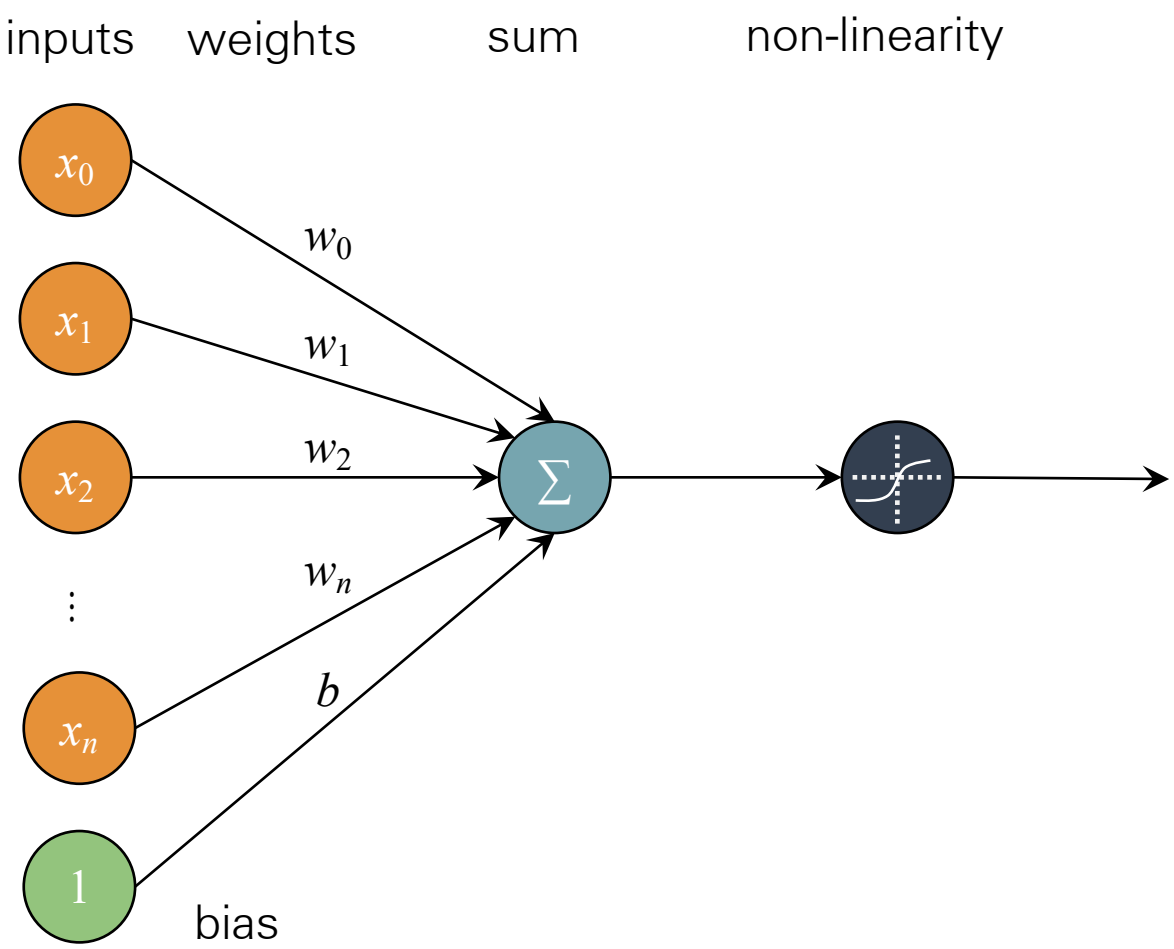
Linear Activation Function

$$h(\mathbf{x}) = g(a(\mathbf{x})) = g(b + \sum_i w_i x_i)$$

$$g(a) = a$$



- No nonlinear transformation
- No input squashing

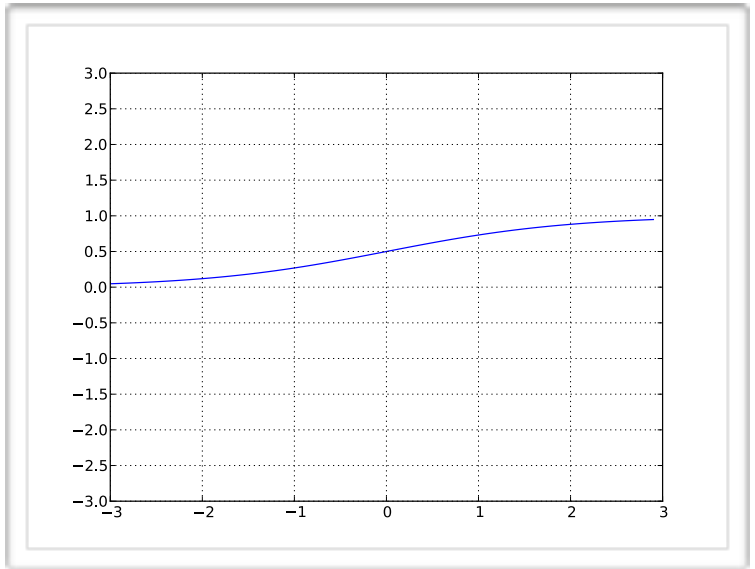


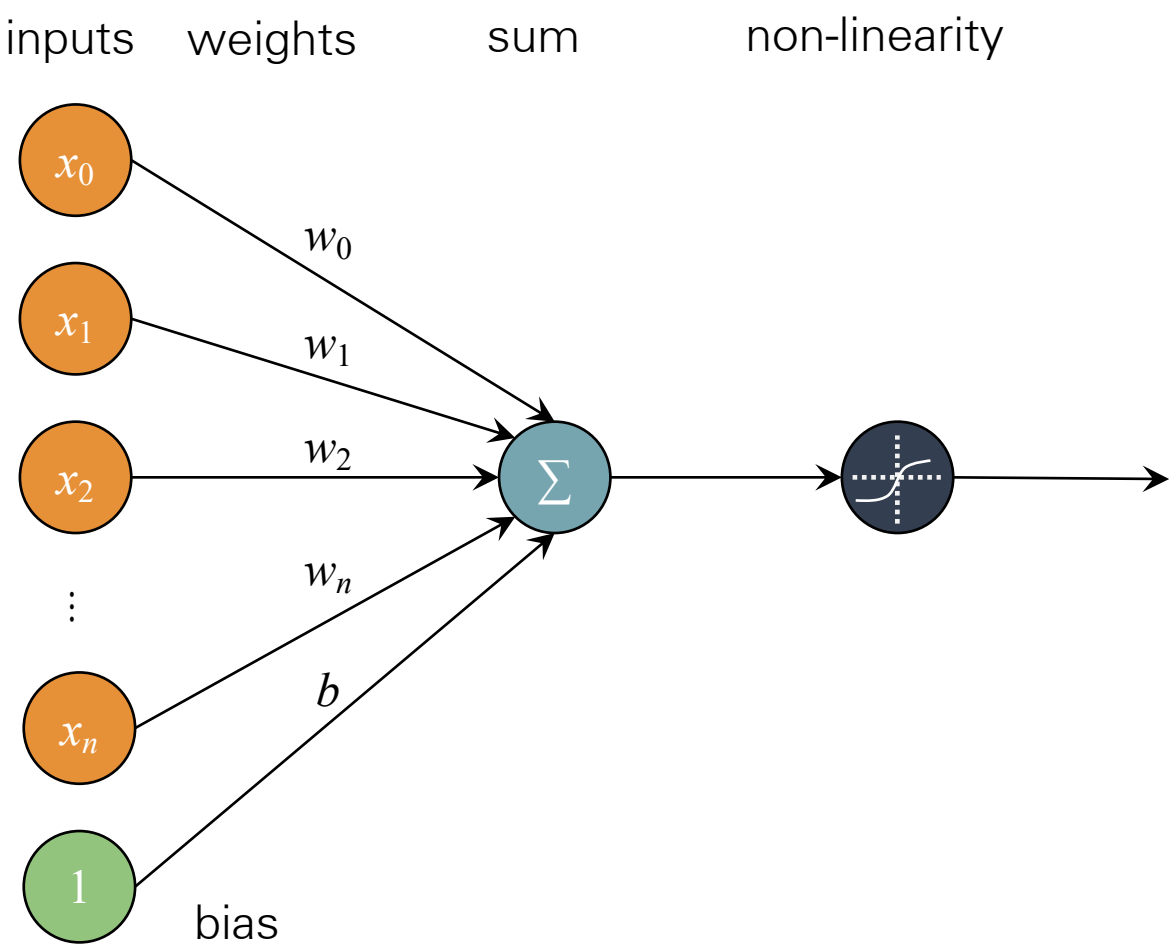
Sigmoid Activation Function

$$h(\mathbf{x}) = g(a(\mathbf{x})) = g(b + \sum_i w_i x_i)$$

$$g(a) = \text{sigm}(a) = \frac{1}{1+\exp(-a)}$$

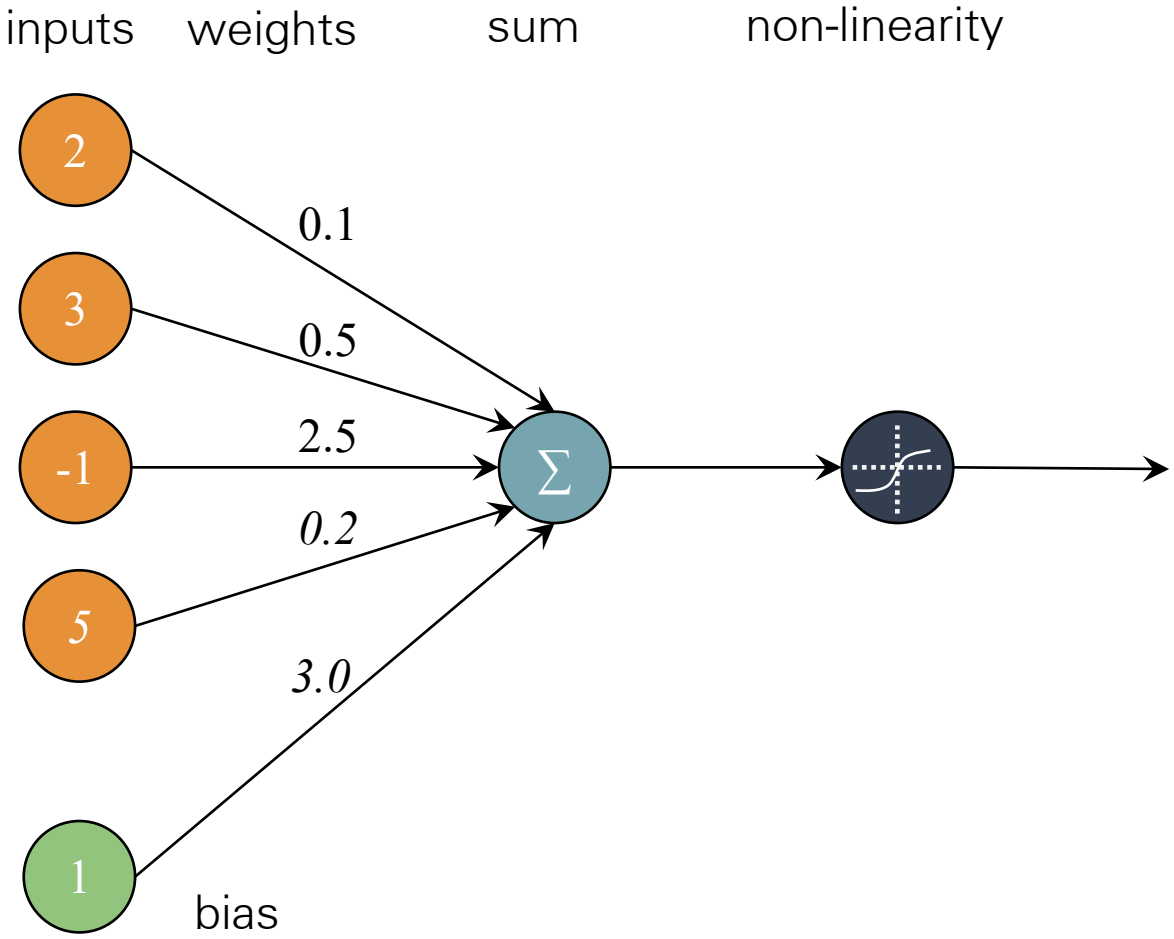
- Squashes the neuron's output between 0 and 1
- Always positive
- Bounded
- Strictly Increasing





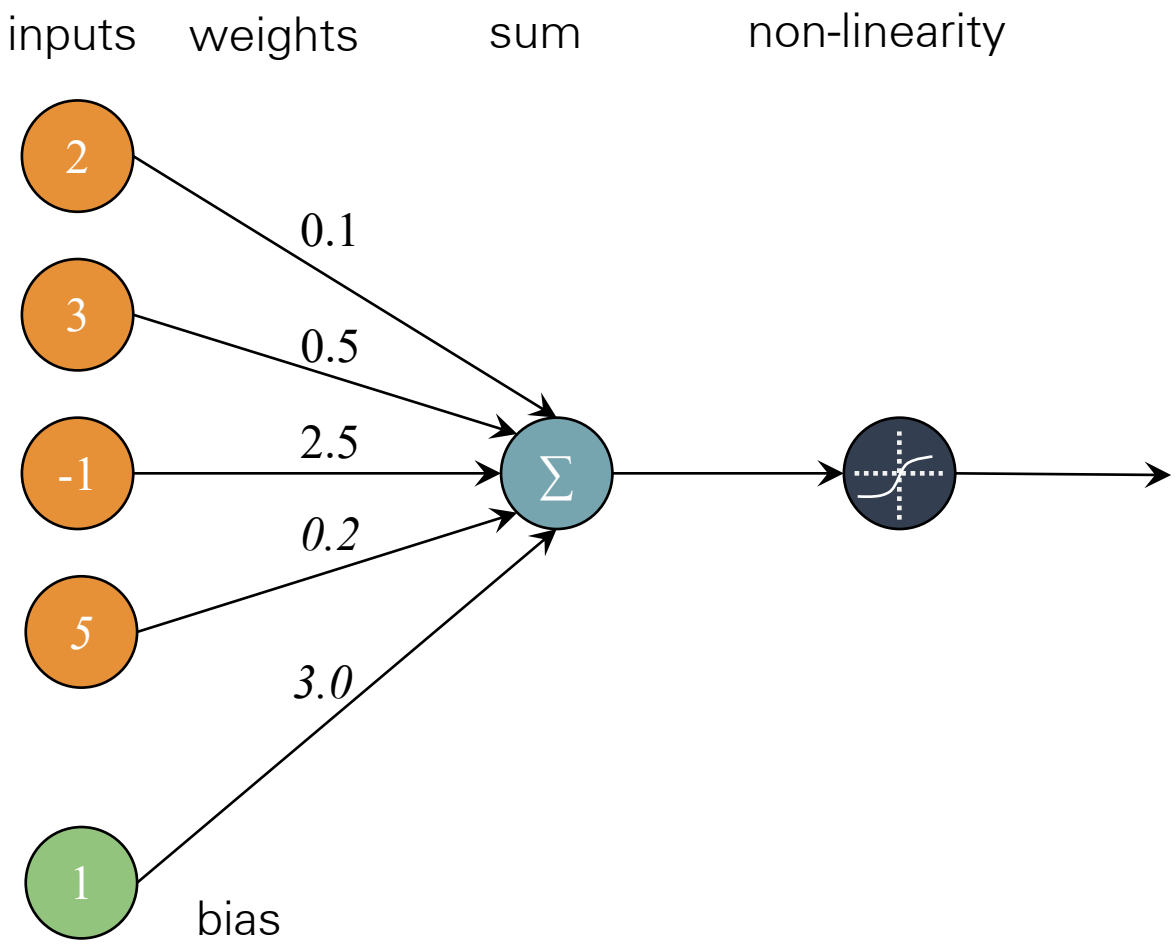
Perceptron Forward Pass

$$h(\mathbf{x}) = g(a(\mathbf{x})) = g(b + \sum_i w_i x_i)$$



Perceptron Forward Pass

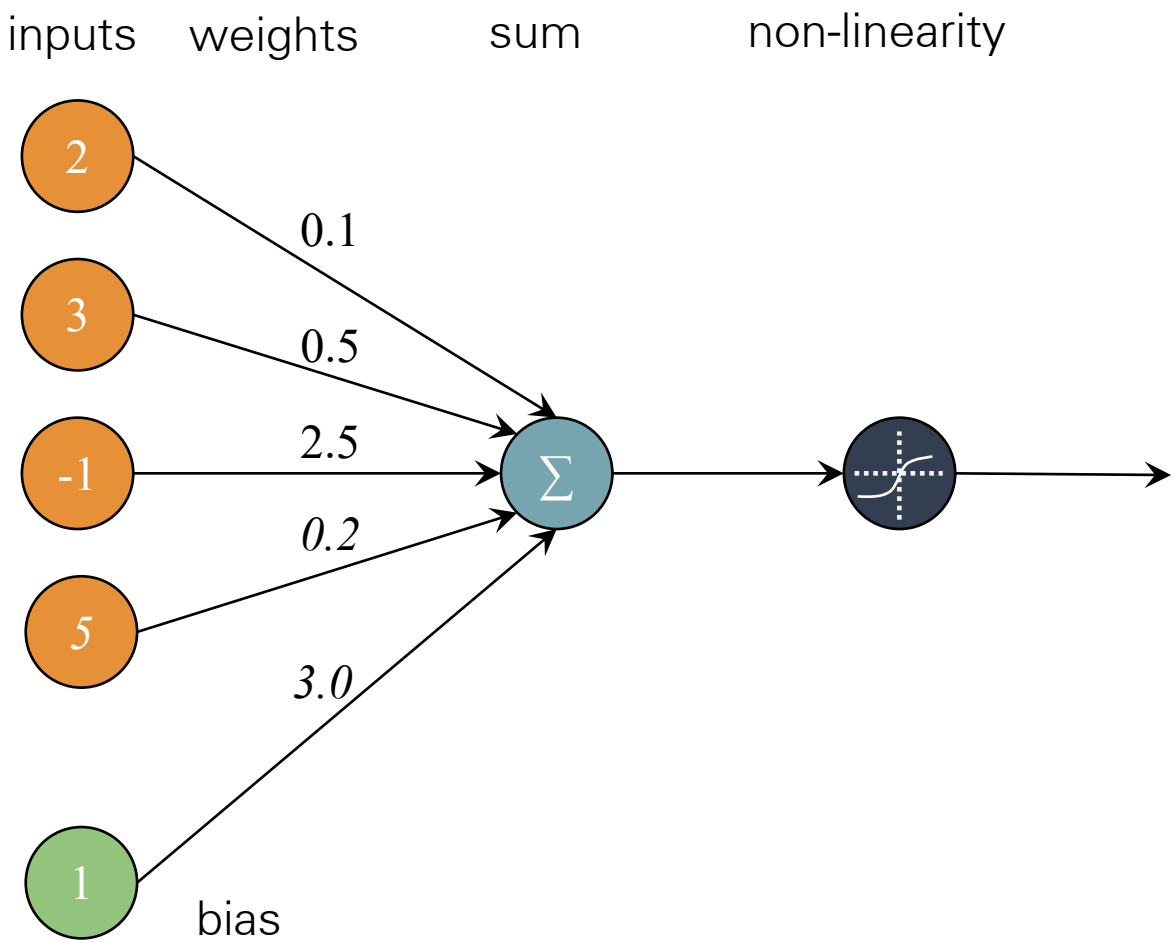
$$h(\mathbf{x}) = g\big((2*0.1) + (3*0.5) + (-1*2.5) + (5*0.2) + (1*3.0)\big)$$



Perceptron Forward Pass

$$h(\mathbf{x}) = g(3.2) = \sigma(3.2)$$

$$\frac{1}{1 + e^{-3.2}} = 0.96$$



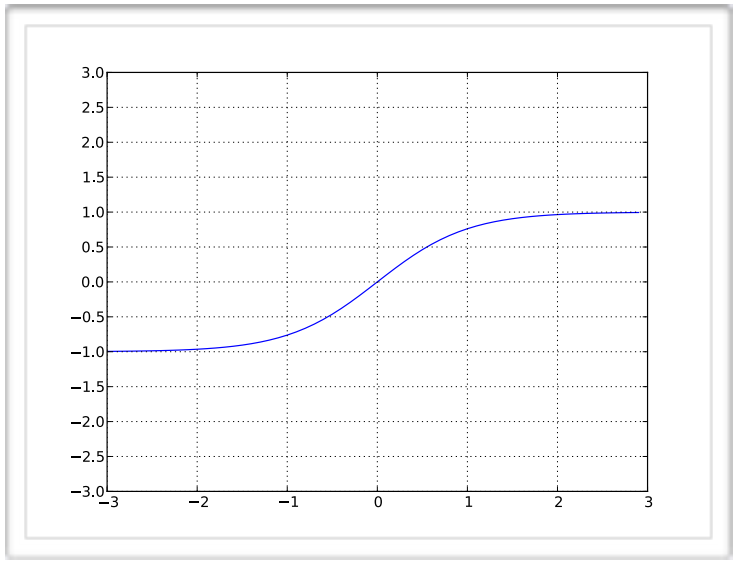
Hyperbolic Tangent (tanh) Activation Function

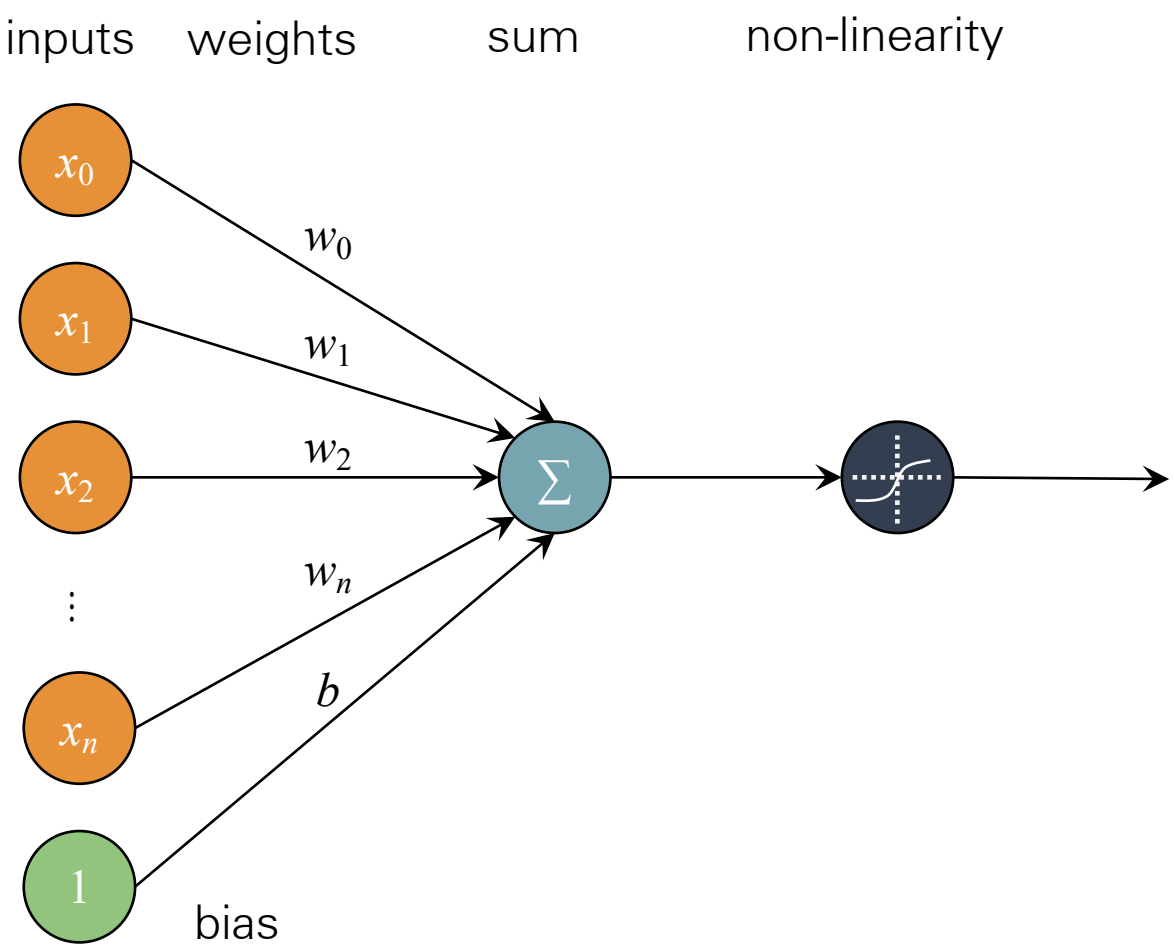
$$h(\mathbf{x}) = g(a(\mathbf{x})) = g(b + \sum_i w_i x_i)$$

$$g(a) = \tanh(a) =$$

$$= \frac{\exp(a) - \exp(-a)}{\exp(a) + \exp(-a)} = \frac{\exp(2a) - 1}{\exp(2a) + 1}$$

- Squashes the neuron's output between -1 and 1
- Can be positive or negative
- Bounded
- Strictly Increasing



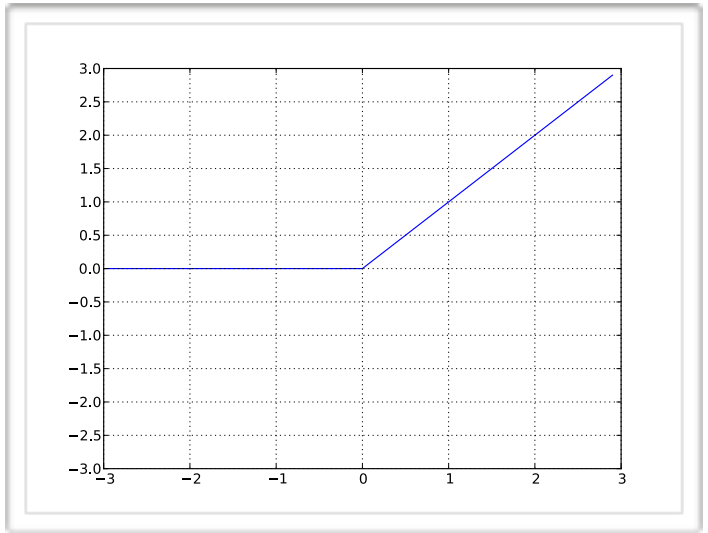


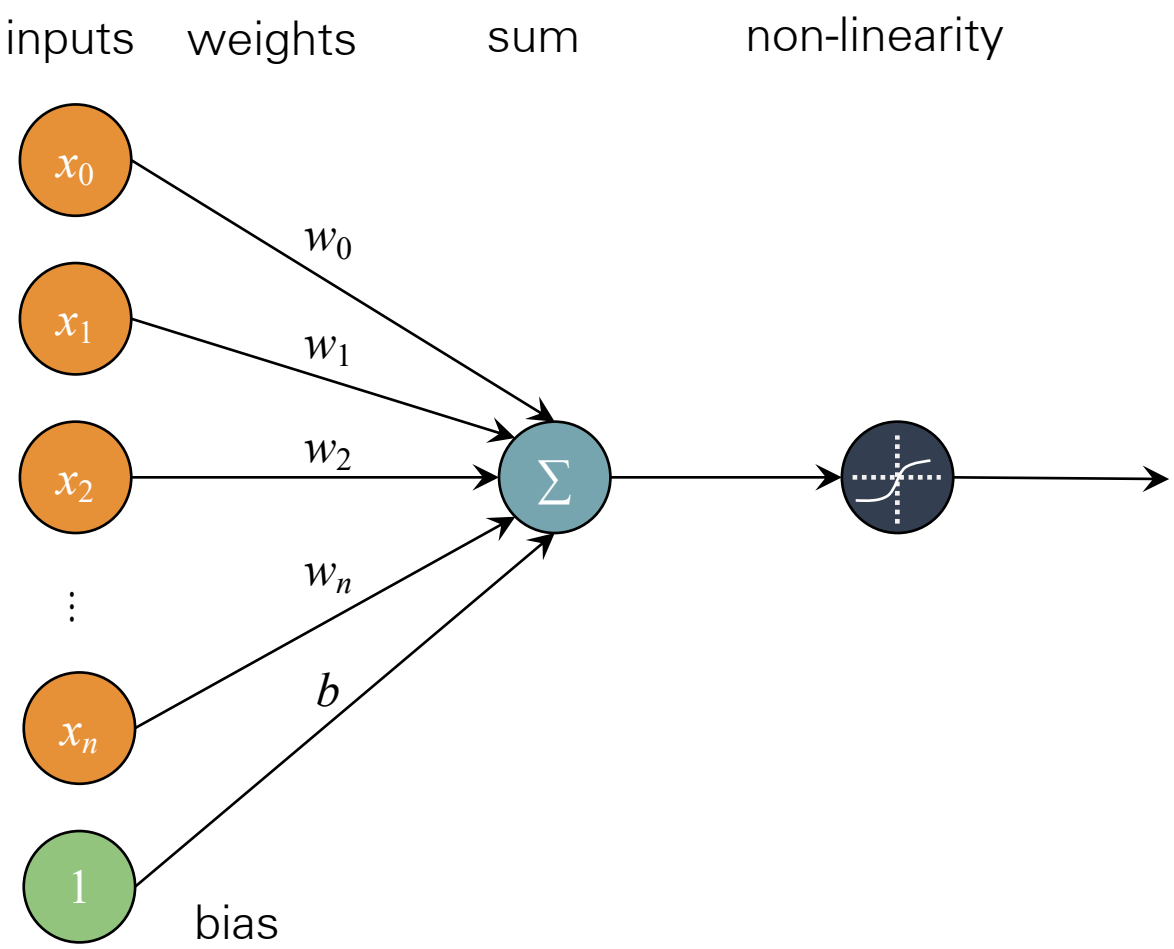
Rectified Linear (ReLU) Activation Function

$$h(\mathbf{x}) = g(a(\mathbf{x})) = g(b + \sum_i w_i x_i)$$

$$g(a) = \text{reclin}(a) = \max(0, a)$$

- Bounded below by 0 (always non-negative)
- Not upper bounded
- Strictly increasing
- Tends to produce units with sparse activities





Decision Boundary of a Neuron

- Could do binary classification:
  - with sigmoid, one can interpret neuron as estimating $p(y = 1 \mid \mathbf{x})$
  - also known as logistic regression classifier

  - if activation is greater than 0.5, predict 1
  - otherwise predict 0

Same idea can be applied to a tanh activation

Decision boundary is linear

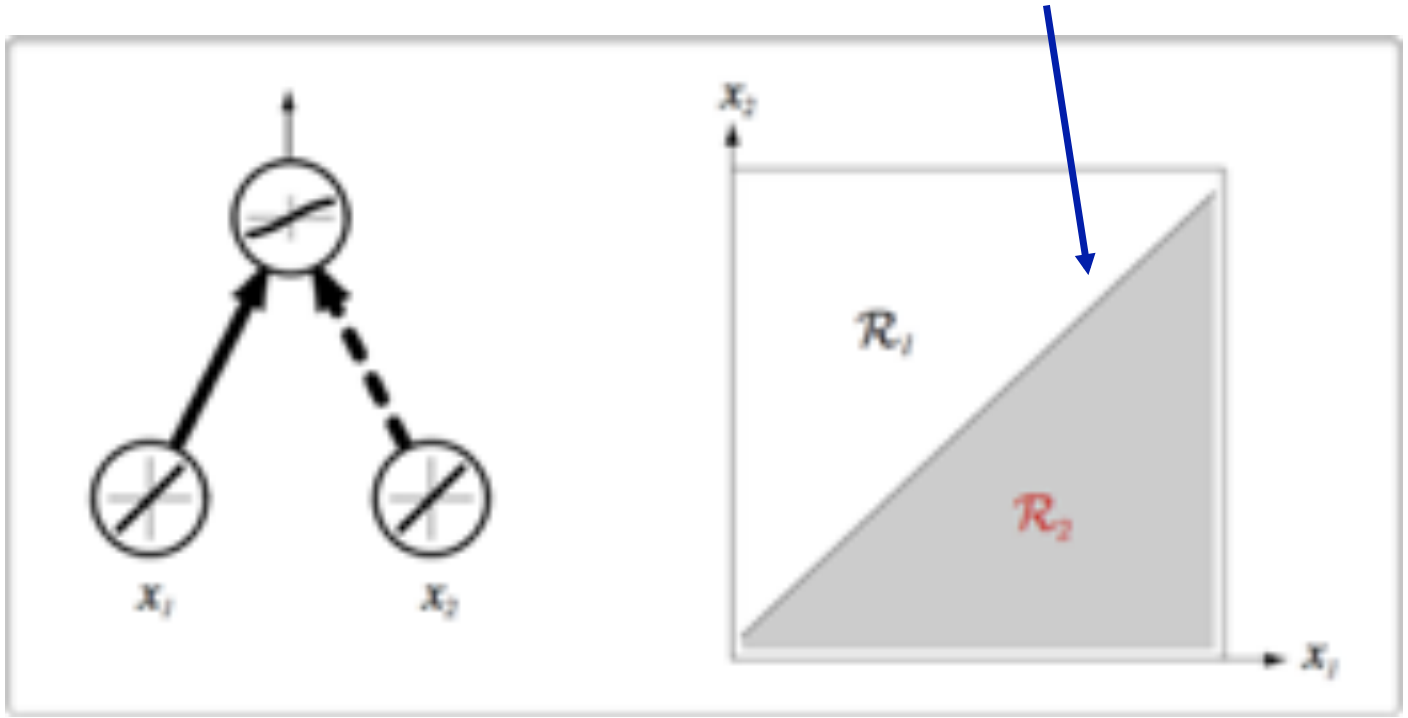
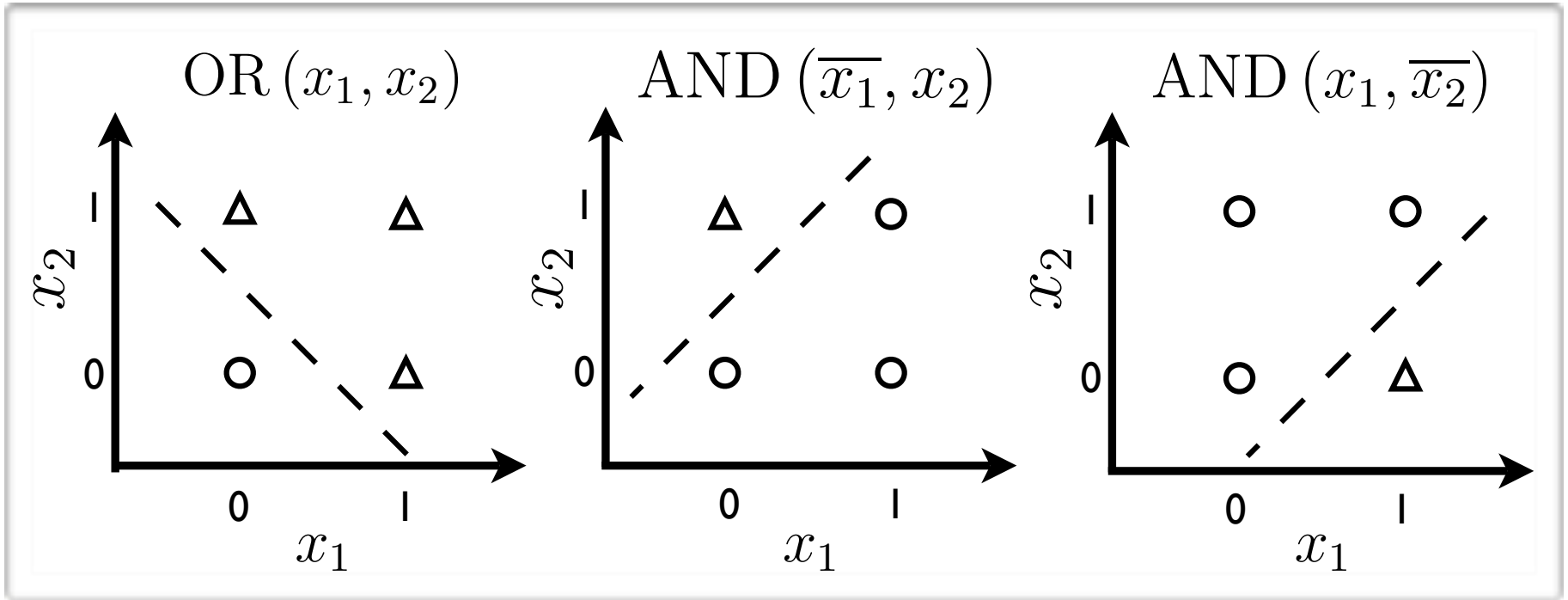


Image credit: Pascal Vincent

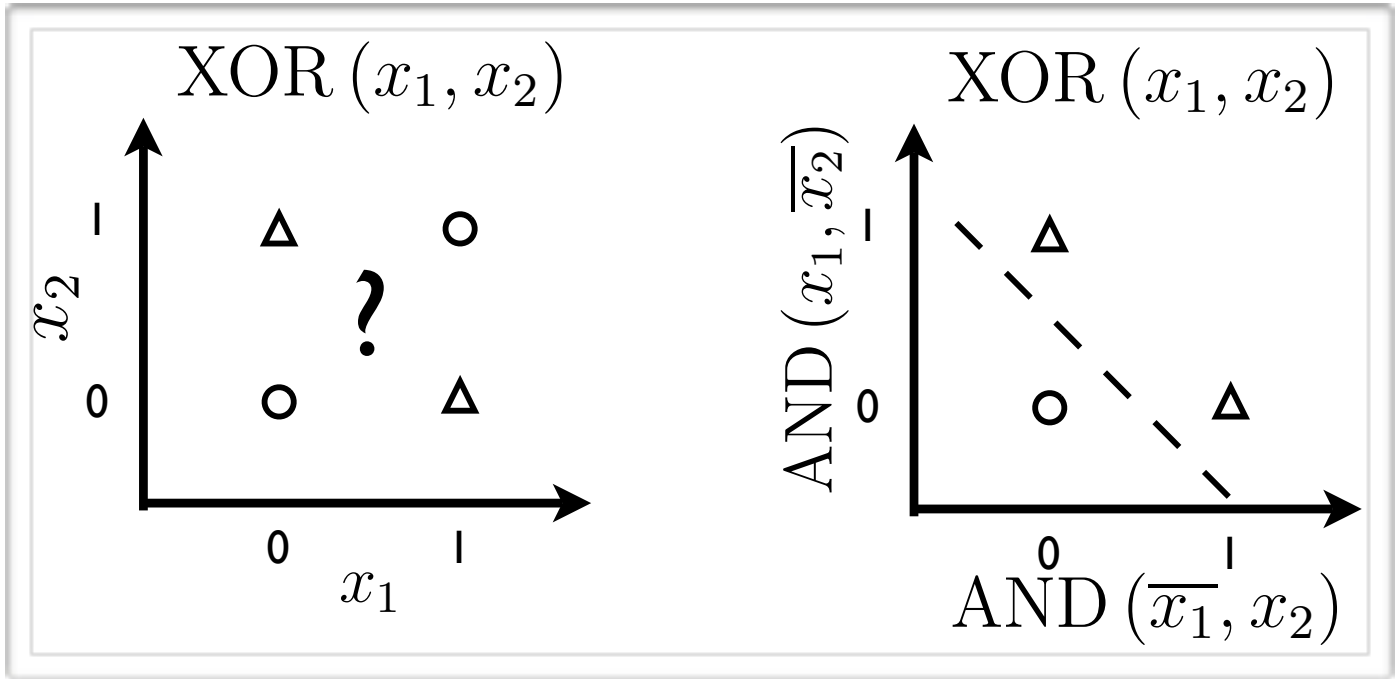
Capacity of Single Neuron

- Can solve linearly separable problems



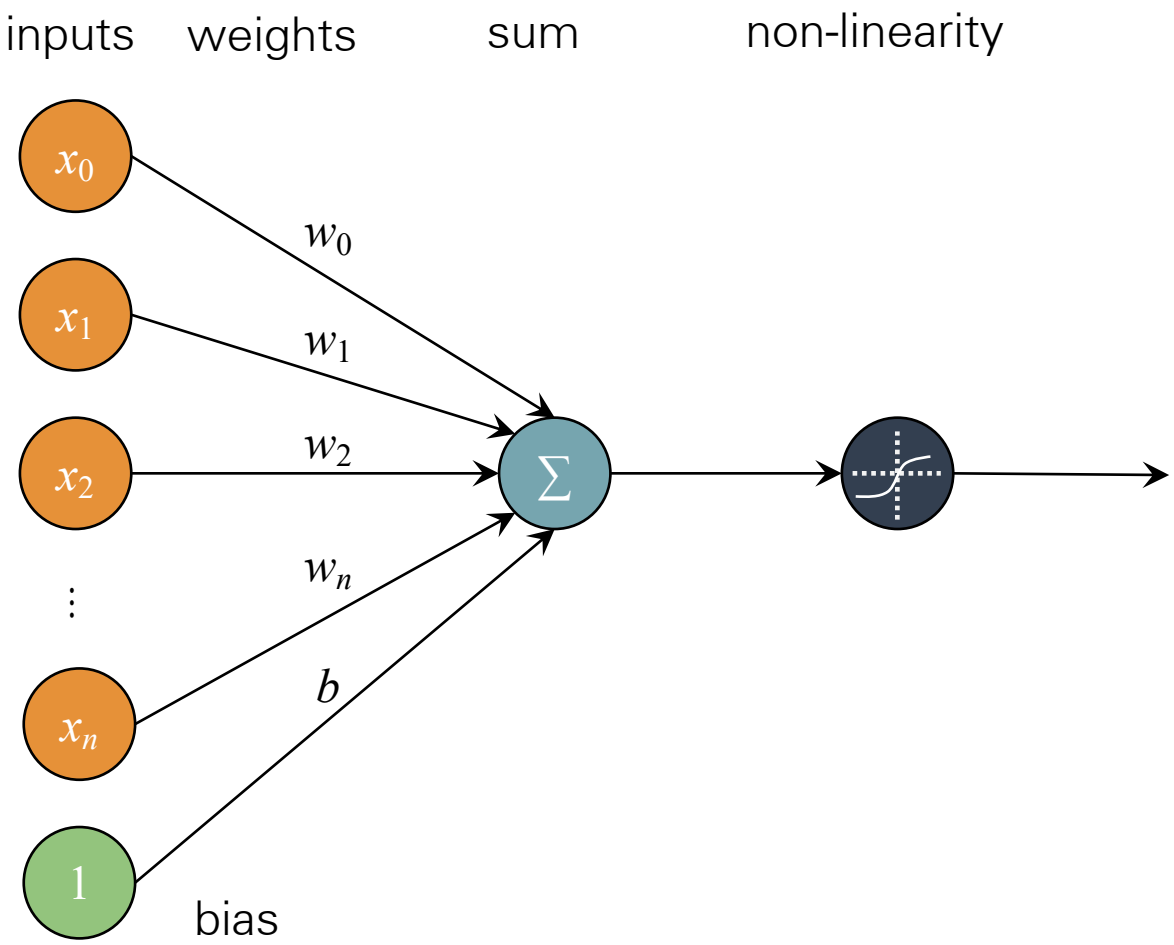
Capacity of Single Neuron

- Can not solve non-linearly separable problems

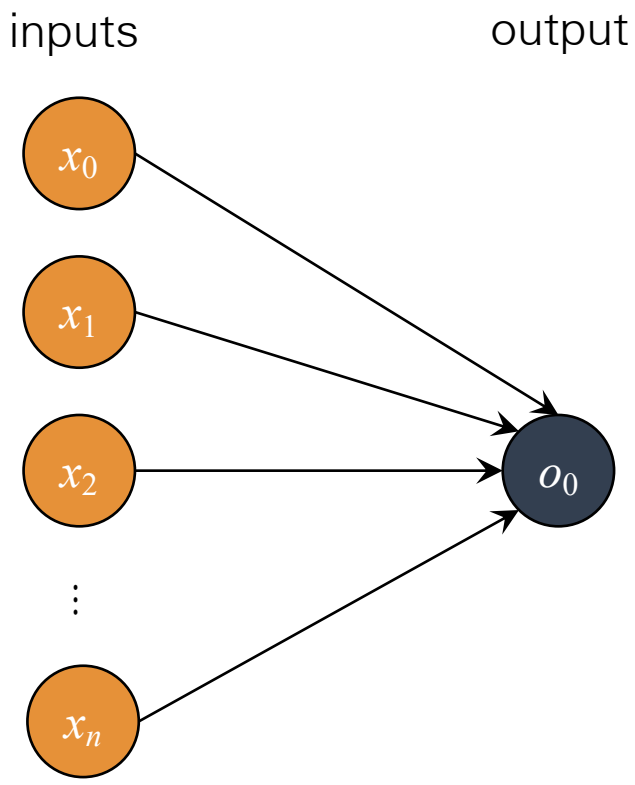


- Need to transform the input into a better representation
- Remember basis functions!

Perceptron Diagram Simplified



Perceptron Diagram Simplified



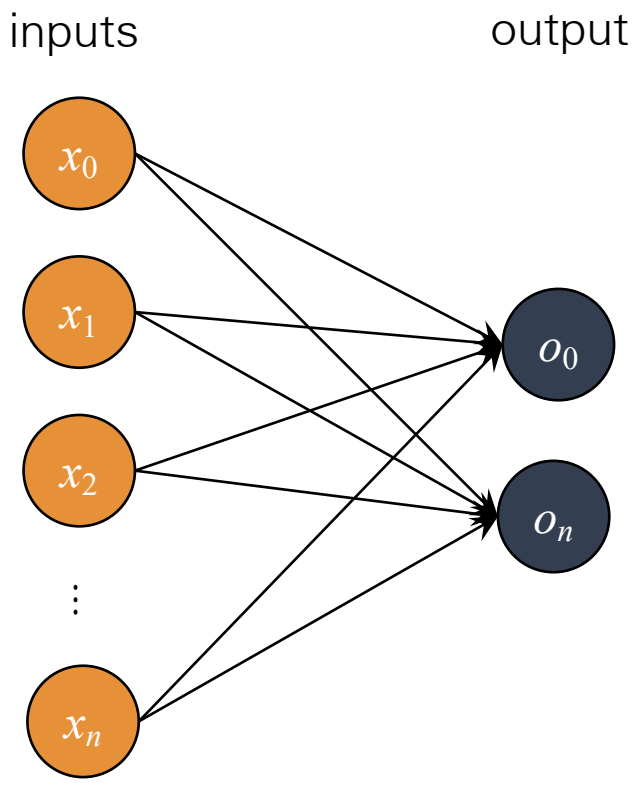
Multi-Output Perceptron

- Remember multi-way classification
  - We need multiple outputs (1 output per class)
  - We need to estimate conditional probability $p(y = \mathbf{c} \mid \mathbf{x})$
  - Discriminative Learning

- Softmax activation function at the output

$$\mathbf{o}(\mathbf{a}) = \mathrm{softmax}(\mathbf{a}) = \left[\frac{\exp(a_1)}{\sum_c \exp(a_c)} \cdots \frac{\exp(a_C)}{\sum_c \exp(a_c)} \right]^\top$$

  - strictly positive
  - sums to one



- Predict class with the highest estimated class conditional probability.

Multi-Layer Perceptron

Single Hidden Layer Neural Network

- Hidden layer pre-activation:

$$\mathbf{a}(\mathbf{x}) = \mathbf{b}^{(1)} + \mathbf{W}^{(1)}\mathbf{x}$$

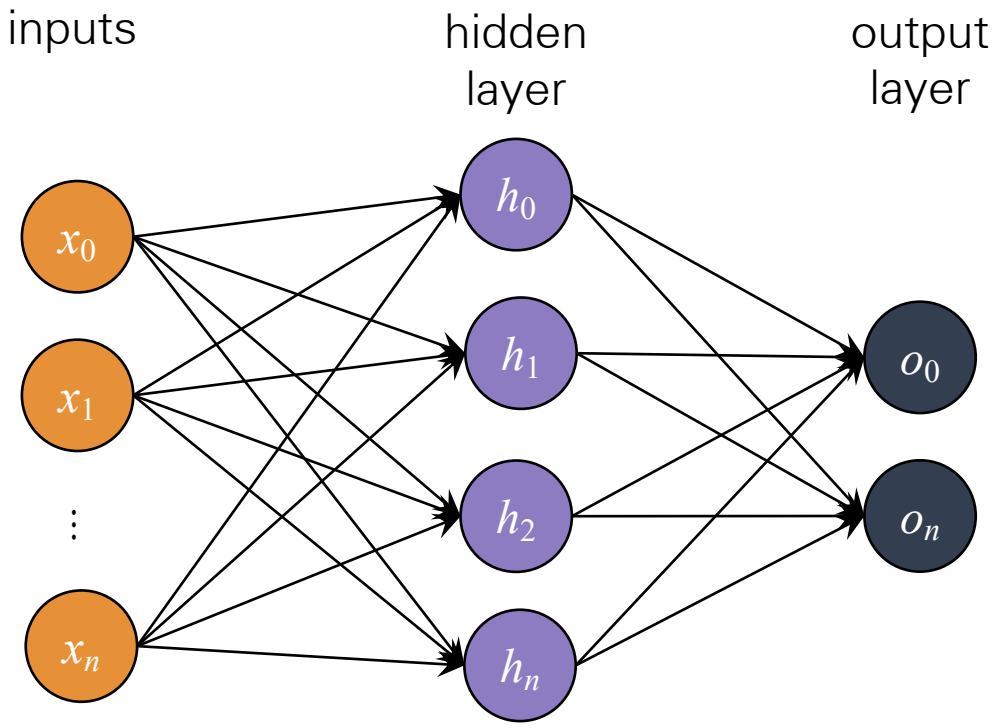
$$\left(a(\mathbf{x})_i = b_i^{(1)} + \sum_j W_{i,j}^{(1)} x_j\right)$$

- Hidden layer activation:

$$\mathbf{h}(\mathbf{x}) = \mathbf{g}(\mathbf{a}(\mathbf{x}))$$

- Output layer activation:

$$\mathbf{o}(\mathbf{x}) = \mathbf{o}\left(b^{(2)} + \mathbf{w}^{(2)\top}\mathbf{h}^{(1)}\mathbf{x}\right)$$



Multi-Layer Perceptron (MLP)

- Consider a network with L hidden layers.
  - layer pre-activation for k>0

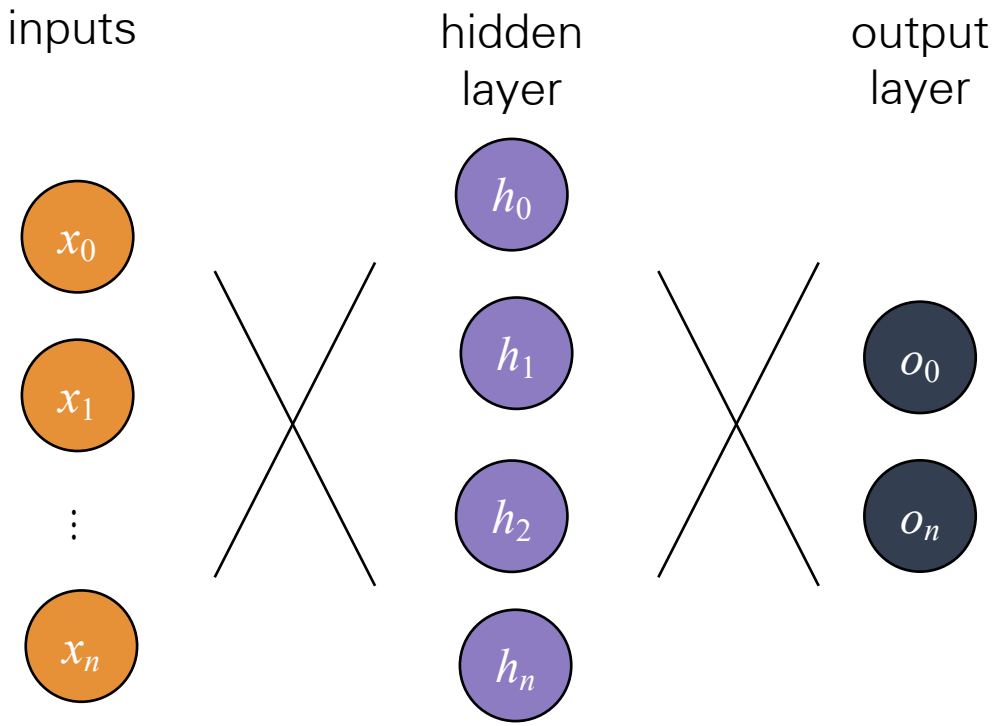
$$\mathbf{a}^{(k)}(\mathbf{x}) = \mathbf{b}^{(k)} + \mathbf{W}^{(k)}\mathbf{h}^{(k-1)}(\mathbf{x})$$

  - hidden layer activation from 1 to L:

$$\mathbf{h}^{(k)}(\mathbf{x}) = \mathbf{g}(\mathbf{a}^{(k)}(\mathbf{x}))$$

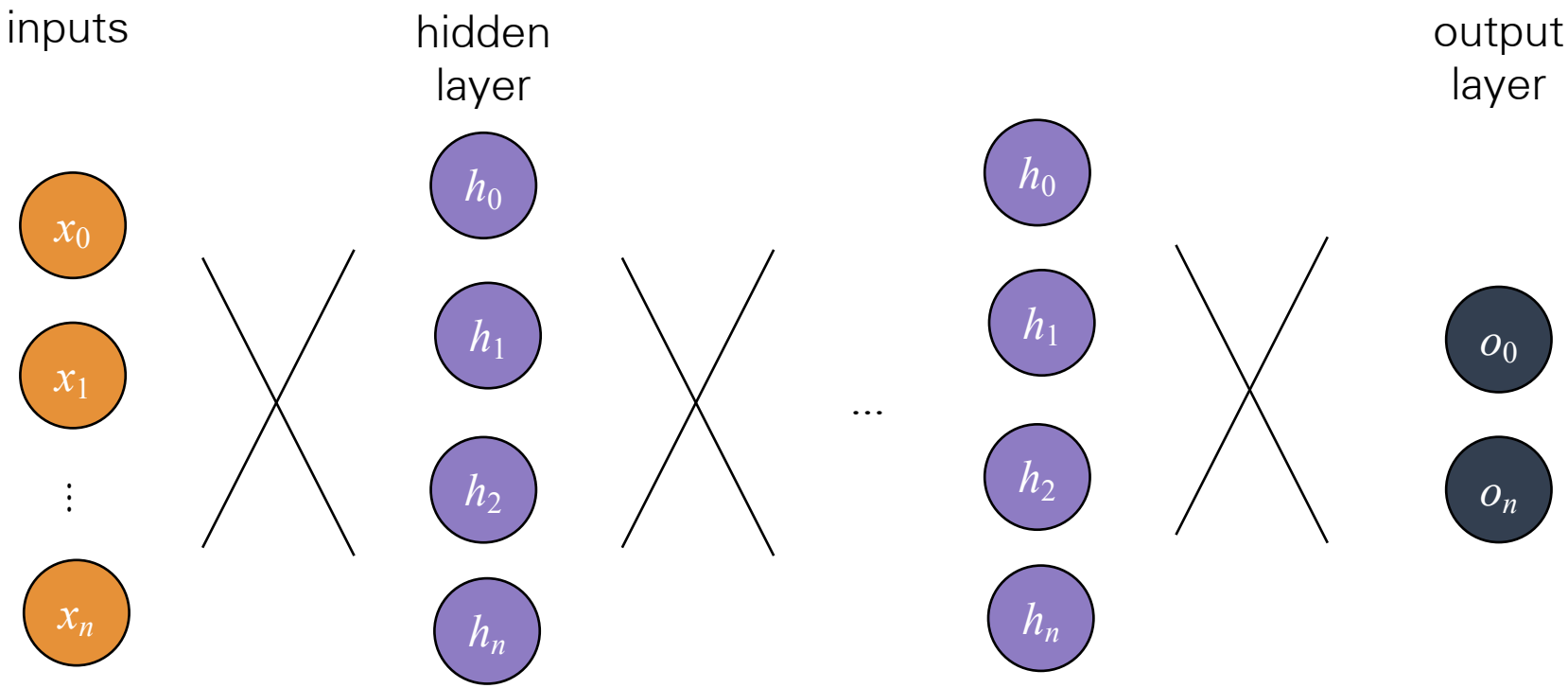
  - output layer activation (k=L+1)

$$\mathbf{h}^{(L+1)}(\mathbf{x}) = \mathbf{o}(\mathbf{a}^{(L+1)}(\mathbf{x})) = \mathbf{f}(\mathbf{x})$$



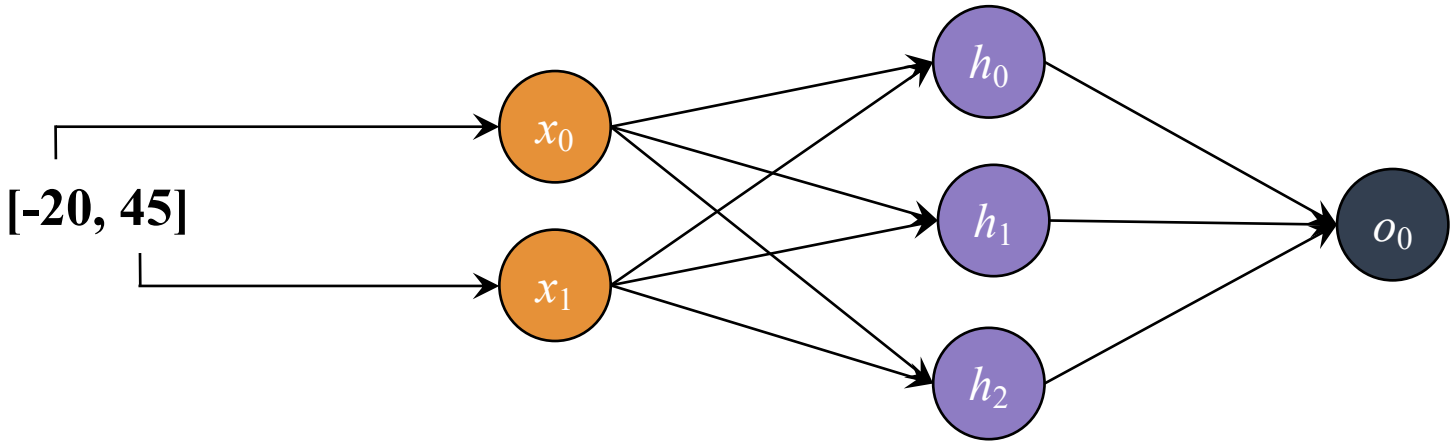
$$(\mathbf{h}^{(0)}(\mathbf{x}) = \mathbf{x})$$

Deep Neural Network



Applying Neural Networks

Quantifying Loss



Predicted: 0.05

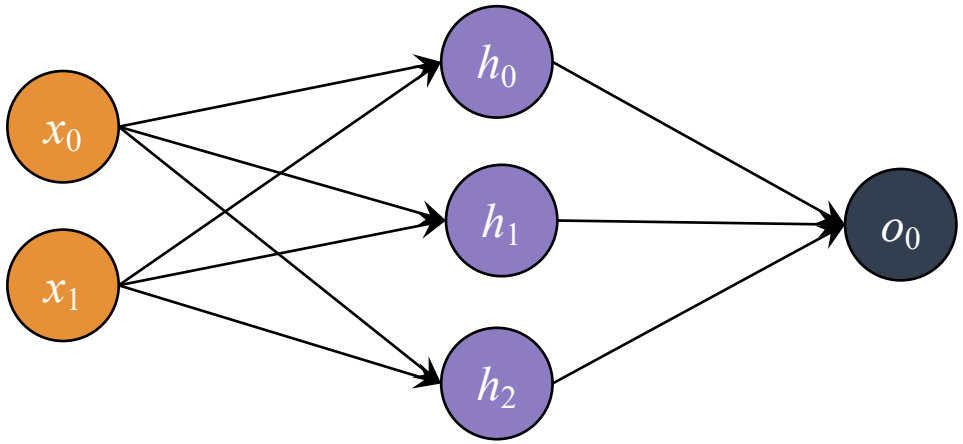
Actual: 1

$$\ell(\underbrace{f(\mathbf{x}^{(i)};\theta)}_{\text{Predicted}}, \underset{\text{Actual}}{y^{(i)}})$$

Total Loss

Input

[
[-20, 45],
[80, 0],
[4, 15],
[45, 60],
]



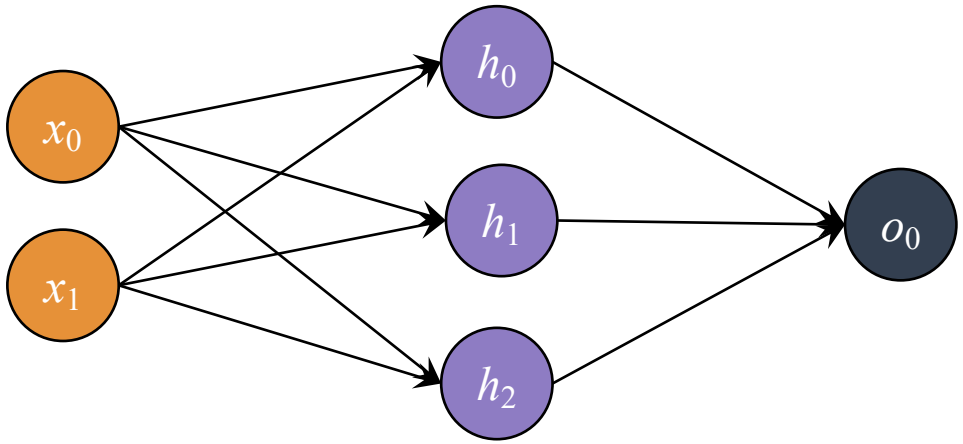
Predicted	Actual
[	[
0.05	1
0.02	0
0.96	1
0.35	1
]	]

$$J(\theta) = \frac{1}{N} \sum_i \ell(\underbrace{f(\mathbf{x}^{(i)}; \theta)}_{\text{Predicted}}, \underbrace{y^{(i)}}_{\text{Actual}})$$

Total Loss

Input

[
[-20, 45],
[80, 0],
[4, 15],
[45, 60],
]



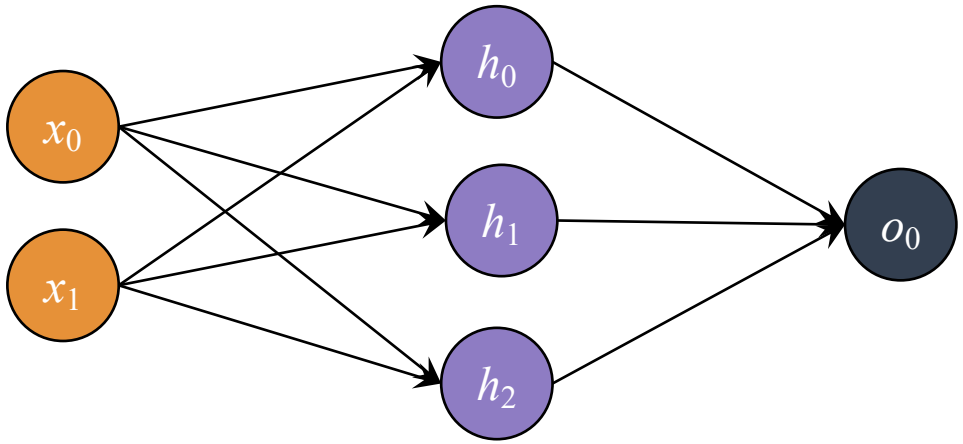
Predicted	Actual
[	[
0.05	1
0.02	0
0.96	1
0.35	1
]	]

$$J(\theta) = \frac{1}{N} \sum_i \ell(\underbrace{f(\mathbf{x}^{(i)}; \theta)}_{\text{Predicted}}, \underbrace{y^{(i)}}_{\text{Actual}})$$

Binary Cross Entropy Loss

Input

[
[-20, 45],
[80, 0],
[4, 15],
[45, 60],
]



Predicted	Actual
[	[
0.05	1
0.02	0
0.96	1
0.35	1
]	]

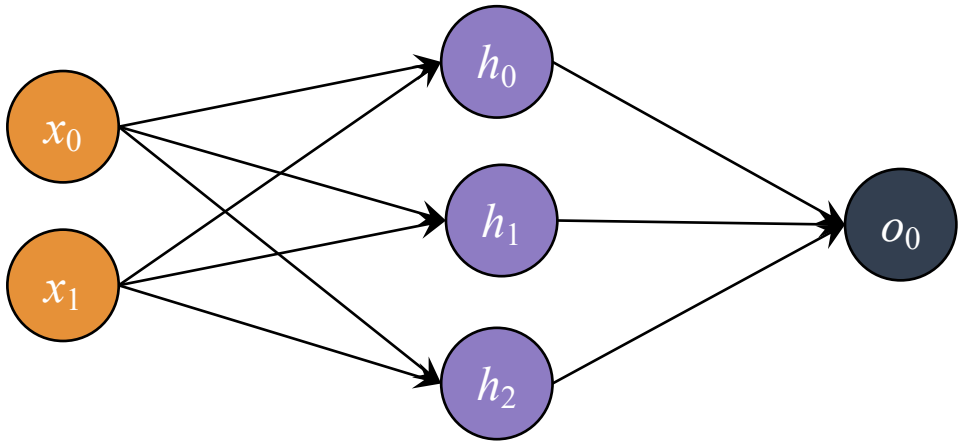
$$J_{\text{cross_entropy}}(\theta) = \frac{1}{N} \sum_i y^{(i)} \log(f(\mathbf{x}^{(i)}; \theta)) + (1 - y^{(i)}) \log(1 - f(\mathbf{x}^{(i)}; \theta)))$$

- For classification problems with a softmax output layer.
- Maximize log-probability of the correct class given an input

Binary Cross Entropy Loss

Input

[
[-20, 45],
[80, 0],
[4, 15],
[45, 60],
]



Predicted	Actual
[	[
0.05	1
0.02	0
0.96	1
0.35	1
]	]

$$J_{\mathrm{MSE}}(\theta) = \frac{1}{N} \sum_i \left(f(\mathbf{x}^{(i)}; \theta) - y^{(i)} \right)^2$$

Training Neural Networks

Training

$$J(\theta) = \arg\min_{\boldsymbol{\theta}} \frac{1}{T} \sum_t \underbrace{l(f(\mathbf{x}^{(t)}; \boldsymbol{\theta}), y^{(t)})}_{\text{Loss function}} + \underbrace{\lambda \Omega(\boldsymbol{\theta})}_{\text{Regularizer}}$$

$$\theta = W_1, W_2 \ldots W_n$$

- Learning is cast as optimization.
  - For classification problems, we would like to minimize classification error
  - Loss function can sometimes be viewed as a surrogate for what we want to optimize (e.g. upper bound)

What is a neural network again?

- A family of parametric, non-linear and hierarchical representation learning functions

- $a_L(x; \theta_{1,\ldots,L}) = h_L(h_{L-1}(\ldots h_1(x, \theta_1), \theta_{L-1}), \theta_L)$
  - x: input, θ_l: parameters for layer l, $a_l = h_l(x, \theta_l)$: (non-)linear function

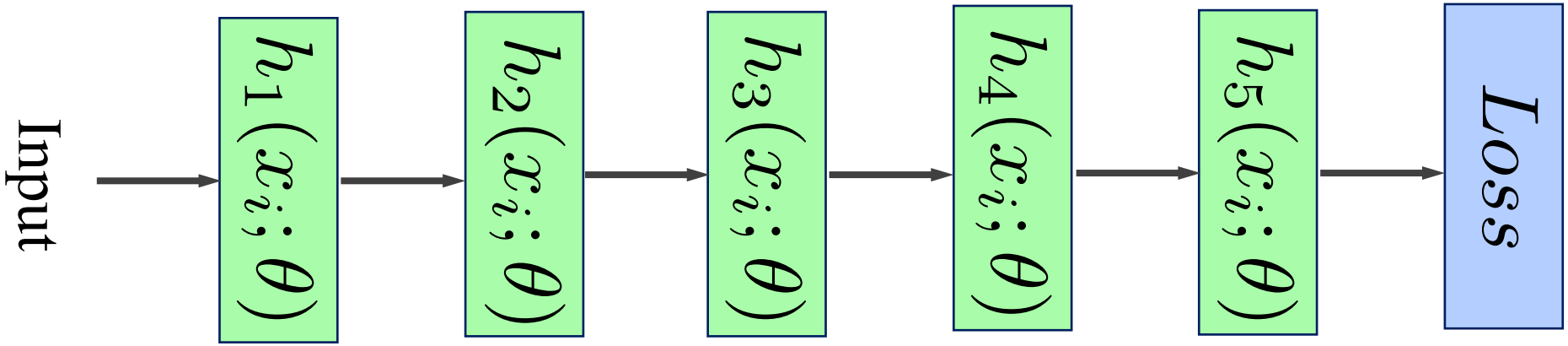
- Given training corpus $\{X, Y\}$ find optimal parameters

$$\theta^* \leftarrow \arg\min_{\theta} \sum_{(x,y)\in(X,Y)} \ell(y, a_L(x; \theta_{1,\ldots,L}))$$

Neural network models

- A neural network model is a series of hierarchically connected functions
- The hierarchy can be very, very complex

Forward connections (Feedforward architecture)



Neural network models

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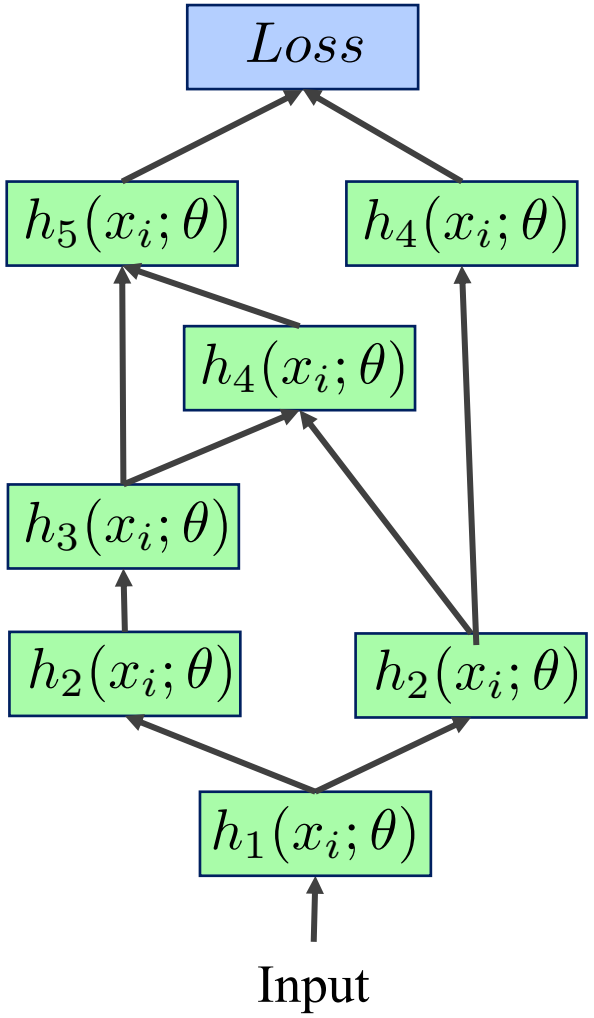
- The hierarchy can be very, very complex

Interweaved connections (Directed Acyclic Graph architecture – DAGNN)



Neural network models

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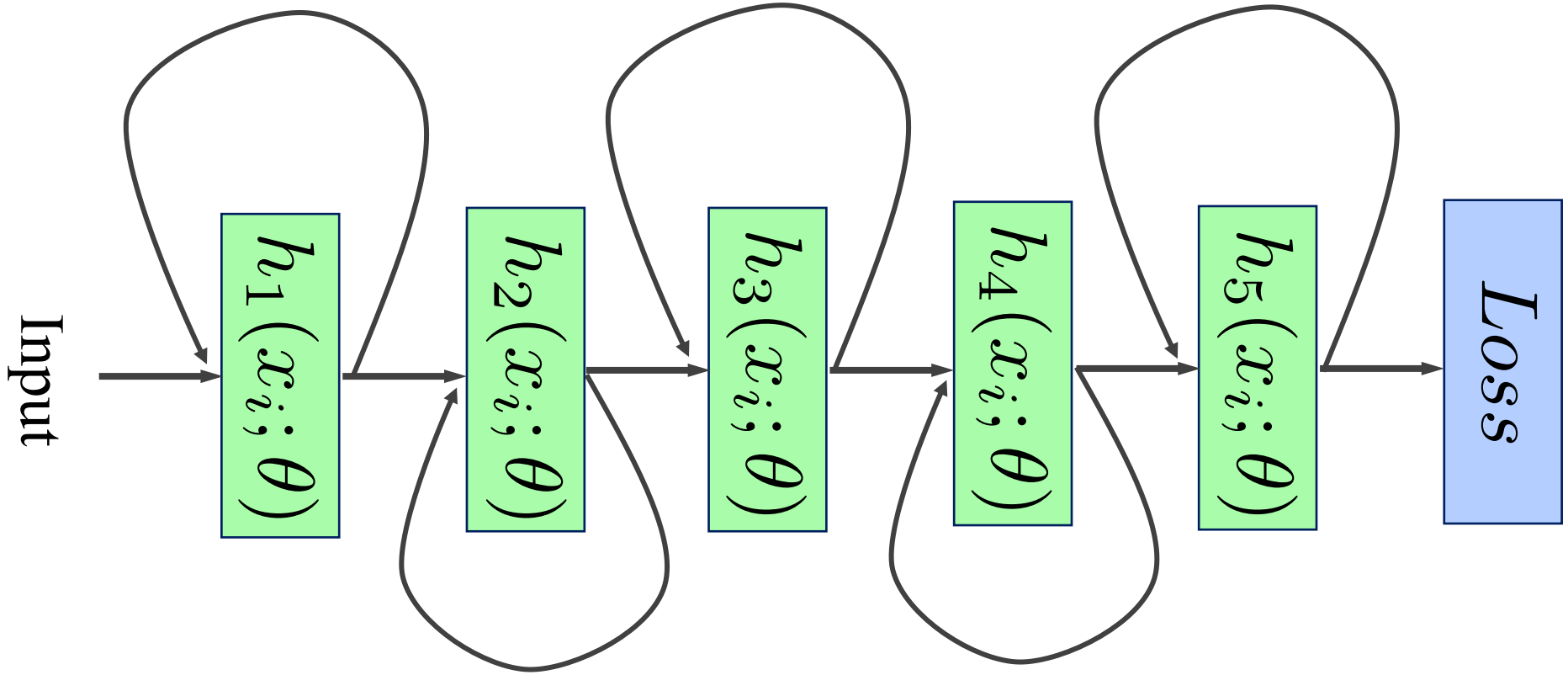
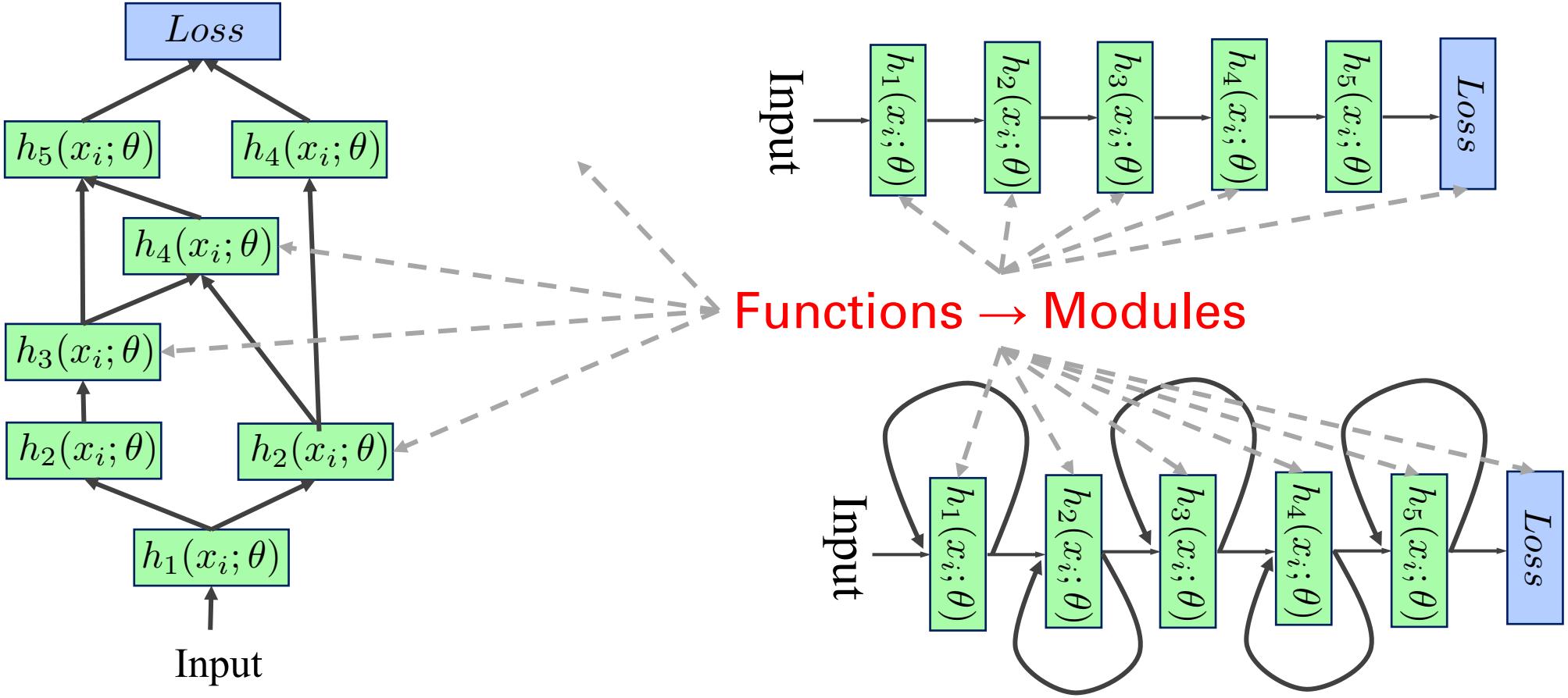


Loopy connections (Recurrent architecture, special care needed)

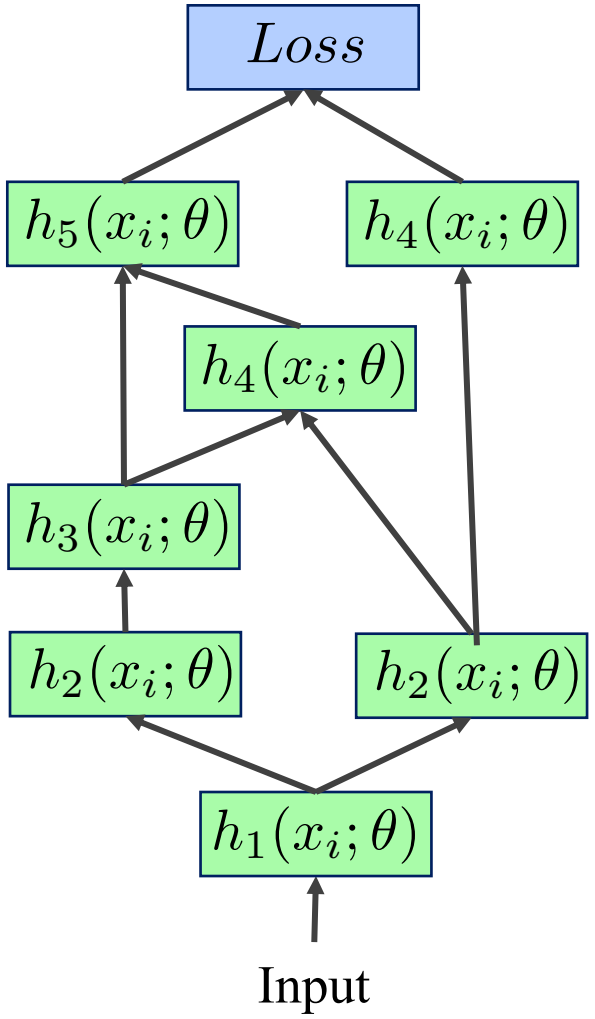
Neural network models

- A neural network model is a series of hierarchically connected functions
- The hierarchy can be very, very complex



What is a module

- A module is a building block for our network
- Each module is an object/function $a = h(x; \theta)$ that
  - Contains trainable parameters (θ)
  - Receives as an argument an input x
  - And returns an output a based on the activation function $h(...)$
- The activation function should be (at least) first order differentiable (almost) everywhere
- For easier/more efficient backpropagation
  $\rightarrow$ <u>store module input</u>
  - easy to get module output fast
  - easy to compute derivatives

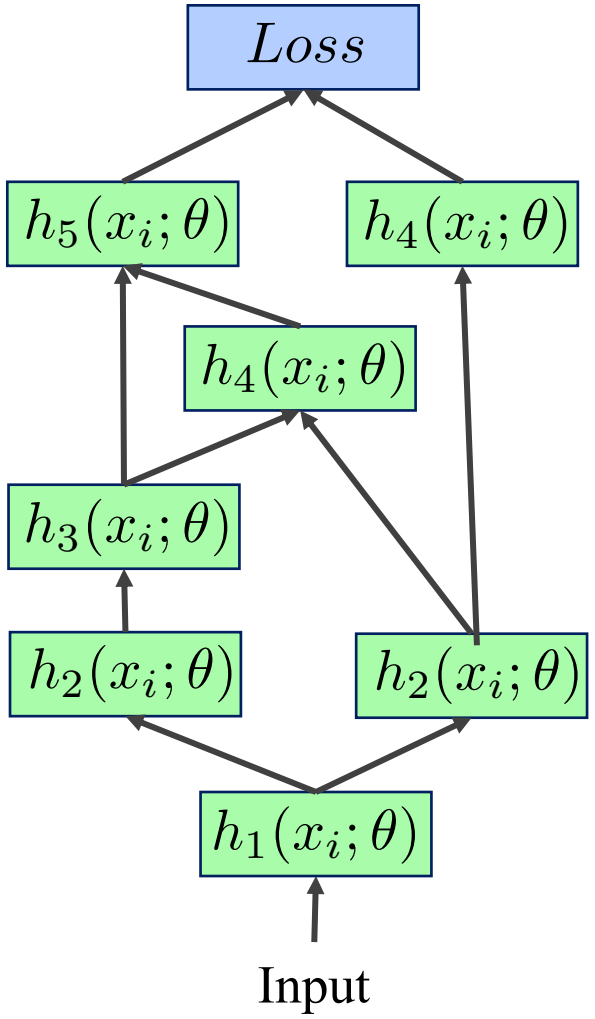


What is a module

- Simply compute the activation of each module in the network

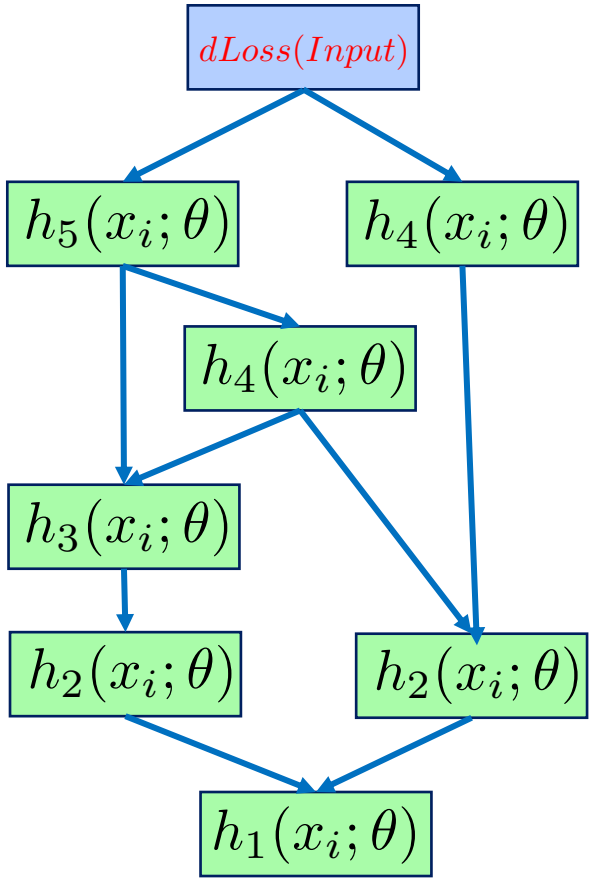
$$a_l = h_l(x_l; \theta) \text{ where } a_l = x_{l+1} \text{ or } x_l = a_{l-1}$$

- We need to know the precise function behind each module $h_l(\dots)$
- Recursive operations
  - One module's output is another's input
- Steps
  - Visit modules one by one starting from the data input
  - Some modules might have several inputs from multiple modules
- Compute modules activations **with the right order**
  - Make sure all the inputs computed at the right time



What is a module

- Simply compute the gradients of each module for our data
  - We need to know the gradient formulation of each module $\partial h_l(x_l;\theta_l)$ w.r.t. their inputs x_l and parameters θ_l
- We need the forward computations first
  - Their result is the sum of losses for our input data
- Then take the reverse network (reverse connections) and traverse it backwards
- Instead of using the activation functions, we use their gradients
- The whole process can be described very neatly and concisely with the backpropagation algorithm



Again, what is a neural network again?

- $a_L(x; \theta_{1,\ldots,L}) = h_L(h_{L-1}(\ldots h_1(x, \theta_1), \theta_{L-1}), \theta_L)$
  - x: input, θ_l: parameters for layer l, $a_l = h_l(x, \theta_l)$: (non-)linear function
- Given training corpus $\{X, Y\}$ find optimal parameters

$$\theta^* \leftarrow \arg\min_{\theta} \sum_{(x,y)\in(X,Y)} \ell(y, a_L(x; \theta_{1,\ldots,L}))$$

- To use any gradient descent based optimization

$$\left(\theta^{t+1} = \theta^t - \eta_t \frac{\partial \mathcal{L}}{\partial \theta^t}\right)$$

we need the gradients

$$\frac{\partial \mathcal{L}}{\partial \theta_l}, l = 1, \ldots, L$$

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- How to compute the gradients for such a complicated function enclosing other functions, like a_L (…)?

How do we compute gradients?

- Numerical Differentiation
- Symbolic Differentiation
- Automatic Differentiation (AutoDiff)

Numerical Differentiation

$\mathbf{1}_i$ - Vector of all zeros, except for one 1 in i-th location

- We can approximate the gradient numerically, using:

$$\frac{\partial f(\mathbf{x})}{\partial x_i} \approx \lim_{h \to 0} \frac{f(\mathbf{x} + h\mathbf{1}_i) - f(\mathbf{x})}{h}$$

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- Even better, we can use central differencing:

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- However, both of these suffer from rounding errors and are not good enough for learning (they are very good tools for checking the correctness of implementation though, e.g., use $h = 0.000001$).

Numerical Differentiation

$\mathbf{1}_i$ - Vector of all zeros, except for one 1 in i-th location

$\mathbf{1}_{ij}$ - Matrix of all zeros, except for one 1 in (i,j)-th location

- We can approximate the gradient numerically, using:

$$\frac{\partial \mathcal{L}(\mathbf{W}, \mathbf{b})}{\partial w_{ij}} \approx \lim_{h \to 0} \frac{\mathcal{L}(\mathbf{W} + h\mathbf{1}_{ij}, \mathbf{b}) - \mathcal{L}(\mathbf{W}, \mathbf{b})}{h} \qquad \frac{\partial \mathcal{L}(\mathbf{W}, \mathbf{b})}{\partial b_j} \approx \lim_{h \to 0} \frac{\mathcal{L}(\mathbf{W}, \mathbf{b} + h\mathbf{1}_j) - \mathcal{L}(\mathbf{W}, \mathbf{b})}{h}$$

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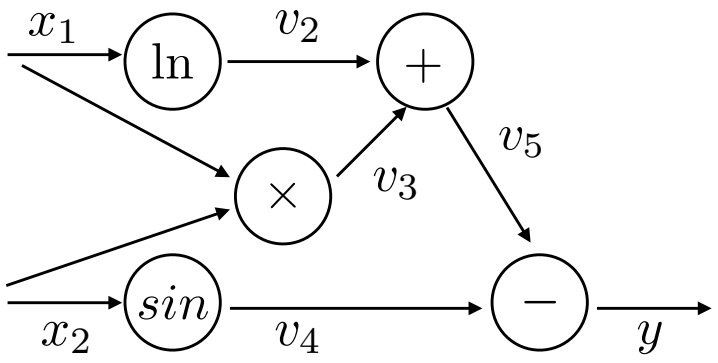
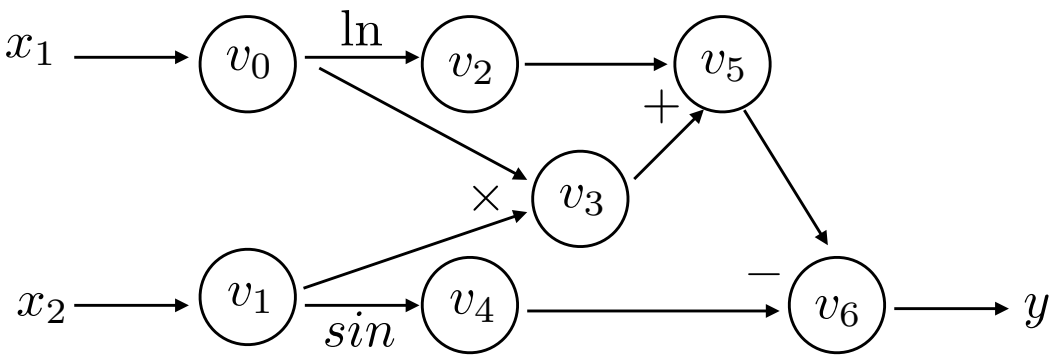
$$y = f(x_1, x_2) = \ln(x_1) + x_1 x_2 - sin(x_2)$$

Symbolic Differentiation

- Input function is represented as **computational graph** (a symbolic tree)





- Implements differentiation rules for composite functions:

Sum Rule

$$\frac{\mathrm{d}\left(f(x) + g(x)\right)}{\mathrm{d}x} = \frac{\mathrm{d}f(x)}{\mathrm{d}x} + \frac{\mathrm{d}g(x)}{\mathrm{d}x}$$

Product Rule

$$\frac{\mathrm{d}\left(f(x) \cdot g(x)\right)}{\mathrm{d}x} = \frac{\mathrm{d}f(x)}{\mathrm{d}x} g(x) + f(x) \frac{\mathrm{d}g(x)}{\mathrm{d}x}$$

Chain Rule

$$\frac{\mathrm{d}(f(g(x)))}{\mathrm{d}x} = \frac{\mathrm{d}f(g(x))}{\mathrm{d}x} \cdot \frac{\mathrm{d}g(x)}{\mathrm{d}x}$$

Problem: For complex functions, expressions can be exponentially large; also difficult to deal with piece-wise functions (creates many symbolic cases)

slide adopted from T. Chen, H. Shen, A. Krishnamurthy

Automatic Differentiation (AutoDiff)

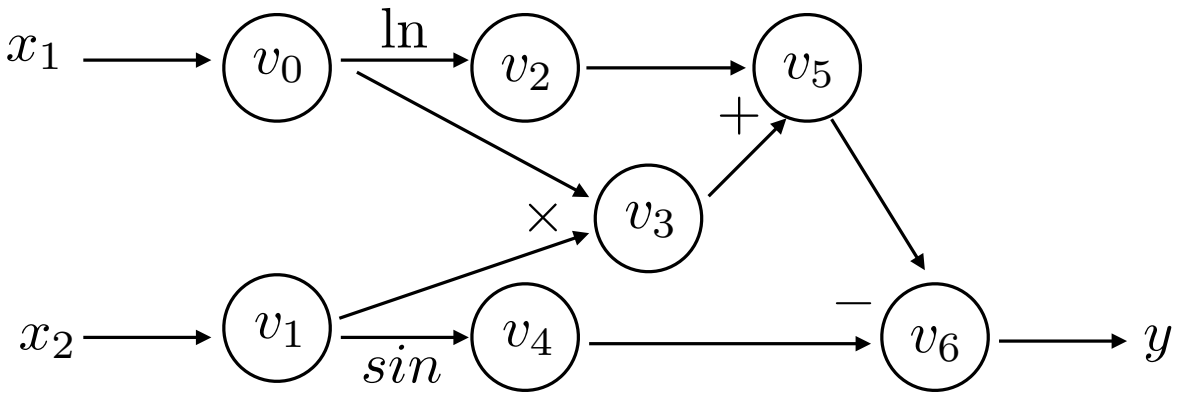
- **Intuition:** Interleave symbolic differentiation and simplification
- **Key Idea:** Apply symbolic differentiation at the elementary operation level, evaluate and keep intermediate results

Success of **deep learning** owes A LOT to success of AutoDiff algorithms
(also to advances in parallel architectures, and large datasets, ...)

slide adopted from T. Chen, H. Shen, A. Krishnamurthy

Automatic Differentiation (AutoDiff)

$$y = f(x_1, x_2) = \ln(x_1) + x_1 x_2 - sin(x_2)$$



- Each **node** is an input, intermediate, or output variable
- **Computational graph** (a DAG) with variable ordering from topological sort.

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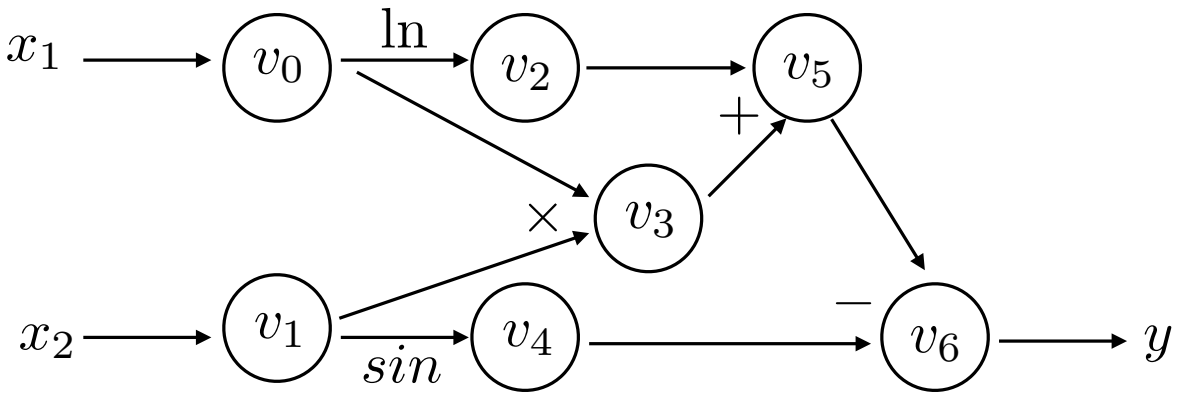

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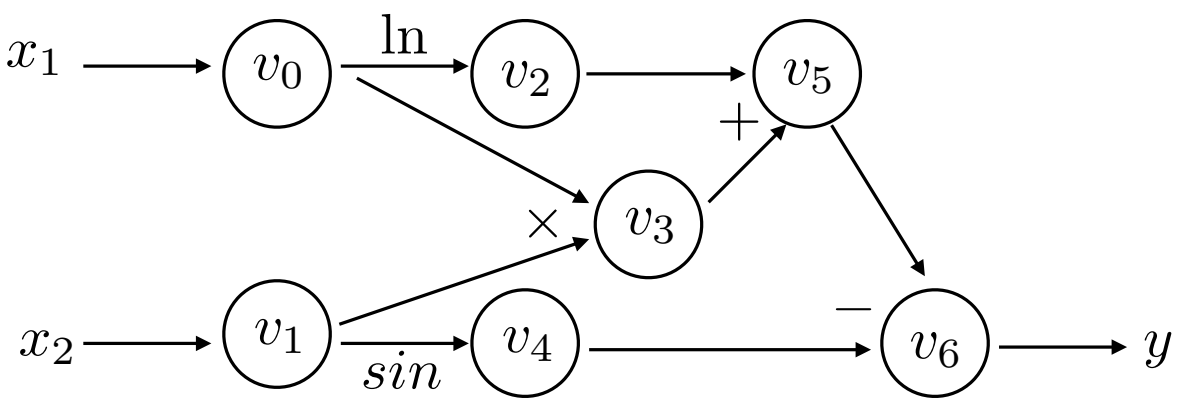
Lets see how we can **evaluate a function** using computational graph (DNN inferences)



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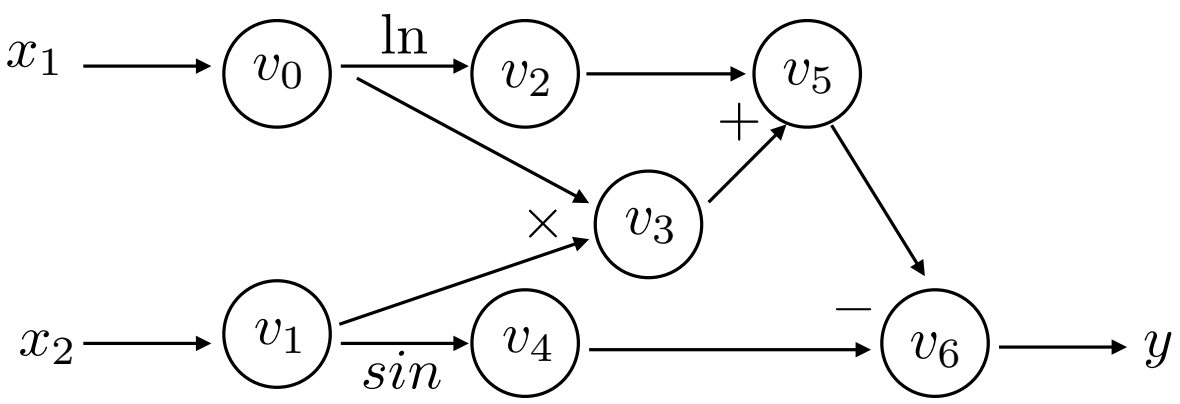

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Forward Evaluation

Trace:

	$f(2,5)$
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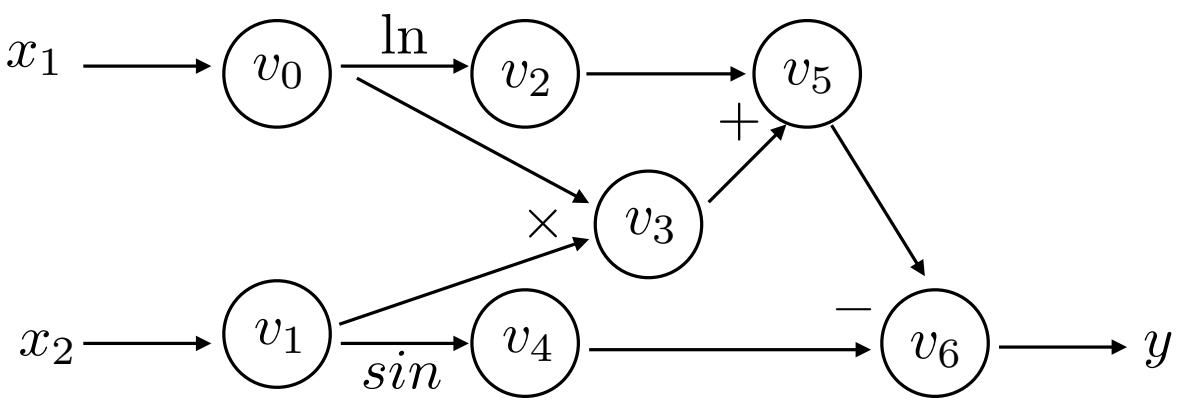

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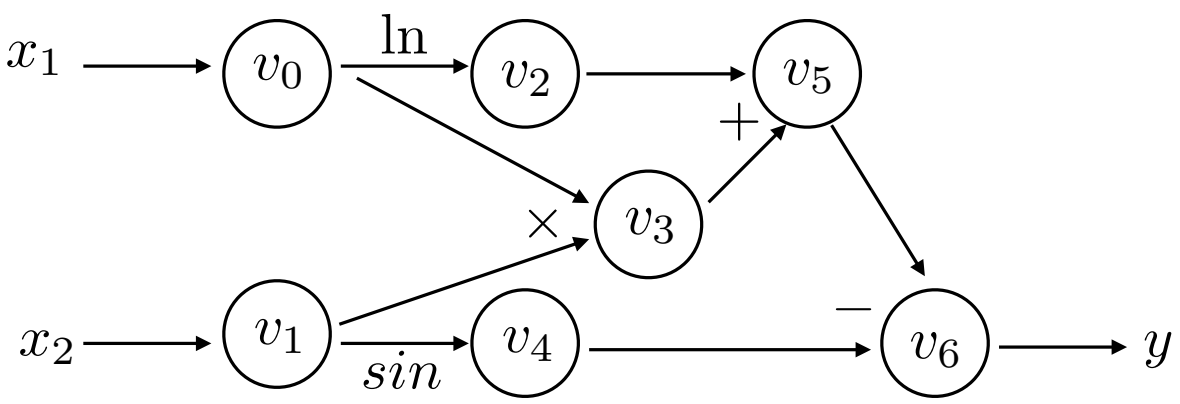

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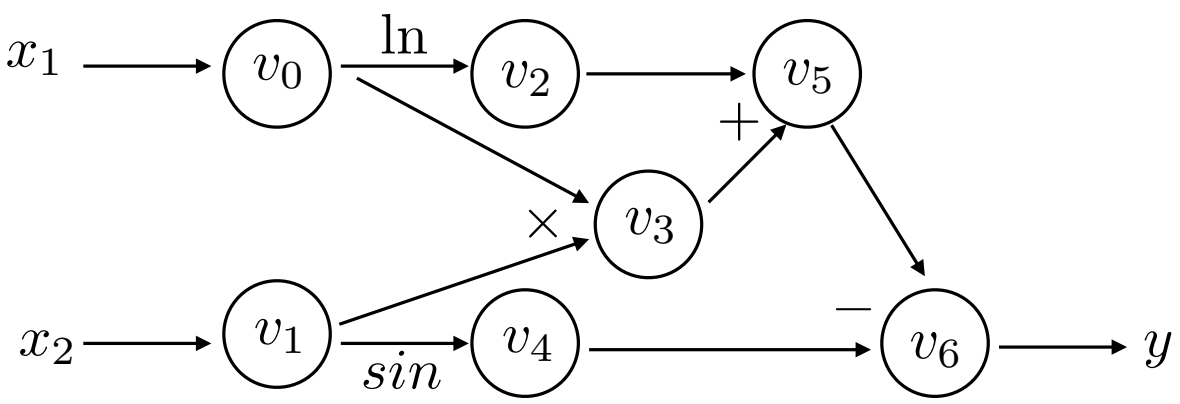

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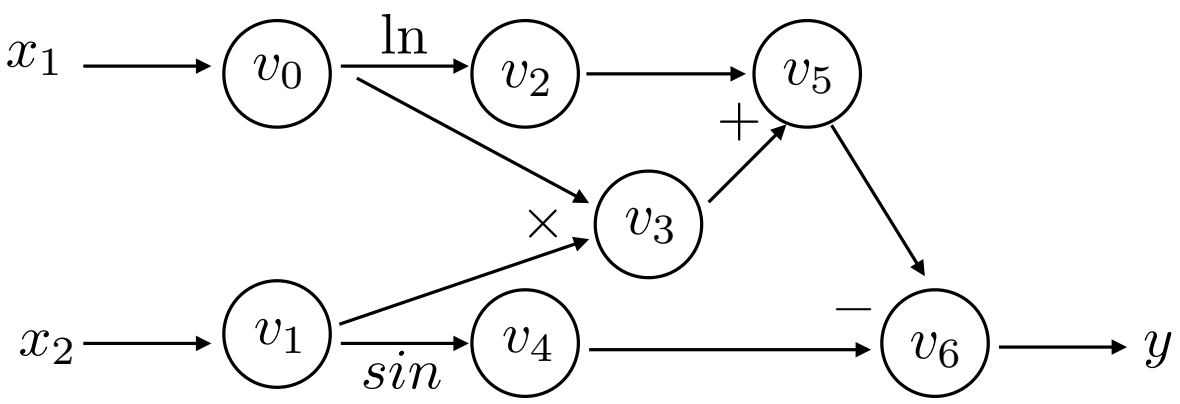

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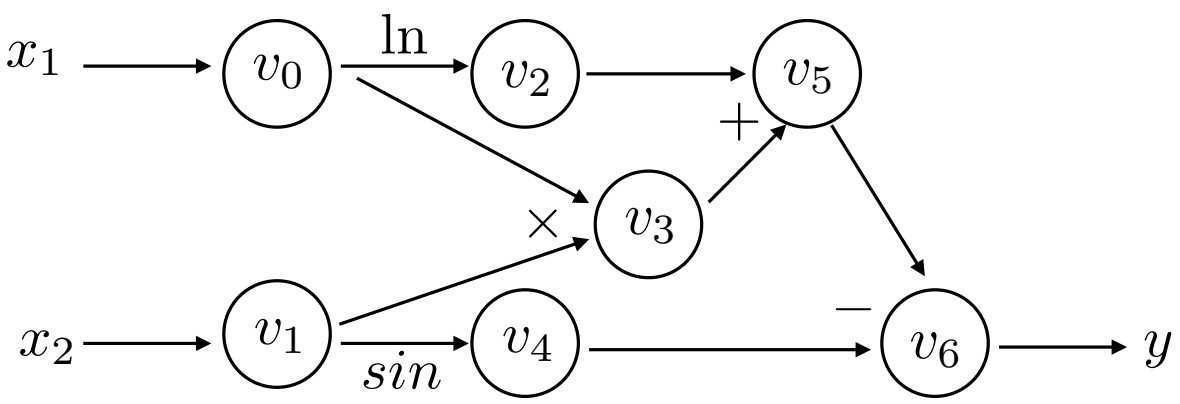

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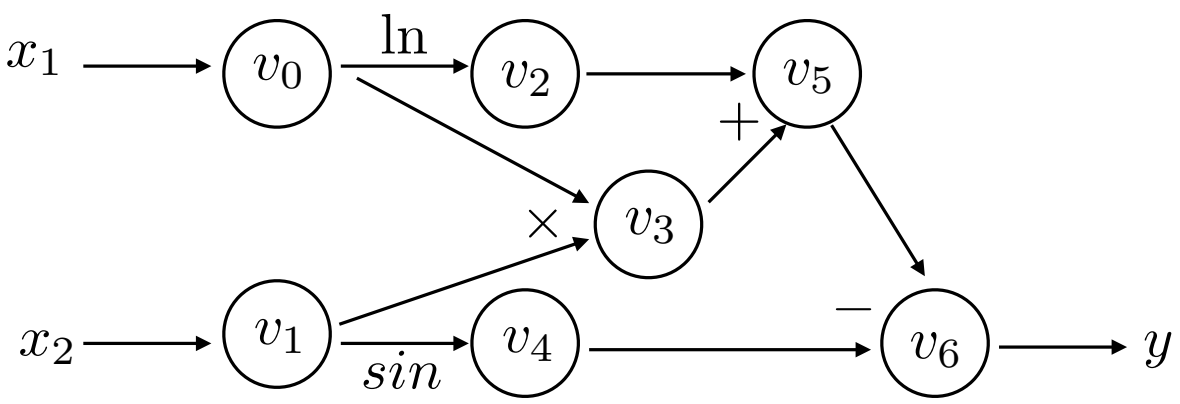

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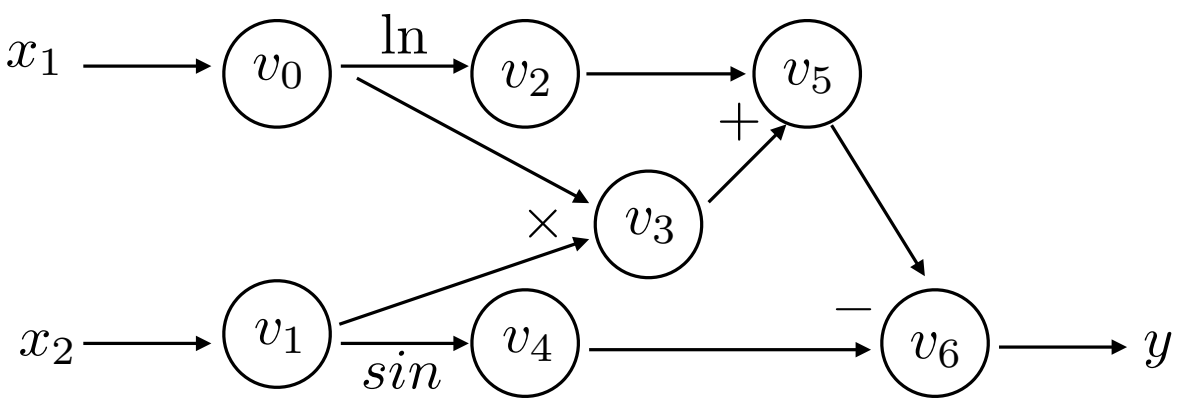

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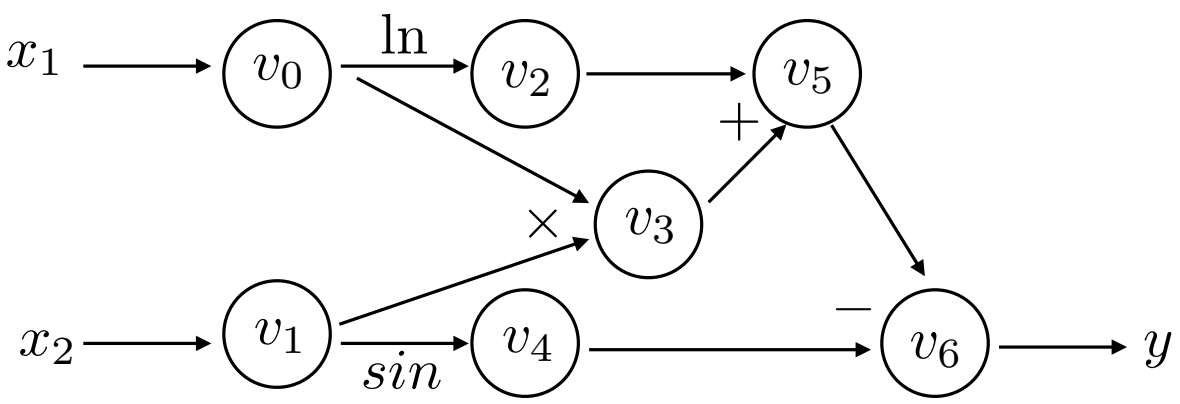

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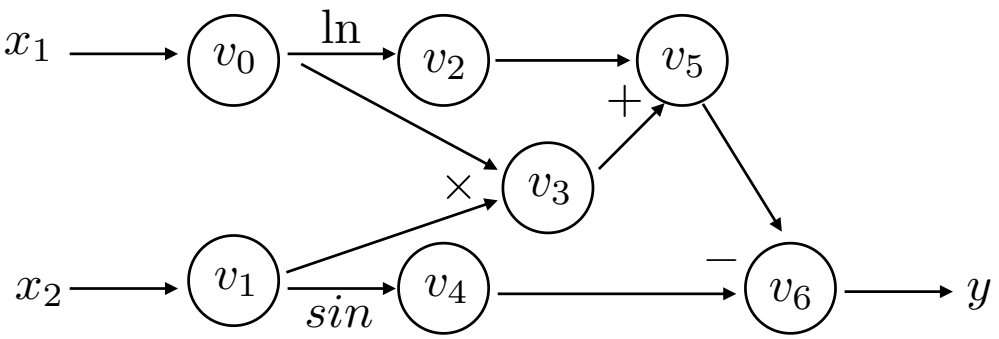

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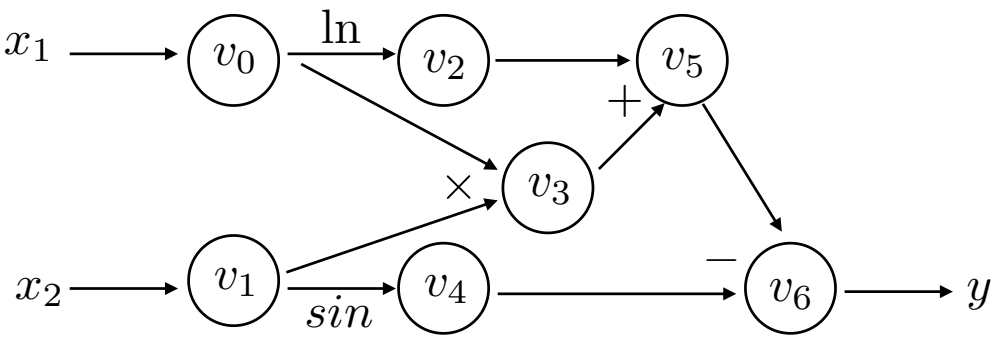

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Lets see how we can **evaluate a function** using computational graph (DNN inferences)

$$\left.\frac{\partial f(x_1, x_2)}{\partial x_1}\right|_{(x_1=2, x_2=5)}$$

We will do this with **forward mode** first, by introducing a derivative of each variable node with respect to the input variable.

Forward Evaluation

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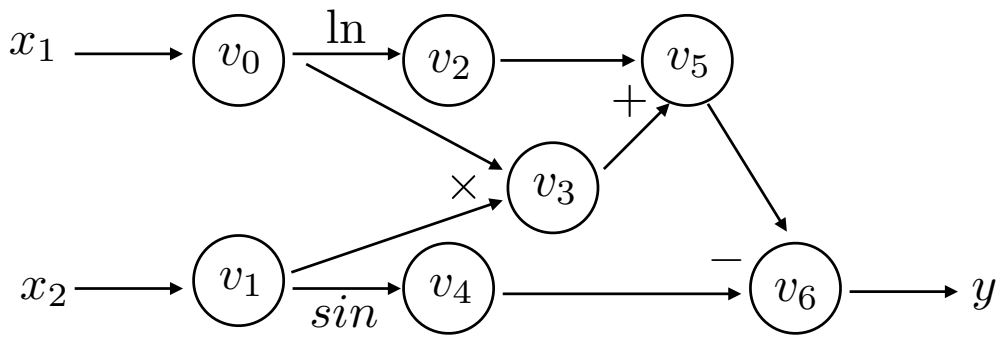

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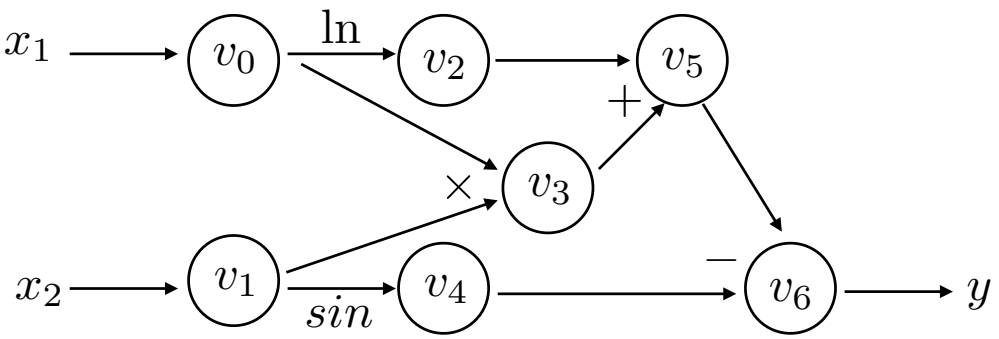
Forward Derivative Trace:

	$\left.\frac{\partial f(x_1, x_2)}{\partial x_1}\right\|_{(x_1=2, x_2=5)}$
$\frac{\partial v_0}{\partial x_1}$	

Automatic Differentiation (AutoDiff)

$$y = f(x_1, x_2) = \ln(x_1) + x_1 x_2 - sin(x_2)$$



Forward Evaluation Trace:

	$f(2,5)$
$v_0 = x_1$	2
$v_1 = x_2$	5
$v_2 = \ln(v_0)$	ln(2) = 0.693
$v_3 = v_0 \cdot v_1$	2 x 5 = 10
$v_4 = sin(v_1)$	sin(5) = -0.959
$v_5 = v_2 + v_3$	0.693 + 10 = 10.693
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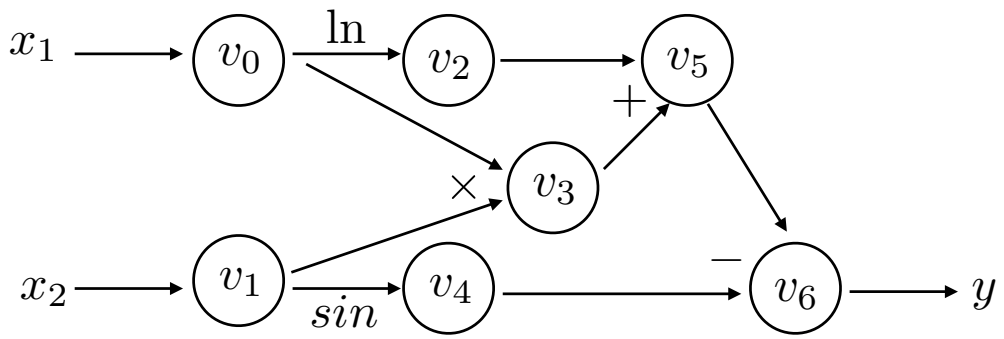
$y = v_6$	11.652

Forward Derivative Trace:

	$\left.\frac{\partial f(x_1, x_2)}{\partial x_1}\right\|_{(x_1=2, x_2=5)}$
$\frac{\partial v_0}{\partial x_1}$	1

Automatic Differentiation (AutoDiff)



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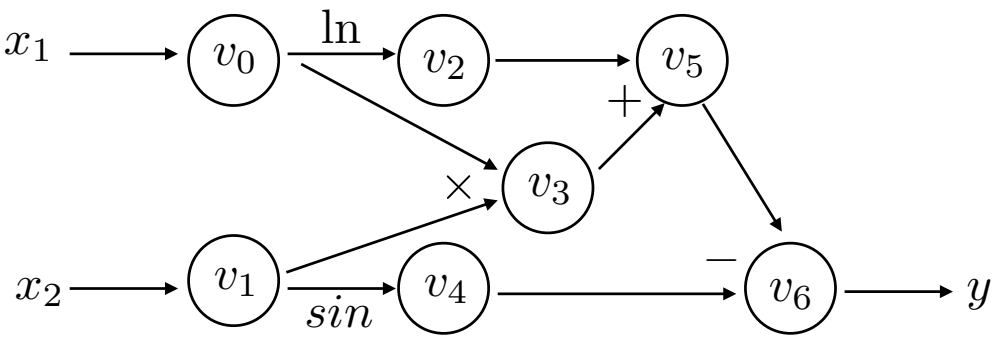

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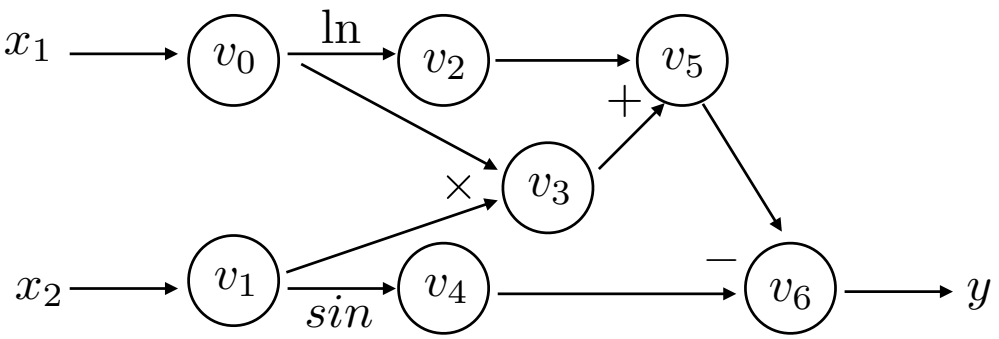

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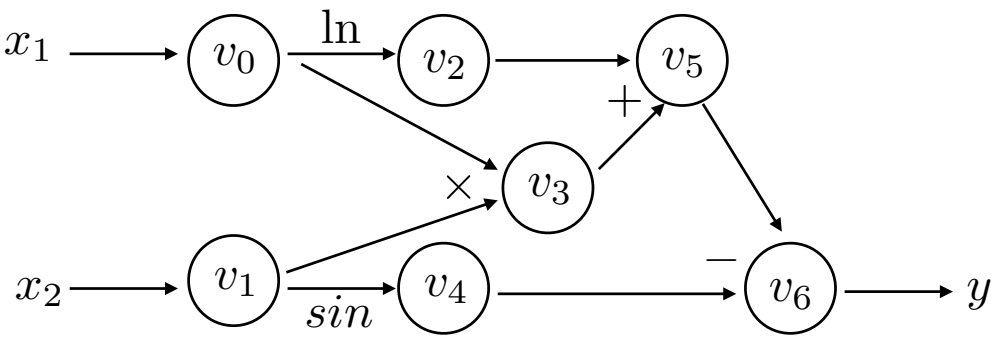

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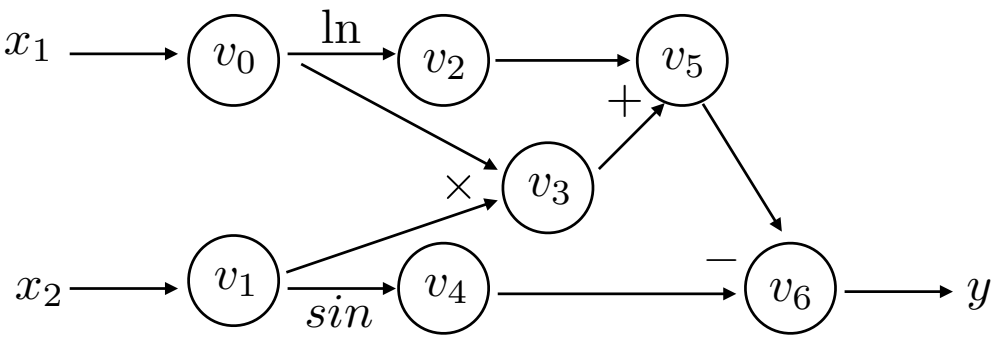
Chain Rule

Automatic Differentiation (AutoDiff)



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$\frac{\partial v_0}{\partial x_1}$	1
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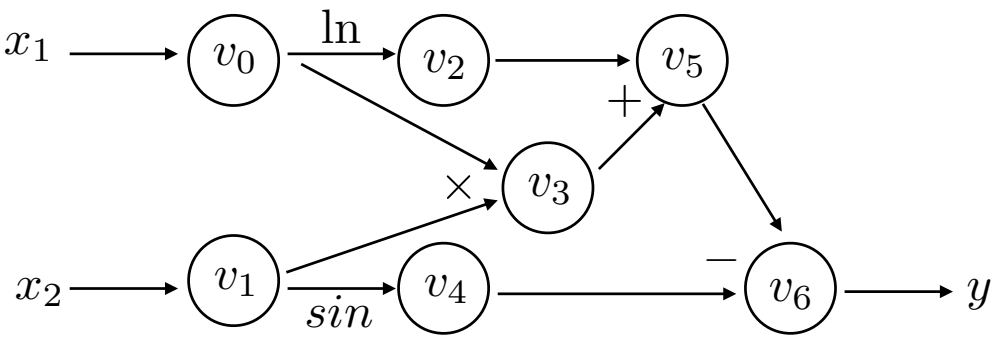
$\frac{\partial v_2}{\partial x_1} = \frac{1}{v_0}\frac{\partial v_0}{\partial x_1}$ Chain Rule	

Automatic Differentiation (AutoDiff)



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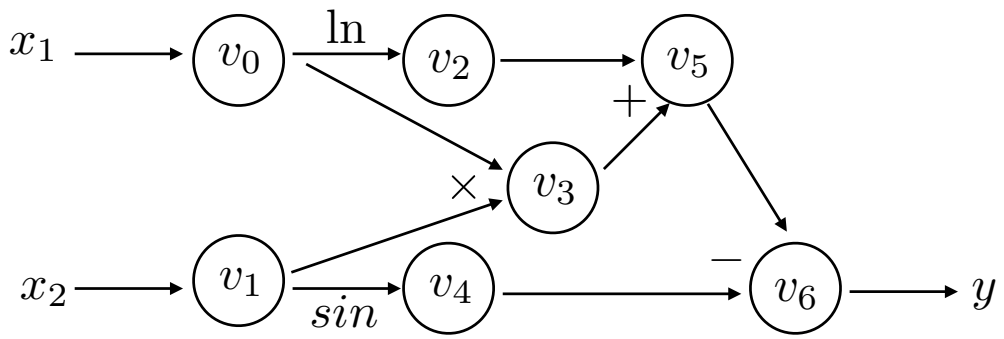
$\frac{\partial v_1}{\partial x_1}$	0
$\frac{\partial v_2}{\partial x_1} = \frac{1}{v_0}\frac{\partial v_0}{\partial x_1}$ Chain Rule	1/2 * 1 = 0.5

Automatic Differentiation (AutoDiff)



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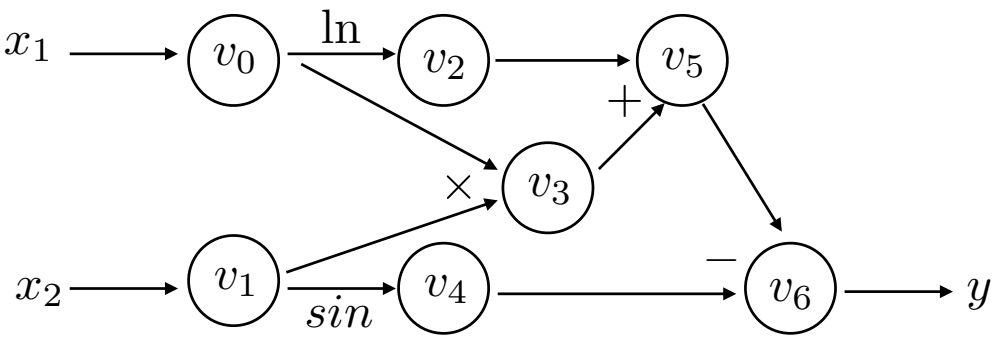

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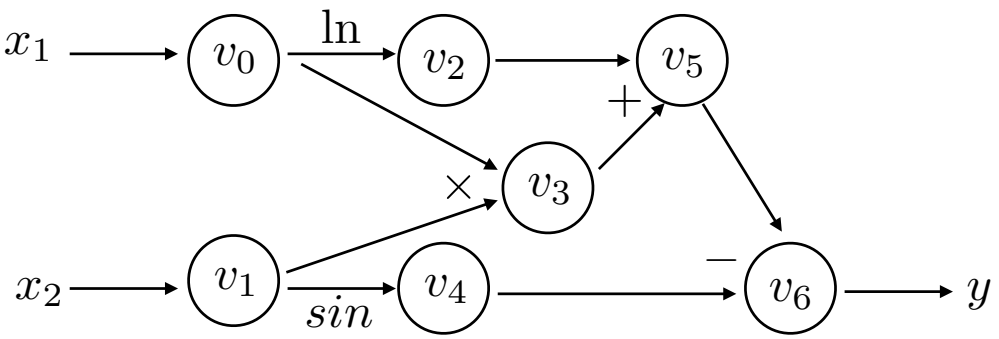
Product Rule

Automatic Differentiation (AutoDiff)



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$\frac{\partial v_2}{\partial x_1} = \frac{1}{v_0}\frac{\partial v_0}{\partial x_1}$	1/2 * 1 = 0.5
$\frac{\partial v_3}{\partial x_1} = \frac{\partial v_0}{\partial x_1} \cdot v_1 + v_0 \cdot \frac{\partial v_1}{\partial x_1}$	

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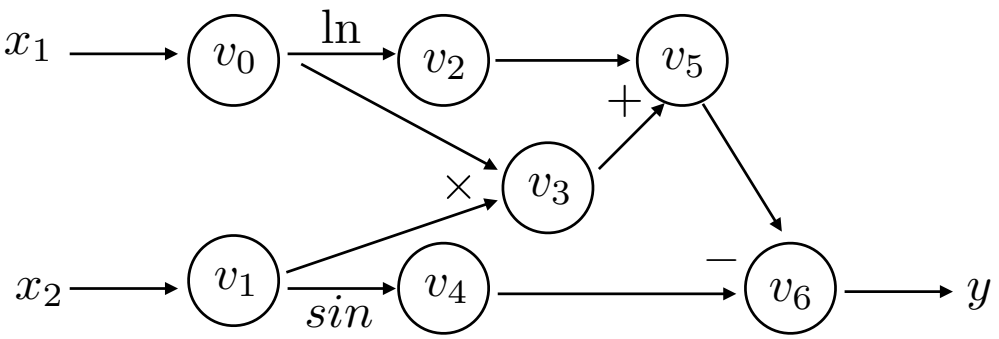

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$\frac{\partial v_3}{\partial x_1} = \frac{\partial v_0}{\partial x_1} \cdot v_1 + v_0 \cdot \frac{\partial v_1}{\partial x_1}$	1*5 + 2*0 = 5

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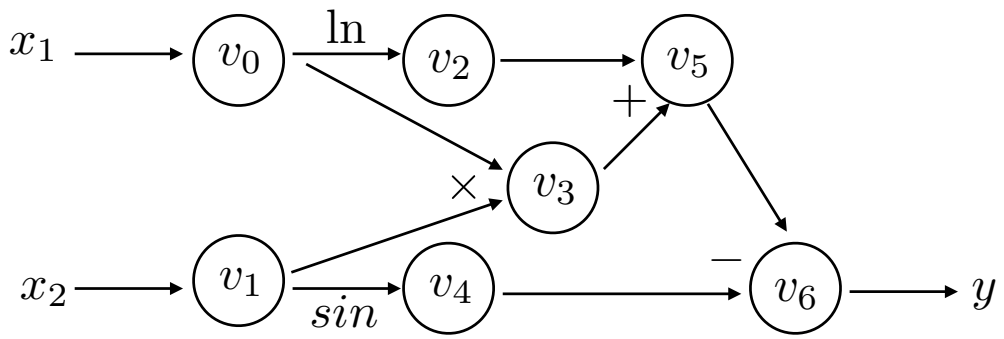

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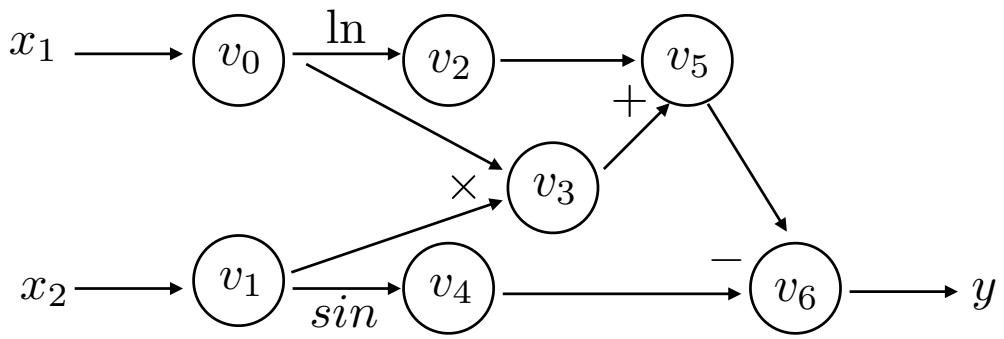
Automatic Differentiation (AutoDiff)



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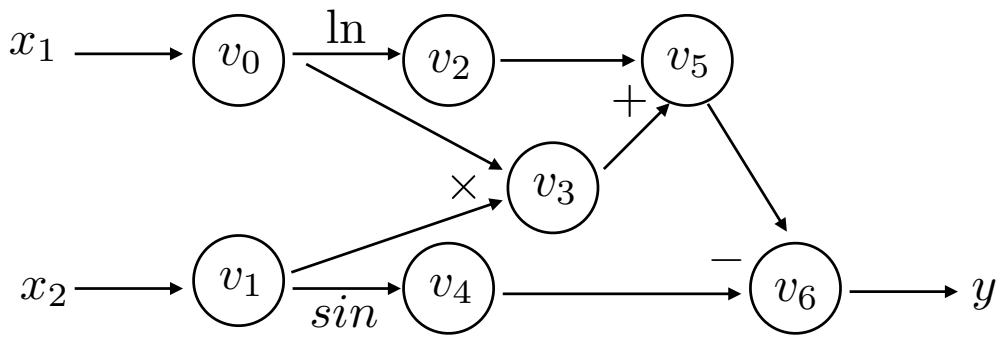

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We now have:

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Still need:

$$\left.\frac{\partial f(x_1, x_2)}{\partial x_2}\right|_{(x_1=2,x_2=5)}$$

AutoDiff: Forward Mode

- **Forward mode** needs m forward passes to get a full Jacobian (all gradients of output with respect to each input), where m is the number of inputs

$$\mathbf{y} = f(\mathbf{x}) : \mathbb{R}^m \to \mathbb{R}^n$$

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Problem: DNN typically has large number of inputs:

image as an input, plus all the weights and biases of layers = millions of inputs!

and very few outputs (many DNNs have $n = 1$)

slide adopted from T. Chen, H. Shen, A. Krishnamurthy

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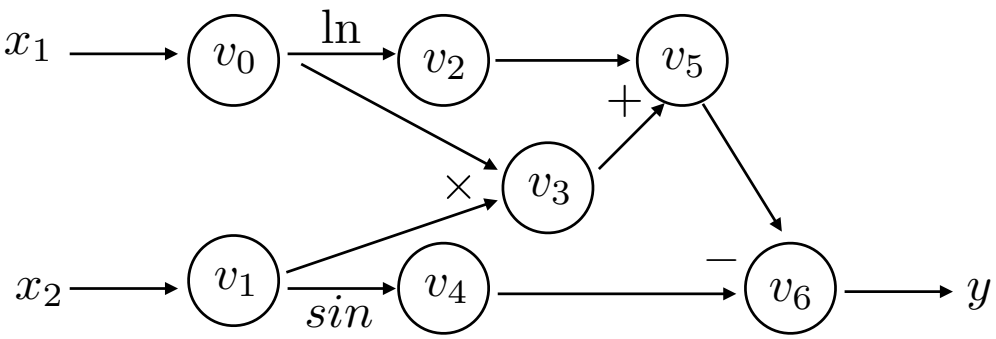
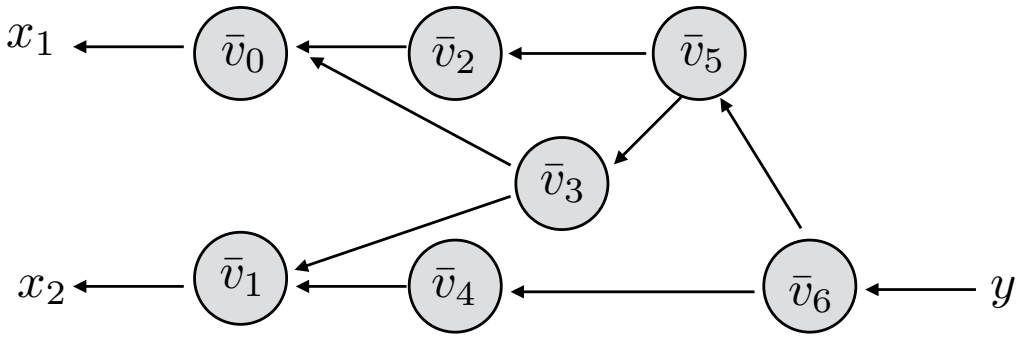
- Automatic differentiation in **reverse mode** computes all gradients in n backwards passes (so for most DNNs in a single back pass — **back propagation**)

slide adopted from T. Chen, H. Shen, A. Krishnamurthy

AutoDiff: Reverse Mode





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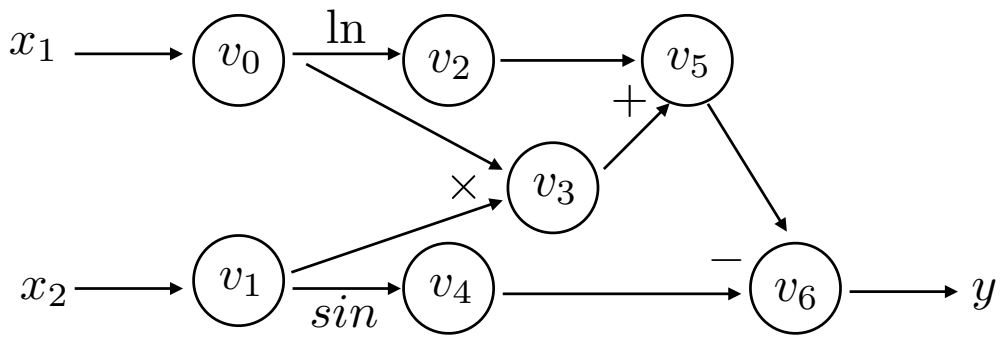
$v_5 = v_2 + v_3$	0.693 + 10 = 10.693
$v_6 = v_5 - v_4$	10.693 + 0.959 = 11.652
$y = v_6$	11.652

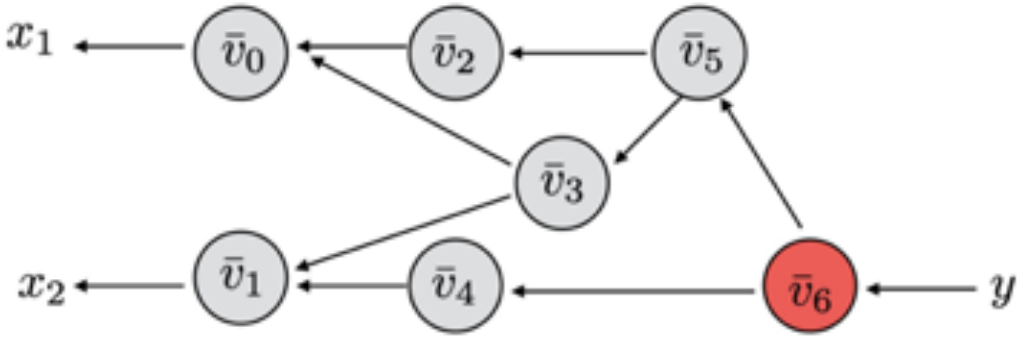
Traverse the original graph in the reverse topological order and for each node in the original graph introduce an **adjoint node**, which computes derivative of the output with respect to the local node (using Chain rule):

$$\bar{v}_i = \frac{\partial y_j}{\partial v_i} = \sum_{k \in \mathrm{pa}(i)} \frac{\partial v_k}{\partial v_i} \frac{\partial y_j}{\partial v_k} = \sum_{k \in \mathrm{pa}(i)} \frac{\partial v_k}{\partial v_i} \bar{v}_k$$

"local" derivative

AutoDiff: Reverse Mode





Forward Evaluation Trace:

	$f(2,5)$
$v_0 = x_1$	2
$v_1 = x_2$	5
$v_2 = \ln(v_0)$	ln(2) = 0.693
$v_3 = v_0 \cdot v_1$	2 x 5 = 10
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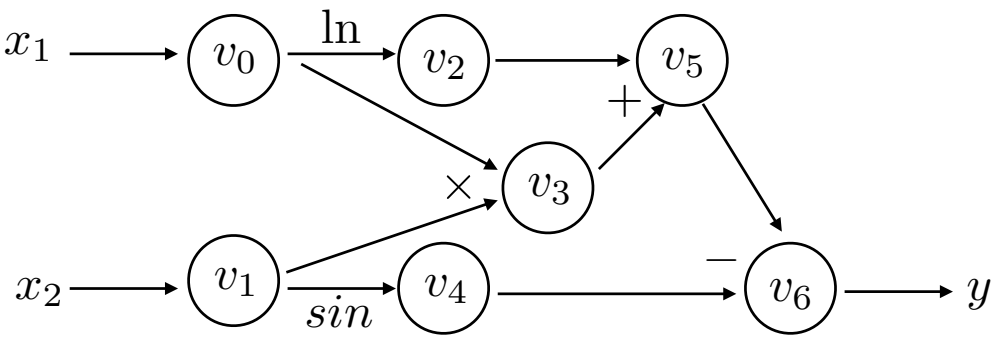
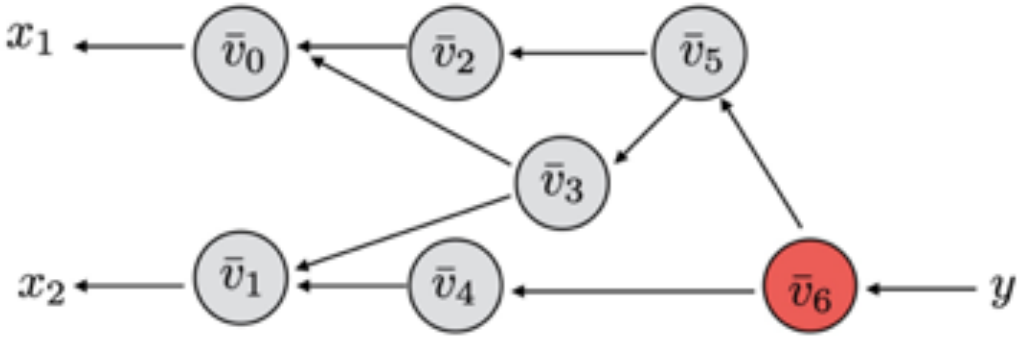
$y = v_6$	11.652

Backwards Derivative Trace:

$$\bar{v}_6 = \frac{\partial y}{\partial v_6}$$

AutoDiff: Reverse Mode





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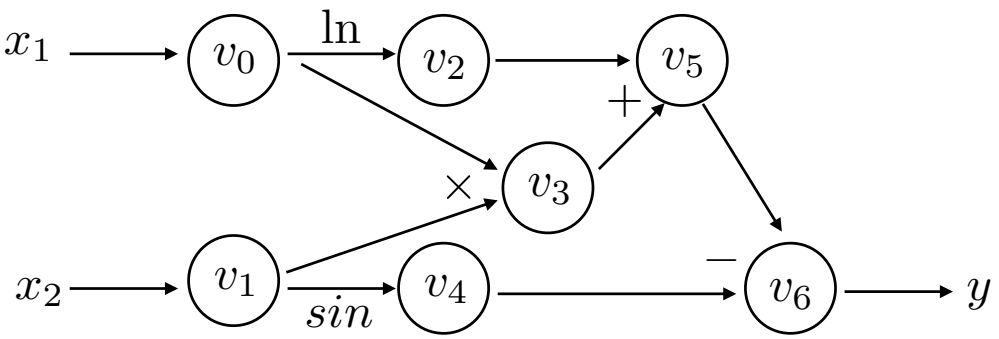

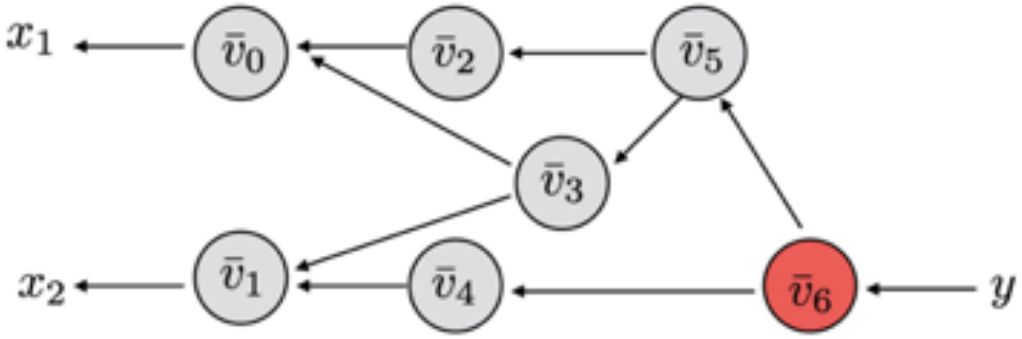

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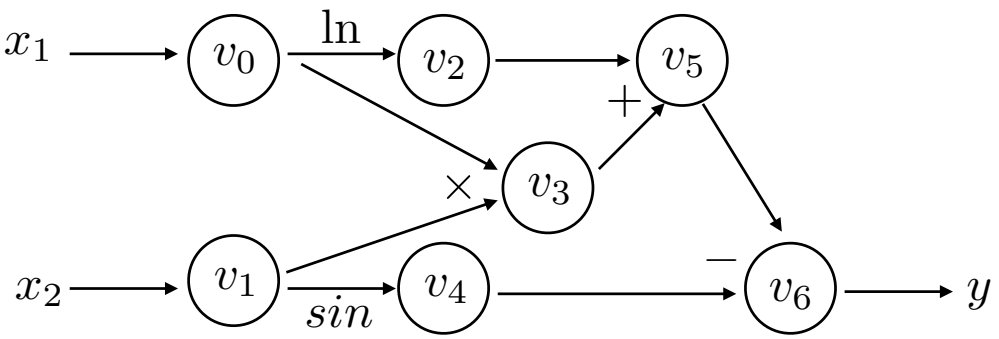
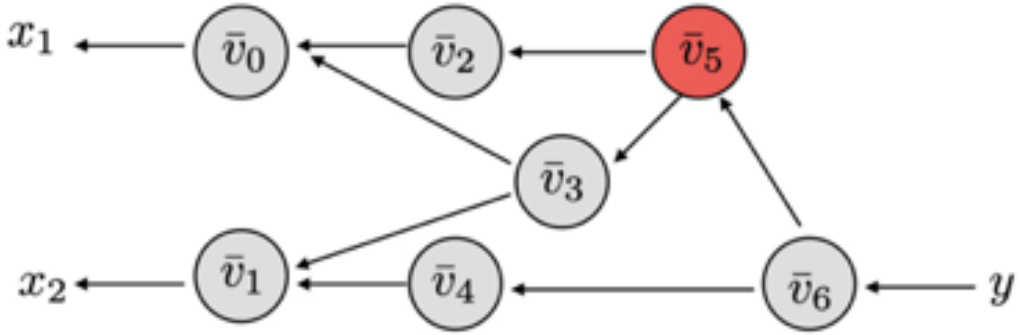
Backwards Derivative Trace:

$\bar{v}_6 = \dfrac{\partial y}{\partial v_6}$	1

AutoDiff: Reverse Mode





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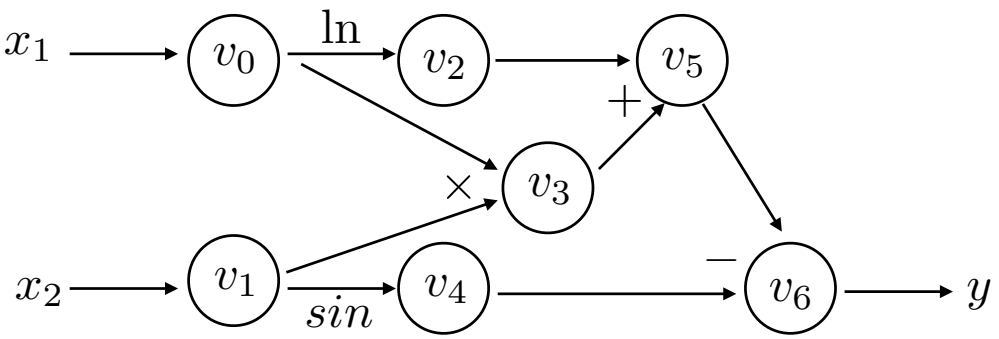
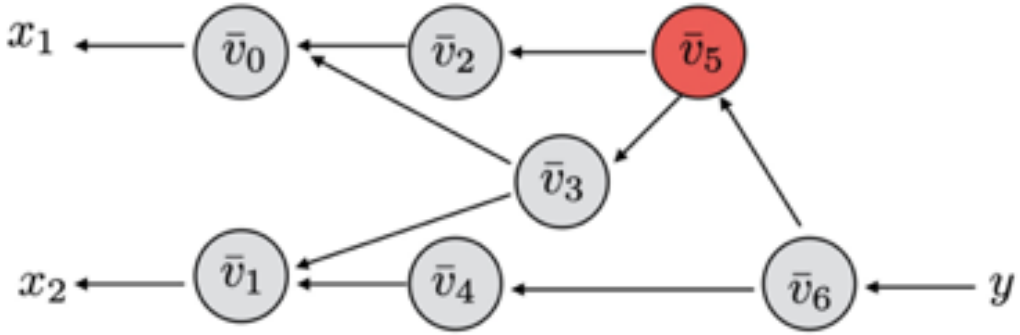
Backwards Derivative Trace:

$\bar{v}_5 = \bar{v}_6 \dfrac{\partial v_6}{\partial v_5}$	
$\bar{v}_6 = \dfrac{\partial y}{\partial v_6}$	1

AutoDiff: Reverse Mode





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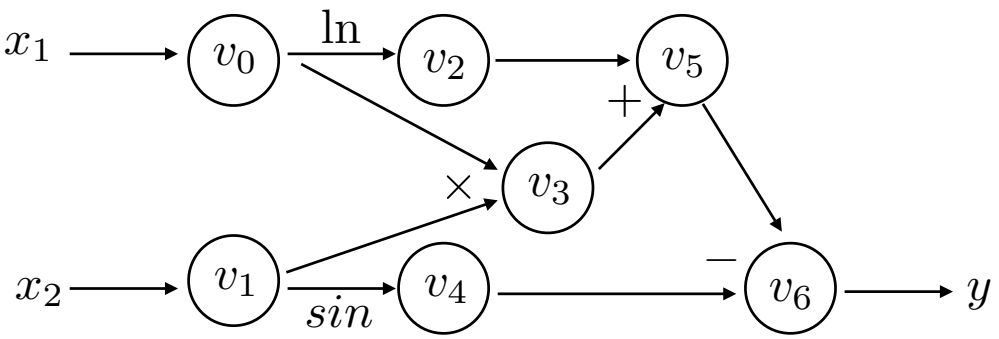

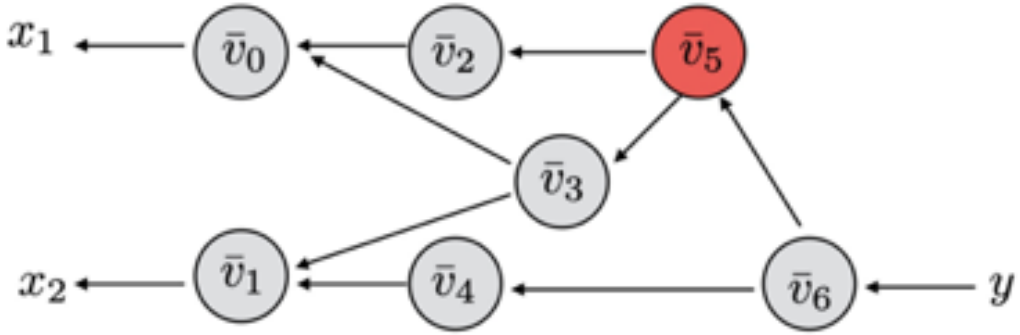

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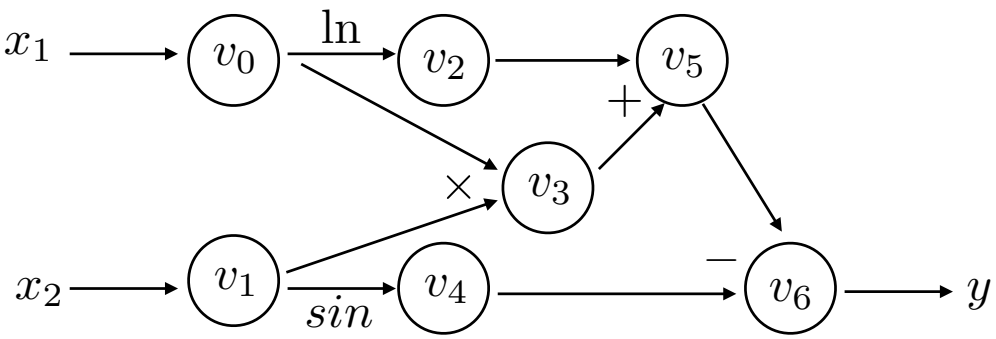
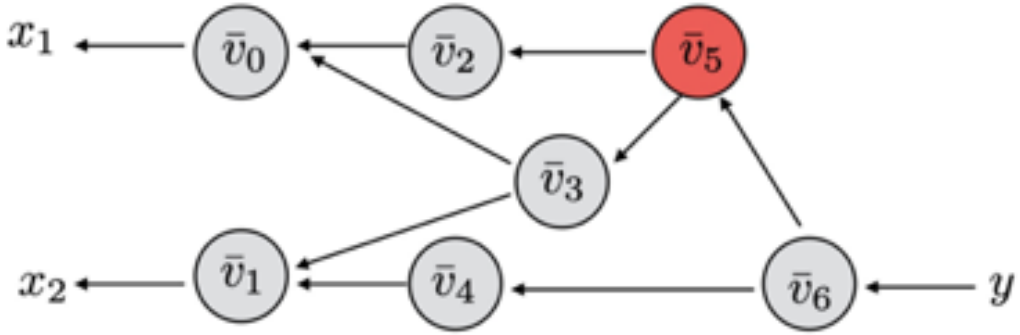
Backwards Derivative Trace:

$\bar{v}_5 = \bar{v}_6 \dfrac{\partial v_6}{\partial v_5} = \bar{v}_6 \cdot 1$	
$\bar{v}_6 = \dfrac{\partial y}{\partial v_6}$	1

AutoDiff: Reverse Mode





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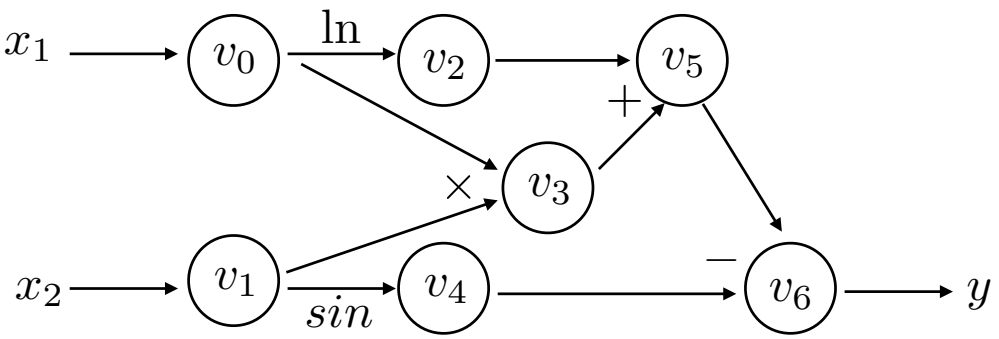

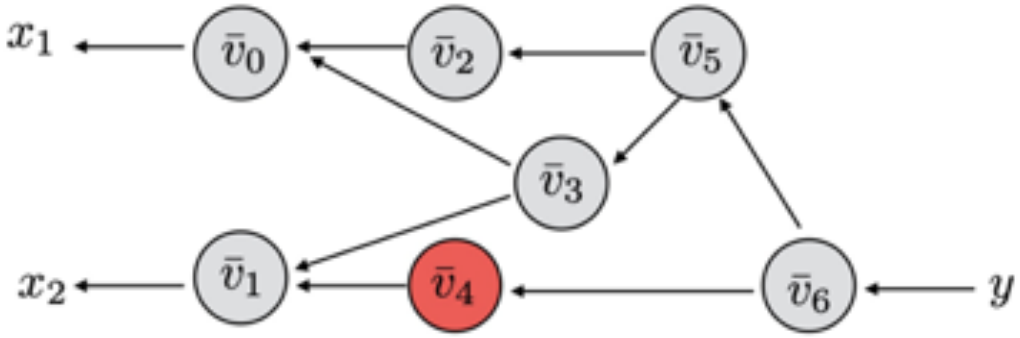

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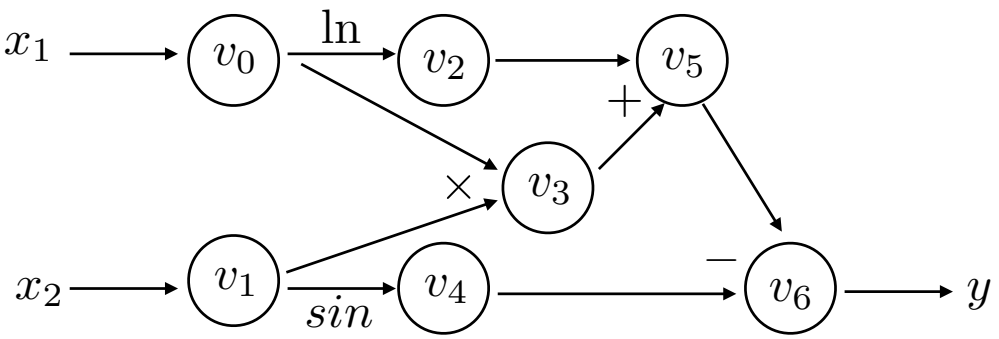
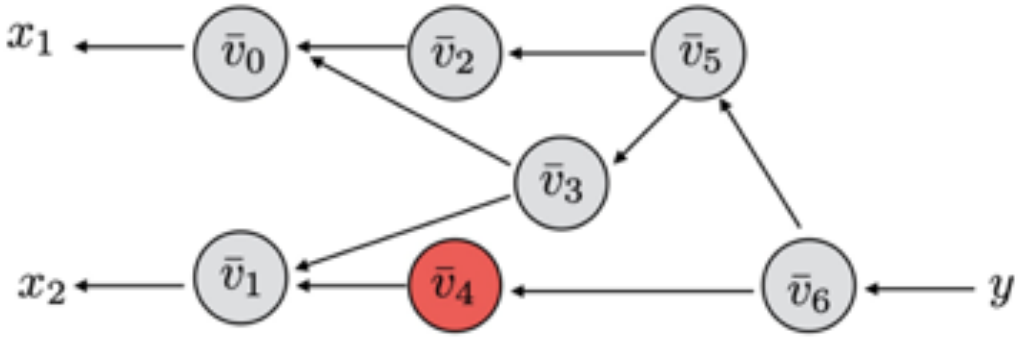
AutoDiff: Reverse Mode





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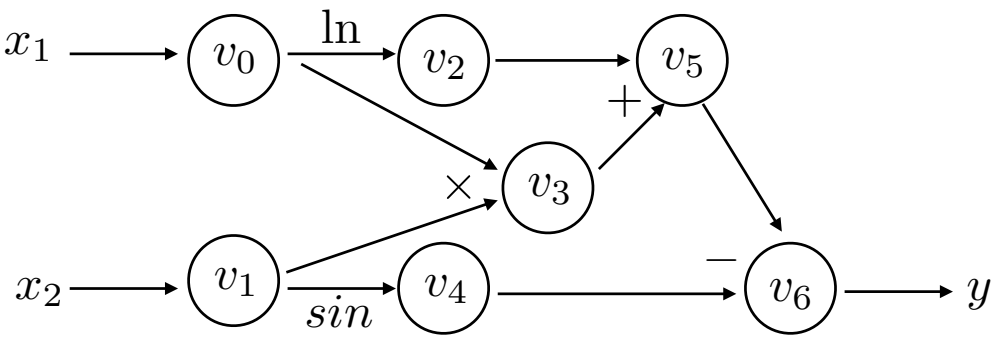

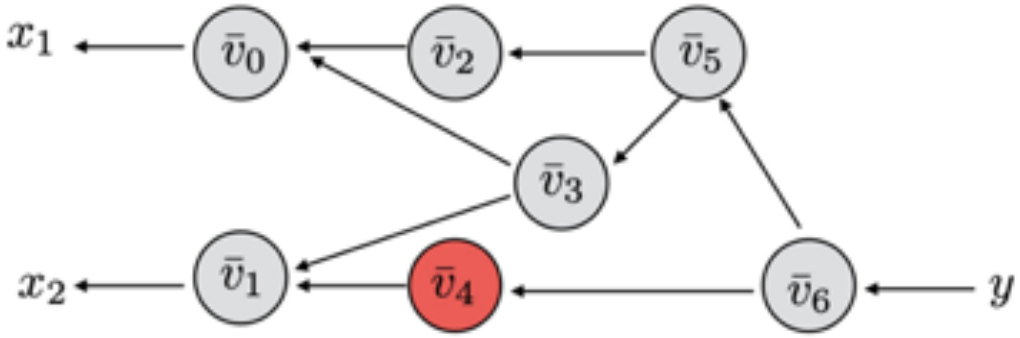

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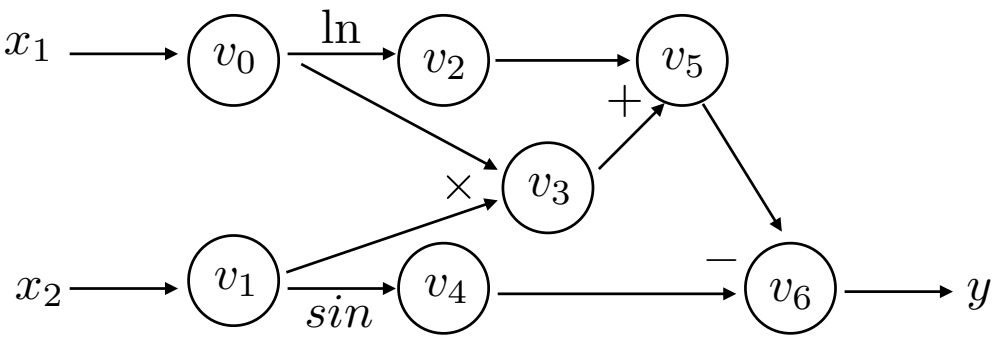

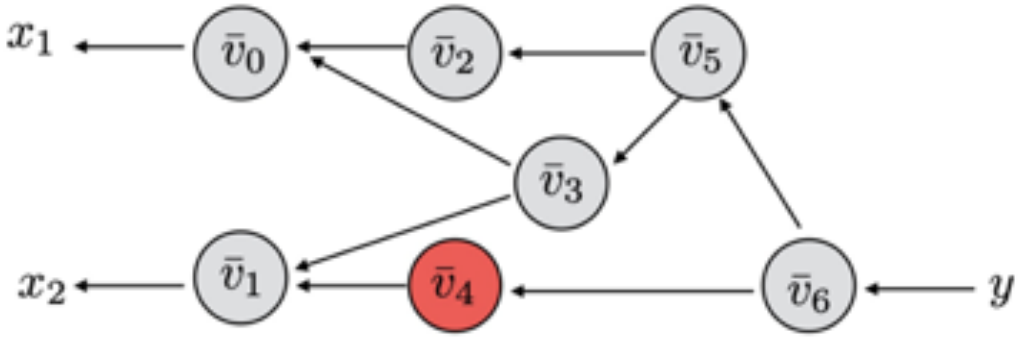

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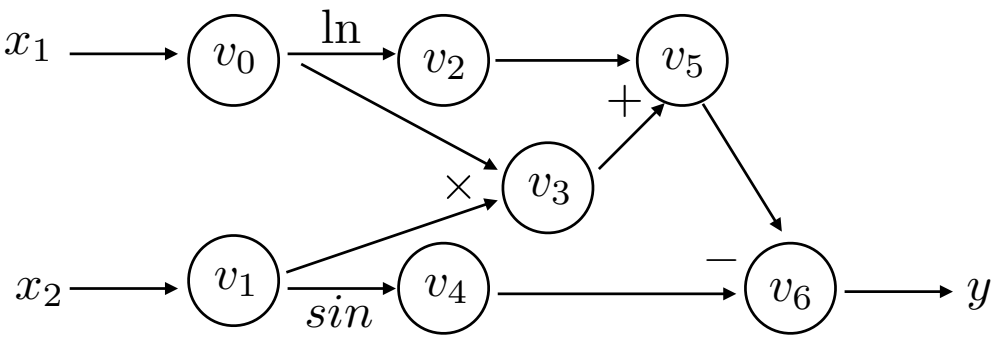

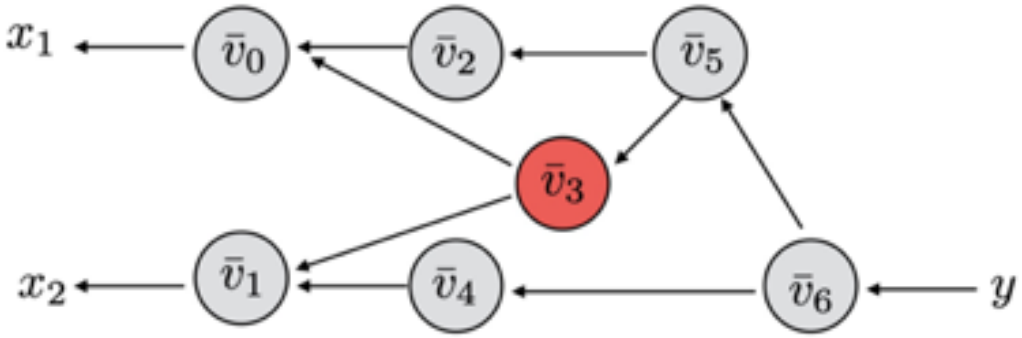

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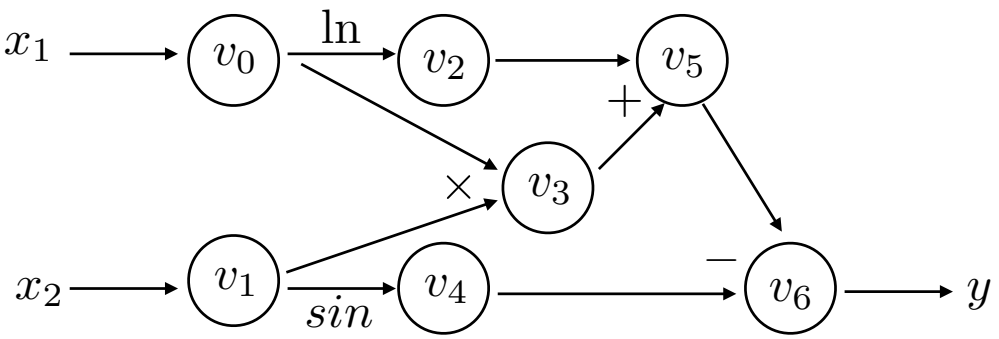

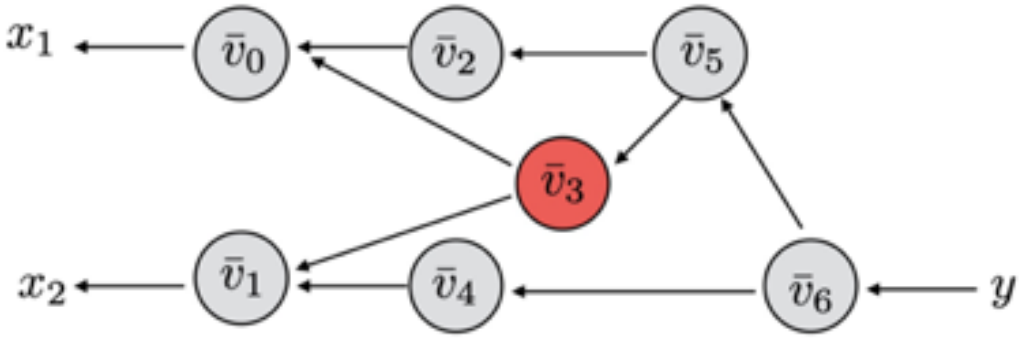

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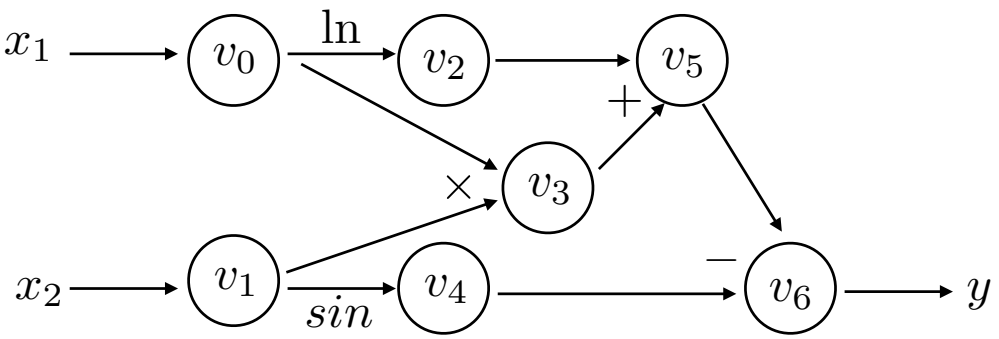

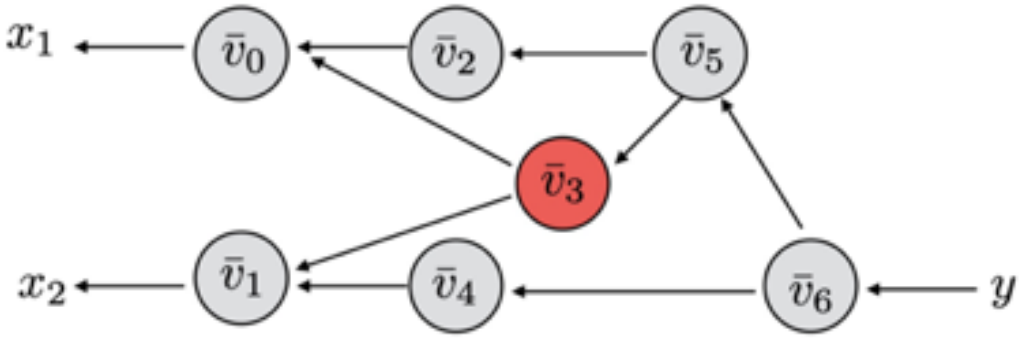

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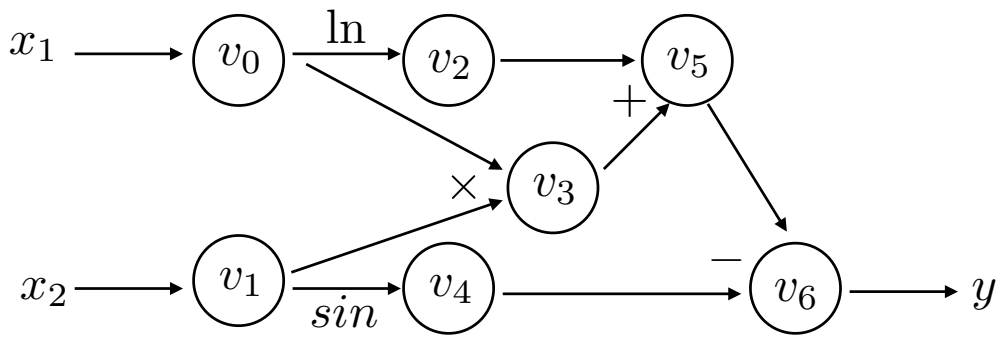
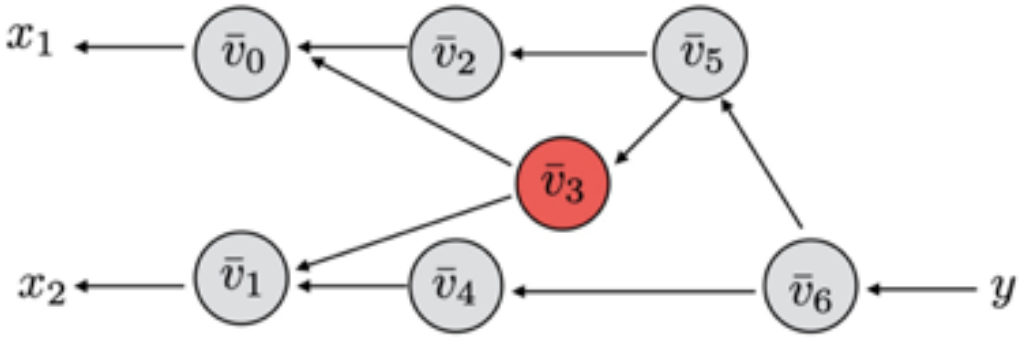
$\bar{v}_6 = \dfrac{\partial y}{\partial v_6}$	1

AutoDiff: Reverse Mode





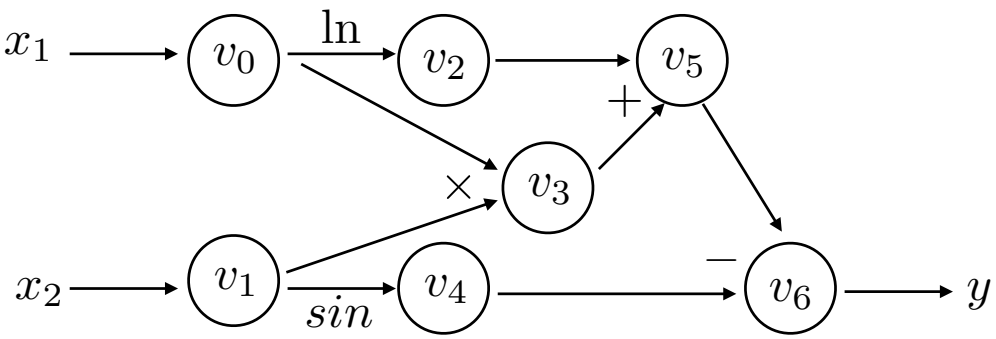
Forward Evaluation Trace:

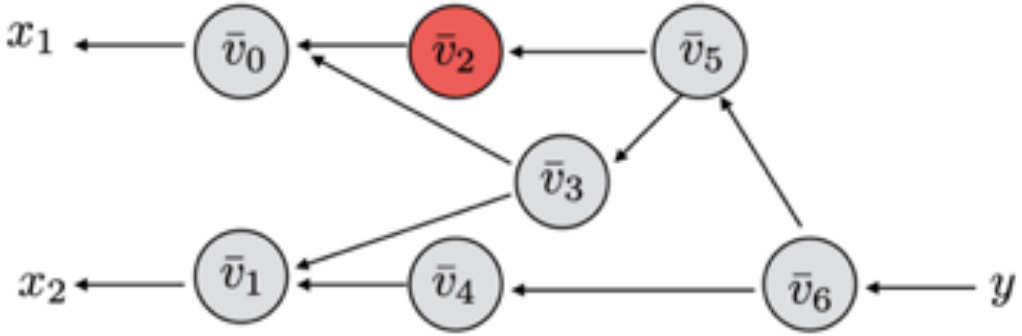
	$f(2,5)$
$v_0 = x_1$	2
$v_1 = x_2$	5
$v_2 = \ln(v_0)$	ln(2) = 0.693
$v_3 = v_0 \cdot v_1$	2 x 5 = 10
$v_4 = sin(v_1)$	sin(5) = -0.959
$v_5 = v_2 + v_3$	0.693 + 10 = 10.693
$v_6 = v_5 - v_4$	10.693 + 0.959 = 11.652
$y = v_6$	11.652

Backwards Derivative Trace:

$\bar{v}_3 = \bar{v}_5 \dfrac{\partial v_5}{\partial v_3} = \bar{v}_5 \cdot (1)$	1x1 = 1
$\bar{v}_4 = \bar{v}_6 \dfrac{\partial v_6}{\partial v_4} = \bar{v}_6 \cdot (-1)$	1x-1 = -1
$\bar{v}_5 = \bar{v}_6 \dfrac{\partial v_6}{\partial v_5} = \bar{v}_6 \cdot 1$	1x1 = 1
$\bar{v}_6 = \dfrac{\partial y}{\partial v_6}$	1

AutoDiff: Reverse Mode





Forward Evaluation Trace:

	$f(2,5)$
$v_0 = x_1$	2
$v_1 = x_2$	5
$v_2 = \ln(v_0)$	ln(2) = 0.693
$v_3 = v_0 \cdot v_1$	2 x 5 = 10
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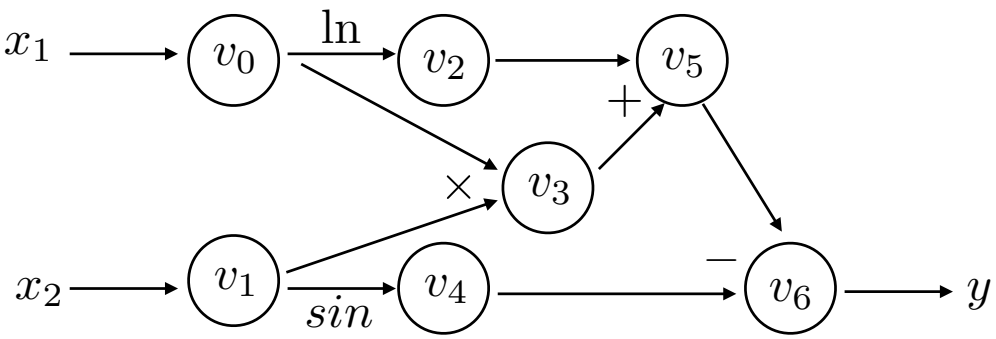
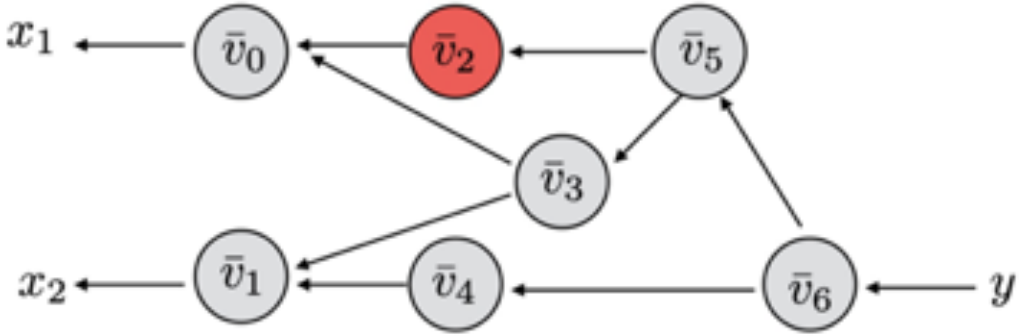
$v_6 = v_5 - v_4$	10.693 + 0.959 = 11.652
$y = v_6$	11.652

Backwards Derivative Trace:

$\bar{v}_2 = \bar{v}_5 \dfrac{\partial v_5}{\partial v_2}$	
$\bar{v}_3 = \bar{v}_5 \dfrac{\partial v_5}{\partial v_3} = \bar{v}_5 \cdot (1)$	1x1 = 1
$\bar{v}_4 = \bar{v}_6 \dfrac{\partial v_6}{\partial v_4} = \bar{v}_6 \cdot (-1)$	1x-1 = -1
$\bar{v}_5 = \bar{v}_6 \dfrac{\partial v_6}{\partial v_5} = \bar{v}_6 \cdot 1$	1x1 = 1
$\bar{v}_6 = \dfrac{\partial y}{\partial v_6}$	1

AutoDiff: Reverse Mode





Forward Evaluation

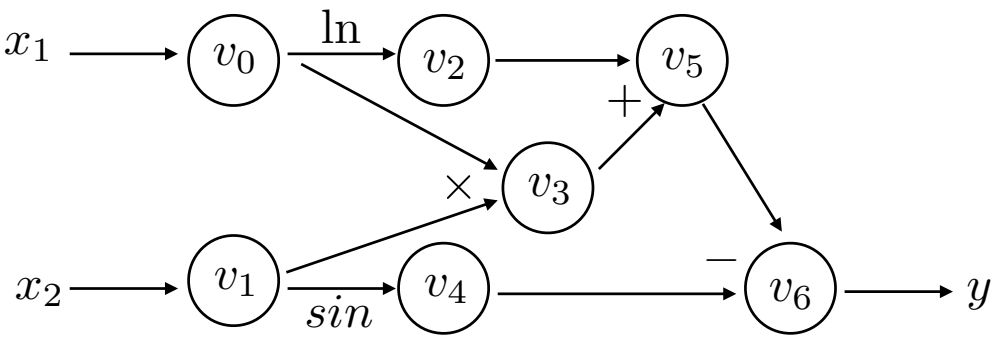
Trace:

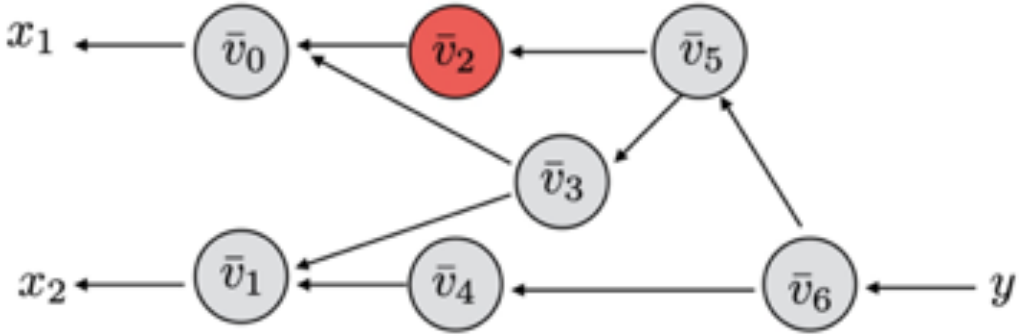
	$f(2,5)$
$v_0 = x_1$	2
$v_1 = x_2$	5
$v_2 = \ln(v_0)$	ln(2) = 0.693
$v_3 = v_0 \cdot v_1$	2 x 5 = 10
$v_4 = sin(v_1)$	sin(5) = -0.959
$v_5 = v_2 + v_3$	0.693 + 10 = 10.693
$v_6 = v_5 - v_4$	10.693 + 0.959 = 11.652
$y = v_6$	11.652

Backwards Derivative Trace:

$\bar{v}_2 = \bar{v}_5 \frac{\partial v_5}{\partial v_2} = \bar{v}_5 \cdot (1)$	
$\bar{v}_3 = \bar{v}_5 \frac{\partial v_5}{\partial v_3} = \bar{v}_5 \cdot (1)$	1x1 = 1
$\bar{v}_4 = \bar{v}_6 \frac{\partial v_6}{\partial v_4} = \bar{v}_6 \cdot (-1)$	1x-1 = -1
$\bar{v}_5 = \bar{v}_6 \frac{\partial v_6}{\partial v_5} = \bar{v}_6 \cdot 1$	1x1 = 1
$\bar{v}_6 = \frac{\partial y}{\partial v_6}$	1

AutoDiff: Reverse Mode





Forward Evaluation

Trace:

	$f(2,5)$
$v_0 = x_1$	2
$v_1 = x_2$	5
$v_2 = \ln(v_0)$	ln(2) = 0.693
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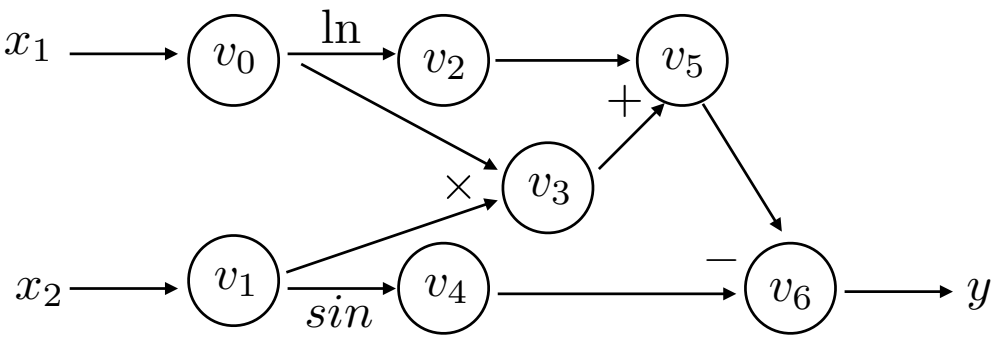
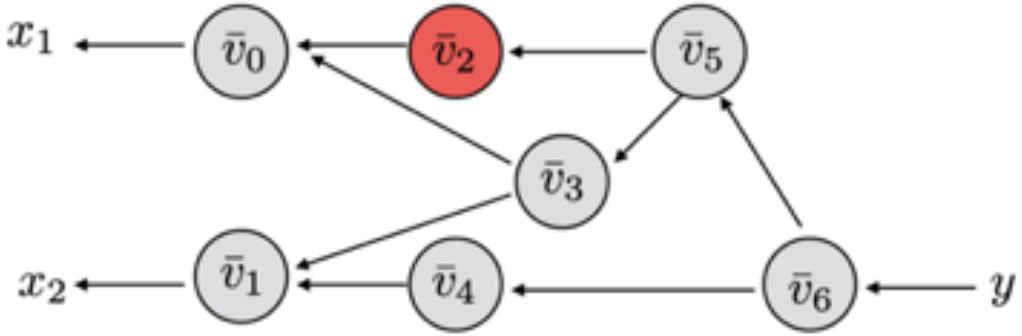
$v_5 = v_2 + v_3$	0.693 + 10 = 10.693
$v_6 = v_5 - v_4$	10.693 + 0.959 = 11.652
$y = v_6$	11.652

Backwards Derivative Trace:

$\bar{v}_2 = \bar{v}_5 \frac{\partial v_5}{\partial v_2} = \bar{v}_5 \cdot (1)$	
$\bar{v}_3 = \bar{v}_5 \frac{\partial v_5}{\partial v_3} = \bar{v}_5 \cdot (1)$	1x1 = 1
$\bar{v}_4 = \bar{v}_6 \frac{\partial v_6}{\partial v_4} = \bar{v}_6 \cdot (-1)$	1x-1 = -1
$\bar{v}_5 = \bar{v}_6 \frac{\partial v_6}{\partial v_5} = \bar{v}_6 \cdot 1$	1x1 = 1
$\bar{v}_6 = \frac{\partial y}{\partial v_6}$	1

AutoDiff: Reverse Mode





Forward Evaluation

Trace:

	$f(2,5)$
$v_0 = x_1$	2
$v_1 = x_2$	5
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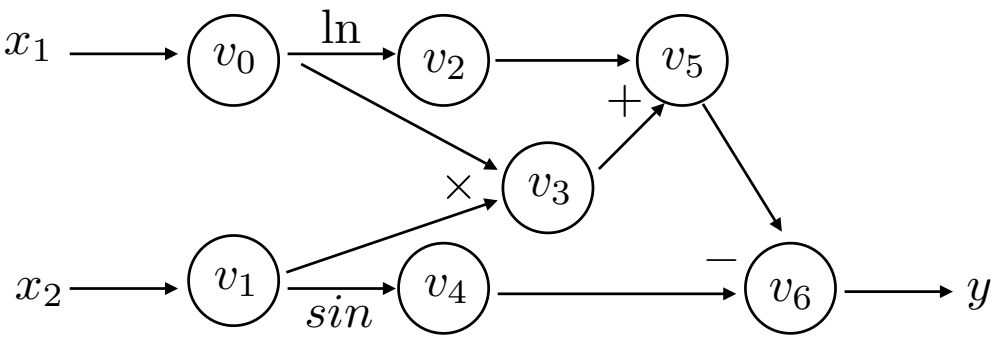
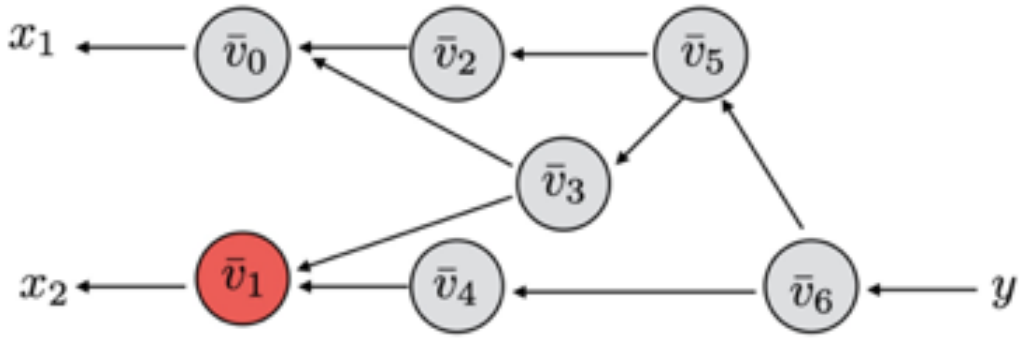
$v_6 = v_5 - v_4$	10.693 + 0.959 = 11.652
$y = v_6$	11.652

Backwards Derivative Trace:

$\bar{v}_2 = \bar{v}_5 \frac{\partial v_5}{\partial v_2} = \bar{v}_5 \cdot (1)$	1x1 = 1
$\bar{v}_3 = \bar{v}_5 \frac{\partial v_5}{\partial v_3} = \bar{v}_5 \cdot (1)$	1x1 = 1
$\bar{v}_4 = \bar{v}_6 \frac{\partial v_6}{\partial v_4} = \bar{v}_6 \cdot (-1)$	1x-1 = -1
$\bar{v}_5 = \bar{v}_6 \frac{\partial v_6}{\partial v_5} = \bar{v}_6 \cdot 1$	1x1 = 1
$\bar{v}_6 = \frac{\partial y}{\partial v_6}$	1

AutoDiff: Reverse Mode





Forward Evaluation Trace:

	$f(2,5)$
$v_0 = x_1$	2
$v_1 = x_2$	5
$v_2 = \ln(v_0)$	ln(2) = 0.693
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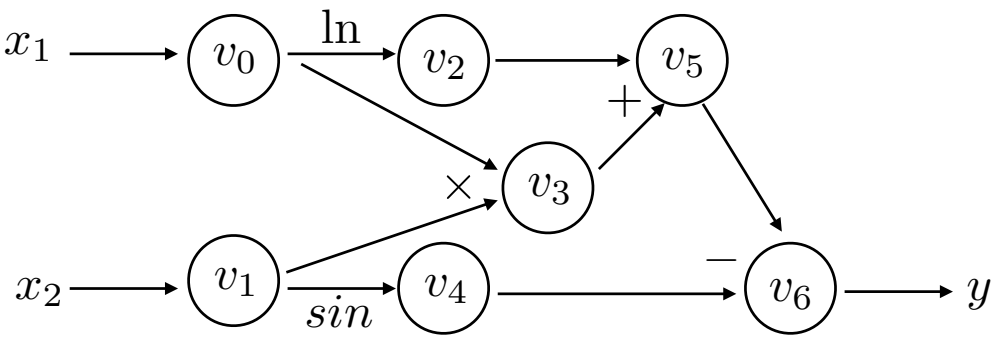
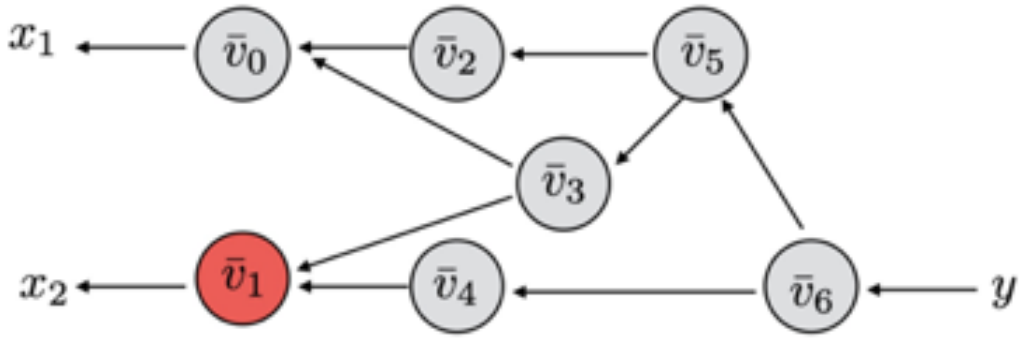
$v_6 = v_5 - v_4$	10.693 + 0.959 = 11.652
$y = v_6$	11.652

Backwards Derivative Trace:

$\bar{v}_1$	
$\bar{v}_2 = \bar{v}_5 \dfrac{\partial v_5}{\partial v_2} = \bar{v}_5 \cdot (1)$	1x1 = 1
$\bar{v}_3 = \bar{v}_5 \dfrac{\partial v_5}{\partial v_3} = \bar{v}_5 \cdot (1)$	1x1 = 1
$\bar{v}_4 = \bar{v}_6 \dfrac{\partial v_6}{\partial v_4} = \bar{v}_6 \cdot (-1)$	1x-1 = -1
$\bar{v}_5 = \bar{v}_6 \dfrac{\partial v_6}{\partial v_5} = \bar{v}_6 \cdot 1$	1x1 = 1
$\bar{v}_6 = \dfrac{\partial y}{\partial v_6}$	1

AutoDiff: Reverse Mode





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	$f(2,5)$
$v_0 = x_1$	2
$v_1 = x_2$	5
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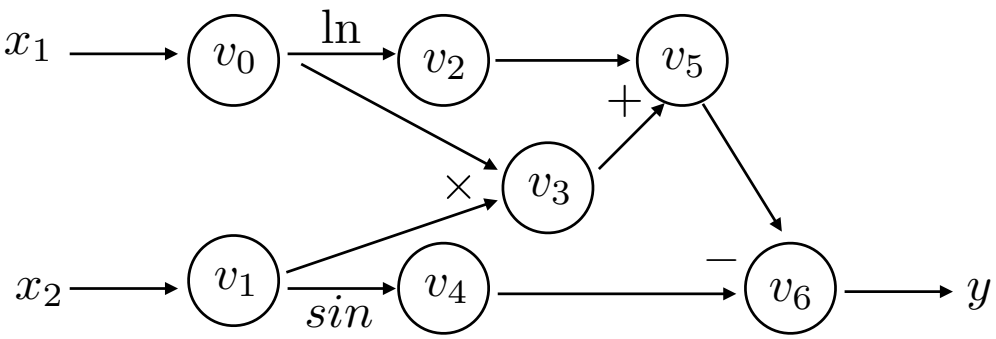
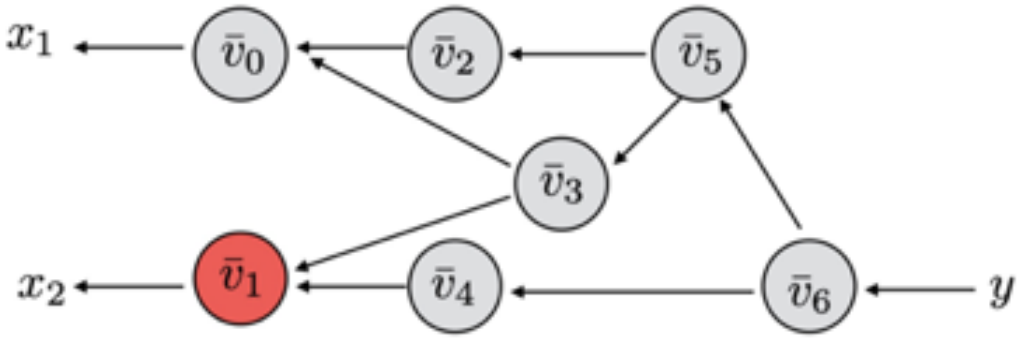
$v_6 = v_5 - v_4$	10.693 + 0.959 = 11.652
$y = v_6$	11.652

Backwards Derivative Trace:

$\bar{v}_1 = \bar{v}_3 \frac{\partial v_3}{\partial v_1} + \bar{v}_4 \frac{\partial v_4}{\partial v_1}$	
$\bar{v}_2 = \bar{v}_5 \frac{\partial v_5}{\partial v_2} = \bar{v}_5 \cdot (1)$	1x1 = 1
$\bar{v}_3 = \bar{v}_5 \frac{\partial v_5}{\partial v_3} = \bar{v}_5 \cdot (1)$	1x1 = 1
$\bar{v}_4 = \bar{v}_6 \frac{\partial v_6}{\partial v_4} = \bar{v}_6 \cdot (-1)$	1x-1 = -1
$\bar{v}_5 = \bar{v}_6 \frac{\partial v_6}{\partial v_5} = \bar{v}_6 \cdot 1$	1x1 = 1
$\bar{v}_6 = \frac{\partial y}{\partial v_6}$	1

AutoDiff: Reverse Mode





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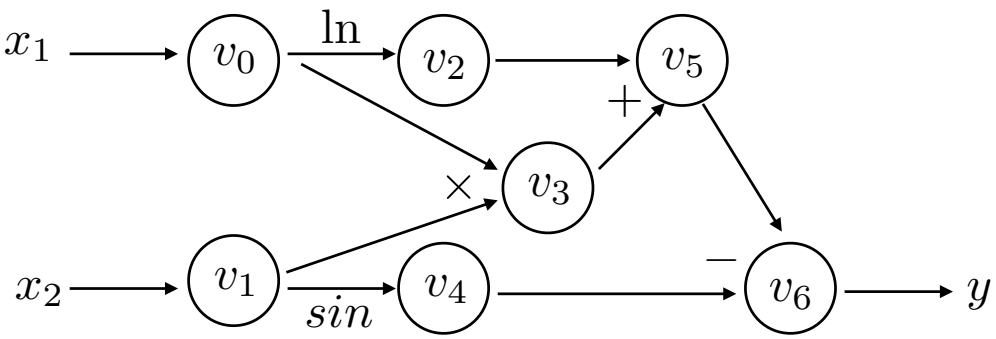
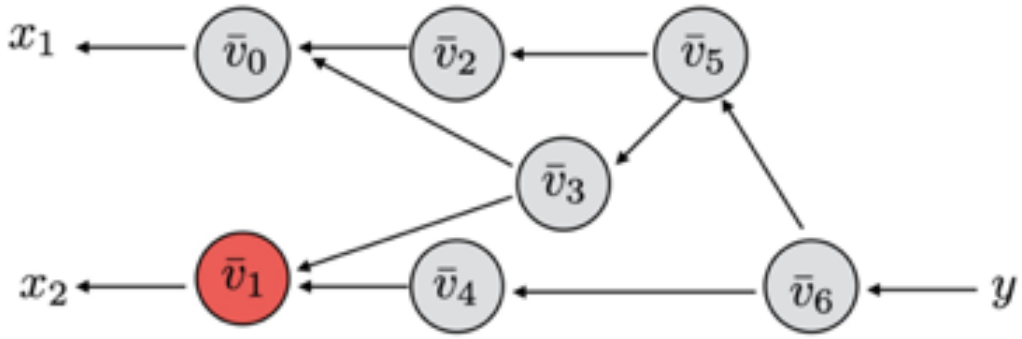
Backwards Derivative Trace:

$\bar{v}_1 = \bar{v}_3 \frac{\partial v_3}{\partial v_1} + \bar{v}_4 \frac{\partial v_4}{\partial v_1}$	
$\bar{v}_2 = \bar{v}_5 \frac{\partial v_5}{\partial v_2} = \bar{v}_5 \cdot (1)$	1x1 = 1
$\bar{v}_3 = \bar{v}_5 \frac{\partial v_5}{\partial v_3} = \bar{v}_5 \cdot (1)$	1x1 = 1
$\bar{v}_4 = \bar{v}_6 \frac{\partial v_6}{\partial v_4} = \bar{v}_6 \cdot (-1)$	1x-1 = -1
$\bar{v}_5 = \bar{v}_6 \frac{\partial v_6}{\partial v_5} = \bar{v}_6 \cdot 1$	1x1 = 1
$\bar{v}_6 = \frac{\partial y}{\partial v_6}$	1

AutoDiff: Reverse Mode





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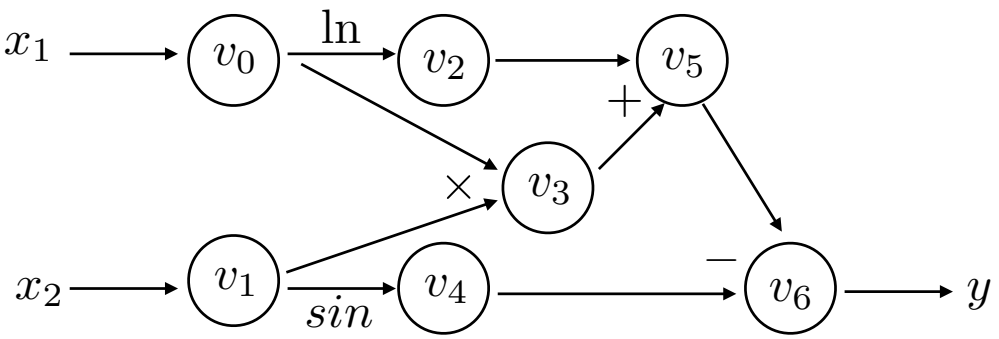
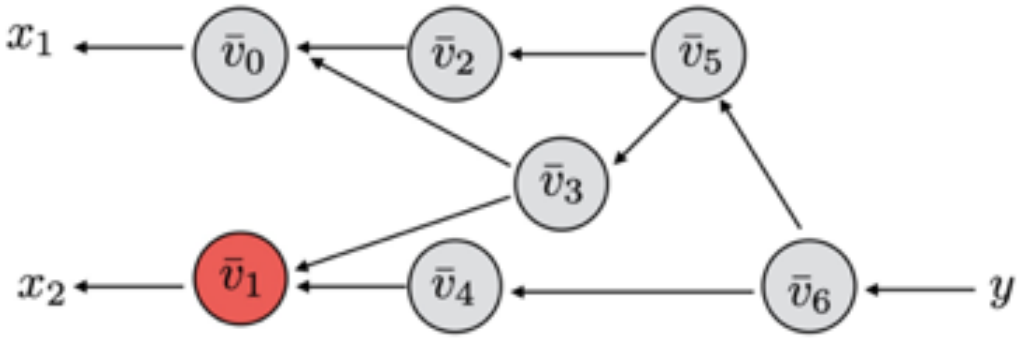
Backwards Derivative Trace:

$\bar{v}_1 = \bar{v}_3 \frac{\partial v_3}{\partial v_1} + \bar{v}_4 \frac{\partial v_4}{\partial v_1} = \bar{v}_3 v_0 + \bar{v}_4 cos(v_1)$	
$\bar{v}_2 = \bar{v}_5 \frac{\partial v_5}{\partial v_2} = \bar{v}_5 \cdot (1)$	1x1 = 1
$\bar{v}_3 = \bar{v}_5 \frac{\partial v_5}{\partial v_3} = \bar{v}_5 \cdot (1)$	1x1 = 1
$\bar{v}_4 = \bar{v}_6 \frac{\partial v_6}{\partial v_4} = \bar{v}_6 \cdot (-1)$	1x-1 = -1
$\bar{v}_5 = \bar{v}_6 \frac{\partial v_6}{\partial v_5} = \bar{v}_6 \cdot 1$	1x1 = 1
$\bar{v}_6 = \frac{\partial y}{\partial v_6}$	1

AutoDiff: Reverse Mode





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Backwards Derivative Trace:

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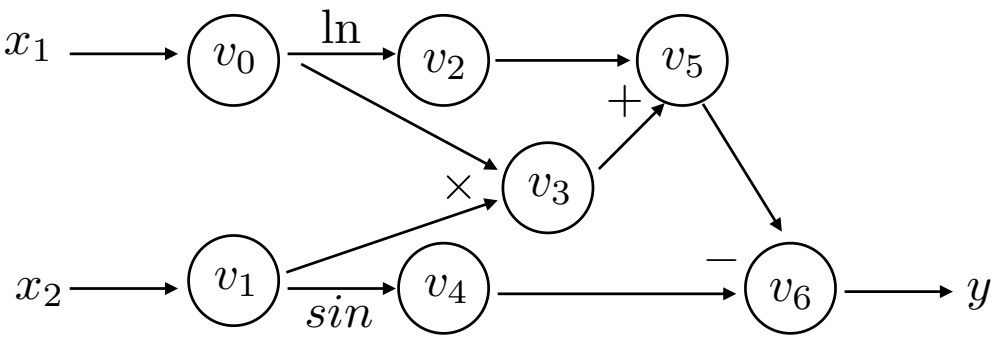
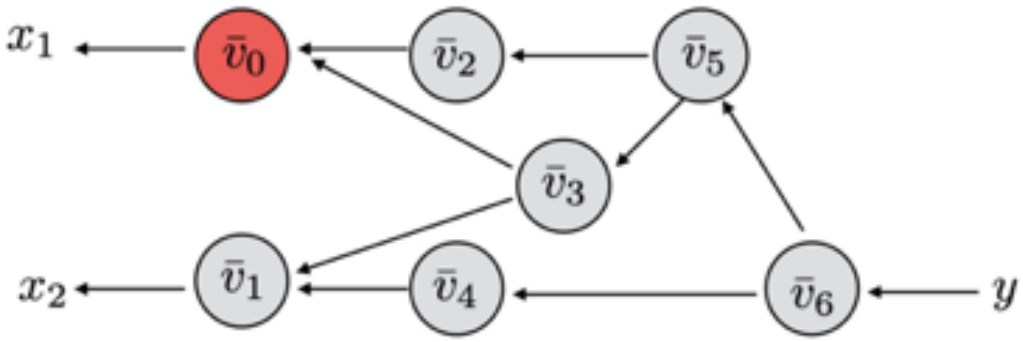
$\bar{v}_2 = \bar{v}_5 \frac{\partial v_5}{\partial v_2} = \bar{v}_5 \cdot (1)$	1x1 = 1
$\bar{v}_3 = \bar{v}_5 \frac{\partial v_5}{\partial v_3} = \bar{v}_5 \cdot (1)$	1x1 = 1
$\bar{v}_4 = \bar{v}_6 \frac{\partial v_6}{\partial v_4} = \bar{v}_6 \cdot (-1)$	1x-1 = -1
$\bar{v}_5 = \bar{v}_6 \frac{\partial v_6}{\partial v_5} = \bar{v}_6 \cdot 1$	1x1 = 1
$\bar{v}_6 = \frac{\partial y}{\partial v_6}$	1

AutoDiff: Reverse Mode





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	$f(2,5)$
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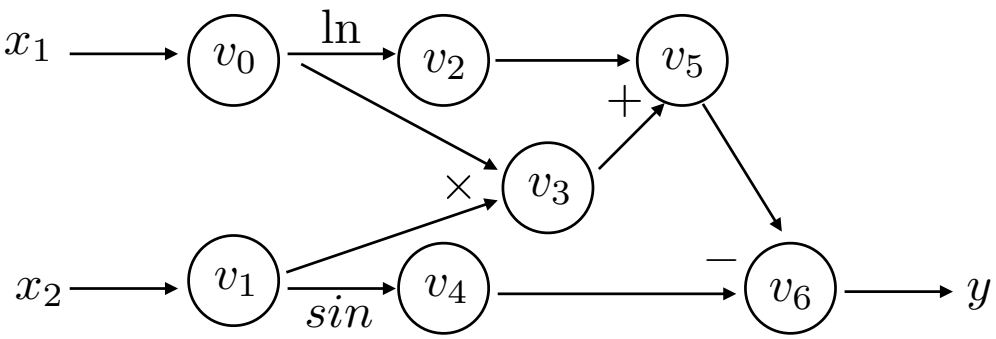
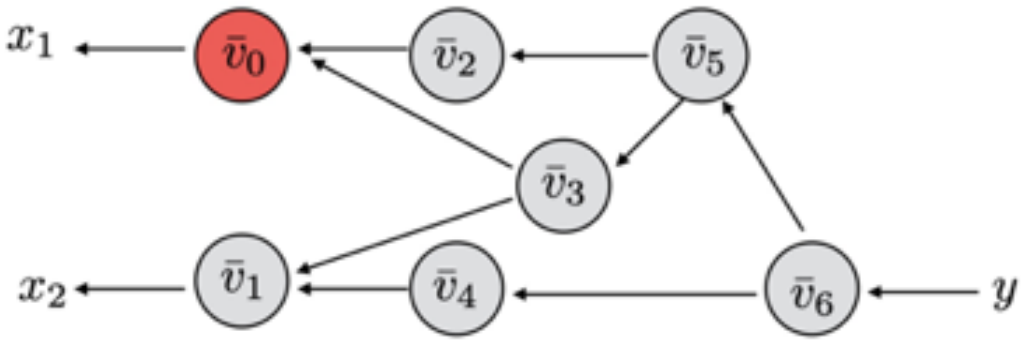
Backwards Derivative Trace:

$\bar{v}_0 = \bar{v}_3 \frac{\partial v_3}{\partial v_0} + \bar{v}_2 \frac{\partial v_2}{\partial v_0} = \bar{v}_3 v_1 + \bar{v}_2 \frac{1}{v_0}$	5.5
$\bar{v}_1 = \bar{v}_3 \frac{\partial v_3}{\partial v_1} + \bar{v}_4 \frac{\partial v_4}{\partial v_1} = \bar{v}_3 v_0 + \bar{v}_4 cos(v_1)$	1.716
$\bar{v}_2 = \bar{v}_5 \frac{\partial v_5}{\partial v_2} = \bar{v}_5 \cdot (1)$	1x1 = 1
$\bar{v}_3 = \bar{v}_5 \frac{\partial v_5}{\partial v_3} = \bar{v}_5 \cdot (1)$	1x1 = 1
$\bar{v}_4 = \bar{v}_6 \frac{\partial v_6}{\partial v_4} = \bar{v}_6 \cdot (-1)$	1x-1 = -1
$\bar{v}_5 = \bar{v}_6 \frac{\partial v_6}{\partial v_5} = \bar{v}_6 \cdot 1$	1x1 = 1
$\bar{v}_6 = \frac{\partial y}{\partial v_6}$	1

AutoDiff: Reverse Mode





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	$f(2,5)$
$v_0 = x_1$	2
$v_1 = x_2$	5
$v_2 = \ln(v_0)$	ln(2) = 0.693
$v_3 = v_0 \cdot v_1$	2 x 5 = 10
$v_4 = sin(v_1)$	sin(5) = -0.959
$v_5 = v_2 + v_3$	0.693 + 10 = 10.693
$v_6 = v_5 - v_4$	10.693 + 0.959 = 11.652
$y = v_6$	11.652

Backwards Derivative Trace:

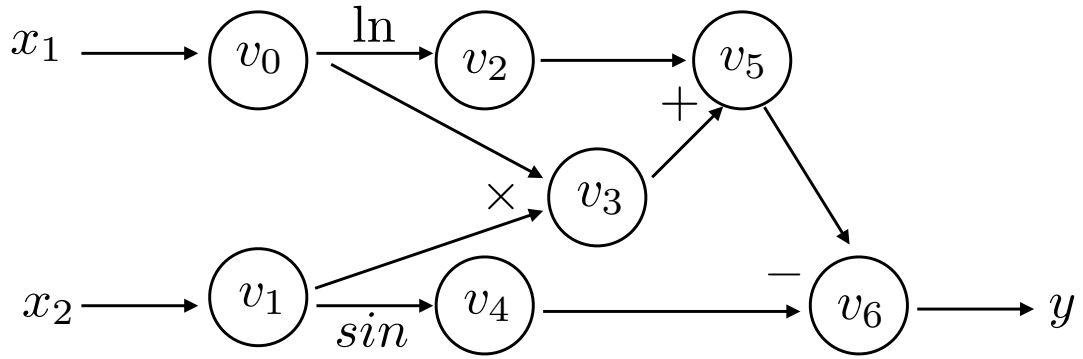
$\bar{v}_0 = \bar{v}_3 \frac{\partial v_3}{\partial v_0} + \bar{v}_2 \frac{\partial v_2}{\partial v_0} = \bar{v}_3 v_1 + \bar{v}_2 \frac{1}{v_0}$	5.5
$\bar{v}_1 = \bar{v}_3 \frac{\partial v_3}{\partial v_1} + \bar{v}_4 \frac{\partial v_4}{\partial v_1} = \bar{v}_3 v_0 + \bar{v}_4 cos(v_1)$	1.716
$\bar{v}_2 = \bar{v}_5 \frac{\partial v_5}{\partial v_2} = \bar{v}_5 \cdot (1)$	1x1 = 1
$\bar{v}_3 = \bar{v}_5 \frac{\partial v_5}{\partial v_3} = \bar{v}_5 \cdot (1)$	1x1 = 1
$\bar{v}_4 = \bar{v}_6 \frac{\partial v_6}{\partial v_4} = \bar{v}_6 \cdot (-1)$	1x-1 = -1
$\bar{v}_5 = \bar{v}_6 \frac{\partial v_6}{\partial v_5} = \bar{v}_6 \cdot 1$	1x1 = 1
$\bar{v}_6 = \frac{\partial y}{\partial v_6}$	1

Automatic Differentiation (AutoDiff)

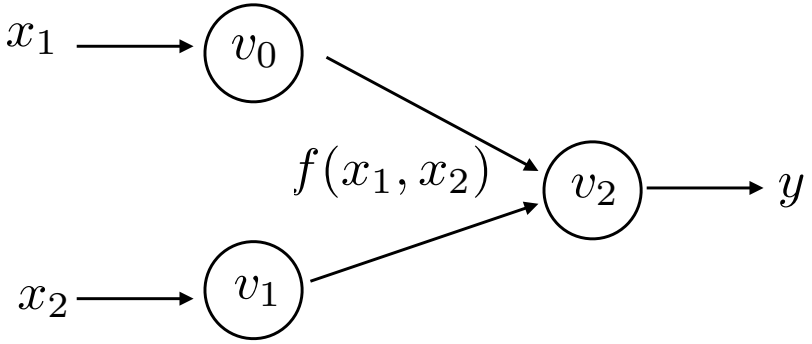
$$y = f(x_1, x_2) = \ln(x_1) + x_1 x_2 - sin(x_2)$$

- AutoDiff can be done at various **granularities**

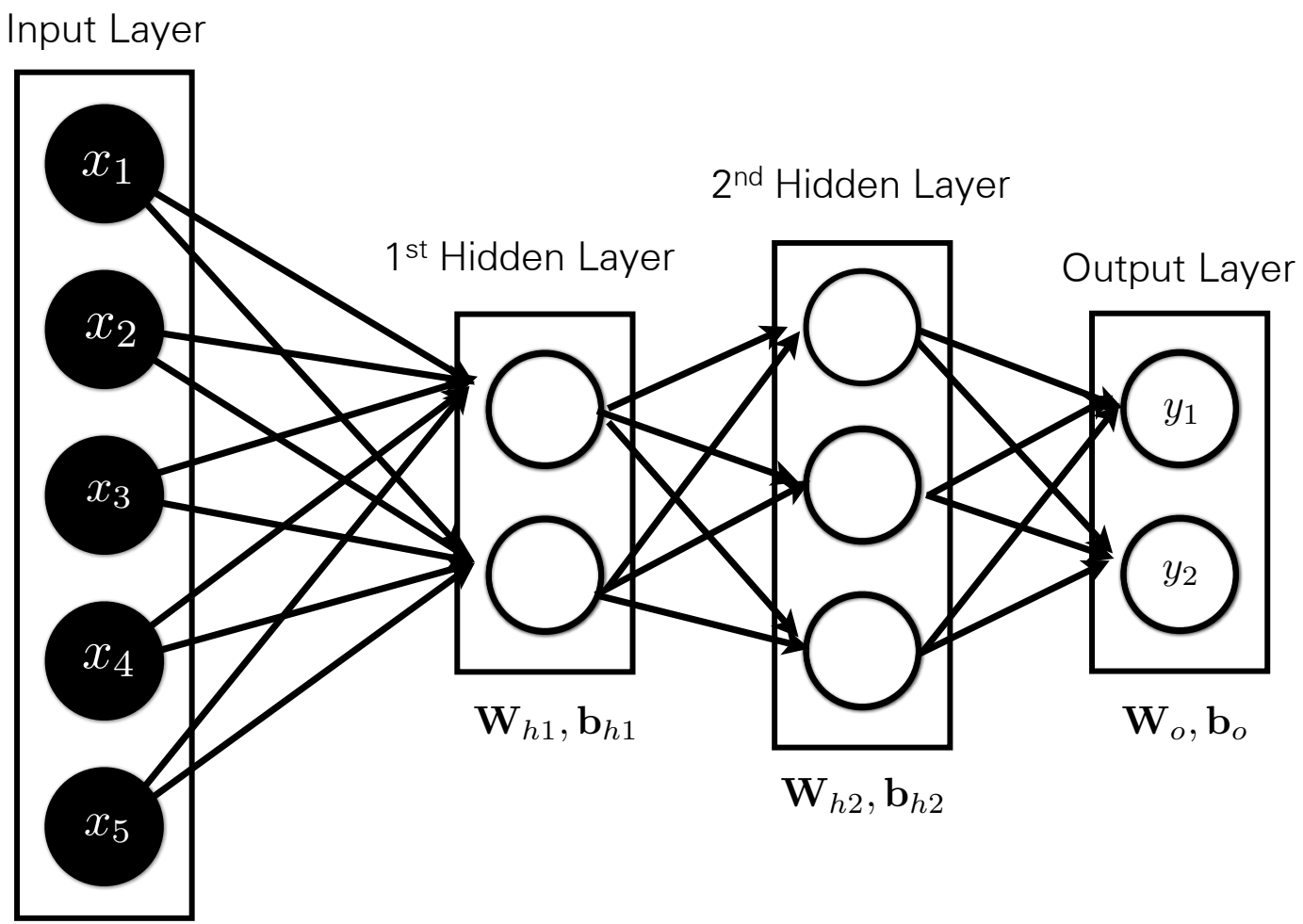
Elementary function granularity:



Complex function granularity:



Backpropagation: Practical Issues



Easier to deal with in vector form

Jacobian of Sigmoid layer

$\mathbf{x}, \mathbf{y} \in \mathbb{R}^{2048}$

- Element-wise sigmoid layer:

Jacobian of Sigmoid layer

$\mathbf{x}, \mathbf{y} \in \mathbb{R}^{2048}$

- Element-wise sigmoid layer:

  - What is the dimension of **Jacobian**?

Jacobian of Sigmoid layer

$\mathbf{x}, \mathbf{y} \in \mathbb{R}^{2048}$

- Element-wise sigmoid layer:

  - What is the dimension of **Jacobian**?
  - What does it look like?

Jacobian of Sigmoid layer

$\mathbf{x}, \mathbf{y} \in \mathbb{R}^{2048}$

- Element-wise sigmoid layer:

  - What is the dimension of **Jacobian**?
  - What does it look like?

    If we are working with a mini batch of 100 inputs-output pairs, Jacobian is a matrix 204,800 x 204,800!

Backpropagation: Common questions

- **Question:** Does BackProp only work for certain layers?

  Answer: No, for any differentiable functions

- **Question:** What is computational cost of BackProp?

  Answer: On average about twice the forward pass

- **Question:** Is BackProp a dual of forward propagation?

  Answer: Yes

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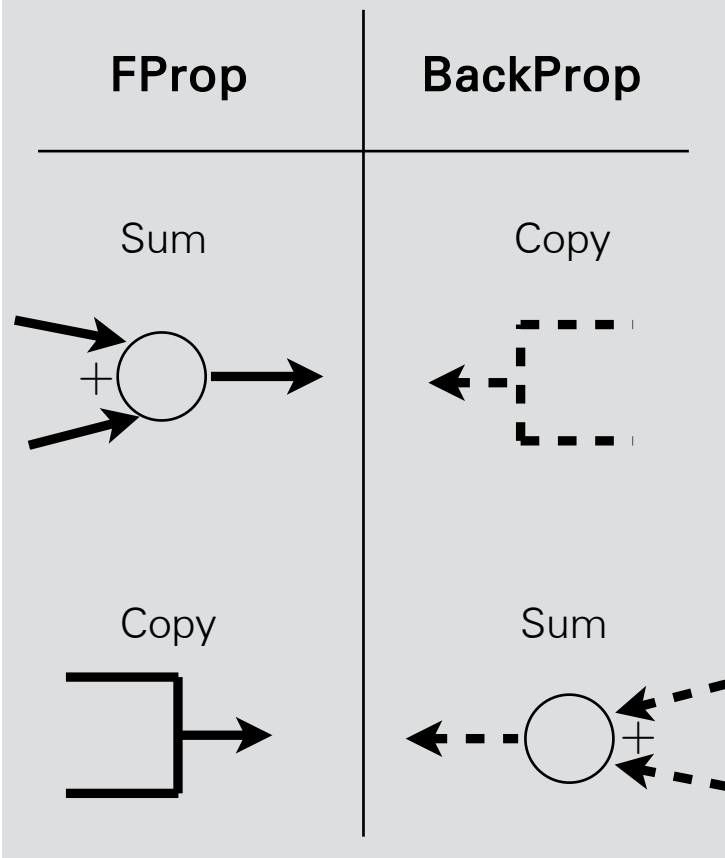


slide adopted from Marc'Aurelio Ranzato

From symbolic to distributed word representations

- The vast majority of rule-based or statistical NLP and IR work regarded words as atomic symbols: **hotel**, **conference**, **walk**
- In vector space terms, this is a vector with one 1 and a lot of zeroes

"hotel"

0	0	0	0	0	0	0	0	0	0	**1**	0	0	0	0

- We now call this a **one-hot** representation.

Window based co-occurence matrix

- Example corpus:
  - I like deep learning.
  - I like NLP.
  - I enjoy flying.

counts	I	like	enjoy	deep	learning	NLP	flying	.
I	0	2	1	0	0	0	0	0
like	2	0	0	1	0	1	0	0
enjoy	1	0	0	0	0	0	1	0
deep	0	1	0	0	1	0	0	0
learning	0	0	0	1	0	0	0	1
NLP	0	1	0	0	0	0	0	1
flying	0	0	1	0	0	0	0	1
.	0	0	0	0	1	1	1	0

- Increase in size with vocabulary
- Very high dimensional: require a lot of storage
- Subsequent classification models have sparsity issues
- Models are less robust

Prediction-based models: An alternative way to get dense vectors

- **Skip-gram** (Mikolov et al. 2013a), **CBOW** (Mikolov et al. 2013b)
- Learn embeddings as part of the process of word prediction.
- Train a neural network to predict neighboring words
  - Inspired by **neural net language models**.
  - In so doing, learn dense embeddings for the words in the training corpus.
- Advantages:
  - Fast, easy to train (much faster than SVD)
  - Available online in the `word2vec` package
  - Including sets of pretrained embeddings!

Basic idea of learning neural network word embeddings

- We define some model that aims to predict a word based on other words in its context

$$\mathrm{argmax}_w w \cdot \left(\left(w_{j-1} + w_{j+1} \right) / 2 \right)$$

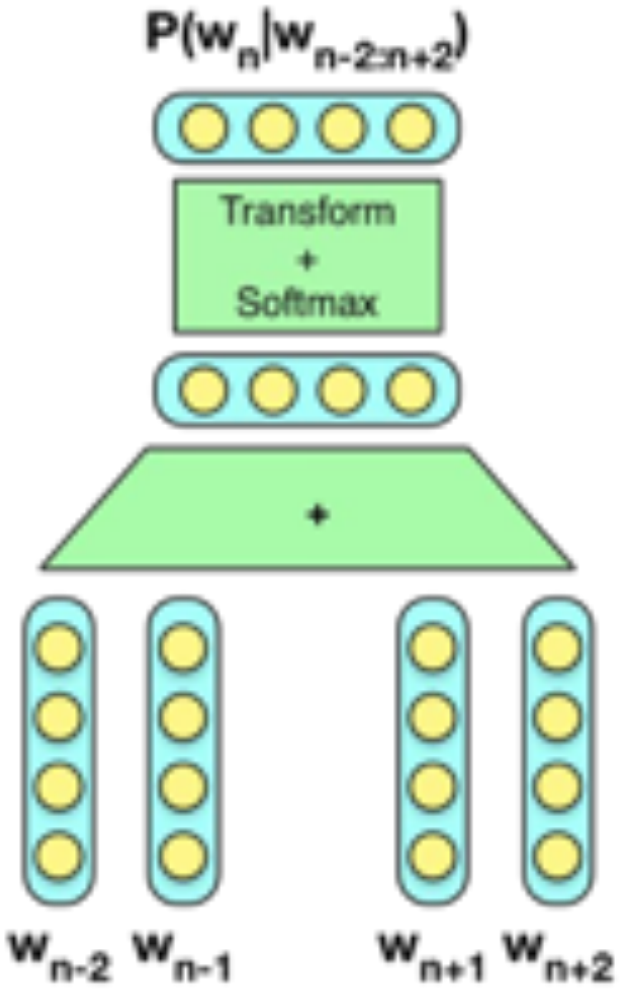
which has a loss function, e.g.,

$$J(\theta) = 1 - w_j \cdot \left(\left(w_{j-1} + w_{j+1} \right) / 2 \right)$$

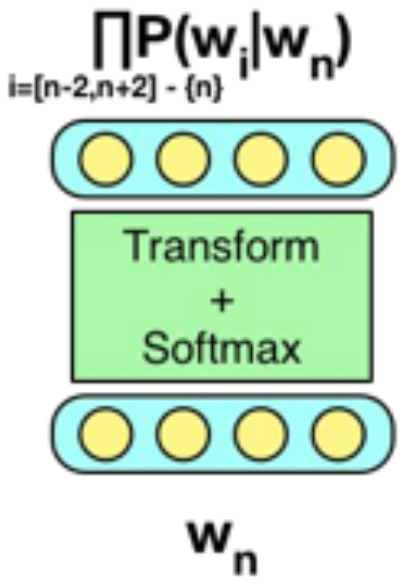
Unit norm vectors

- We look at many samples from a big language corpus
- We keep adjusting the vector representations of words to minimize this loss

Neural Embedding Models (Mikolov et al. 2013)



CBoW model



Skip-gram model

Distributed representations of words and phrases and their compositionality [Mikolov vd.'13]

Image credit: Ed Grefenstette

Details of `word2vec`

- Predict surrounding words in a window of length m of every word.
- **Objective function:** Maximize the log probability of any context word given the current center word:

$$J(\theta) = \frac{1}{T} \sum_{t=1}^{T} \sum_{-m \leq j \leq m, j \neq 0} \log p(w_{t+j} | w_t)$$

where θ represents all variables we optimize

Distributed representations of words and phrases and their compositionality [Mikolov vd.'13]

Details of `word2vec`

- Predict surrounding words in a window of length m of every word.
- For $p(w_{t+j}|w_t)$ the simplest first formulation is

$$p(o|c) = \frac{\exp(u_o^T v_c)}{\sum_{w=1}^{W} \exp(u_w^T v_c)}$$

where o is the outside (or output) word id,

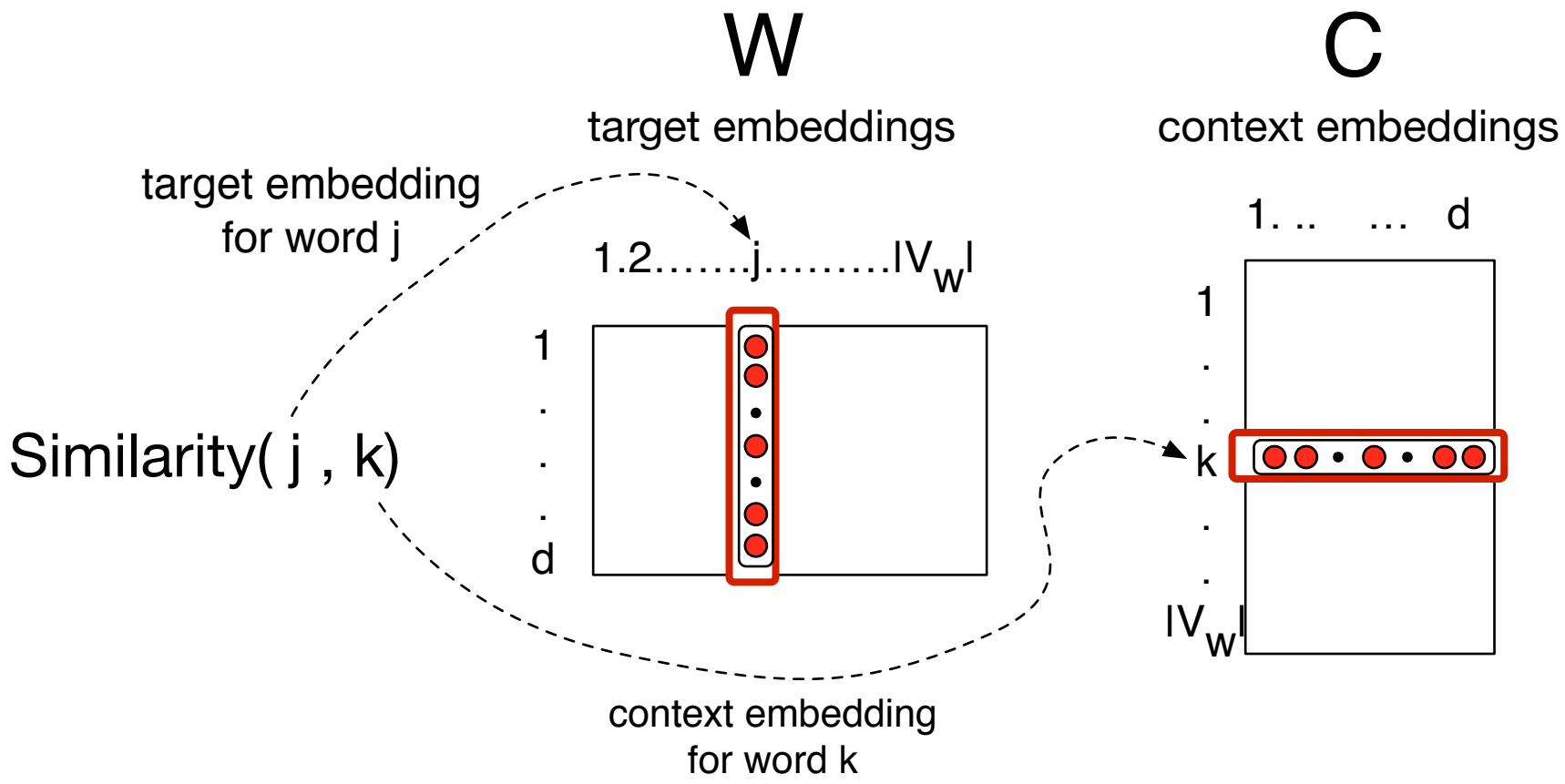
c is the center word id,

u and v are "center" and "outside" vectors of o and c

- Every word has two vectors!
- This is essentially "dynamic" logistic regression

Distributed representations of words and phrases and their compositionality [Mikolov vd.'13]

Intuition: similarity as dot-product between a target vector and context vector



- Similarity(j,k) = $c_k \cdot v_j$
- We use softmax to turn into probabilities

$$p(w_k|w_j) = \frac{exp(c_k \cdot v_j)}{\sum_{i \in |V|} exp(c_i \cdot v_j)}$$

Details of `word2vec`

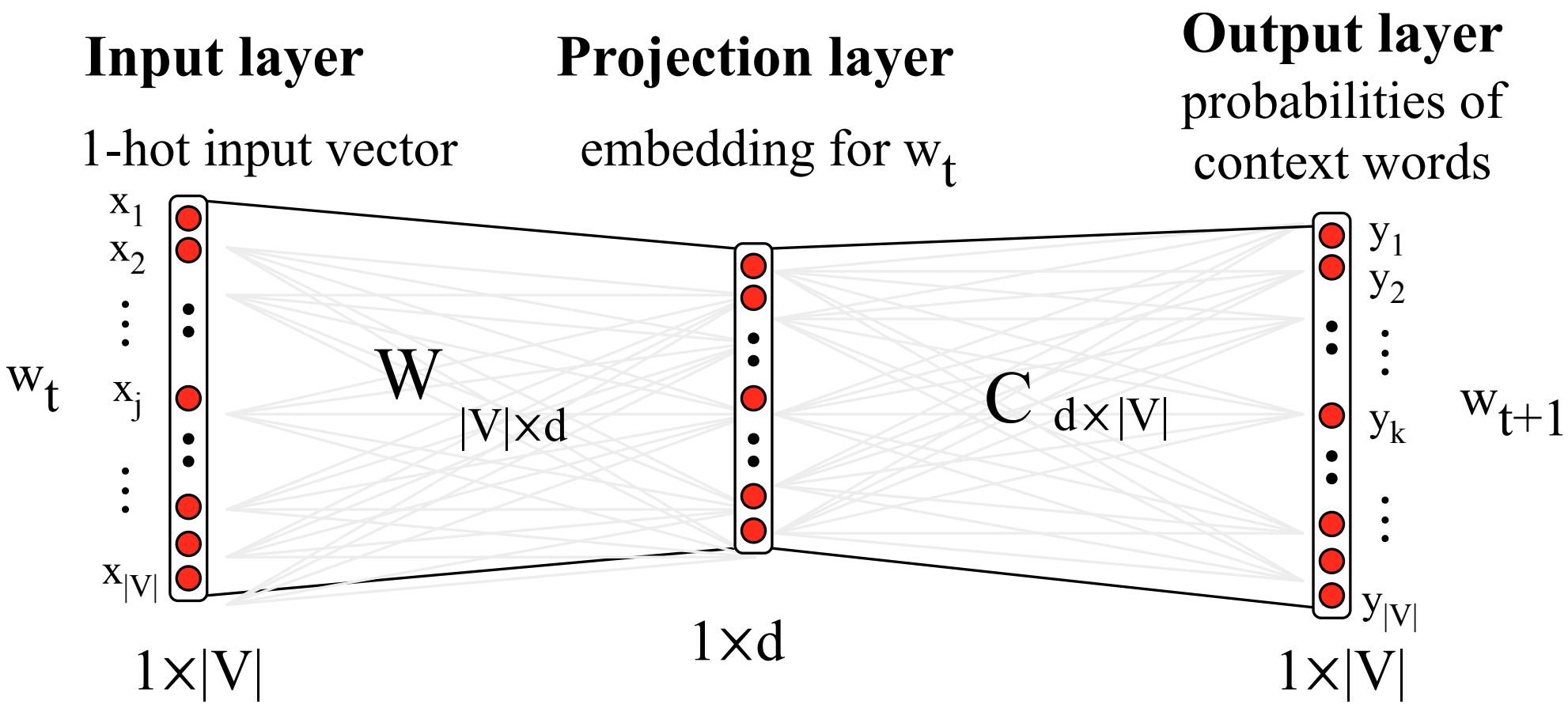
- Predict surrounding words in a window of length m of every word.
- For $p(w_{t+j}|w_t)$ the simplest first formulation is

$$p(o|c) = \frac{\exp(u_o^T v_c)}{\sum_{w=1}^{W} \exp(u_w^T v_c)}$$

- Every word has two vectors!
- We can either:
  - Just use v_j
  - Sum them
  - Concatenate them to make a double-length embedding

Distributed representations of words and phrases and their compositionality [Mikolov vd.'13]

Visualizing W and C as a network for doing error backprop



Problem with the softmax

- The denominator: have to compute over every word in vocabulary

$$p(w_k|w_j) = \frac{exp(c_k \cdot v_j)}{\sum_{i \in |V|} exp(c_i \cdot v_j)}$$

- Instead: just sample a few of those negative words

Goal in learning

- Make the word like the context words

```
lemon,  a [tablespoon of apricot preserves or] jam
           c1         c2    w     c3       c4
```

$$\sigma(x) = \frac{1}{1+e^{x}}$$

- We want this to be high:

$$\sigma(c1 \cdot w) + \sigma(c2 \cdot w) + \sigma(c3 \cdot w) + \sigma(c4 \cdot w)$$

- And not like k randomly selected "noise words"

```
[cement metaphysical dear coaxial    apricot attendant whence forever puddle]
 n1     n2            n3   n4                 n5         n6     n7       n8
```

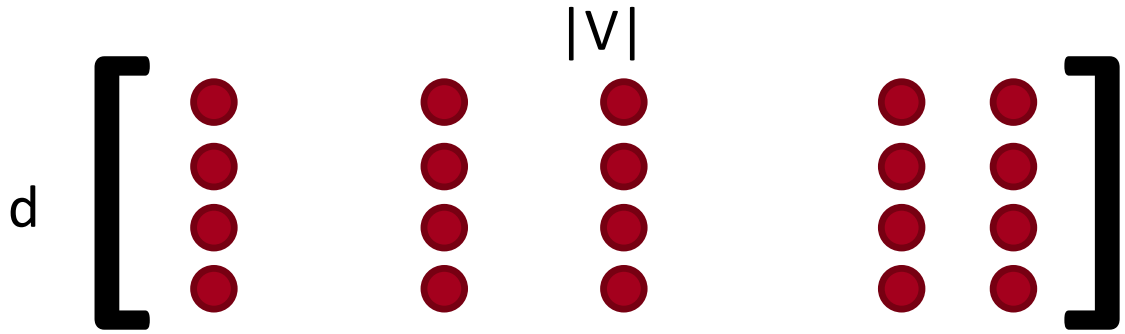
- We want this to be low: $\sigma(n1 \cdot w) + \sigma(n2 \cdot w) + \ldots + \sigma(n8 \cdot w)$

Skipgram with negative sampling: Loss function

$$\log \sigma(c \cdot w) + \sum_{i=1}^{\kappa} \mathbb{E}_{w_i \sim p(w)} \left[\log \sigma(-w_i \cdot w) \right]$$

Stochastic gradients with word vectors!

- We may as well only update the word vectors that actually appear!
- Solution: either keep around hash for word vectors or only update certain columns of full embedding matrix U and V



- Important if you have millions of word vectors and do distributed computing to not have to send gigantic updates around.

Next Lecture:
Training Deep Neural Networks