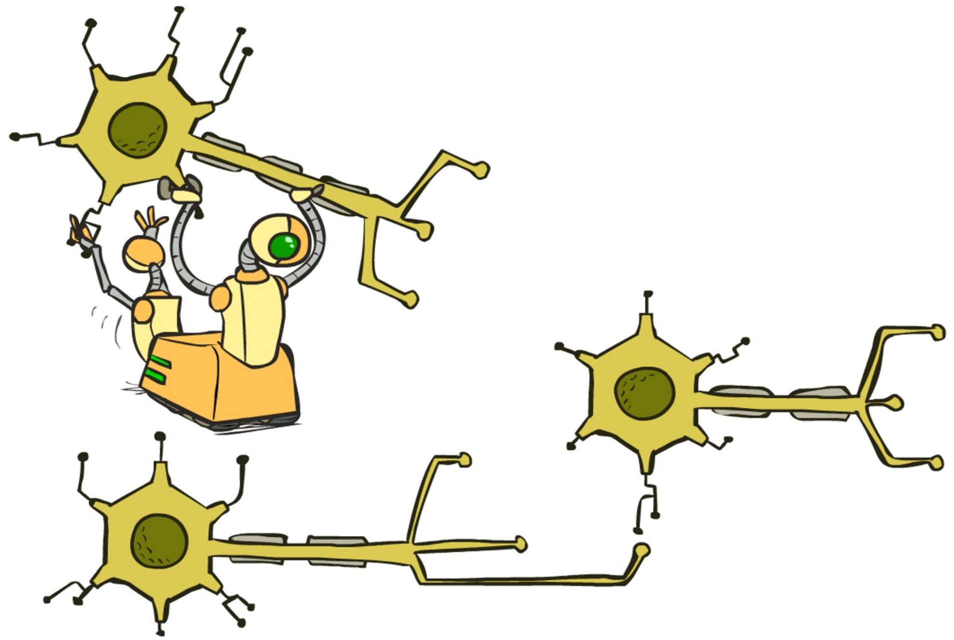
# Artificial Intelligence - INFOF311

## Gradient ascent and neural networks

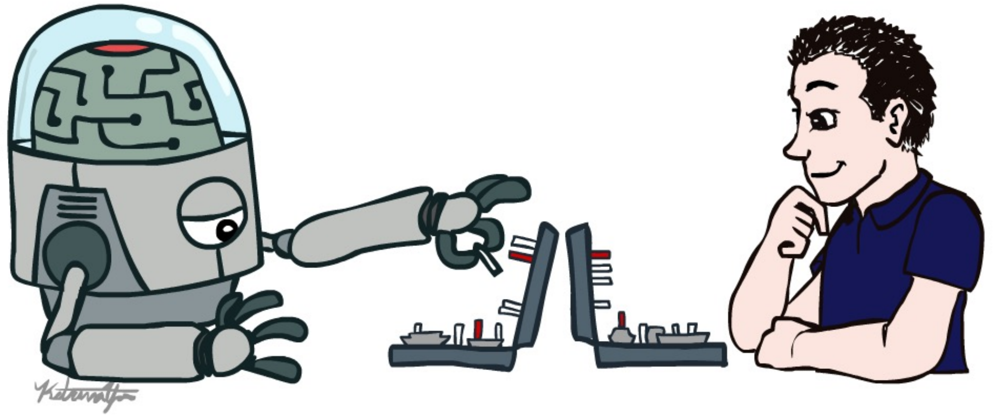


Instructor : Tom Lenaerts

## Acknowledgement

We thank Stuart Russell for his generosity in allowing us to use the slide set of the UC Berkeley Course CS188, Introduction to Artificial Intelligence. These slides were created by Dan Klein, Pieter Abbeel and Anca Dragan for CS188 Intro to AI at UC Berkeley. All CS188 materials are available at http://ai.berkeley.edu.]

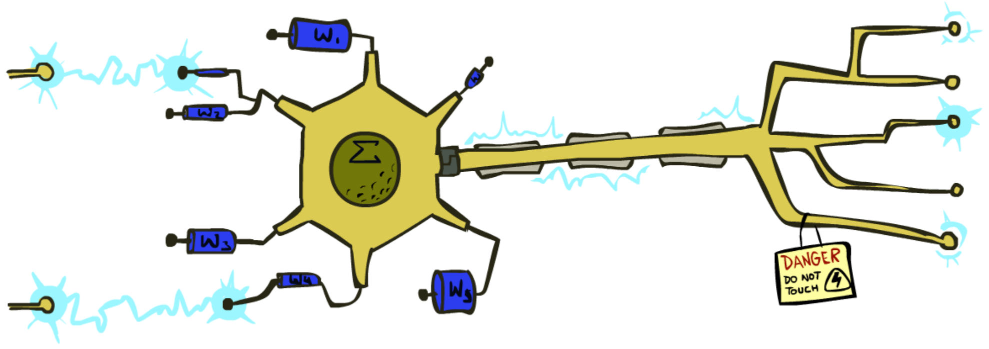
CHAI Center for Human-Compatible Artificial Intelligence



The slides for INFOF311 are slightly modified versions of the slides of the spring and summer CS188 sessions in 2021 and 2022

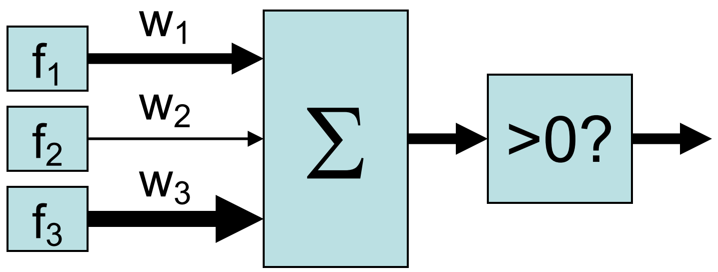
# Reminder : Linear Classifiers

- Inputs are feature values
- Each feature has a weight
- Sum is the activation



$$\text{activation}_w(x) = \sum_i w_i \cdot f_i(x) = w \cdot f(x)$$

- If the activation is:
  - Positive, output +1
  - Negative, output -1

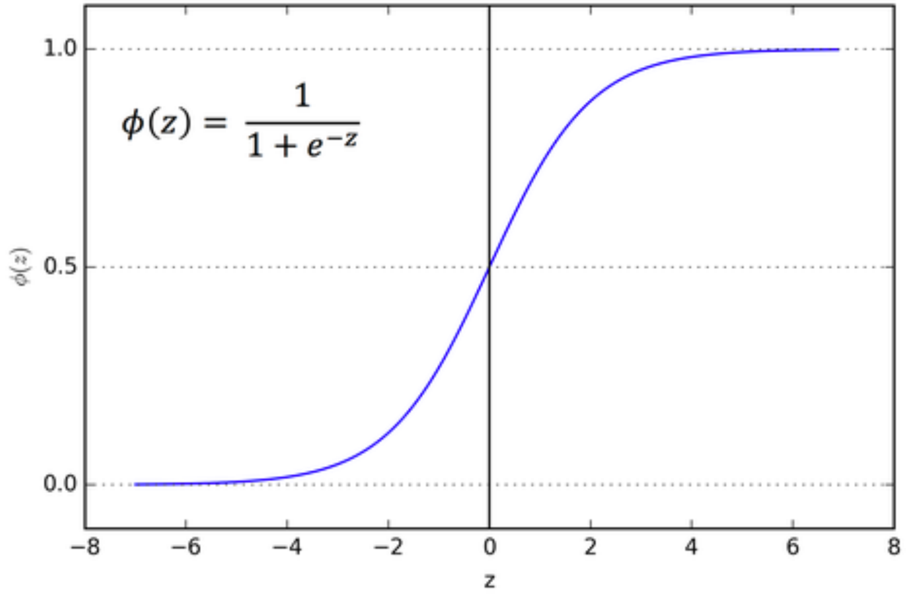


# How to get probabilistic decisions?

- Perceptron scoring: $z = w \cdot f(x)$
- If $z = w \cdot f(x)$ very positive → want probability going to 1
- If $z = w \cdot f(x)$ very negative → want probability going to 0

- Sigmoid function

$$\phi(z) = \frac{1}{1 + e^{-z}}$$



## Best w?

- Maximum likelihood estimation:

$$\max_w \quad ll(w) = \max_w \quad \sum_i \log P(y^{(i)}|x^{(i)}; w)$$

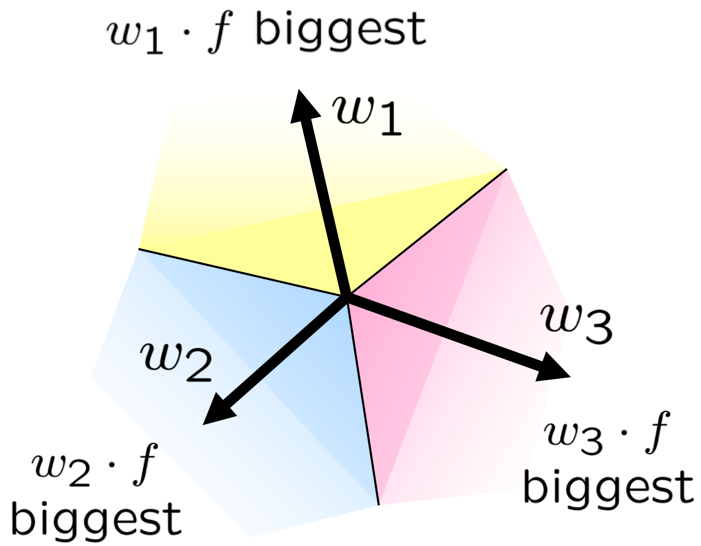
with: $$P(y^{(i)} = +1|x^{(i)}; w) = \frac{1}{1 + e^{-w \cdot f(x^{(i)})}}$$

$$P(y^{(i)} = -1|x^{(i)}; w) = 1 - \frac{1}{1 + e^{-w \cdot f(x^{(i)})}}$$

**= Logistic Regression**

# Multiclass Logistic Regression

- Recall Perceptron:
  - A weight vector for each class: $w_y$
  - Score (activation) of a class y: $w_y \cdot f(x)$
  - Prediction highest score wins $y = \arg\max_y \; w_y \cdot f(x)$



- How to make the scores into probabilities?

$$\underbrace{z_1, z_2, z_3}_{\text{original activations}} \rightarrow \underbrace{\frac{e^{z_1}}{e^{z_1}+e^{z_2}+e^{z_3}}, \frac{e^{z_2}}{e^{z_1}+e^{z_2}+e^{z_3}}, \frac{e^{z_3}}{e^{z_1}+e^{z_2}+e^{z_3}}}_{\text{softmax activations}}$$

## Best w?

- Maximum likelihood estimation:

$$\max_w \quad ll(w) = \max_w \quad \sum_i \log P(y^{(i)}|x^{(i)}; w)$$

with: $$P(y^{(i)}|x^{(i)}; w) = \frac{e^{w_{y^{(i)}} \cdot f(x^{(i)})}}{\sum_y e^{w_y \cdot f(x^{(i)})}}$$

**= Multi-Class Logistic Regression**

# What's next …

## Optimization

i.e., how do we solve:

$$\max_w \quad ll(w) = \max_w \quad \sum_i \log P(y^{(i)}|x^{(i)}; w)$$

## Review: Derivatives and Gradients

- What is the derivative of the functi$g(x) = x^2 + 3$?

$$\frac{dg}{dx} = 2x$$

- What is the derivative of g(x) at x=5?

$$\frac{dg}{dx}\Big|_{x=5} = 10$$

# Review: Derivatives and Gradients

- What is the gradient of the functi $g(x, y) = x^2 y$ ?
  - Recall: Gradient is a vector of partial derivatives with respect to each variable

$$\nabla g = \begin{bmatrix} \frac{\partial f}{\partial x} \\ \\ \frac{\partial f}{\partial y} \end{bmatrix} = \begin{bmatrix} 2xy \\ \\ x^2 \end{bmatrix}$$

- What is the derivative of g(x, y) at x=0.5, y=0.5?

$$\nabla g|_{x=0.5, y=0.5} = \begin{bmatrix} 2(0.5)(0.5) \\ (0.5^2) \end{bmatrix} = \begin{bmatrix} 0.5 \\ 0.25 \end{bmatrix}$$

# Hill Climbing

## Recall from local search lecture: simple, general idea

Start wherever

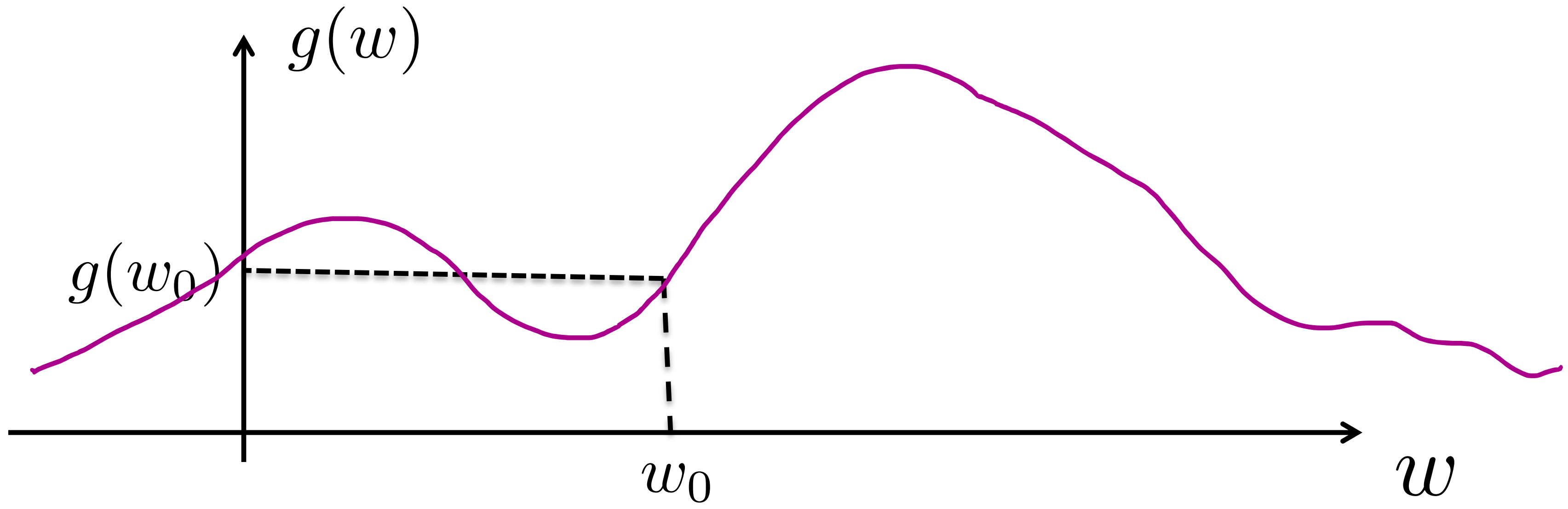
Repeat: move to the best neighboring state

If no neighbors better than current, quit

## What's particularly tricky when hill-climbing for multiclass logistic regression?

- Optimization over a continuous space
  - Infinitely many neighbors!
  - How to do this efficiently?

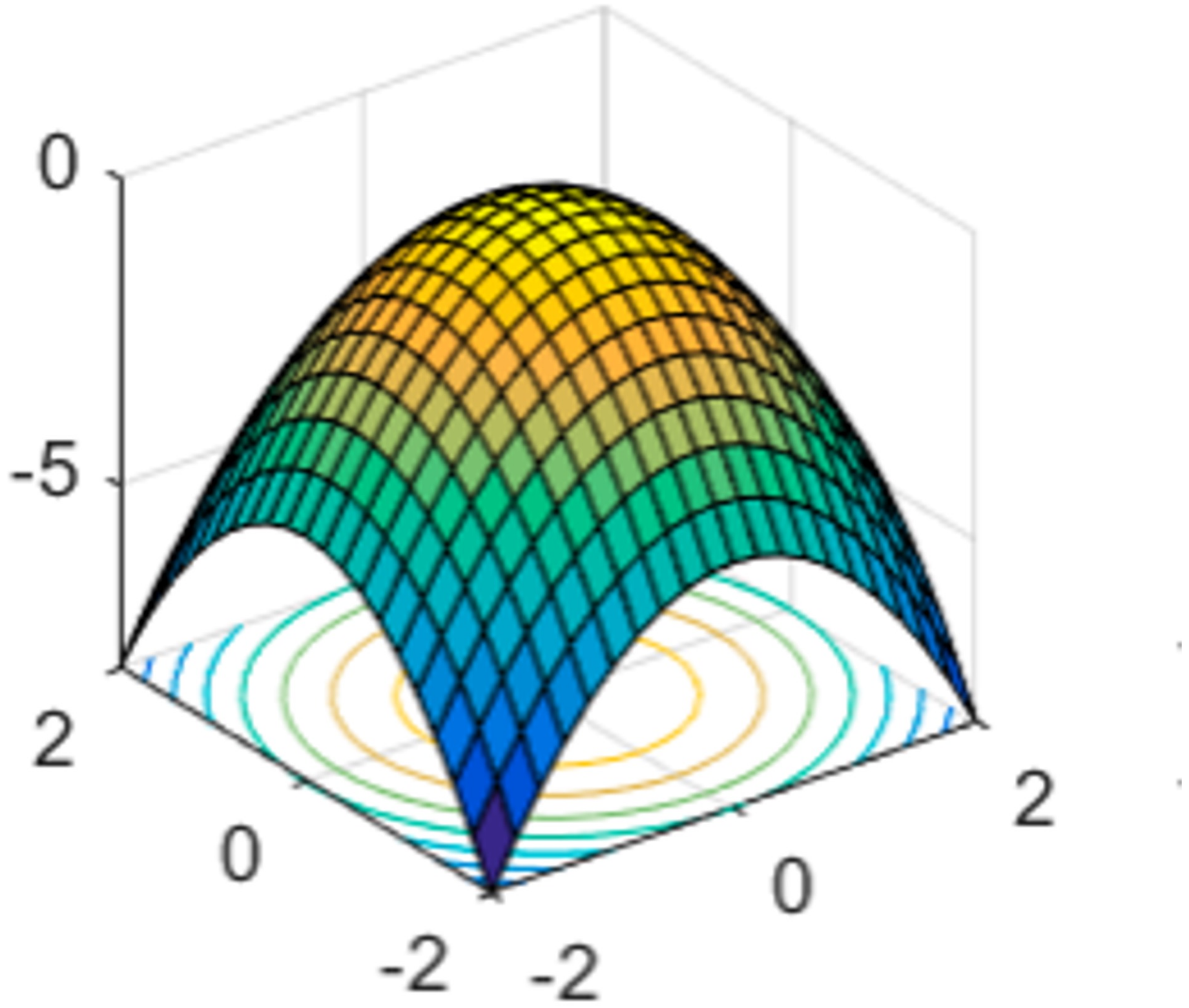
# 1-D Optimization



- Could evaluate $g(w_0 + h)$ and $g(w_0 - h)$
  - Then step in best direction

- Or, evaluate derivative: $\dfrac{\partial g(w_0)}{\partial w} = \lim_{h \to 0} \dfrac{g(w_0 + h) - g(w_0 - h)}{2h}$
  - Tells which direction to step into

## 2-D Optimization



Source: offconvex.org

## Gradient Ascent

Perform update in uphill direction for each coordinate

The steeper the slope (i.e. the higher the derivative) the bigger the step for that coordinate

E.g., consider: $g(w_1, w_2)$

Updates:

$$w_1 \leftarrow w_1 + \alpha * \frac{\partial g}{\partial w_1}(w_1, w_2)$$

$$w_2 \leftarrow w_2 + \alpha * \frac{\partial g}{\partial w_2}(w_1, w_2)$$

- Updates in vector notation:

$$w \leftarrow w + \alpha * \nabla_w g(w)$$

with: $\nabla_w g(w) = \begin{bmatrix} \frac{\partial g}{\partial w_1}(w) \\ \frac{\partial g}{\partial w_2}(w) \end{bmatrix}$ **= gradient**

# Gradient Ascent

Idea:

Start somewhere

Repeat: Take a step in the gradient direction

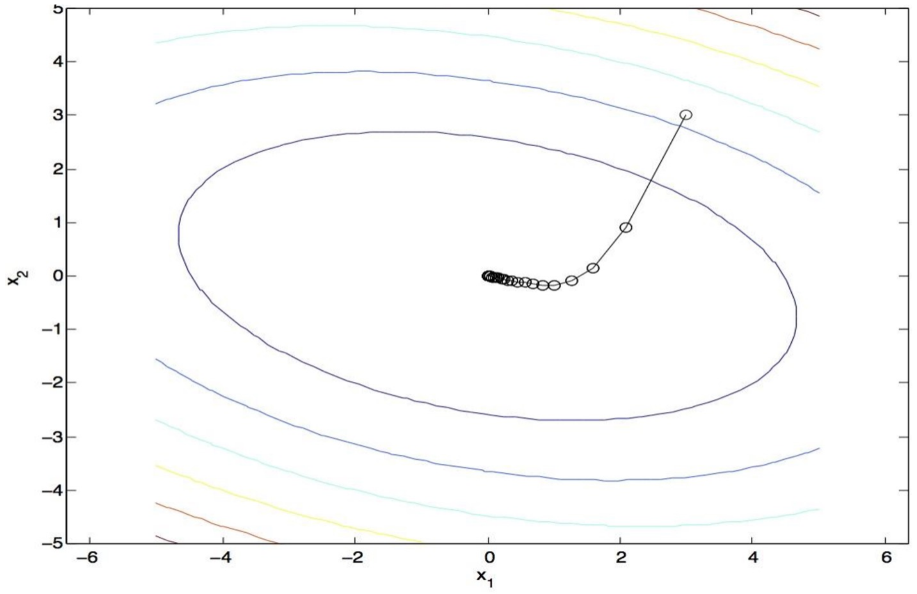
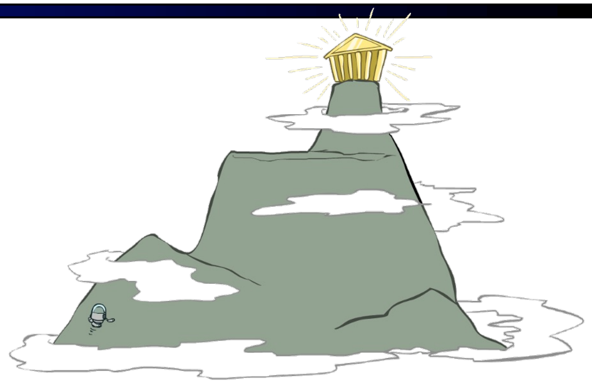


Figure source: Mathworks

# What is the Steepest Direction?

$$\max_{\Delta:\Delta_1^2+\Delta_2^2\leq\varepsilon} \quad g(w+\Delta)$$



- First-Order Taylor Expansion: $g(w+\Delta) \approx g(w) + \frac{\partial g}{\partial w_1}\Delta_1 + \frac{\partial g}{\partial w_2}\Delta_2$
- Steepest Ascent Direction: $\max_{\Delta:\Delta_1^2+\Delta_2^2\leq\varepsilon} \quad g(w) + \frac{\partial g}{\partial w_1}\Delta_1 + \frac{\partial g}{\partial w_2}\Delta_2$
- Recall: $\max_{\Delta:\|\Delta\|\leq\varepsilon} \Delta^\top a$ → $\Delta = \varepsilon\frac{a}{\|a\|}$
- Hence, solution: $\Delta = \varepsilon\frac{\nabla g}{\|\nabla g\|}$ **Gradient direction = steepest direction!** $\nabla g = \begin{bmatrix} \frac{\partial g}{\partial w_1} \\ \frac{\partial g}{\partial w_2} \end{bmatrix}$

## Gradient in n dimensions

$$\nabla g = \begin{bmatrix} \frac{\partial g}{\partial w_1} \\ \frac{\partial g}{\partial w_2} \\ \cdots \\ \frac{\partial g}{\partial w_n} \end{bmatrix}$$

# Optimization Procedure: Gradient Ascent

```
init $w$
for iter = 1, 2, …
        $w \leftarrow w + \alpha * \nabla g(w)$
```

- $\alpha$ : learning rate --- tweaking parameter that needs to be chosen carefully
- https://distill.pub/2017/momentum/

# Gradient Ascent with momentum

- Use momentum to improve gradient ascent convergence

```
init $w$
for iter = 1, 2, …
    $w \leftarrow w + \alpha \nabla g(w)$
```

**Gradient ascent**

```
init $w$
for iter = 1, 2, …
        $z \leftarrow \beta z + \nabla g(w)$
        $w \leftarrow w + \alpha z$
```

**Gradient ascent with momentum**

- One interpretation: $w$ moves like a particle with mass
- Another : exponential average on gradient
- E.g. Adam algorithm in deep learning

## Batch Gradient Ascent on the Log Likelihood Objective

$$\max_w \quad ll(w) = \max_w \quad \underbrace{\sum_i \log P(y^{(i)}|x^{(i)}; w)}_{g(w)}$$

```
init $w$
for iter = 1, 2, …
$w \leftarrow w + \alpha * \sum_i \nabla \log P(y^{(i)}|x^{(i)}; w)$
```

## Stochastic Gradient Ascent on the Log Likelihood Objective

$$\max_w \quad ll(w) = \max_w \quad \sum_i \log P(y^{(i)}|x^{(i)};w)$$

**Observation:** once gradient on one training example has been computed, might as well incorporate before computing next one

```
init $w$
for iter = 1, 2, …
    pick random j
    $w \leftarrow w + \alpha * \nabla \log P(y^{(j)}|x^{(j)};w)$
```

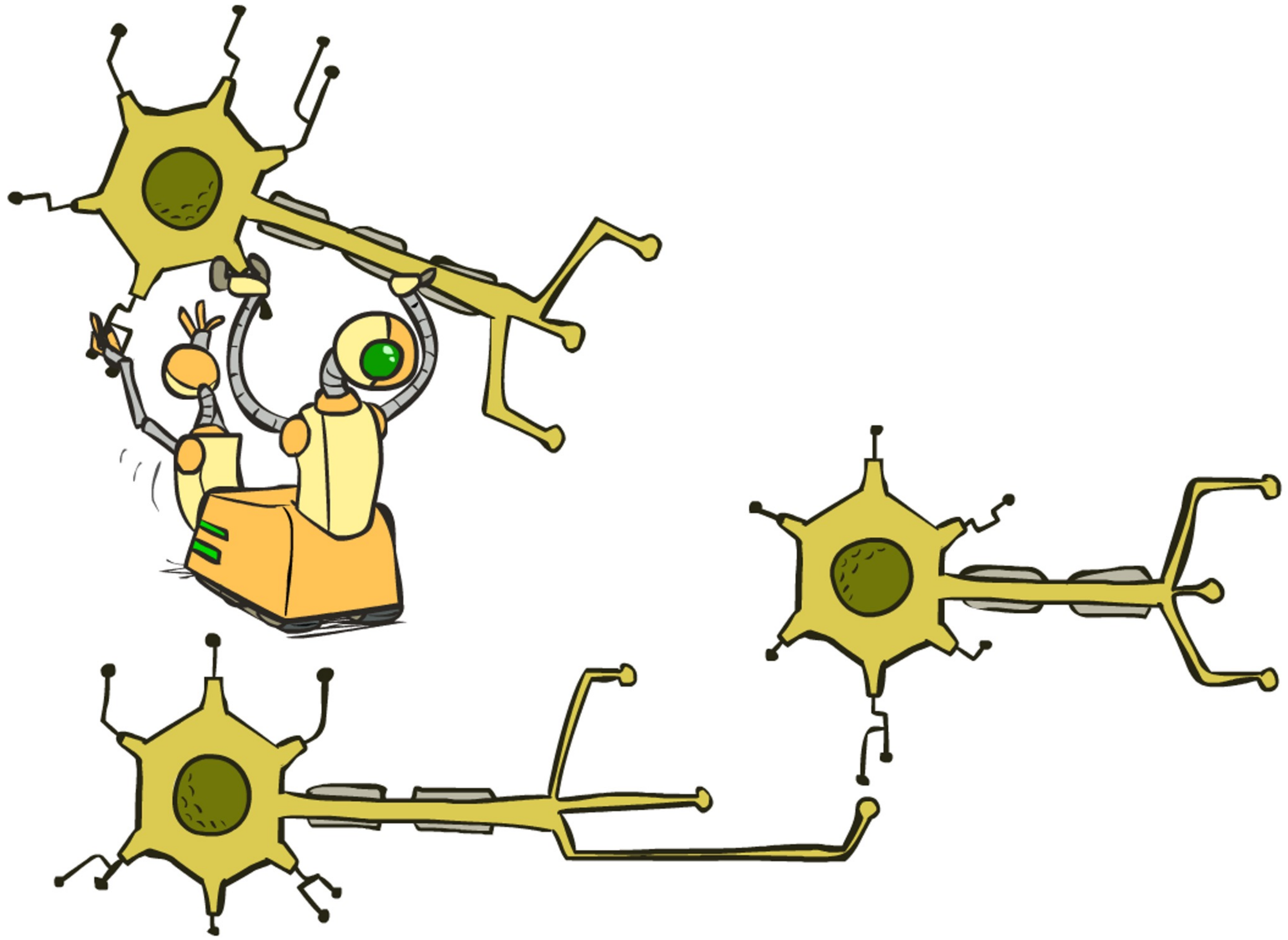
## Mini-Batch Gradient Ascent on the Log Likelihood Objective

$$\max_w \quad ll(w) = \max_w \quad \sum_i \log P(y^{(i)}|x^{(i)}; w)$$

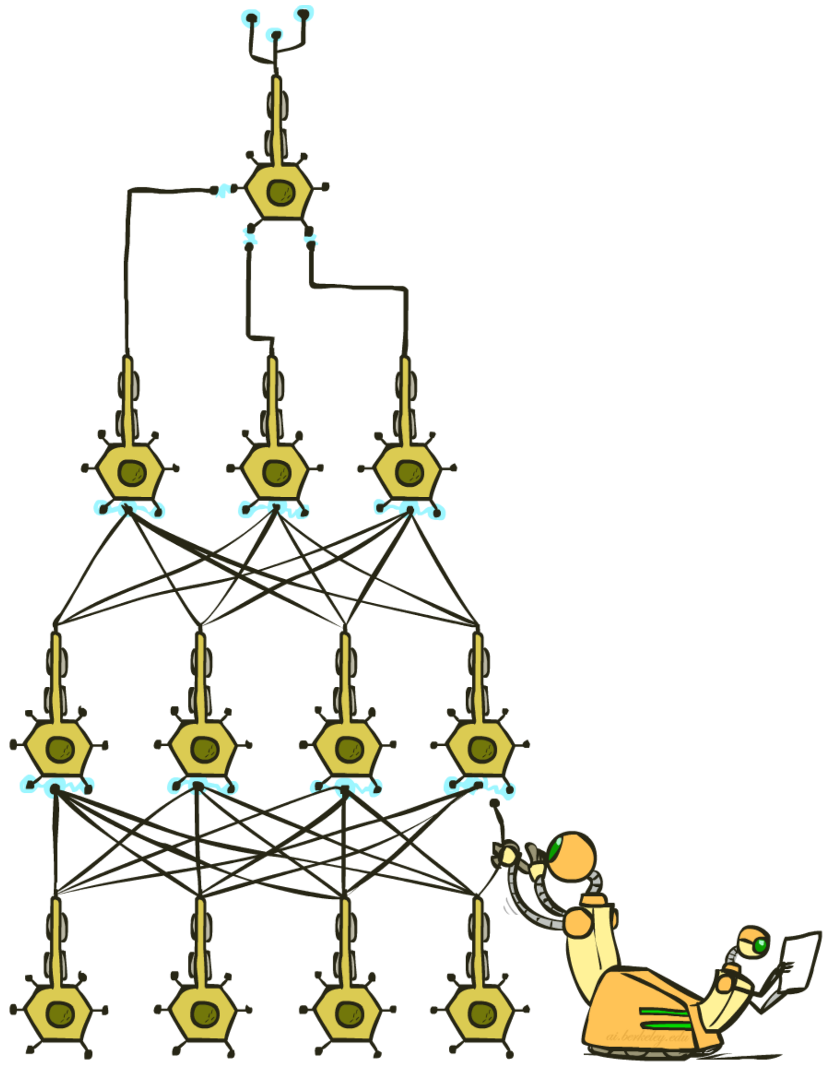
**Observation:** gradient over small set of training examples (=mini-batch) can be computed in parallel, might as well do that instead of a single one

```
init $w$
for iter = 1, 2, …
  pick random subset of training examples J
    $w \leftarrow w + \alpha * \sum_{j \in J} \nabla \log P(y^{(j)}|x^{(j)}; w)$
```

# Neural Networks



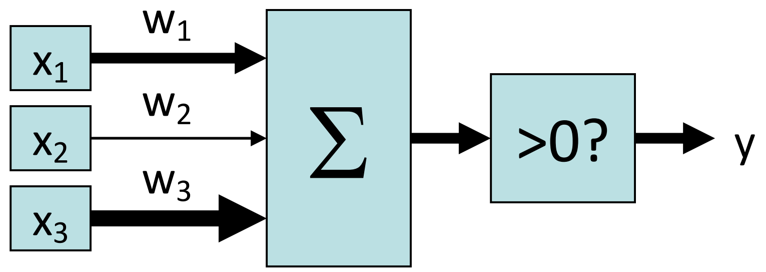
# Manual Feature Design vs. Deep Learning



- Manual feature design requires:
  - Domain-specific expertise
  - Domain-specific effort

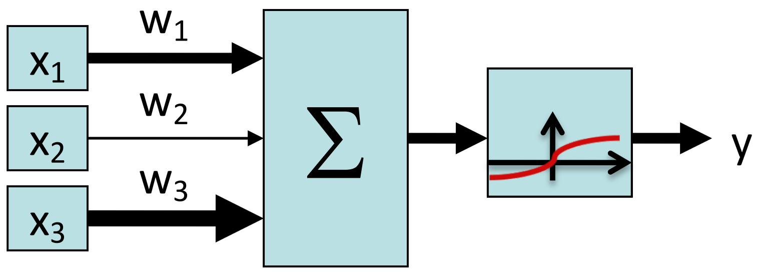
- What if we could learn the features, too?
  - **Deep Learning**

# Review: Perceptron



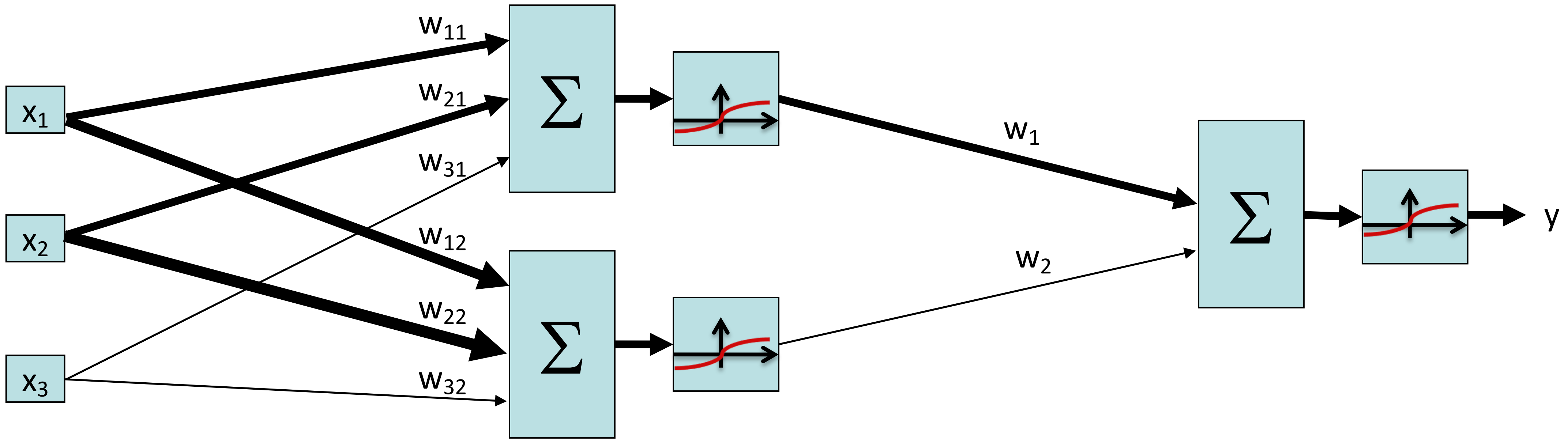
$$y = \begin{cases} 1 & w_1 x_1 + w_2 x_2 + w_3 x_3 > 0 \\ 0 & \text{otherwise} \end{cases}$$

# Review: Perceptron with Sigmoid Activation

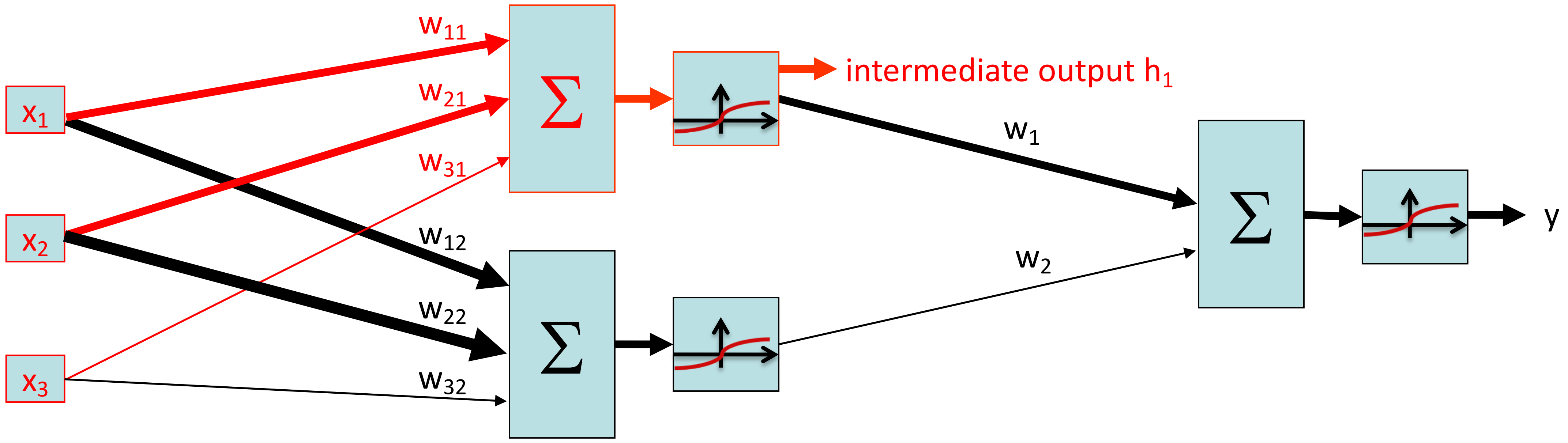


$$y = \phi(w_1x_1 + w_2x_2 + w_3x_3)$$
$$= \frac{1}{1 + e^{-(w_1x_1 + w_2x_2 + w_3x_3)}}$$

# 2-Layer, 2-Neuron Neural Network

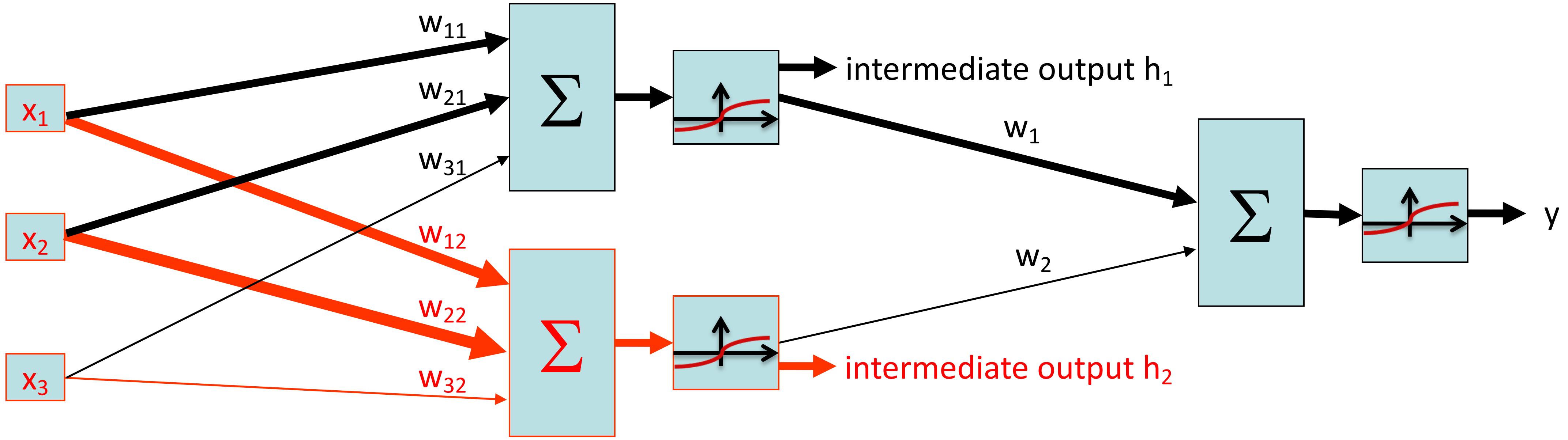


# 2-Layer, 2-Neuron Neural Network



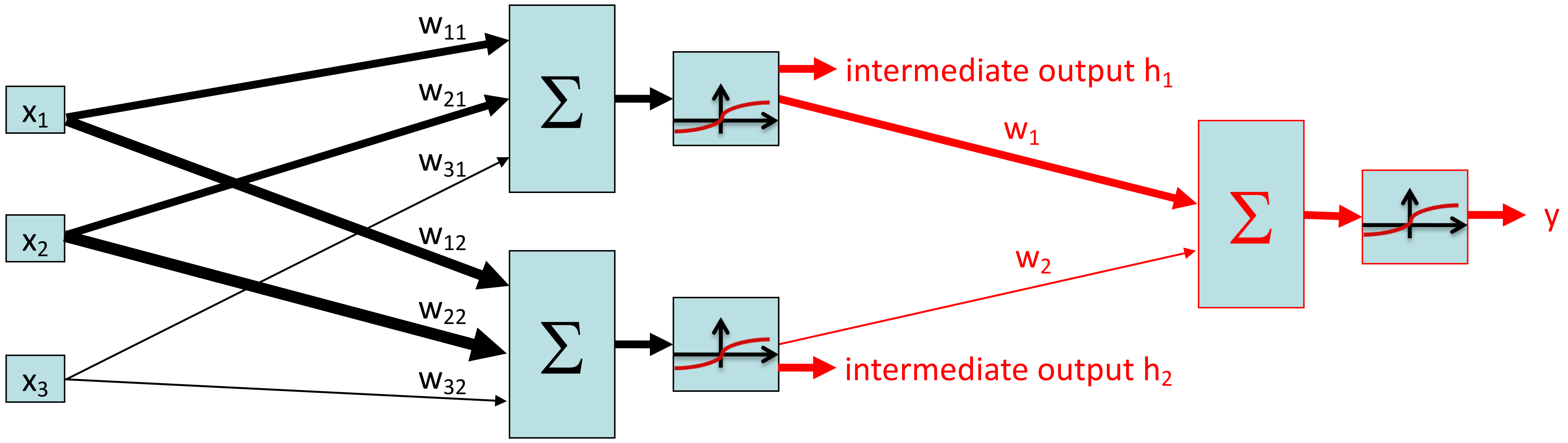
$$\text{intermediate output } h_1 = \phi(w_{11}x_1 + w_{21}x_2 + w_{31}x_3)$$
$$= \frac{1}{1 + e^{-(w_{11}x_1 + w_{21}x_2 + w_{31}x_3)}}$$

# 2-Layer, 2-Neuron Neural Network



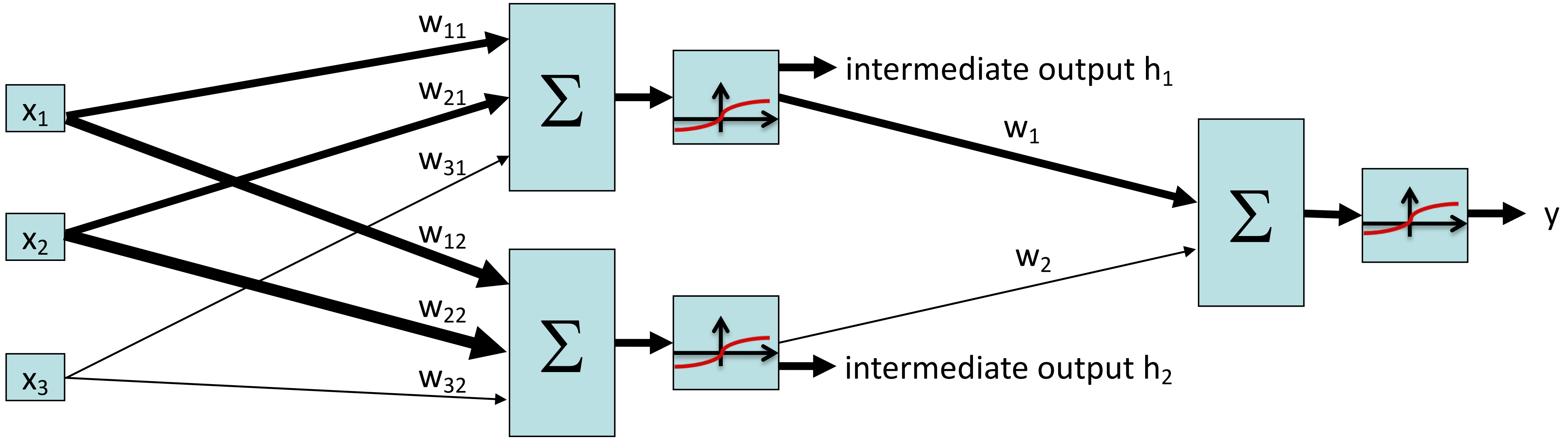
$$\text{intermediate output } h_2 = \phi(w_{12}x_1 + w_{22}x_2 + w_{32}x_3)$$
$$= \frac{1}{1 + e^{-(w_{12}x_1 + w_{22}x_2 + w_{32}x_3)}}$$

# 2-Layer, 2-Neuron Neural Network



$$y = \phi(w_1 h_1 + w_2 h_2)$$
$$= \frac{1}{1 + e^{-(w_1 h_1 + w_2 h_2)}}$$

# 2-Layer, 2-Neuron Neural Network



$$
\begin{aligned}
y &= \phi(w_1 h_1 + w_2 h_2) \\
&= \phi(w_1 \phi(w_{11}x_1 + w_{21}x_2 + w_{31}x_3) + w_2 \phi(w_{12}x_1 + w_{22}x_2 + w_{32}x_3))
\end{aligned}
$$

# 2-Layer, 2-Neuron Neural Network

$$\begin{aligned} y &= \phi(w_1 h_1 + w_2 h_2) \\ &= \phi(w_1 \phi(w_{11}x_1 + w_{21}x_2 + w_{31}x_3) + w_2 \phi(w_{12}x_1 + w_{22}x_2 + w_{32}x_3)) \end{aligned}$$

The same equation, formatted with matrices:

$$\begin{aligned} &\phi\left( \begin{bmatrix} x_1 & x_2 & x_3 \end{bmatrix} \begin{bmatrix} w_{11} & w_{12} \\ w_{21} & w_{22} \\ w_{31} & w_{32} \end{bmatrix} \right) \\ = \; &\phi\left( \begin{bmatrix} w_{11}x_1 + w_{21}x_2 + w_{31}x_3 & w_{12}x_1 + w_{22}x_2 + w_{32}x_3 \end{bmatrix} \right) \\ = \; &\begin{bmatrix} h_1 & h_2 \end{bmatrix} \end{aligned}$$

$$\phi\left( \begin{bmatrix} h_1 & h_2 \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \end{bmatrix} \right) = \phi\left(w_1 h_1 + w_2 h_2\right) = y$$

The same equation, formatted more compactly by introducing variables representing each matrix:

$$\phi(x \times W_{\text{layer 1}}) = h \qquad \phi(h \times W_{\text{layer 2}}) = y$$

## 2-Layer, 2-Neuron Neural Network

$$\phi(x \times W_{\text{layer 1}}) = h$$

Shape (1, 3).
Input feature vector.

Shape (3, 2).
Weights to be learned.

Shape (1, 2).
Outputs of layer 1,
inputs to layer 2.

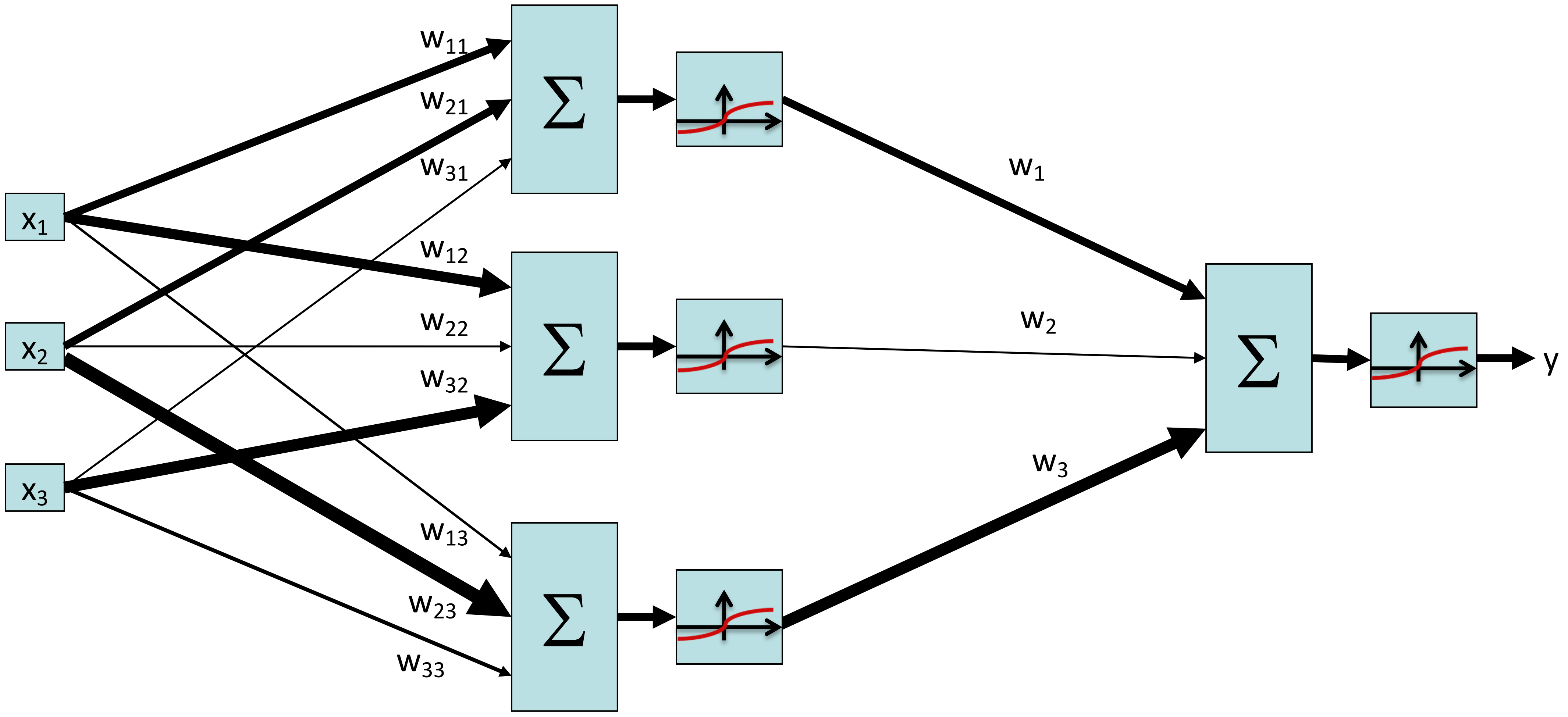
$$\phi(h \times W_{\text{layer 2}}) = y$$

Shape (1, 2).
Outputs of layer 1,
inputs to layer 2.

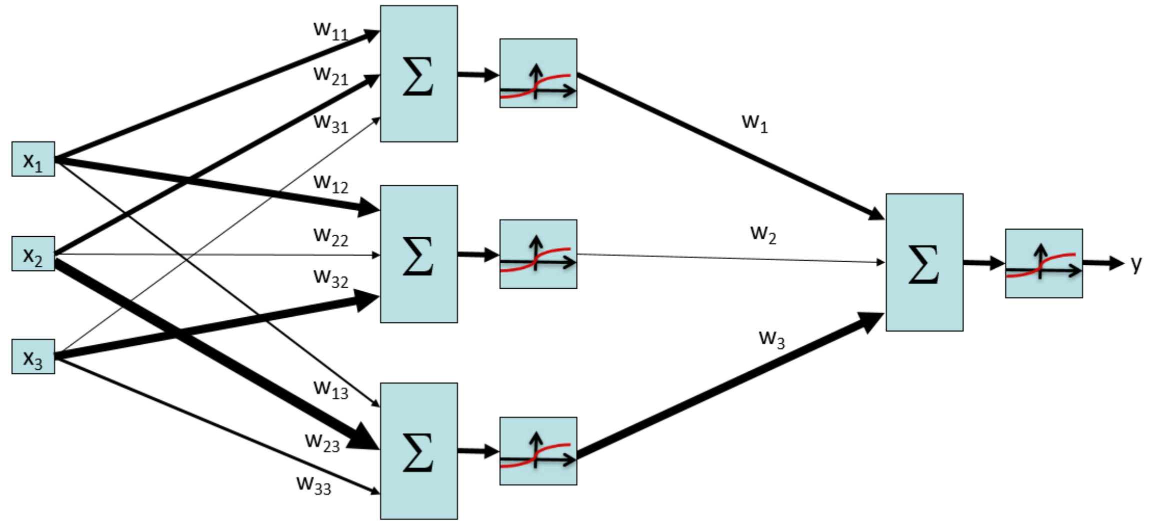
Shape (2, 1).
Weights to be learned.

Shape (1, 1).
Output of network.

# 2-Layer, 3-Neuron Neural Network



# 2-Layer, 3-Neuron Neural Network



$$\phi\left(\begin{bmatrix} x_1 & x_2 & x_3 \end{bmatrix}\begin{bmatrix} w_{11} & w_{12} & w_{13} \\ w_{21} & w_{22} & w_{23} \\ w_{31} & w_{32} & w_{33} \end{bmatrix}\right)$$

$$= \phi\left(\begin{bmatrix} w_{11}x_1 + w_{21}x_2 + w_{31}x_3 & w_{12}x_1 + w_{22}x_2 + w_{32}x_3 & w_{13}x_1 + w_{23}x_2 + w_{33}x_3 \end{bmatrix}\right)$$

$$= \begin{bmatrix} h_1 & h_2 & h_3 \end{bmatrix}$$

$$\phi\left(\begin{bmatrix} h_1 & h_2 & h_3 \end{bmatrix}\begin{bmatrix} w_1 \\ w_2 \\ w_3 \end{bmatrix}\right) = \phi\left(w_1h_1 + w_2h_2 + w_3h_3\right) = y$$

## 2-Layer, 3-Neuron Neural Network

$$\phi(x \times W_{\text{layer 1}}) = h$$

Shape (1, 3).
Input feature vector.

Shape (3, 3).
Weights to be learned

Shape (1, 3).
Outputs of layer 1,
inputs to layer 2.

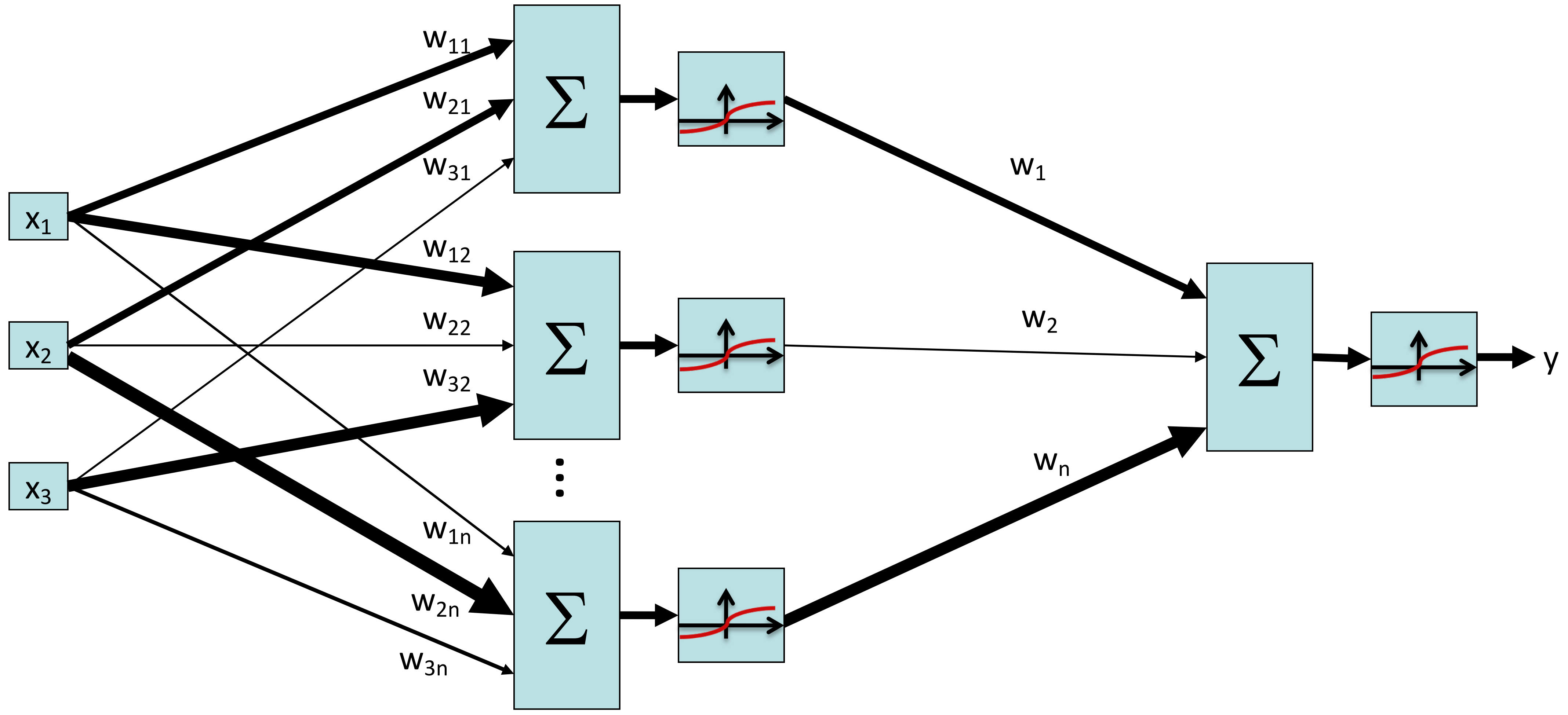
$$\phi(h \times W_{\text{layer 2}}) = y$$

Shape (1, 3).
Outputs of layer 1,
inputs to layer 2.

Shape (3, 1).
Weights to be learned.

Shape (1, 1).
Output of network.

# Generalize: Number of hidden neurons



The hidden layer doesn't necessarily need to have 3 neurons; it could have any arbitrary number *n* neurons.

# Generalize: Number of hidden neurons

$$\phi(x \times W_{\text{layer 1}}) = h$$

Shape (1, 3).
Input feature vector.

Shape (3, *n*).
Weights to be learned

Shape (1, *n*).
Outputs of layer 1,
inputs to layer 2.

$$\phi(h \times W_{\text{layer 2}}) = y$$

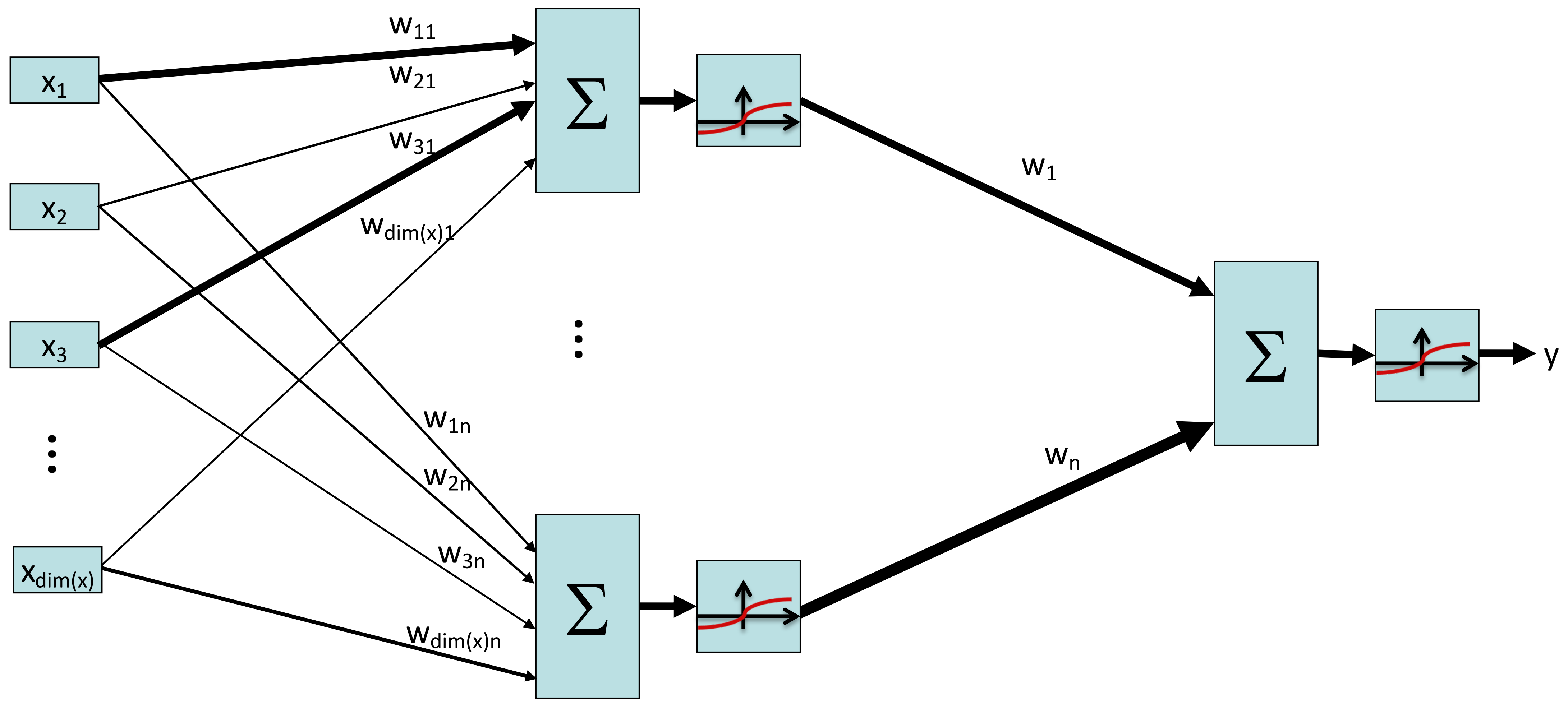
Shape (1, *n*).
Outputs of layer 1,
inputs to layer 2.

Shape (*n*, 1).
Weights to be learned.

Shape (1, 1).
Output of network.

The hidden layer doesn't necessarily need to have 3 neurons; it could have any arbitrary number *n* neurons.

# Generalize: Number of input features



The input feature vector doesn't necessarily need to have 3 features; it could have some arbitrary number *dim(x)* of features.

# Generalize: Number of input features

$$\phi(x \times W_{\text{layer 1}}) = h$$

Shape (1, *dim(x)*). Input feature vector.

Shape (*dim(x)*, *n*). Weights to be learned

Shape (1, *n*). Outputs of layer 1, inputs to layer 2.

$$\phi(h \times W_{\text{layer 2}}) = y$$

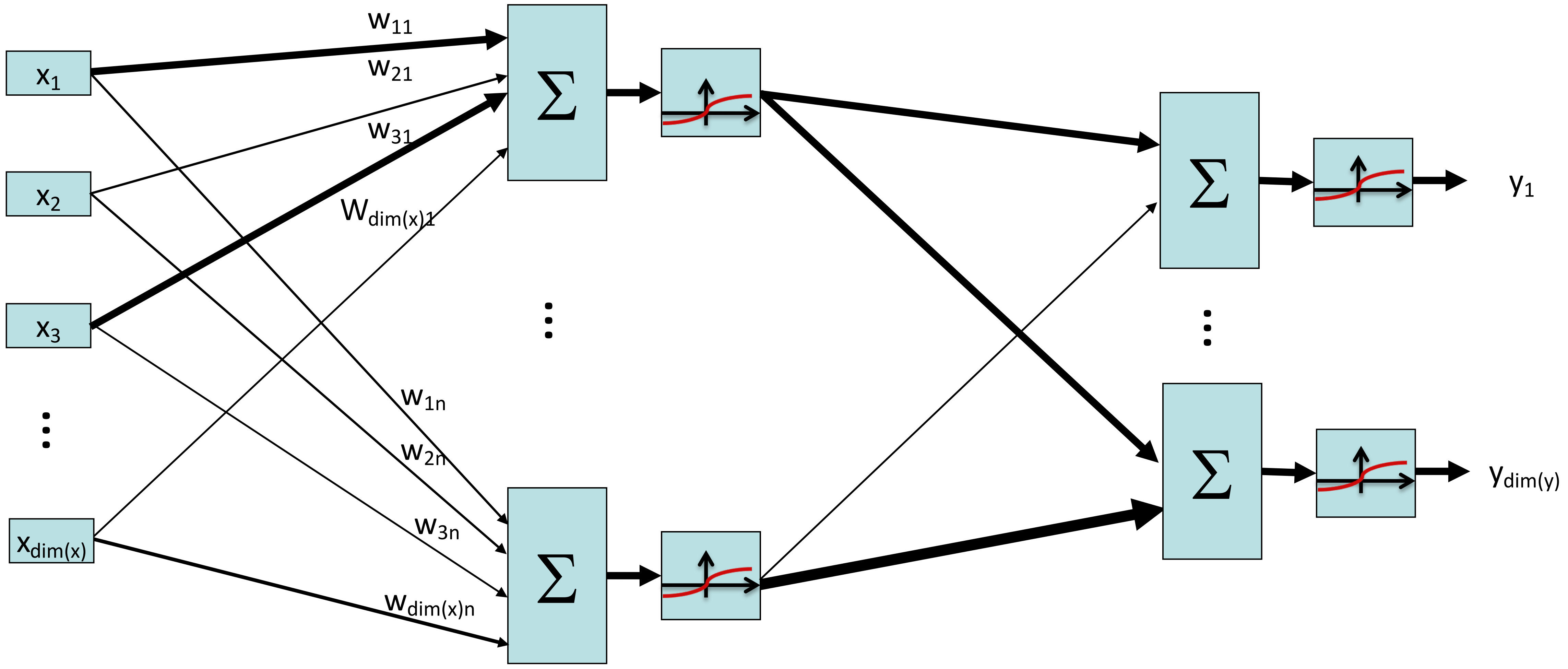
Shape (1, *n*). Outputs of layer 1, inputs to layer 2.

Shape (*n*, 1). Weights to be learned.

Shape (1, 1). Output of network.

The input feature vector doesn't necessarily need to have 3 features; it could have some arbitrary number *dim(x)* of features.

# Generalize: Number of outputs



The output doesn’t necessarily need to be just one number; it could be some arbitrary *dim(y)* length vector.

# Generalize: Number of input features

$$\phi(x \times W_{\text{layer 1}}) = h$$

Shape (1, *dim(x)*).
Input feature vector.

Shape (*dim(x)*, *n*).
Weights to be learned

Shape (1, *n*).
Outputs of layer 1,
inputs to layer 2.

$$\phi(h \times W_{\text{layer 2}}) = y$$

Shape (1, *n*).
Outputs of layer 1,
inputs to layer 2.

Shape (*n*, *dim(y)*).
Weights to be learned.

Shape (1, *dim(y)*).
Output of network.

The output doesn't necessarily need to be just one number; it could be some arbitrary *dim(y)* length vector.

# Generalized 2-Layer Neural Network

$$\phi(x \times W_{\text{layer 1}}) = h$$

Shape (1, *dim(x)*).
Input feature vector.

Shape (*dim(x)*, *n*).
Weights to be learned

Shape (1, *n*).
Outputs of layer 1,
inputs to layer 2.

Layer 1 has weight matrix with shape (*dim(x)*, *n*). These are the weights for *n* neurons, each taking *dim(x)* features as input.

This transforms a *dim(x)*-dimensional input vector into an *n*-dimensional output vector.

$$\phi(h \times W_{\text{layer 2}}) = y$$

Shape (1, *n*).
Outputs of layer 1,
inputs to layer 2.

Shape (*n*, *dim(y)*).
Weights to be learned.

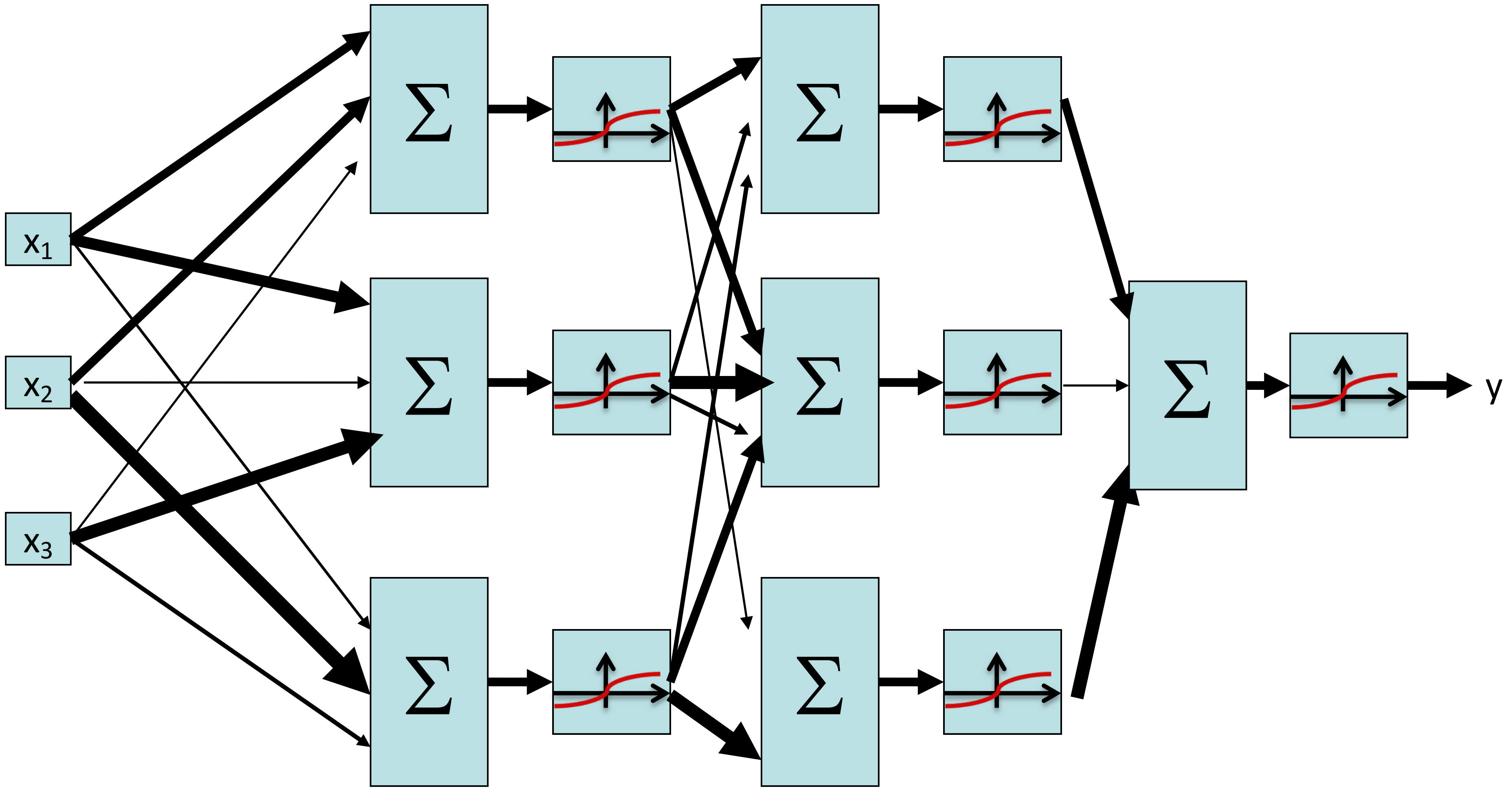
Shape (1, *dim(y)*).
Output of network.

Layer 2 has weight matrix with shape *(n, dim(y)*). These are the weights for *dim(y)* neurons, each taking *n* features as input.

This transforms an *n*-dimensional input vector into a *dim(y)*-dimensional output vector.

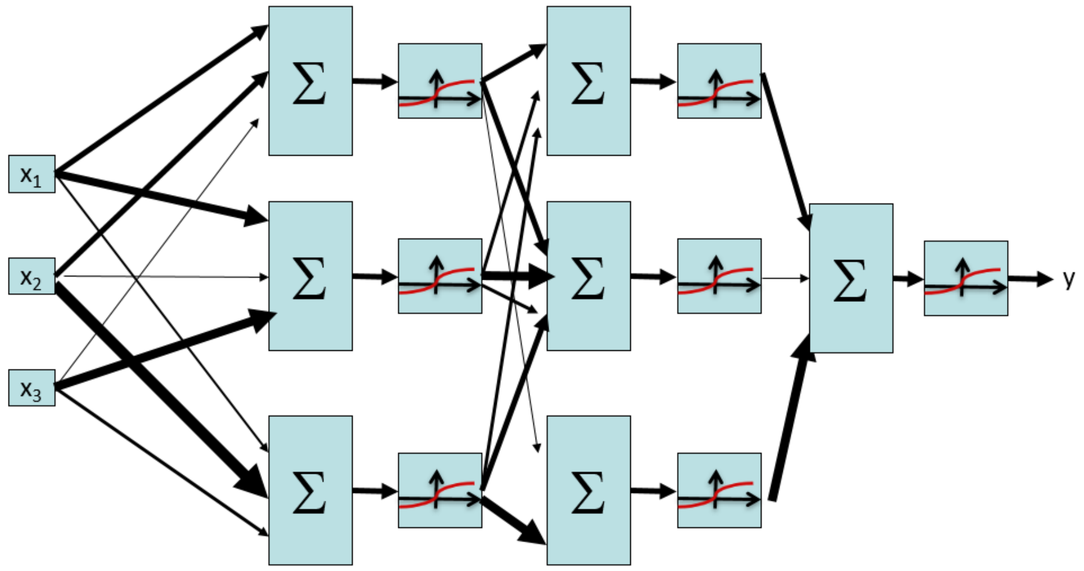
Big idea: The shape of a weight matrix is determined by the dimensions of the input and output of that layer.

# 3-Layer, 3-Neuron Neural Network



# 3-Layer, 3-Neuron Neural Network

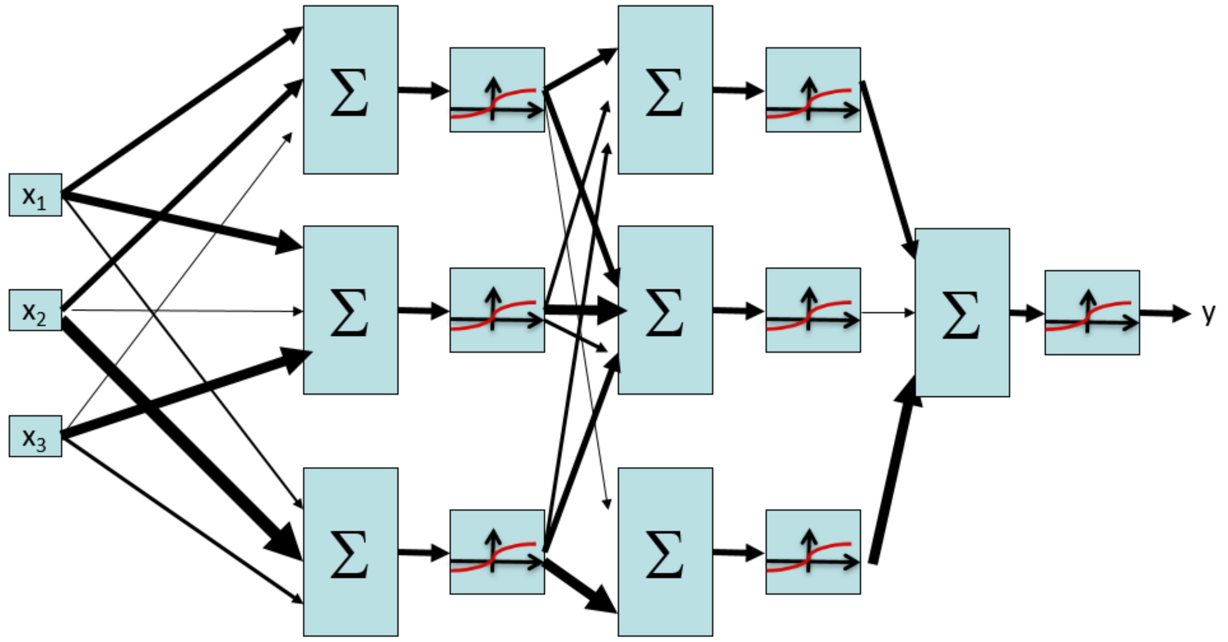
- Layer 1:
  - x has shape (1, 3). Input vector, 3-dimensional.
  - $W_{\text{layer 1}}$ has shape (3, 3). Weights for 3 neurons, each taking in a 3-dimensional input vector.
  - $h_{\text{layer 1}}$ has shape (1, 3). Outputs of the 3 neurons at this layer.
- Layer 2:
  - $h_{\text{layer 1}}$ has shape (1, 3). Outputs of the 3 neurons from the previous layer.
  - $W_{\text{layer 2}}$ has shape (3, 3). Weights for 3 new neurons, each taking in the 3 previous perceptron outputs.
  - $h_{\text{layer 2}}$ has shape (1, 3). Outputs of the 3 new neurons at this layer.
- Layer 3:
  - $h_{\text{layer 2}}$ has shape (1, 3). Outputs from the previous layer.
  - $W_{\text{layer 3}}$ has shape (3, 1). Weights for 1 final neuron, taking in the 3 previous perceptron outputs.
  - y has shape (1, 1). Output of the final neuron.



$$\phi(x \times W_{\text{layer 1}}) = h_{\text{layer 1}}$$
$$\phi(h_{\text{layer 1}} \times W_{\text{layer 2}}) = h_{\text{layer 2}}$$
$$\phi(h_{\text{layer 2}} \times W_{\text{layer 3}}) = y$$

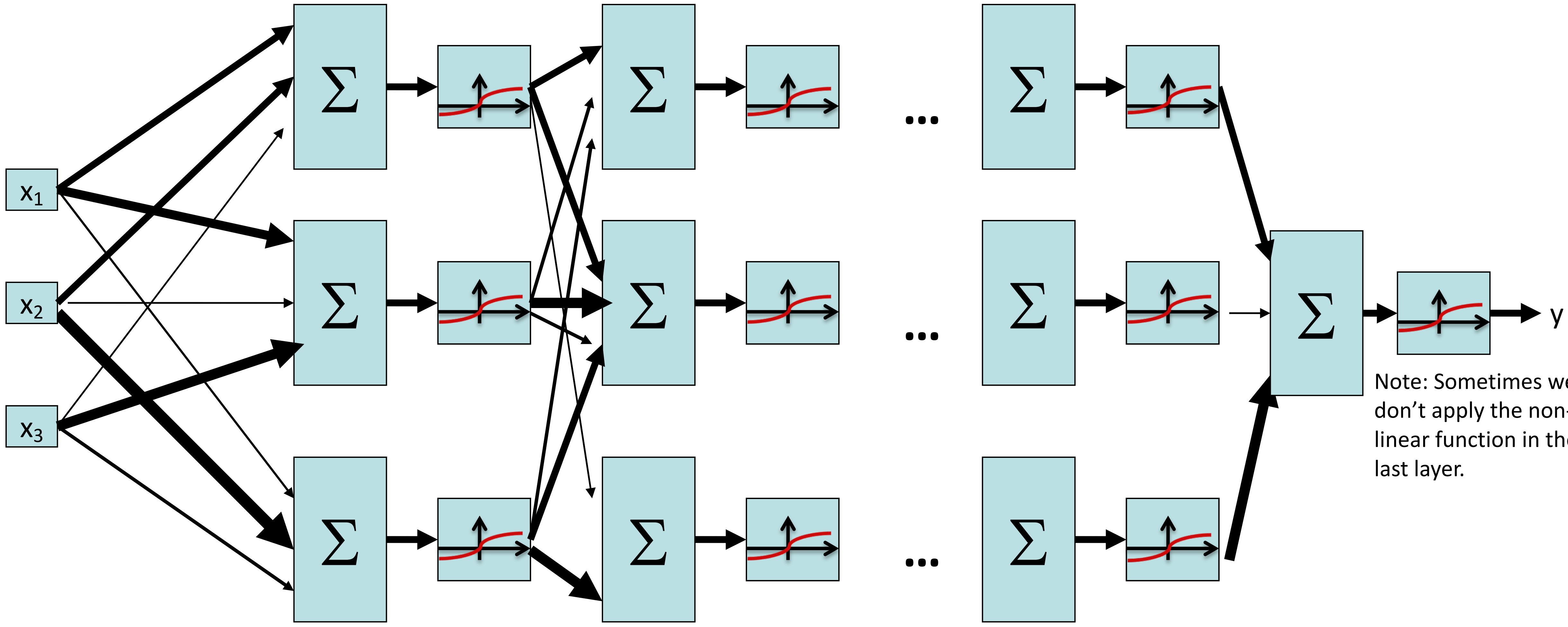
# Generalized 3-Layer Neural Network

- Layer 1:
  - x has shape (1, *dim(x)*)
  - $W_{\text{layer 1}}$ has shape (*dim(x), dim(L1)*)
  - $h_{\text{layer 1}}$ has shape (1, *dim(L1)*)
- Layer 2:
  - $h_{\text{layer 1}}$ has shape (1, *dim(L1)*)
  - $W_{\text{layer 2}}$ has shape (*dim(L1), dim(L2)*)
  - $h_{\text{layer 2}}$ has shape (1, *dim(L2)*)
- Layer 3:
  - $h_{\text{layer 2}}$ has shape (1, *dim(L2)*)
  - $W_{\text{layer 3}}$ has shape (*dim(L2), dim(y)*)
  - y has shape (1, *dim(y)*)



$$\phi(x \times W_{\text{layer 1}}) = h_{\text{layer 1}}$$
$$\phi(h_{\text{layer 1}} \times W_{\text{layer 2}}) = h_{\text{layer 2}}$$
$$\phi(h_{\text{layer 2}} \times W_{\text{layer 3}}) = y$$

# Multi-Layer Neural Network



Note: Sometimes we don't apply the non-linear function in the last layer.

# Multi-Layer Neural Network

- Input to a layer: some *dim(x)*-dimensional input vector
- Output of a layer: some *dim(y)*-dimensional output vector
  - *dim(y)* is the number of neurons in the layer (1 output per neuron)
- Process of converting input to output:
  - Multiply the (1, *dim(x)*) input vector with a (*dim(x)*, *dim(y)*) weight vector.
    The result has shape (1, *dim(y)*).
  - Apply some non-linear function (e.g. sigmoid) to the result.
    The result still has shape (1, *dim(y)*).
- Big idea: Chain layers together
  - The input could come from a previous layer's output
  - The output could be used as the input to the next layer

# Next time: Training Neural Networks