BOSTON UNIVERSITY

Deep Learning for Data Science
DS 542

https://dl4ds.github.io/fa2025/

Shallow Neural Networks

Original slides by Tom Gardos,
other content from Understanding Deep Learning unless otherwise cited

Announcement

Shared Compute Cluster (SCC) Tutorial next class (9/22)

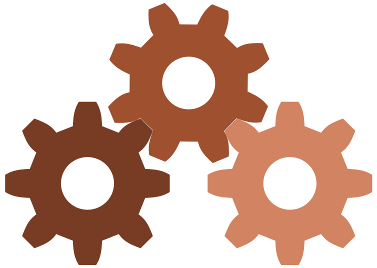
- Bring your laptop next time!
- Will walk through account setup and ways to access the SCC.

Recap: Regression

Real world input | Model input | Model | Model output | Real world output

6000 square feet,
4 bedrooms,
previously sold for
$235K in 2005,
1 parking spot.

$$\begin{bmatrix} 6000 \\ 4 \\ 235 \\ 2005 \\ 1 \end{bmatrix}$$



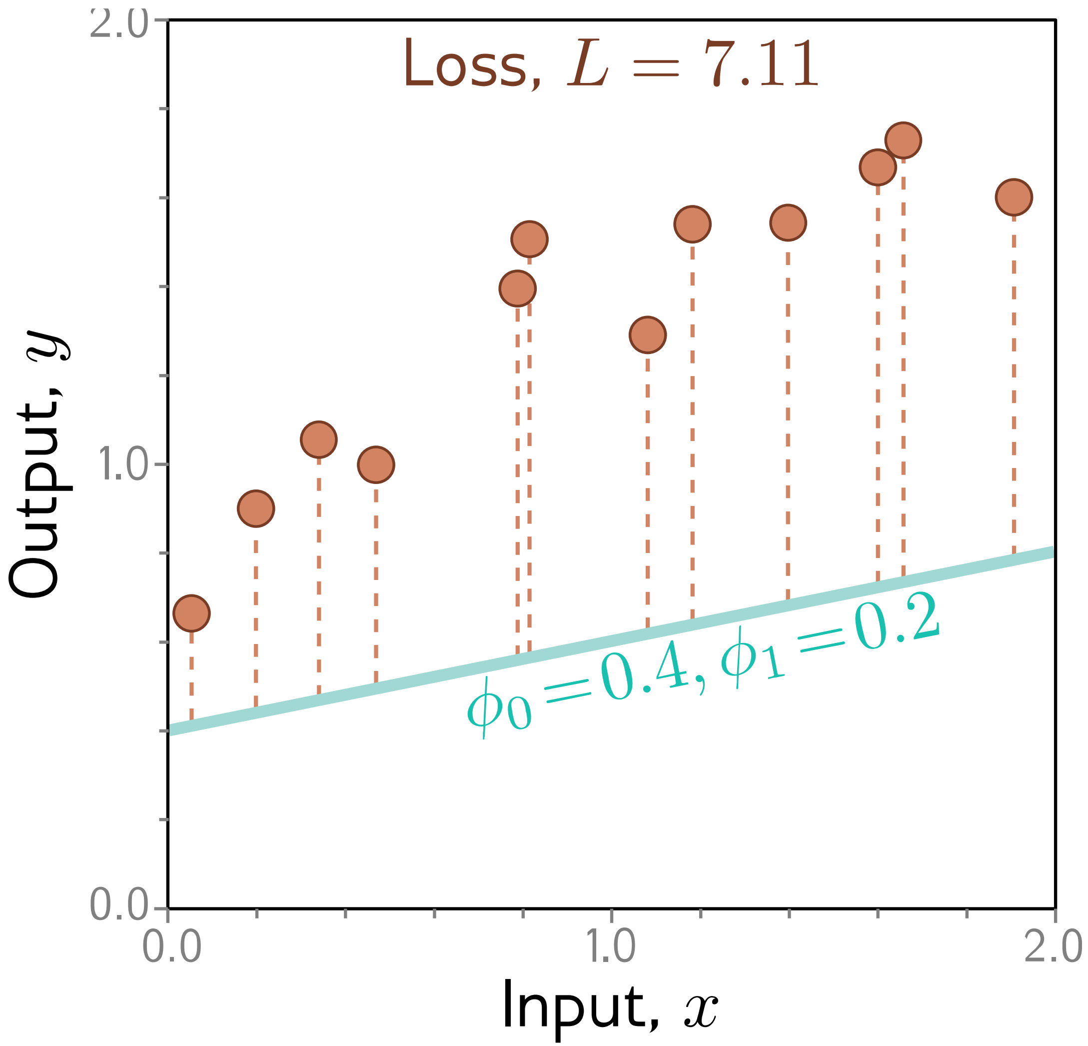
Supervised learning model

$$[340]$$

Predicted price
is $340k

- Univariate regression problem (one output, real value)
- Fully connected network

Recap: 1D Linear regression loss function



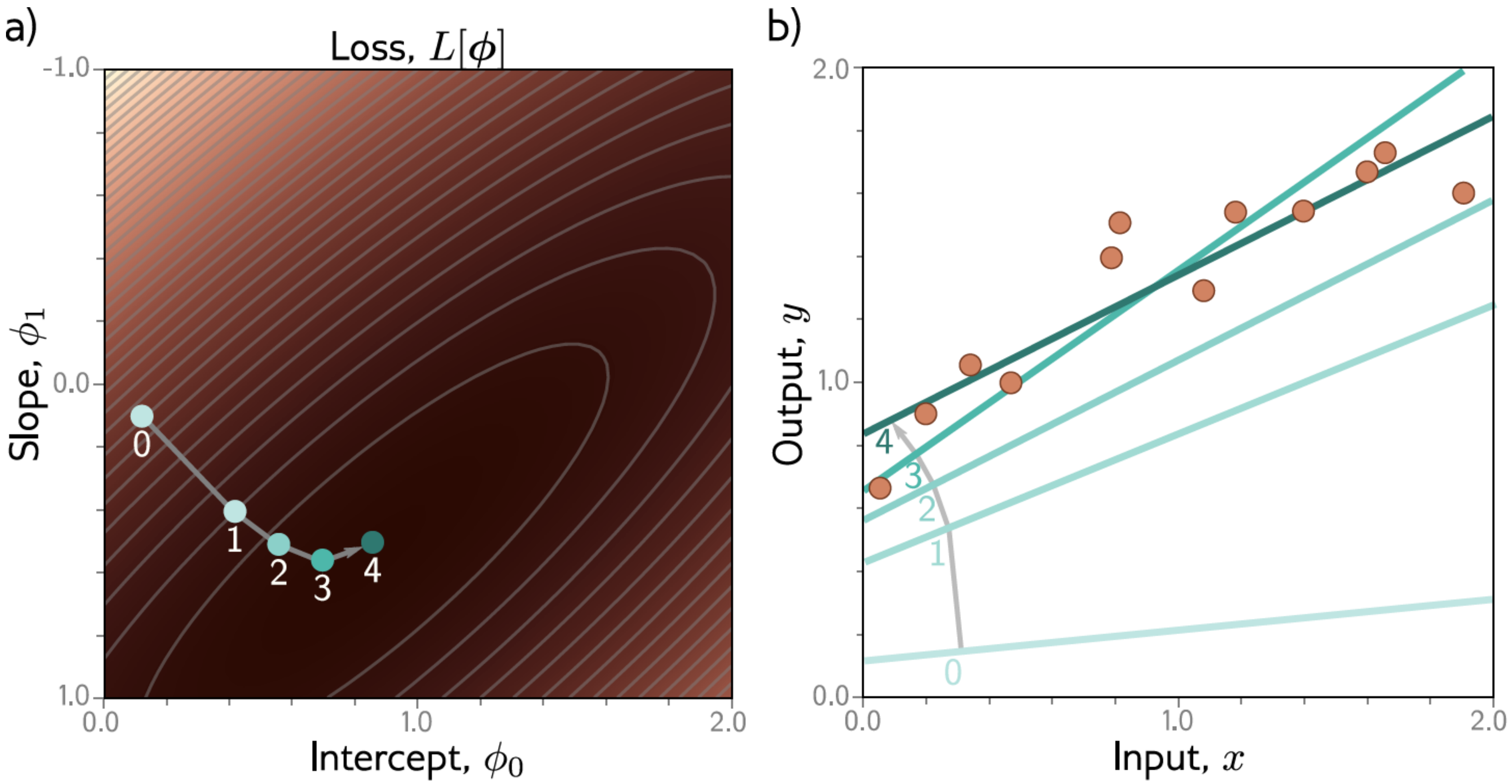
Loss function:

$$L[\boldsymbol{\phi}] = \sum_{i=1}^{I} (\text{f}[x_i, \boldsymbol{\phi}] - y_i)^2$$

$$= \sum_{i=1}^{I} (\phi_0 + \phi_1 x_i - y_i)^2$$

"Least squares loss function"

Recap: 1D Linear regression training



This technique is known as gradient descent

Shallow neural networks

- 1D regression model is obviously limited
  - Want to be able to describe input/output that are not lines
  - Want multiple inputs
  - Want multiple outputs

- Shallow neural networks
  - Flexible enough to describe arbitrarily complex input/output mappings
  - Can have as many inputs as we want
  - Can have as many outputs as we want

Shallow Neural Networks

- Example network, 1 input, 1 output
- Universal approximation theorem
- More than one output
- More than one input
- General case
- Number of regions
- Terminology

1D Linear Regression

$$
\begin{aligned}
y &= \mathrm{f}[x, \boldsymbol{\phi}] \\
&= \phi_0 + \phi_1 x
\end{aligned}
$$

Example shallow network

$$
\begin{aligned}
y &= \mathrm{f}[x, \boldsymbol{\phi}] \\
&= \phi_0 + \phi_1 \mathrm{a}[\theta_{10} + \theta_{11} x] + \phi_2 \mathrm{a}[\theta_{20} + \theta_{21} x] + \phi_3 \mathrm{a}[\theta_{30} + \theta_{31} x]
\end{aligned}
$$

Example shallow network

$$
\begin{aligned}
y &= \mathrm{f}[x, \boldsymbol{\phi}] \\
&= \phi_0 + \phi_1 \mathrm{a}[\theta_{10} + \theta_{11} x] + \phi_2 \mathrm{a}[\theta_{20} + \theta_{21} x] + \phi_3 \mathrm{a}[\theta_{30} + \theta_{31} x]
\end{aligned}
$$

Example shallow network

Activation function

$$
\begin{aligned}
y &= \mathrm{f}[x, \boldsymbol{\phi}] \\
&= \phi_0 + \phi_1 \mathrm{a}[\theta_{10} + \theta_{11}x] + \phi_2 \mathrm{a}[\theta_{20} + \theta_{21}x] + \phi_3 \mathrm{a}[\theta_{30} + \theta_{31}x]
\end{aligned}
$$

Example shallow network

Activation function

$$
\begin{aligned}
y &= \mathrm{f}[x, \boldsymbol{\phi}] \\
&= \phi_0 + \phi_1 \mathrm{a}[\theta_{10} + \theta_{11}x] + \phi_2 \mathrm{a}[\theta_{20} + \theta_{21}x] + \phi_3 \mathrm{a}[\theta_{30} + \theta_{31}x]
\end{aligned}
$$

$$
\mathrm{a}[z] = \mathrm{ReLU}[z] = \begin{cases} 0 & z < 0 \\ z & z \geq 0 \end{cases}.
$$

Rectified Linear Unit

(one type of activation function)

Example shallow network

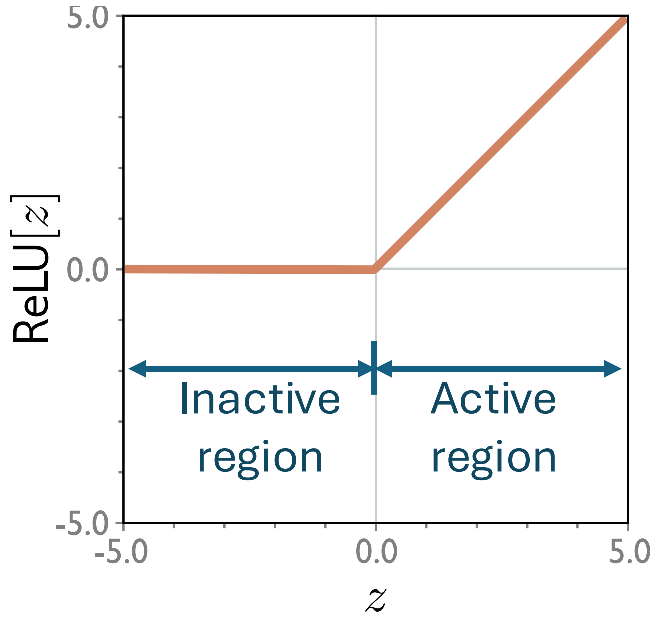
Activation function

$$
\begin{aligned}
y &= \mathrm{f}[x, \boldsymbol{\phi}] \\
&= \phi_0 + \phi_1 \mathrm{a}[\theta_{10} + \theta_{11}x] + \phi_2 \mathrm{a}[\theta_{20} + \theta_{21}x] + \phi_3 \mathrm{a}[\theta_{30} + \theta_{31}x]
\end{aligned}
$$

$$
\mathrm{a}[z] = \mathrm{ReLU}[z] = \begin{cases} 0 & z < 0 \\ z & z \geq 0 \end{cases}.
$$

Rectified Linear Unit

(particular kind of activation function)



Example shallow network

$$
\begin{aligned}
y &= \mathrm{f}[x, \boldsymbol{\phi}] \\
&= \phi_0 + \phi_1 \mathrm{a}[\theta_{10} + \theta_{11} x] + \phi_2 \mathrm{a}[\theta_{20} + \theta_{21} x] + \phi_3 \mathrm{a}[\theta_{30} + \theta_{31} x]
\end{aligned}
$$

This model has 10 parameters:

$$\boldsymbol{\phi} = \{\phi_0, \phi_1, \phi_2, \phi_3, \theta_{10}, \theta_{11}, \theta_{20}, \theta_{21}, \theta_{30}, \theta_{31}\}$$

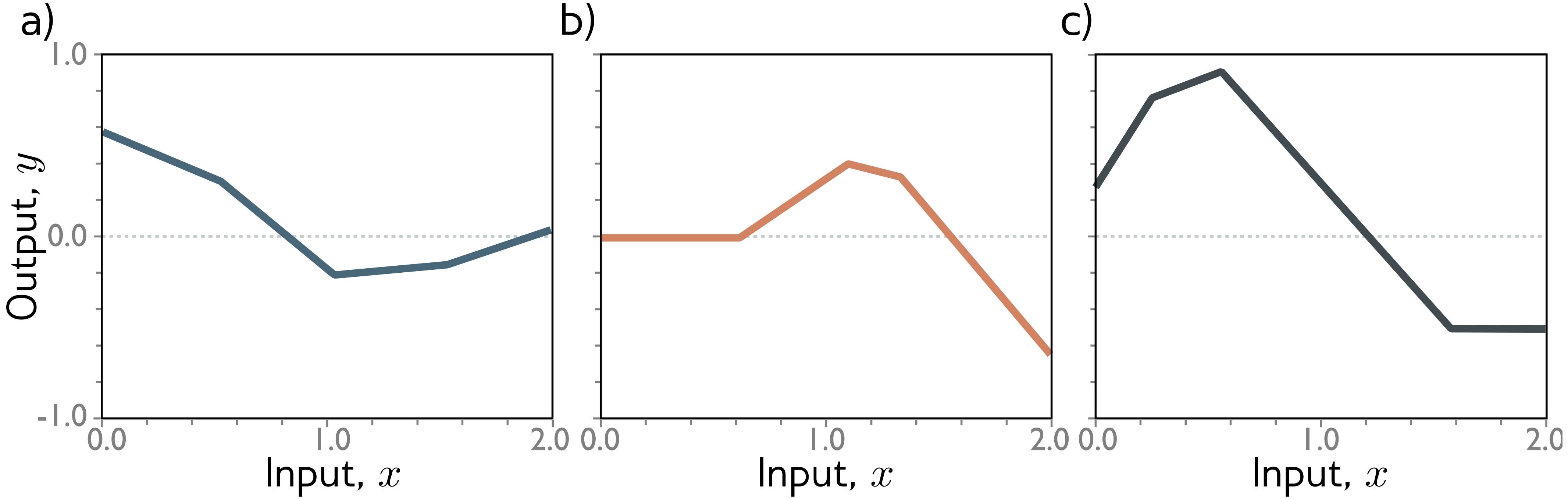
- Represents a family of functions
- Parameters determine a particular function
- Given the parameters, we can perform inference (evaluate the equation)
- Given training dataset $\{\mathbf{x}_i, \mathbf{y}_i\}_{i=1}^{I}$
- Define loss function $L[\boldsymbol{\phi}]$ (least squares)
- Change parameters to minimize loss function

Example shallow network

$$y = \phi_0 + \phi_1 \mathrm{a}[\theta_{10} + \theta_{11}x] + \phi_2 \mathrm{a}[\theta_{20} + \theta_{21}x] + \phi_3 \mathrm{a}[\theta_{30} + \theta_{31}x].$$

Example shallow network

$$y = \phi_0 + \phi_1 \mathrm{a}[\theta_{10} + \theta_{11}x] + \phi_2 \mathrm{a}[\theta_{20} + \theta_{21}x] + \phi_3 \mathrm{a}[\theta_{30} + \theta_{31}x].$$



Piecewise linear functions with three joints

Hidden units

$$y = \phi_0 + \phi_1 \mathrm{a}[\theta_{10} + \theta_{11}x] + \phi_2 \mathrm{a}[\theta_{20} + \theta_{21}x] + \phi_3 \mathrm{a}[\theta_{30} + \theta_{31}x].$$

Break down into two parts:

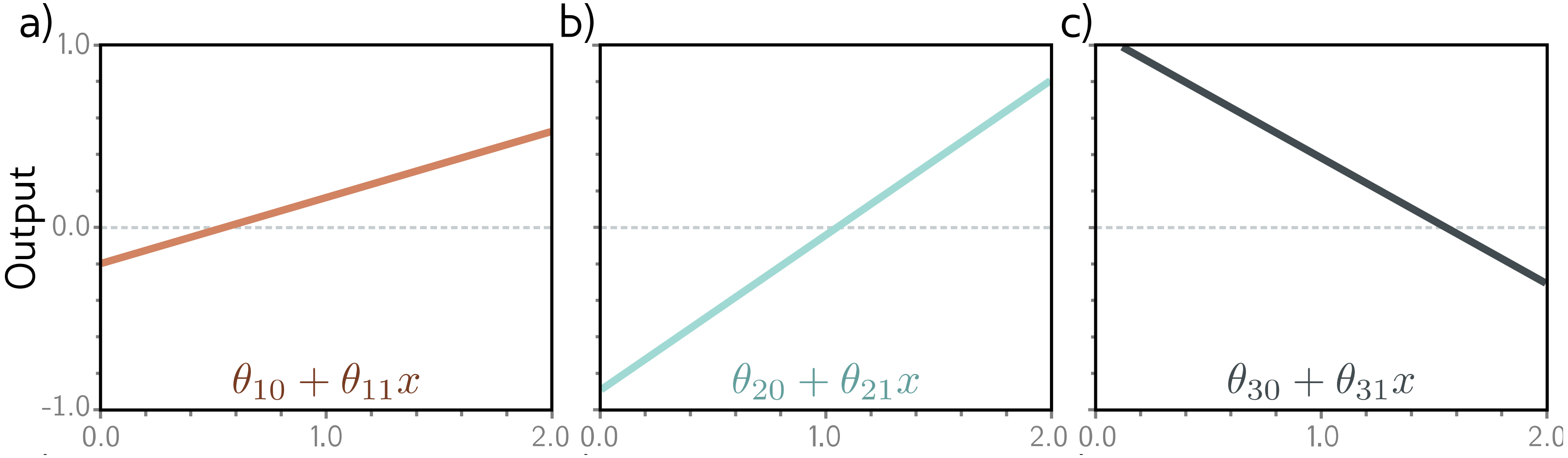
$$y = \phi_0 + \phi_1 h_1 + \phi_2 h_2 + \phi_3 h_3$$

where:

$$\text{Hidden units}\left\{\begin{aligned} h_1 &= \mathrm{a}[\theta_{10} + \theta_{11}x] \\ h_2 &= \mathrm{a}[\theta_{20} + \theta_{21}x] \\ h_3 &= \mathrm{a}[\theta_{30} + \theta_{31}x] \end{aligned}\right.$$

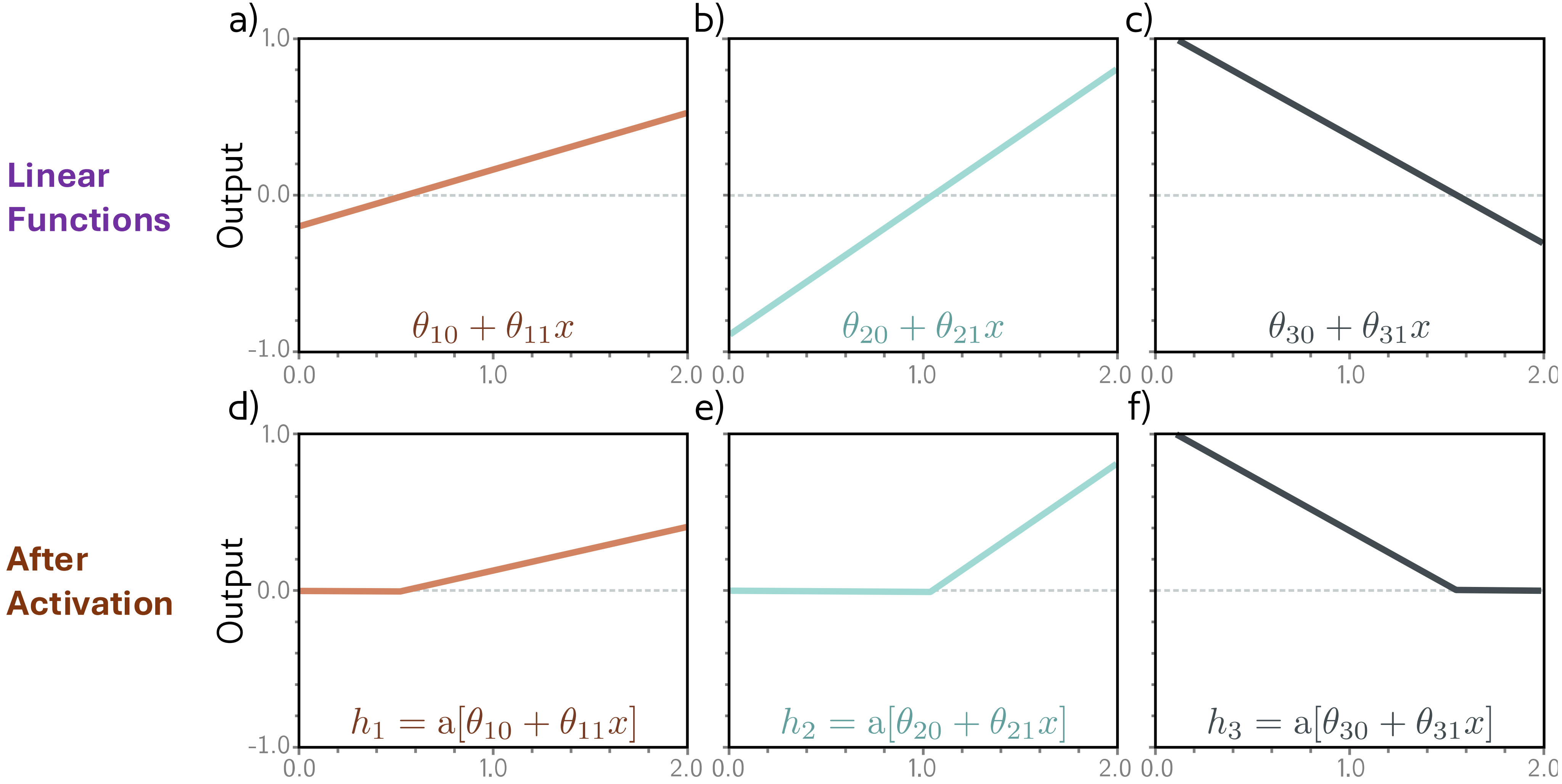
1. compute three linear functions

Linear Functions

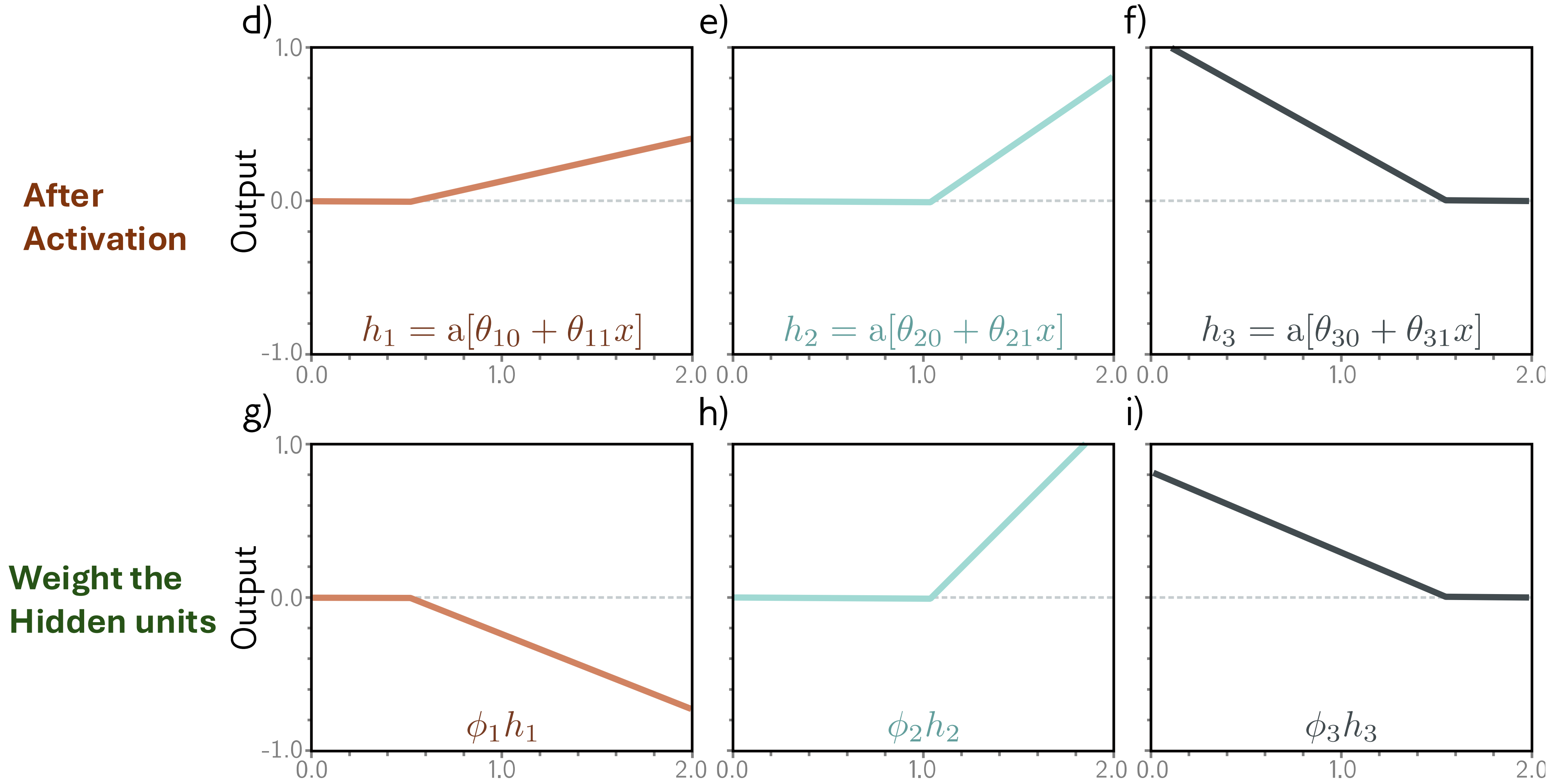


2. Pass through ReLU functions (creates hidden units)

$$h_1 = \mathrm{a}[\theta_{10} + \theta_{11}x]$$
$$h_2 = \mathrm{a}[\theta_{20} + \theta_{21}x]$$
$$h_3 = \mathrm{a}[\theta_{30} + \theta_{31}x],$$



2. Weight the hidden units

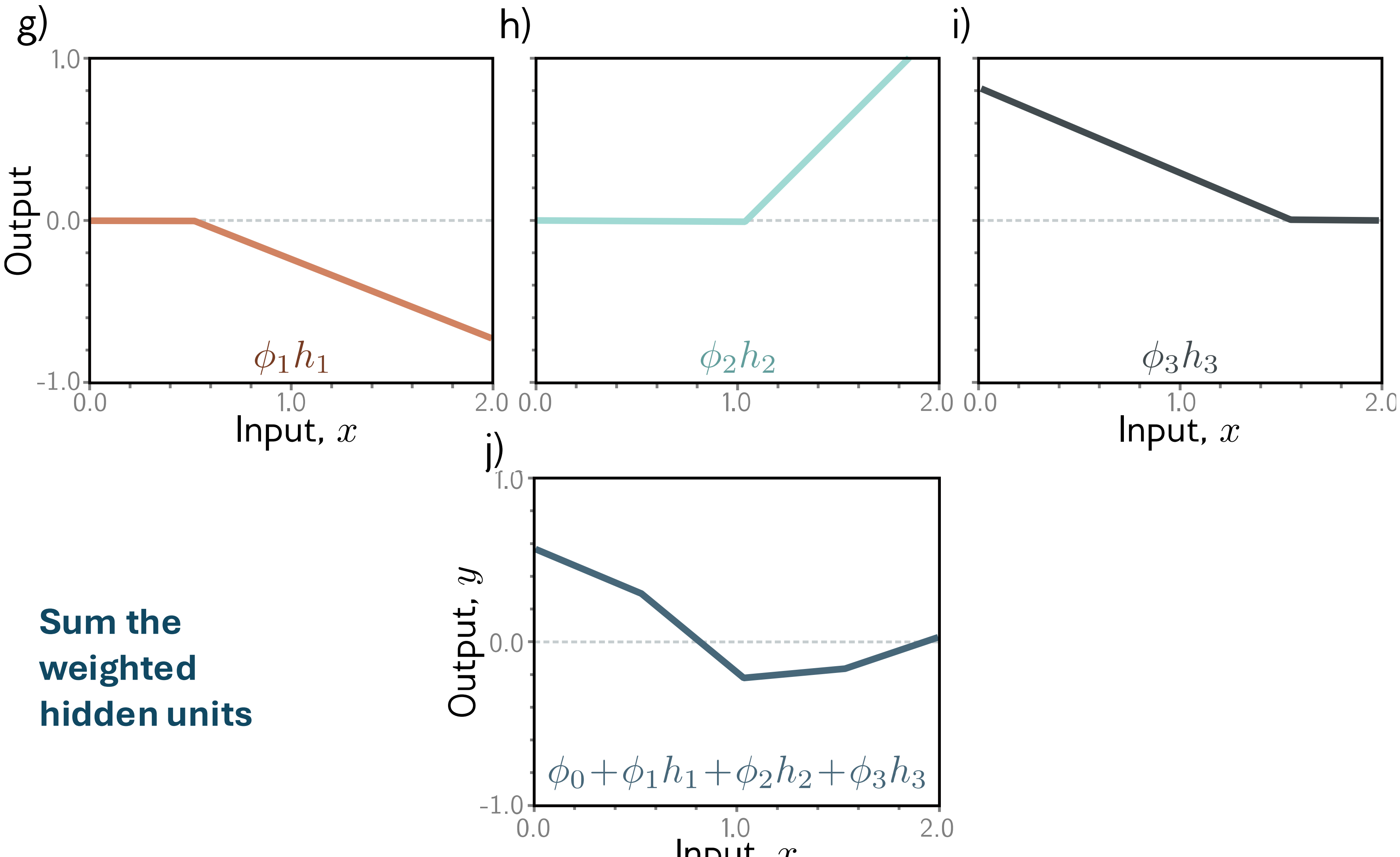


4. Sum the weighted hidden units to create output

$$y = \phi_0 + \phi_1 h_1 + \phi_2 h_2 + \phi_3 h_3$$

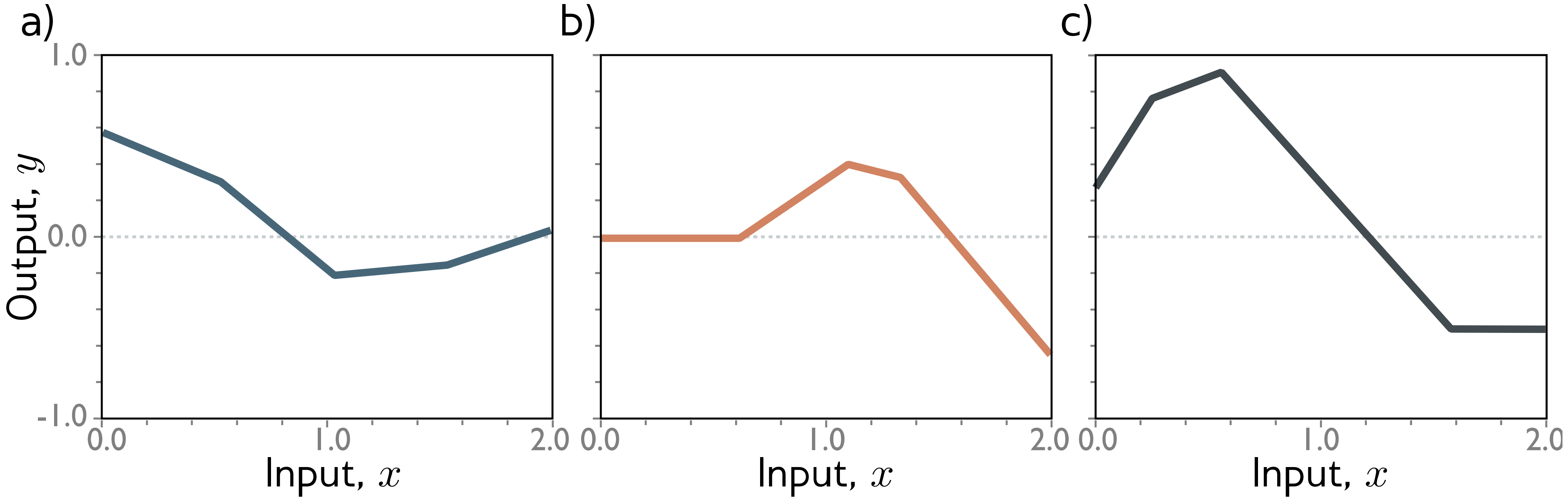
Weight the hidden units

Sum the weighted hidden units



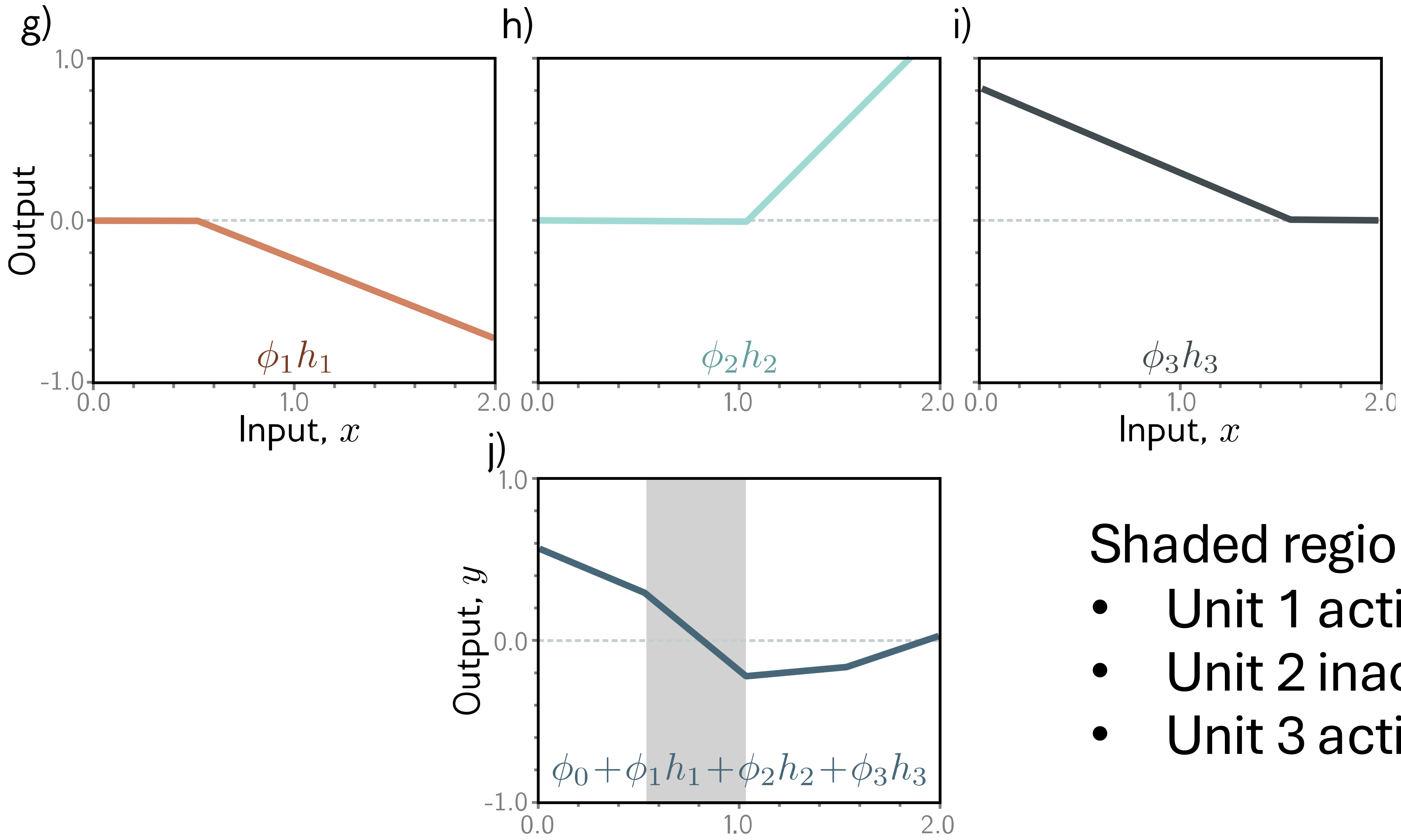
Example: 3 different shallow networks

$$y = \phi_0 + \phi_1 \mathrm{a}[\theta_{10} + \theta_{11}x] + \phi_2 \mathrm{a}[\theta_{20} + \theta_{21}x] + \phi_3 \mathrm{a}[\theta_{30} + \theta_{31}x].$$



Example shallow network = piecewise linear functions
1 “joint” per ReLU function

Activation pattern = which hidden units are activated?



Shaded region:

- Unit 1 active
- Unit 2 inactive
- Unit 3 active

Interactive Figure 3.3a: 1D Shallow Network (ReLU)

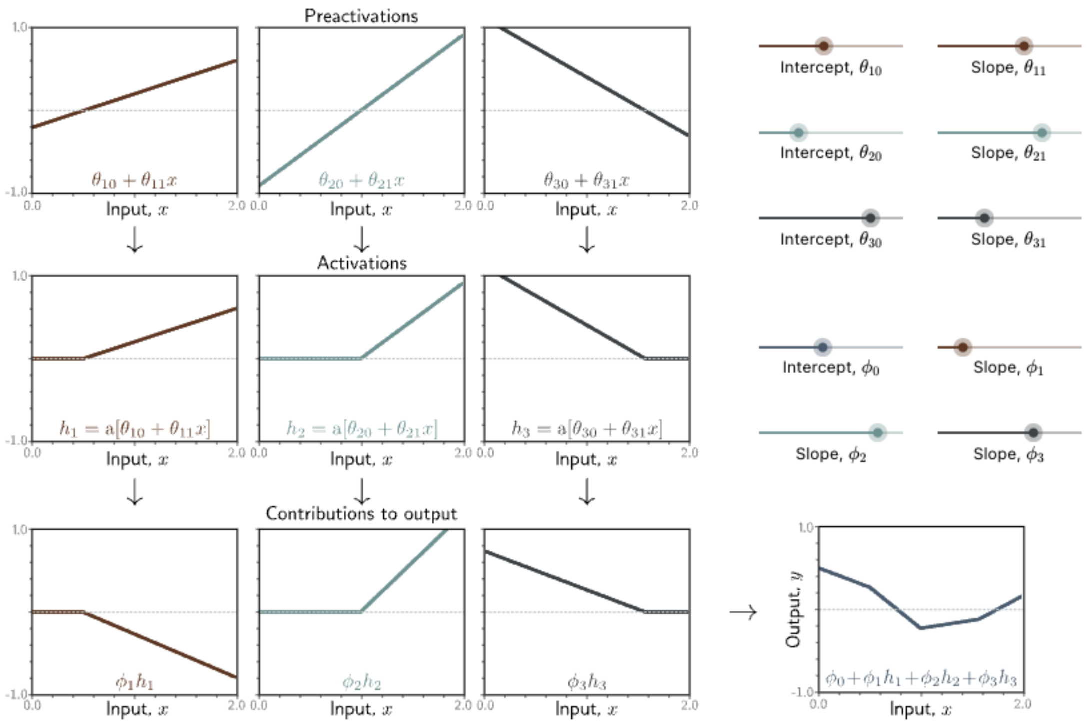


Figure 3.3 Computation for function in figure 3.2a. (Top row) The input x is passed through three linear functions, each with a different y-intercept $\theta_{\bullet 0}$ and slope $\theta_{\bullet 1}$. (Center row) Each line is passed through the ReLU activation function. (Bottom row) The three resulting functions are then weighted (scaled) by ϕ_1, ϕ_2, and ϕ_3, respectively. (Bottom right) Finally, the weighted functions are summed, and an offset ϕ_0 that controls the height is added.

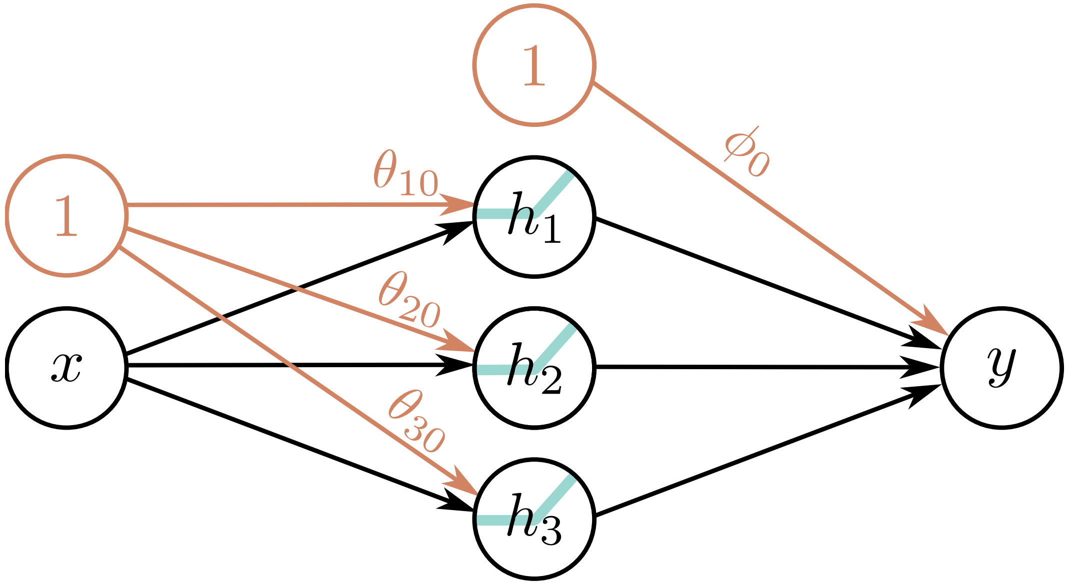
Move the sliders to modify the parameters of the shallow network.

https://udlbook.github.io/udlfigures/

Depicting neural networks

$$h_1 = \mathrm{a}[\theta_{10} + \theta_{11}x]$$
$$h_2 = \mathrm{a}[\theta_{20} + \theta_{21}x]$$
$$h_3 = \mathrm{a}[\theta_{30} + \theta_{31}x]$$

$$y = \phi_0 + \phi_1 h_1 + \phi_2 h_2 + \phi_3 h_3$$



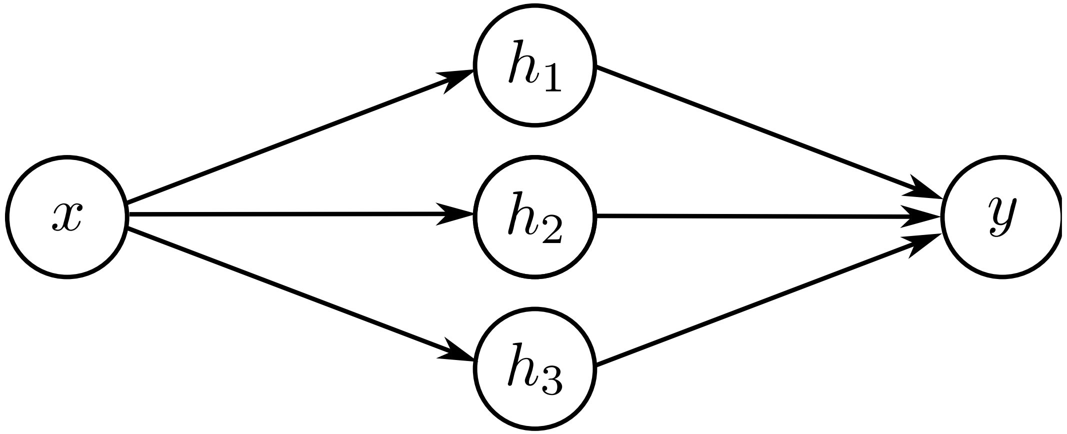
Each parameter multiplies its source and adds to its target

Depicting neural networks

Usually don't show the bias terms

$$
\begin{aligned}
h_1 &= \mathrm{a}[\theta_{10} + \theta_{11}x] \\
h_2 &= \mathrm{a}[\theta_{20} + \theta_{21}x] \\
h_3 &= \mathrm{a}[\theta_{30} + \theta_{31}x]
\end{aligned}
$$

$$y = \phi_0 + \phi_1 h_1 + \phi_2 h_2 + \phi_3 h_3$$



Shallow neural networks

- Example network, 1 input, 1 output
- Universal approximation theorem
- More than one output
- More than one input
- General case
- Number of regions
- Terminology

With 3 hidden units:

$$h_1 = \mathrm{a}[\theta_{10} + \theta_{11}x]$$
$$h_2 = \mathrm{a}[\theta_{20} + \theta_{21}x]$$
$$h_3 = \mathrm{a}[\theta_{30} + \theta_{31}x]$$

$$y = \phi_0 + \phi_1 h_1 + \phi_2 h_2 + \phi_3 h_3$$

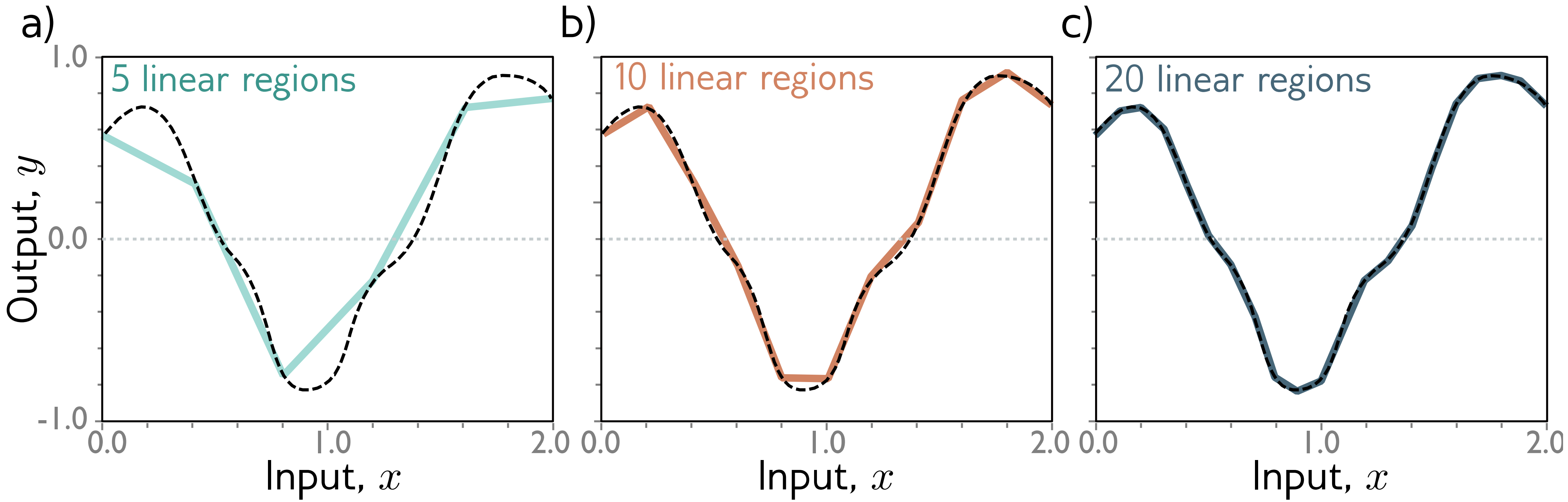
With D hidden units:

$$h_d = \mathrm{a}[\theta_{d0} + \theta_{d1}x]$$

$$y = \phi_0 + \sum_{d=1}^{D} \phi_d h_d$$

With enough hidden units…

… we can describe any 1D function to arbitrary accuracy



Universal approximation theorem

"a formal proof that, with enough hidden units, a shallow neural network can describe any continuous function in R^D to arbitrary precision"

Shallow neural networks

- Example network, 1 input, 1 output
- Universal approximation theorem
- More than one output
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Two outputs

- 1 input, 4 hidden units, 2 outputs

$$
\begin{aligned}
h_1 &= \mathrm{a}[\theta_{10} + \theta_{11}x] \\
h_2 &= \mathrm{a}[\theta_{20} + \theta_{21}x] \\
h_3 &= \mathrm{a}[\theta_{30} + \theta_{31}x] \\
h_4 &= \mathrm{a}[\theta_{40} + \theta_{41}x]
\end{aligned}
$$

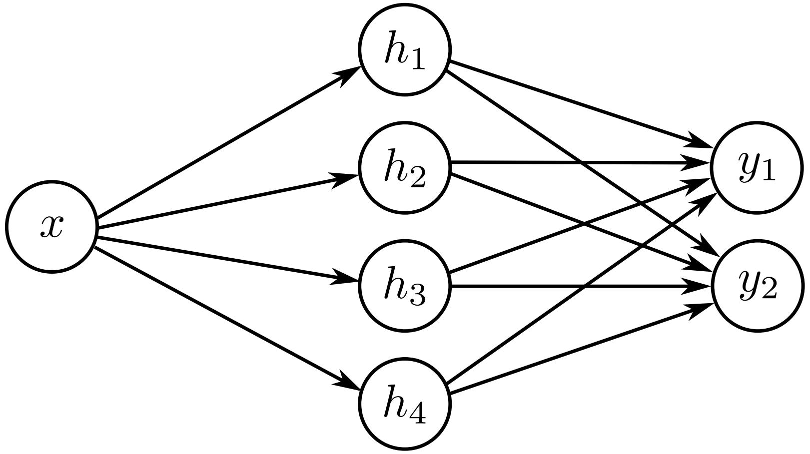
$$
\begin{aligned}
y_1 &= \phi_{10} + \phi_{11}h_1 + \phi_{12}h_2 + \phi_{13}h_3 + \phi_{14}h_4 \\
y_2 &= \phi_{20} + \phi_{21}h_1 + \phi_{22}h_2 + \phi_{23}h_3 + \phi_{24}h_4
\end{aligned}
$$

Two outputs

- 1 input, 4 hidden units, 2 outputs

$$\begin{aligned} h_1 &= \mathrm{a}[\theta_{10} + \theta_{11}x] \\ h_2 &= \mathrm{a}[\theta_{20} + \theta_{21}x] \\ h_3 &= \mathrm{a}[\theta_{30} + \theta_{31}x] \\ h_4 &= \mathrm{a}[\theta_{40} + \theta_{41}x] \end{aligned}$$

$$\begin{aligned} y_1 &= \phi_{10} + \phi_{11}h_1 + \phi_{12}h_2 + \phi_{13}h_3 + \phi_{14}h_4 \\ y_2 &= \phi_{20} + \phi_{21}h_1 + \phi_{22}h_2 + \phi_{23}h_3 + \phi_{24}h_4 \end{aligned}$$

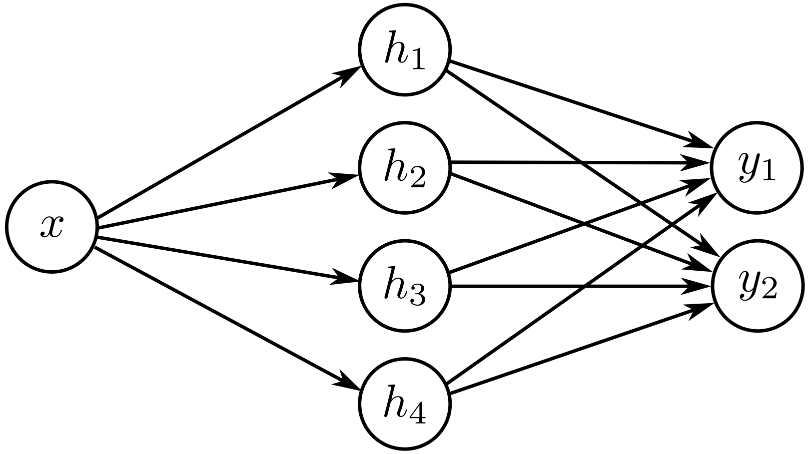


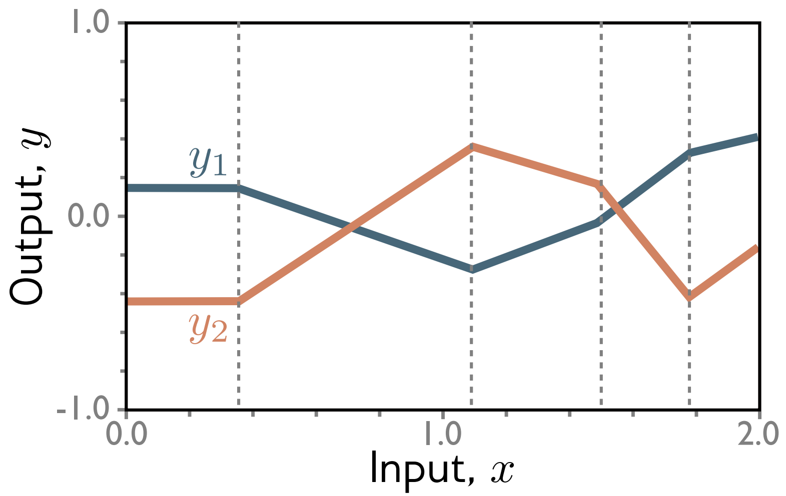
Two outputs

- 1 input, 4 hidden units, 2 outputs

$$\begin{aligned} h_1 &= \mathrm{a}[\theta_{10} + \theta_{11}x] \\ h_2 &= \mathrm{a}[\theta_{20} + \theta_{21}x] \\ h_3 &= \mathrm{a}[\theta_{30} + \theta_{31}x] \\ h_4 &= \mathrm{a}[\theta_{40} + \theta_{41}x] \end{aligned}$$

$$\begin{aligned} y_1 &= \phi_{10} + \phi_{11}h_1 + \phi_{12}h_2 + \phi_{13}h_3 + \phi_{14}h_4 \\ y_2 &= \phi_{20} + \phi_{21}h_1 + \phi_{22}h_2 + \phi_{23}h_3 + \phi_{24}h_4 \end{aligned}$$





Shallow neural networks

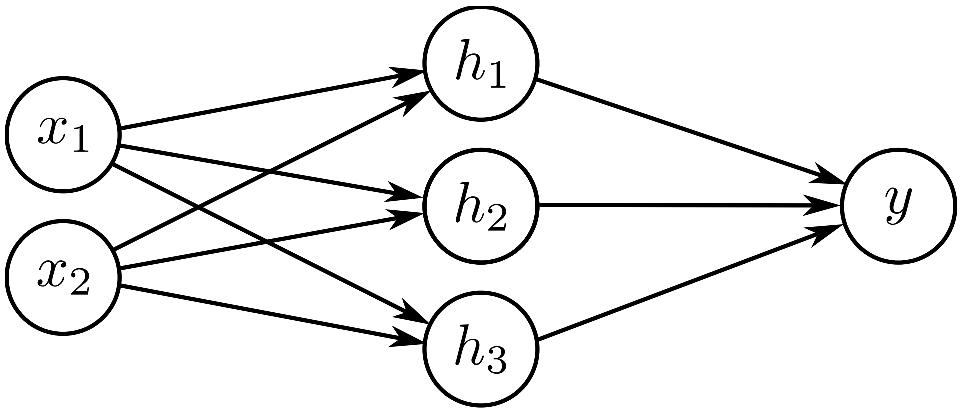
- Example network, 1 input, 1 ouput
- Universal approximation theorem
- More than one output
- More than one input
- General case
- Number of regions
- Terminology

Two inputs

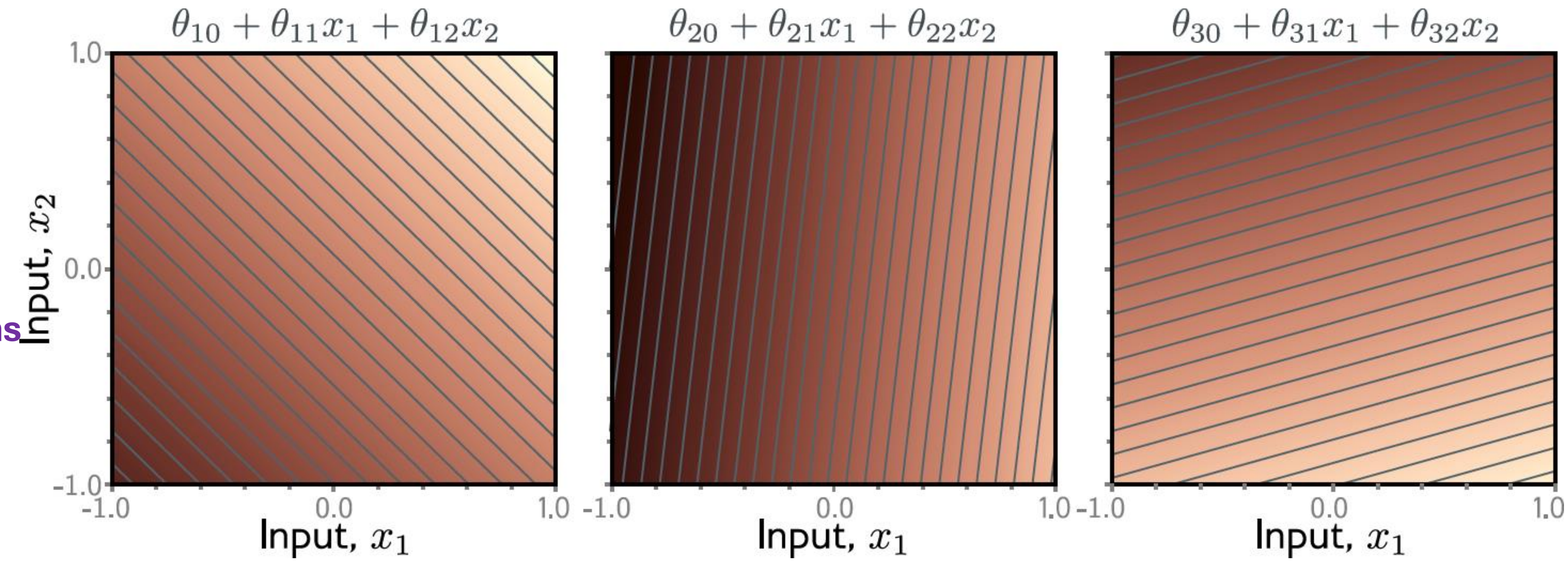
- 2 inputs, 3 hidden units, 1 output

$$
\begin{aligned}
h_1 &= \mathrm{a}[\theta_{10} + \theta_{11}x_1 + \theta_{12}x_2] \\
h_2 &= \mathrm{a}[\theta_{20} + \theta_{21}x_1 + \theta_{22}x_2] \\
h_3 &= \mathrm{a}[\theta_{30} + \theta_{31}x_1 + \theta_{32}x_2]
\end{aligned}
$$

$$y = \phi_0 + \phi_1 h_1 + \phi_2 h_2 + \phi_3 h_3$$



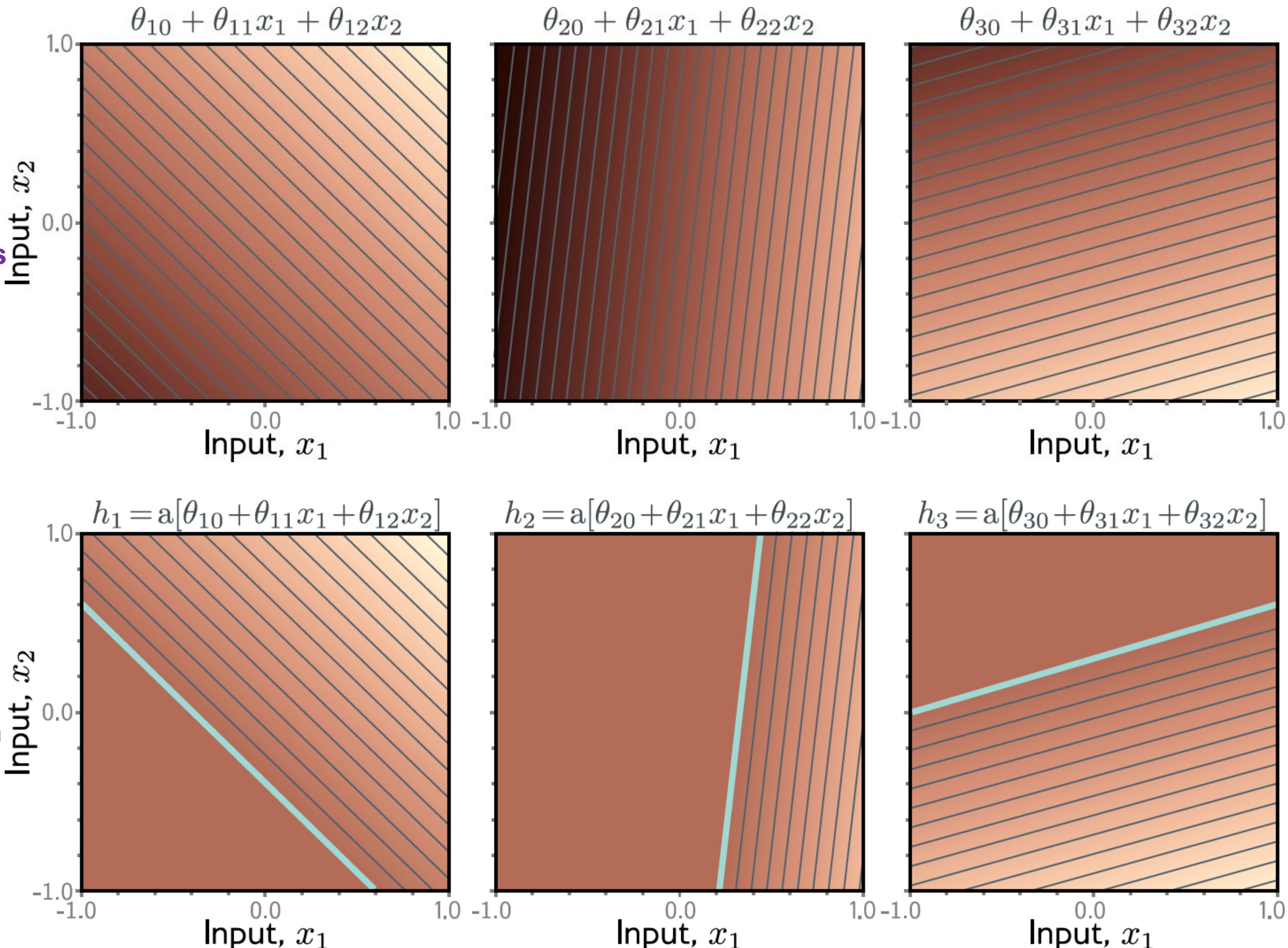
Linear Functions



See Interactive Figure 3.8a https://udlbook.github.io/udlfigures/

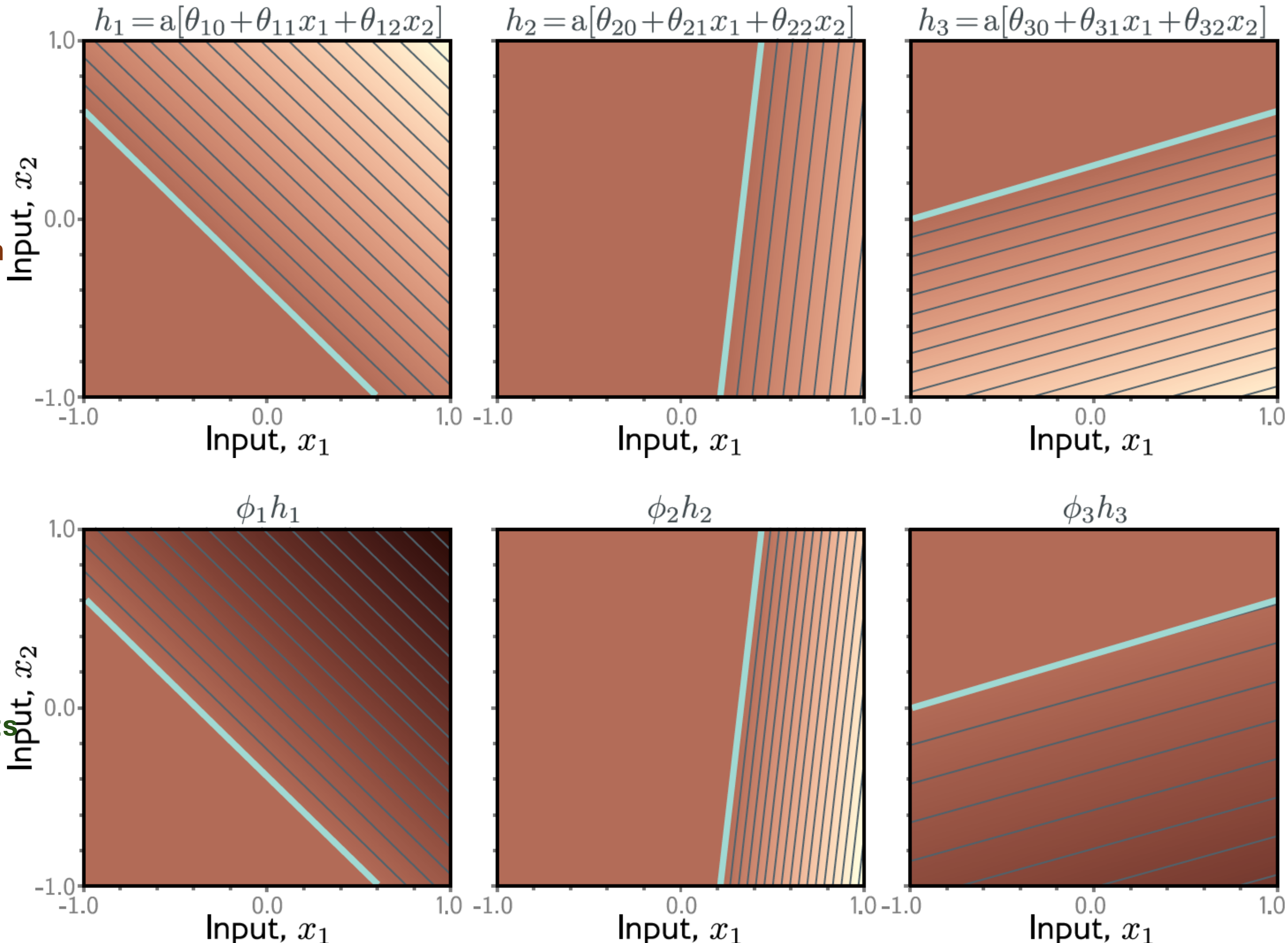
Linear Functions

After Activation

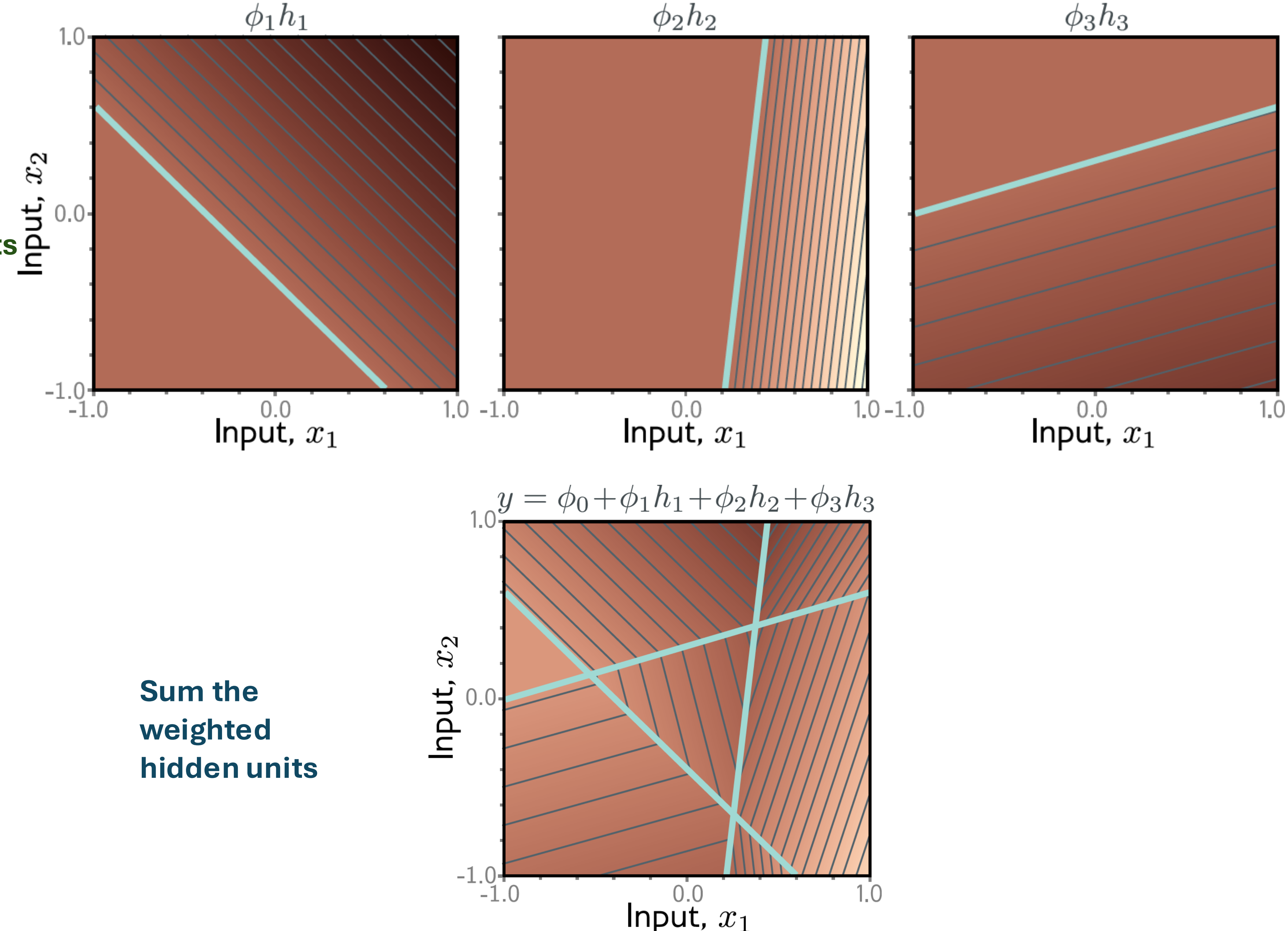


After Activation

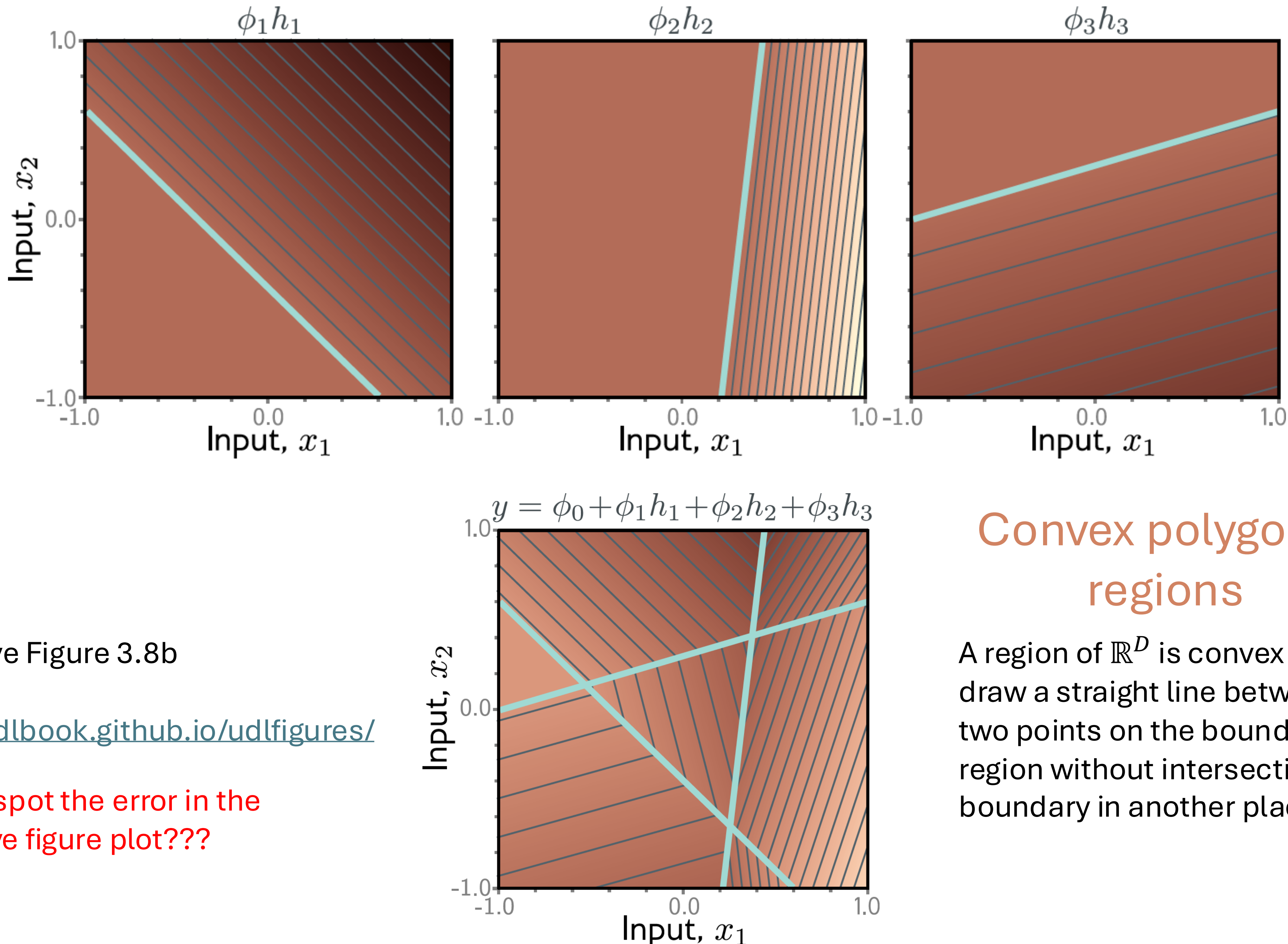
Weight the Hidden units



Weight the hidden units



Sum the weighted hidden units



Interactive Figure 3.8b

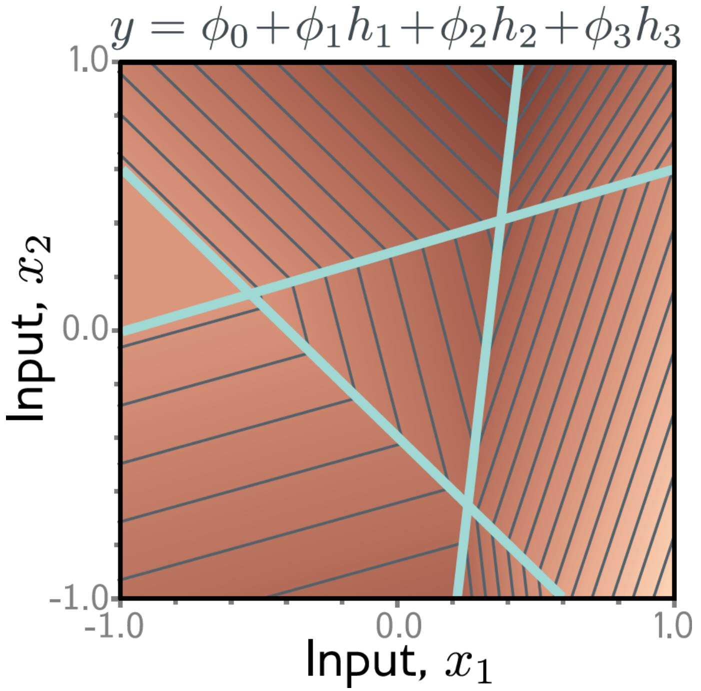
https://udlbook.github.io/udlfigures/

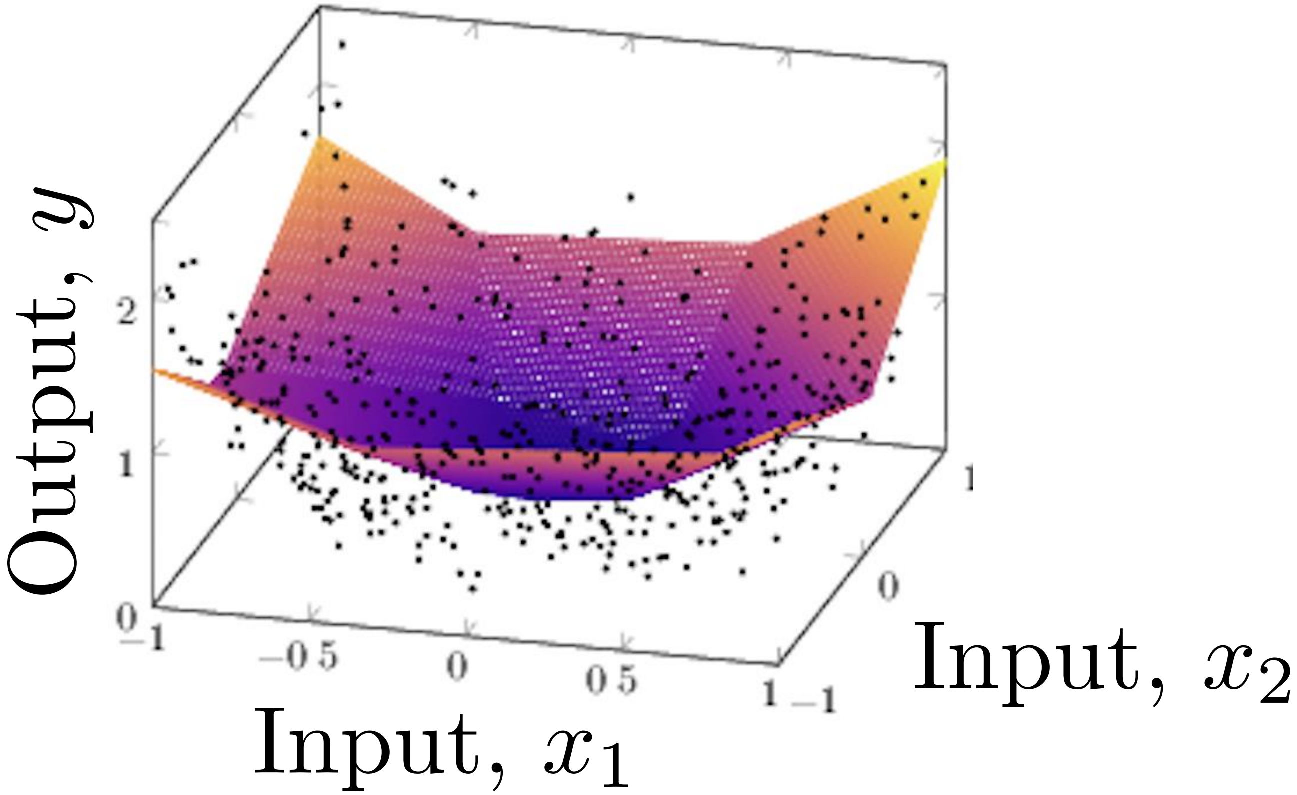
Can you spot the error in the interactive figure plot???

Convex polygonal regions

A region of $\mathbb{R}^D$ is convex if we can draw a straight line between any two points on the boundary of the region without intersecting the boundary in another place.

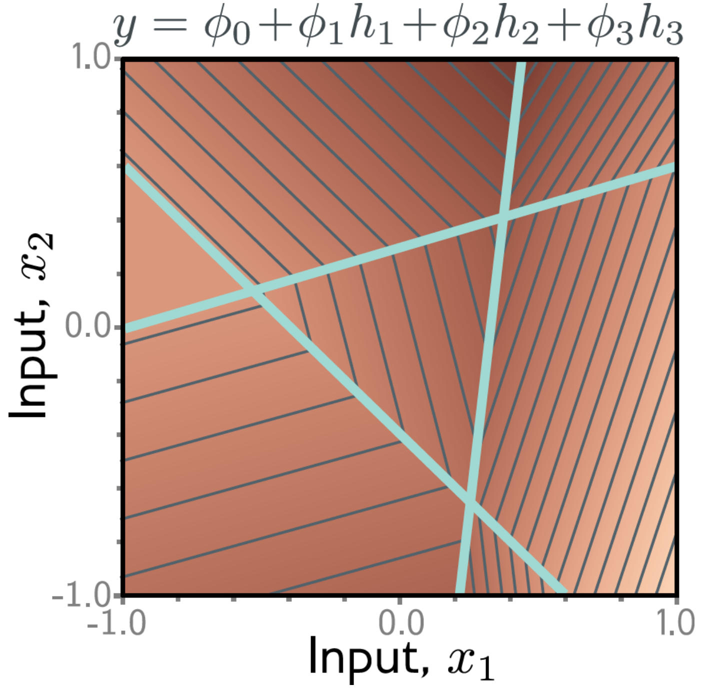
Fitting a dataset where:
each sample has 2 inputs and 1 output





Question:

- For the 2D case, what if there were two outputs?
- If this is one of the outputs, what would the other one look like?



Shallow neural networks

- Example network, 1 input, 1 ouput
- Universal approximation theorem
- More than one output
- More than one input
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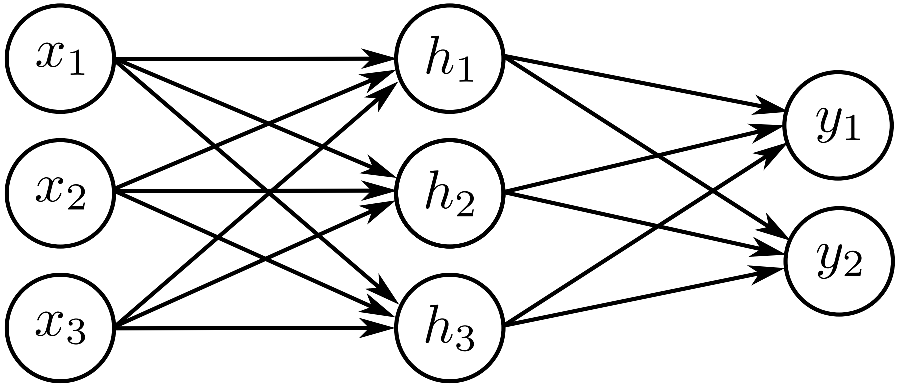
Arbitrary inputs, hidden units, outputs

- D_i inputs, D hidden units, and D_o Outputs

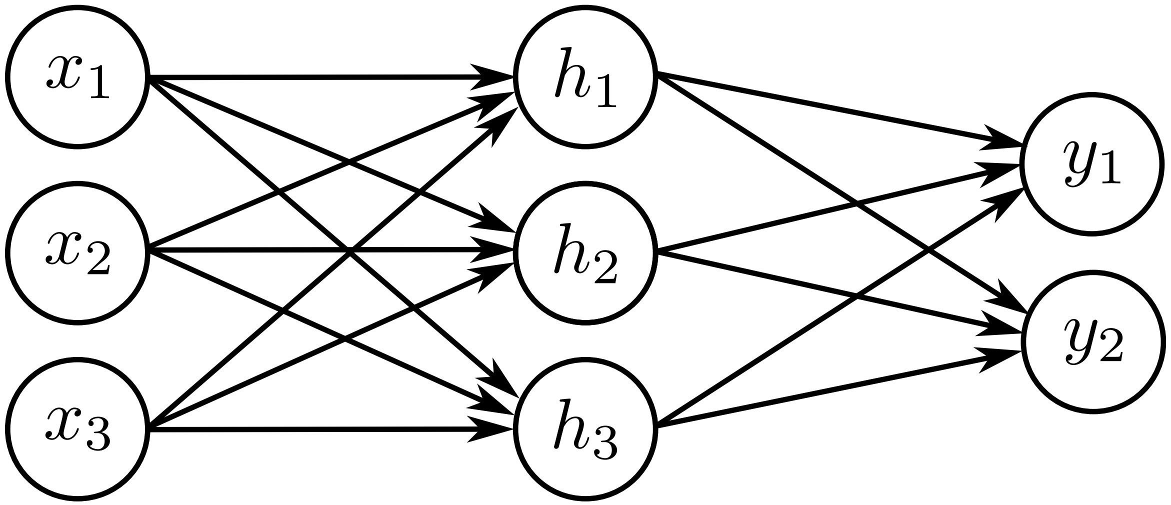
$$h_d = \mathrm{a}\left[\theta_{d0} + \sum_{i=1}^{D_i} \theta_{di} x_i\right] \qquad y_j = \phi_{j0} + \sum_{d=1}^{D} \phi_{jd} h_d$$

- e.g., Three inputs, three hidden units, two outputs



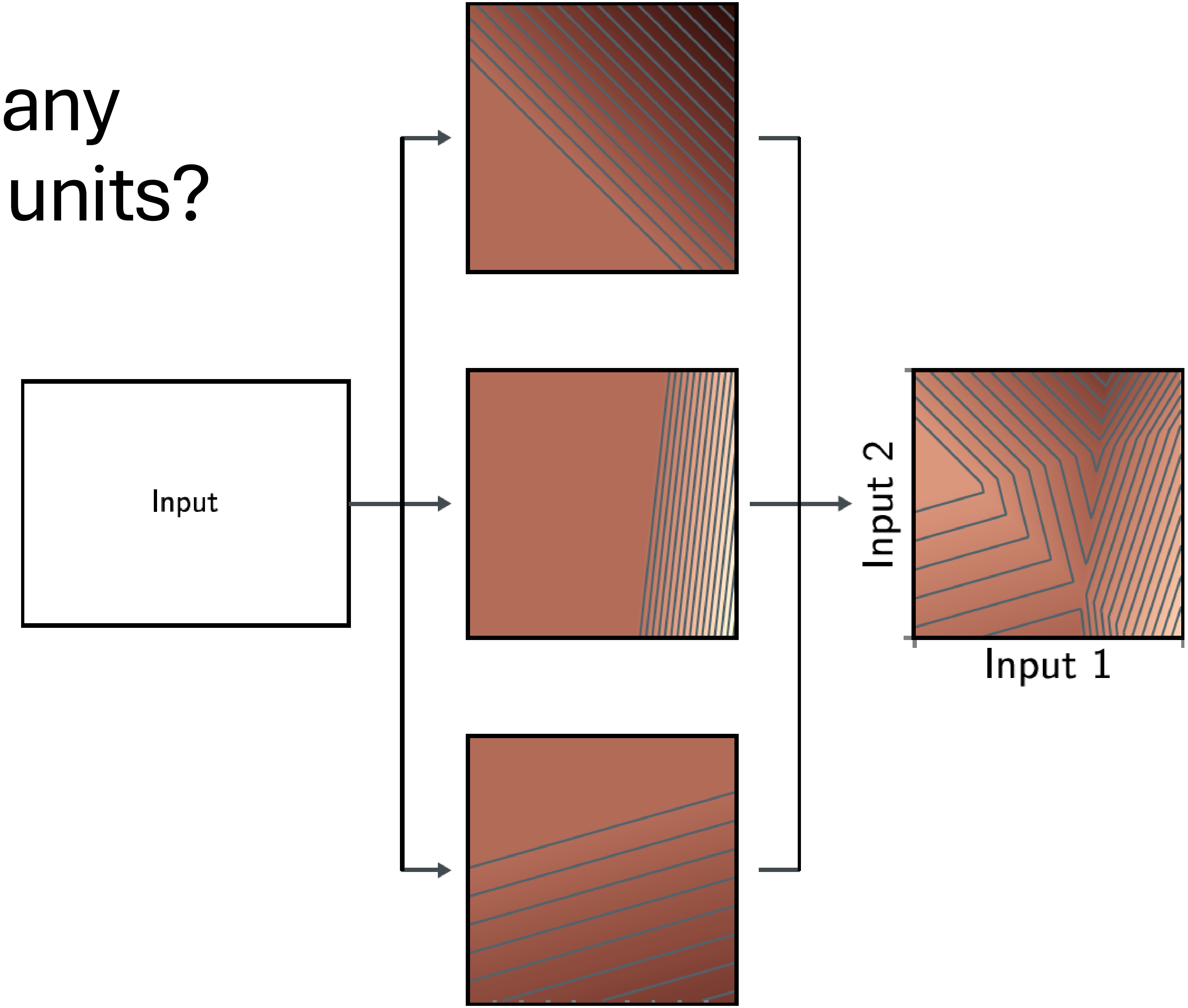
Question:

- How many parameters does this model have?

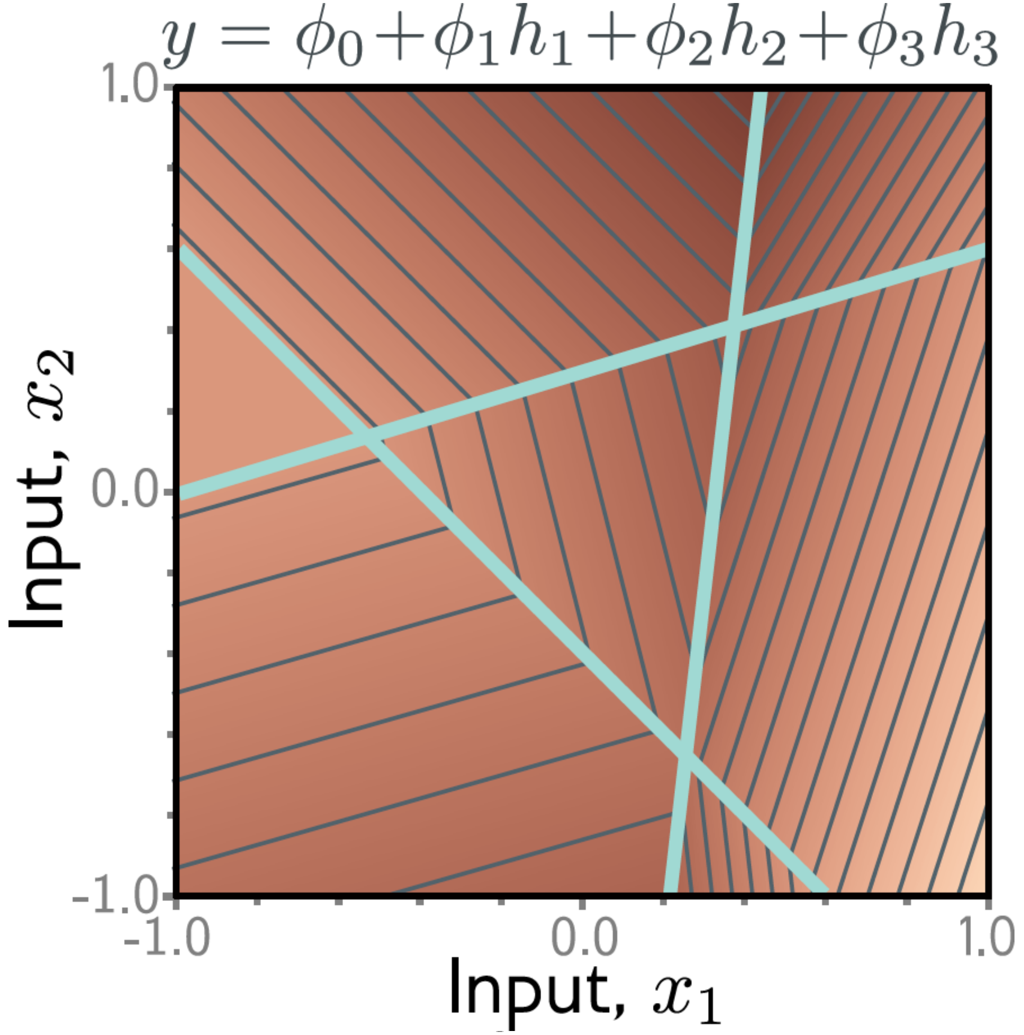


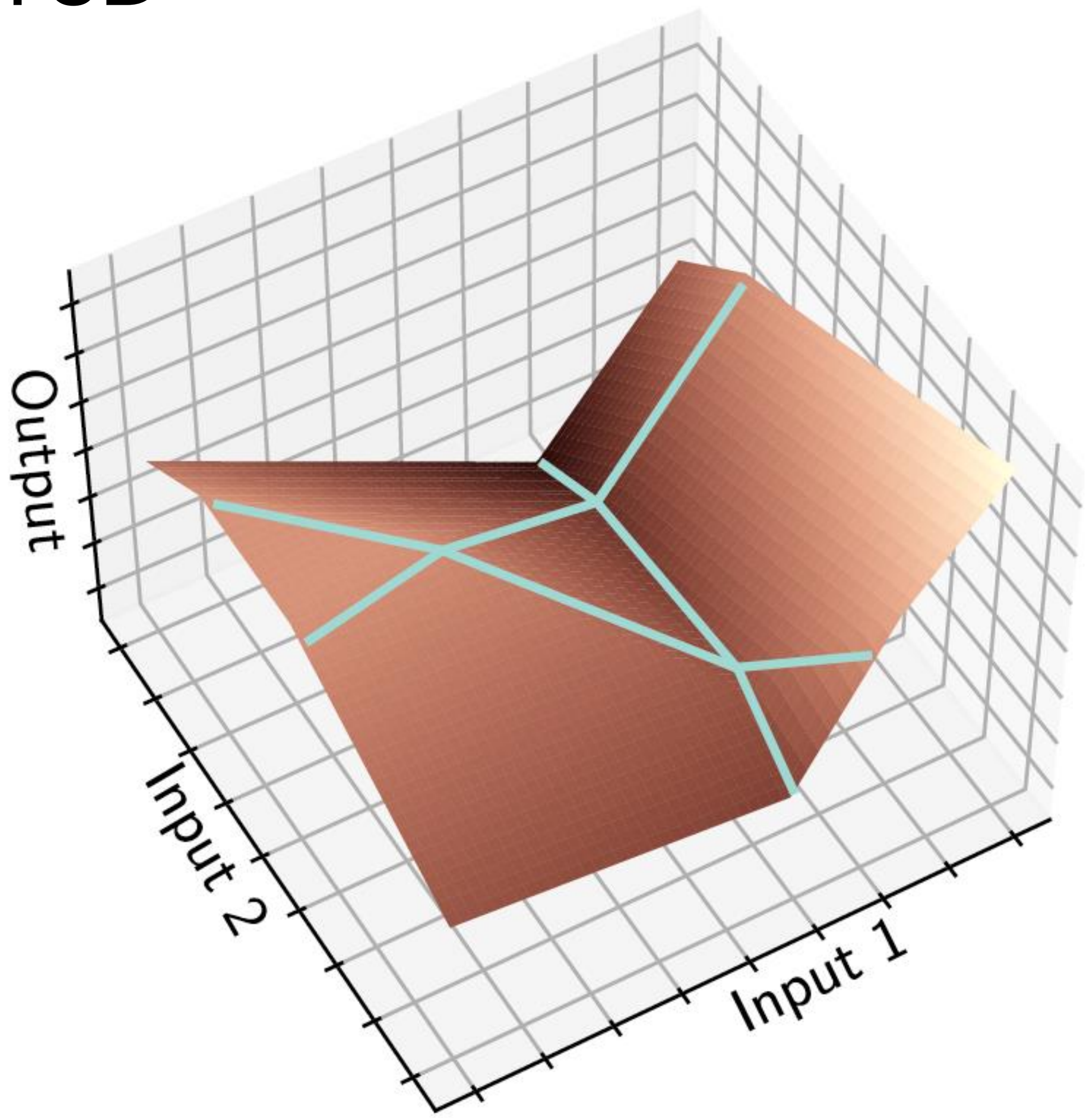
https://piazza.com/class/m5v834h9pcatx/post/19

How many hidden units?

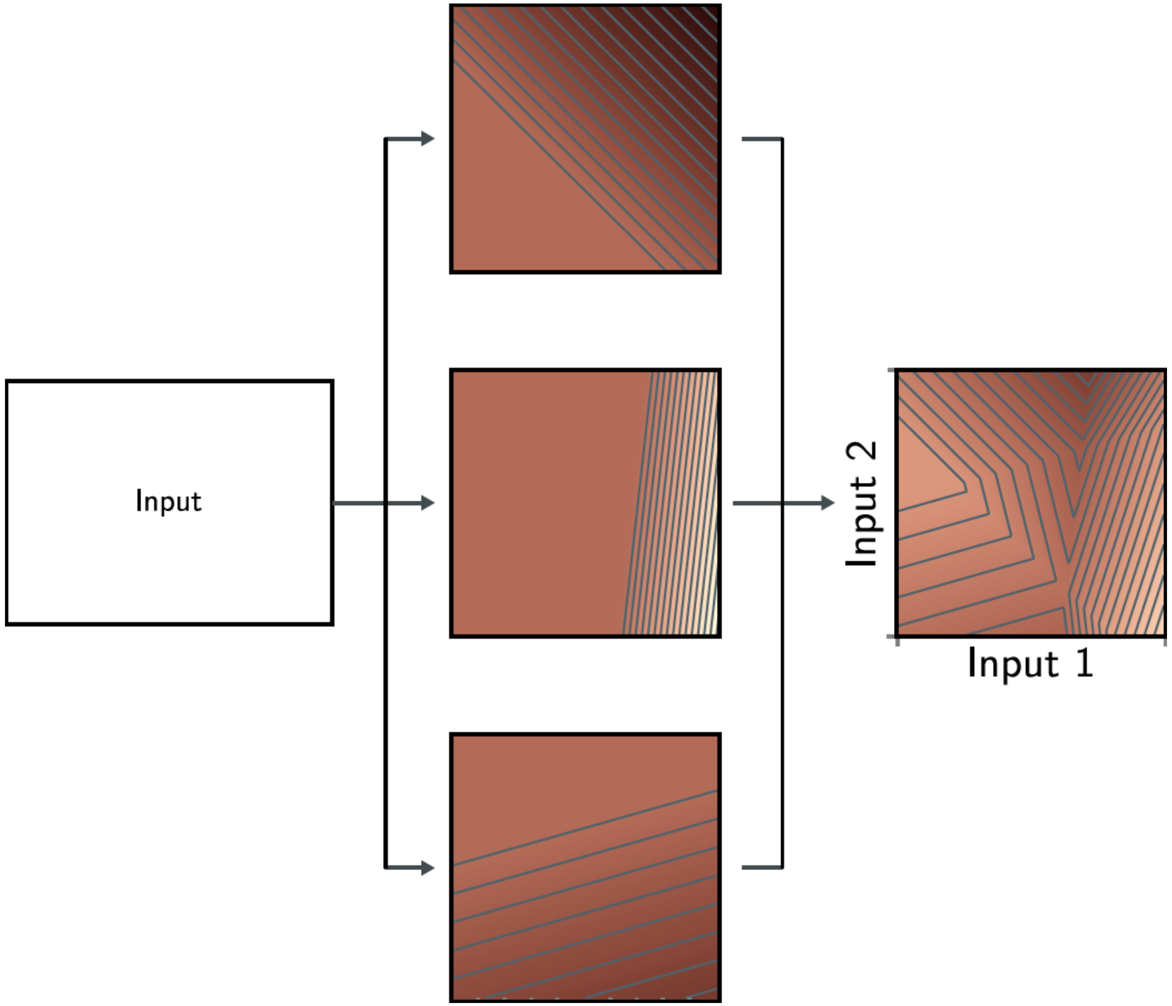


Output with boundaries and in 3D

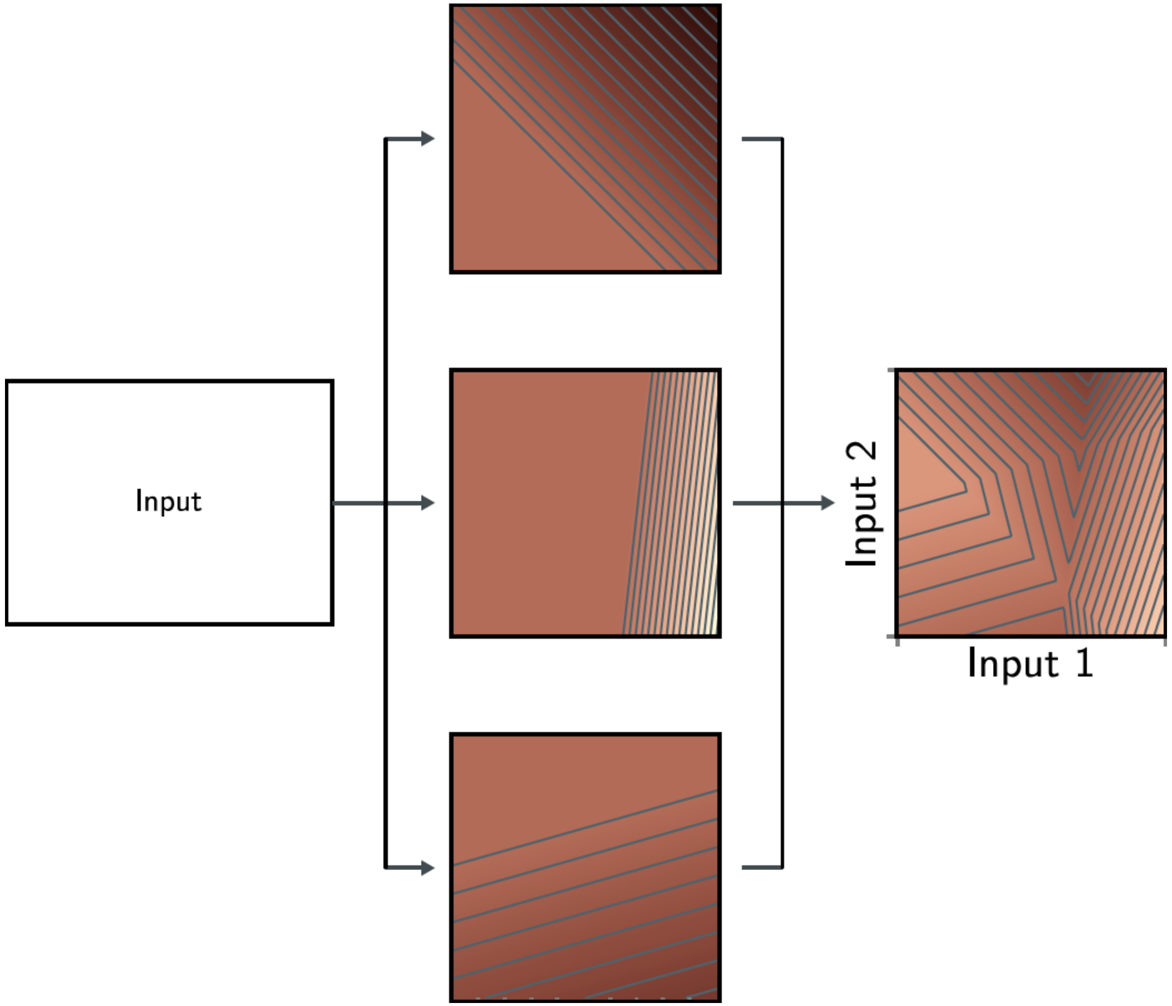


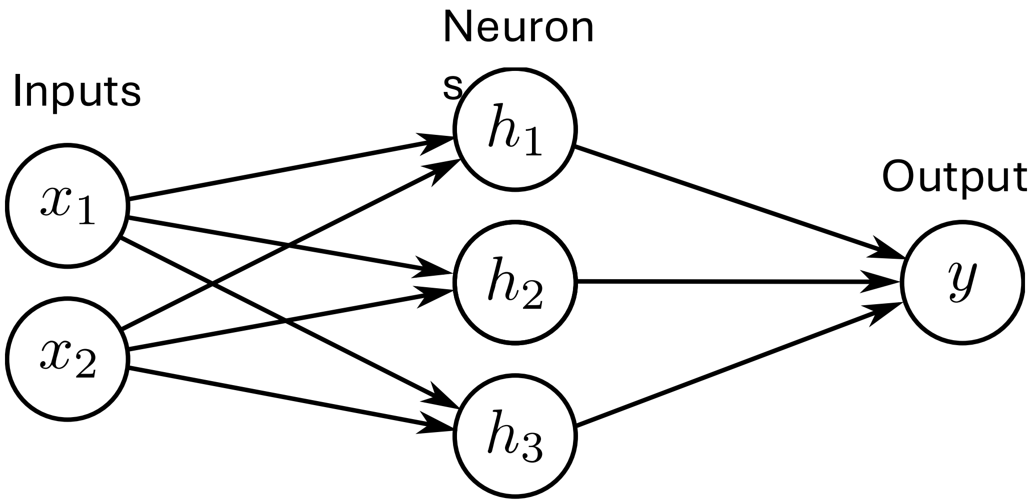


How would you draw and write this neural network?



How would you draw and write this neural network?





"neural network"

$$y = \phi_0 + \phi_1 h_1 + \phi_2 h_2 + \phi_3 h_3$$

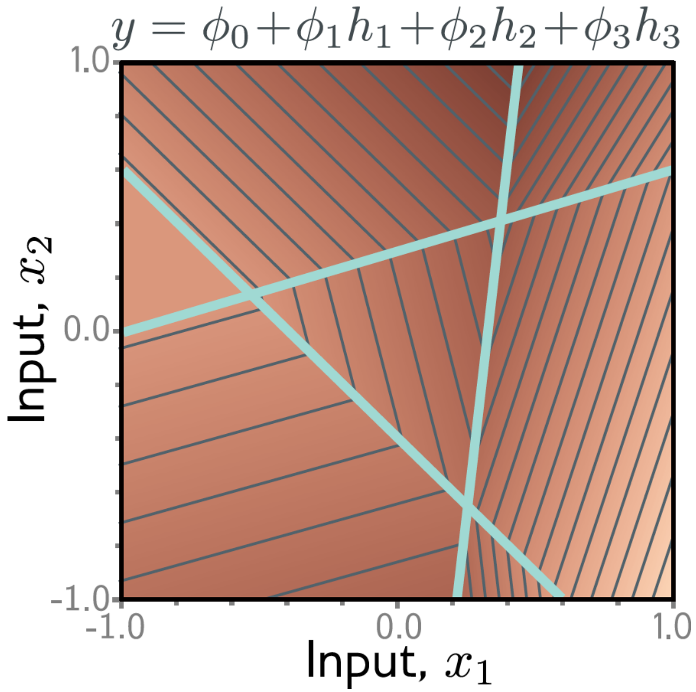
$$h_1 = \mathrm{a}[\theta_{10} + \theta_{11} x_1 + \theta_{12} x_2]$$
$$h_2 = \mathrm{a}[\theta_{20} + \theta_{21} x_1 + \theta_{22} x_2]$$
$$h_3 = \mathrm{a}[\theta_{30} + \theta_{31} x_1 + \theta_{32} x_2]$$

Shallow neural networks

- Example network, 1 input, 1 output
- Universal approximation theorem
- More than one output
- More than one input
- General case
- Number of regions
- Terminology

Number of output regions

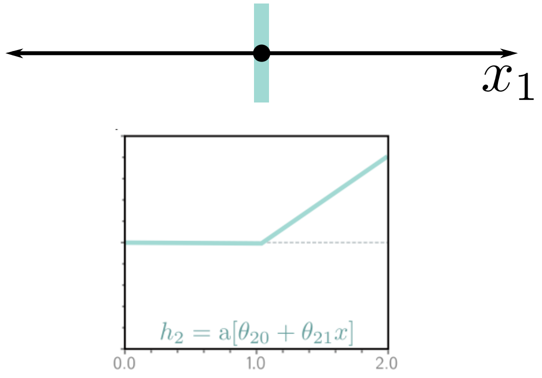
- With ReLU activations, each output consists of multi-dimensional piecewise linear hyperplanes
- With two inputs, and three hidden units, we saw there were seven polygons for each output:



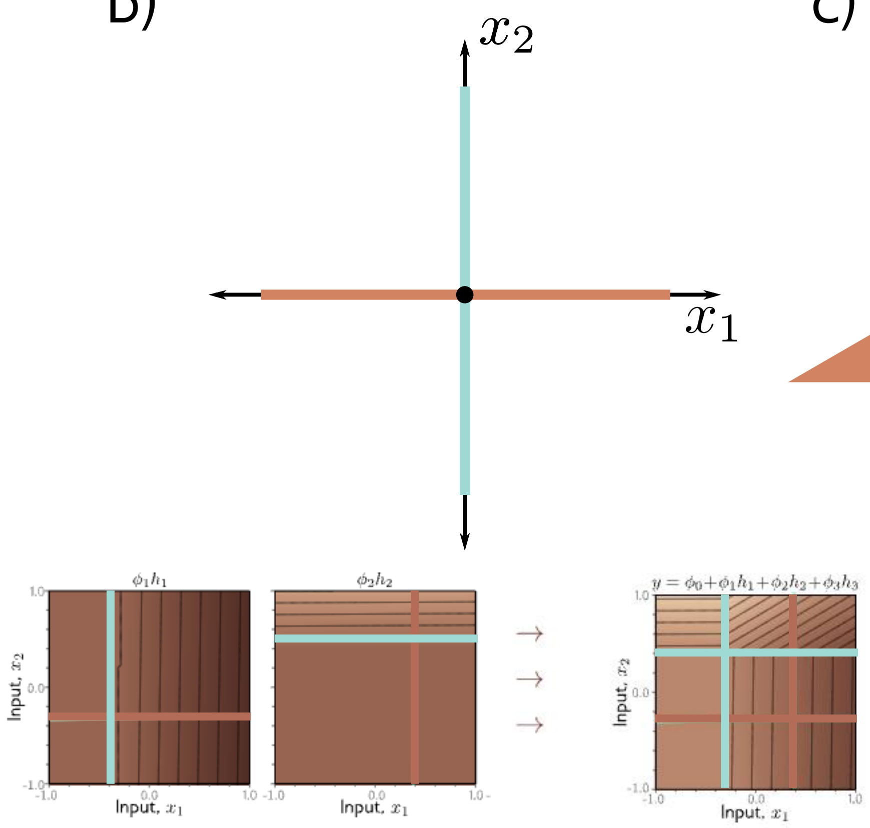
Example with $D = D_i \rightarrow 2^{D_i}$ regions

D_i : # of inputs
D : # of hidden units
D_o : # of outputs

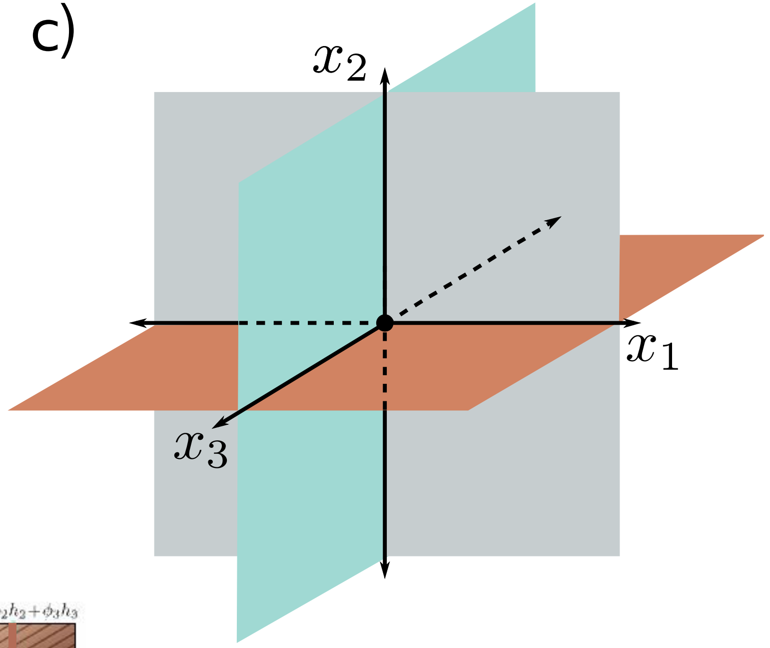
a)



b)



c)



- 1 input (1-dimension)
- 1 hidden unit
- creates two regions (one joint)

- 2 input (2-dimensions) with
- 2 hidden units
- creates four regions (two lines)

- 3 inputs (3-dimensions) with
- 3 hidden units
- creates eight regions (three planes)

Number of regions:

D_i : # of inputs
D : # of hidden units
D_o : # of outputs

- Number of regions created by $D > D_i$ hyper-planes in D_i dimensions was proved by Zaslavsky (1975) to be:

$$\sum_{j=0}^{D_i} \binom{D}{j} = \frac{D!}{j!(D-j)!}$$

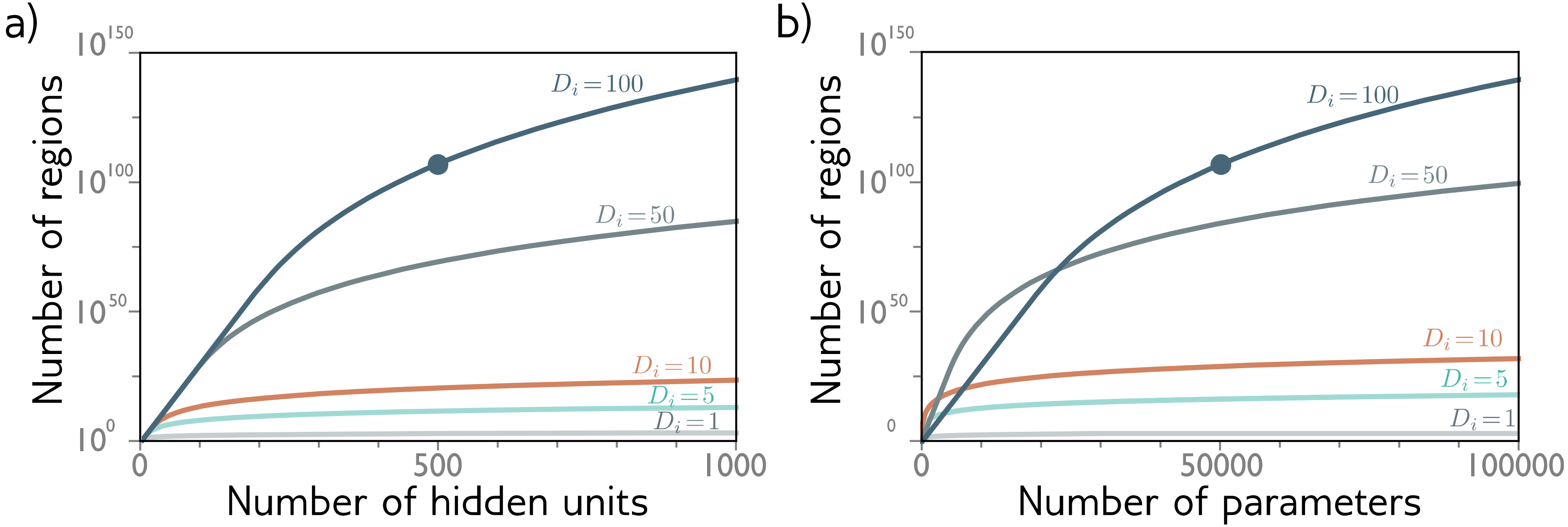
Binomial coefficients!

- How big is this? It's greater than 2^{D_i} but less than 2^D.

Number of output regions

D_i : # of inputs
D : # of hidden units
D_o : # of outputs

- In general, each output consists of D dimensional convex polytopes
- How many?

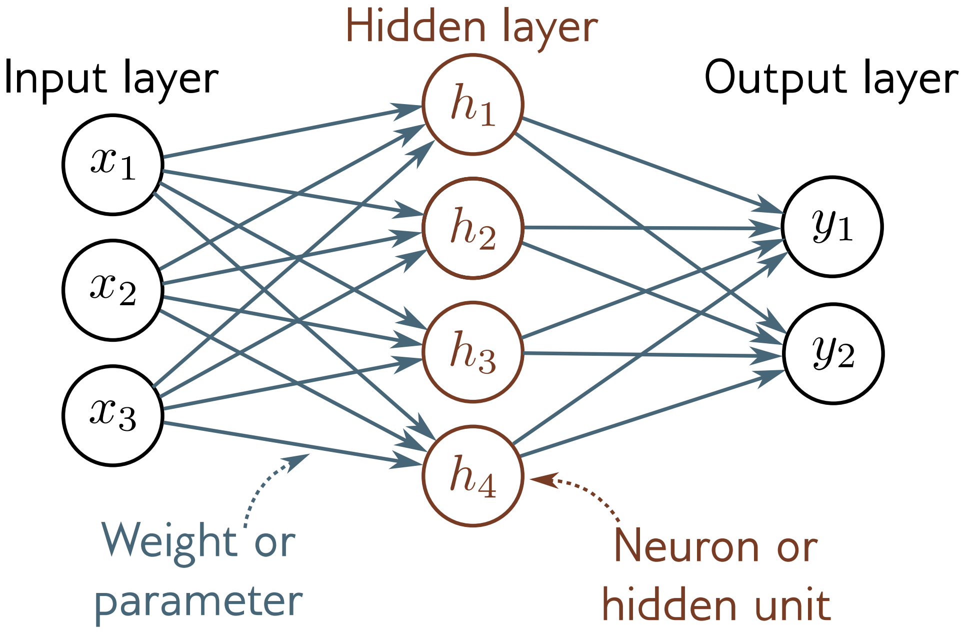


Highlighted point = 500 hidden units or 51,001 parameters

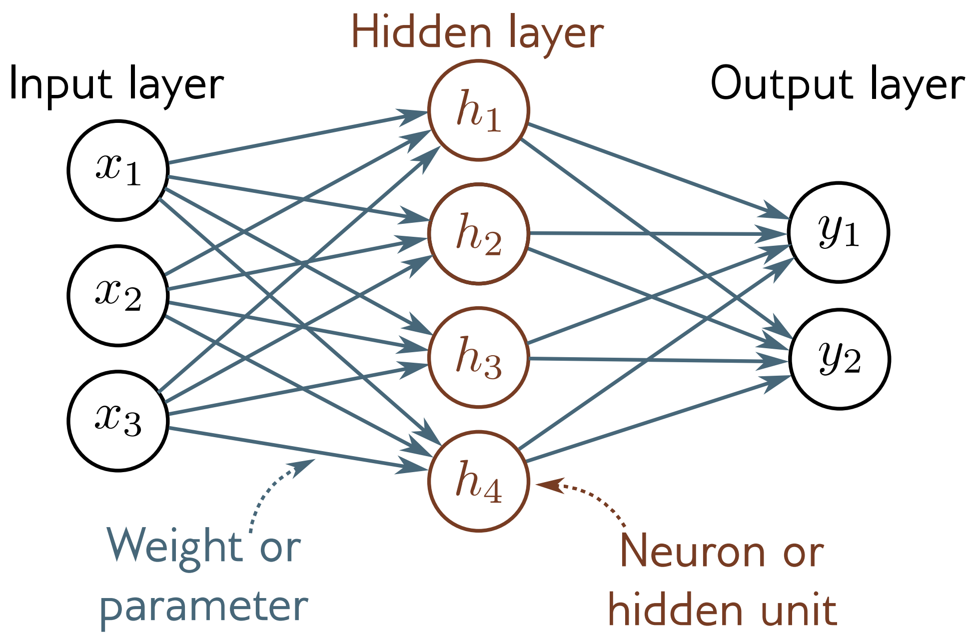
Shallow neural networks

- Example network, 1 input, 1 output
- Universal approximation theorem
- More than one output
- More than one input
- General case
- Number of regions
- Terminology

Nomenclature

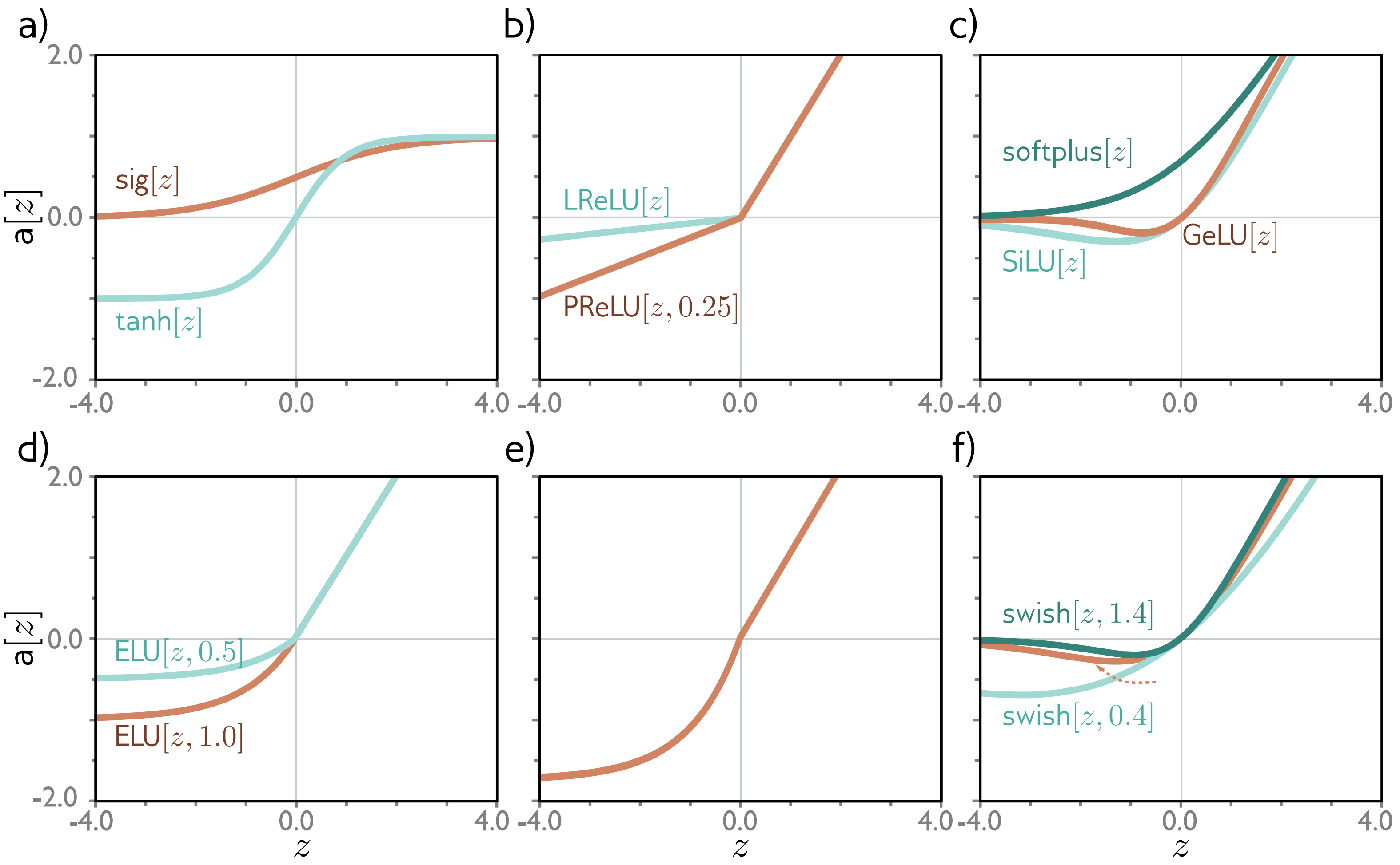


Nomenclature



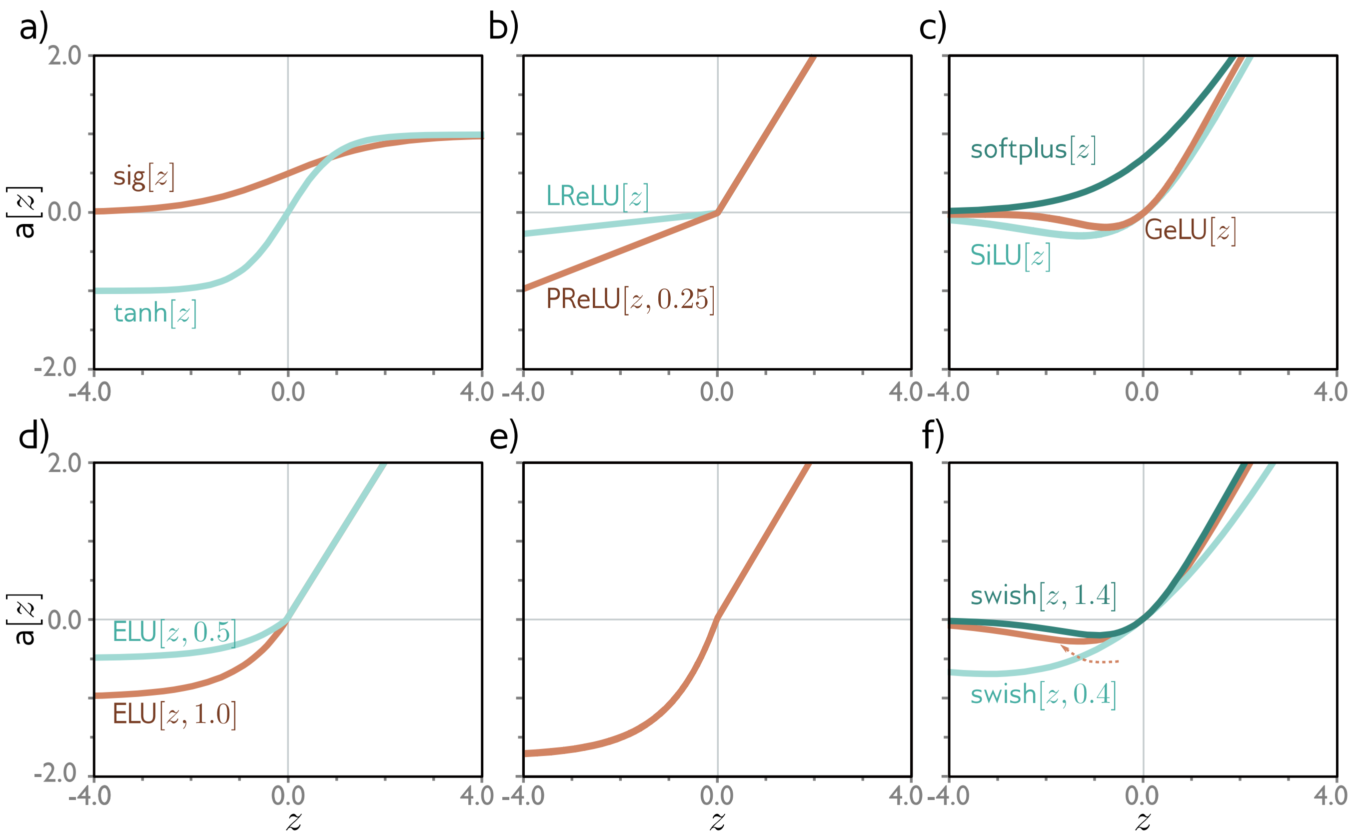
- Y-offsets = biases
- Slopes = weights
- Everything in one layer connected to everything in the next = fully connected network (multi-layer perceptron)
- No loops = feedforward network
- Values after ReLU (activation functions) = activations
- Values before ReLU = pre-activations
- One hidden layer = shallow neural network
- More than one hidden layer = deep neural network
- Number of hidden units ≈ capacity

Other activation functions



Ramachandran, P., Zoph, B., & Le, Q. V. (2017). Searching for activation functions. *arXiv:1710.05941*.

Interactive Figures 3.3b and 3.3c



Also look at

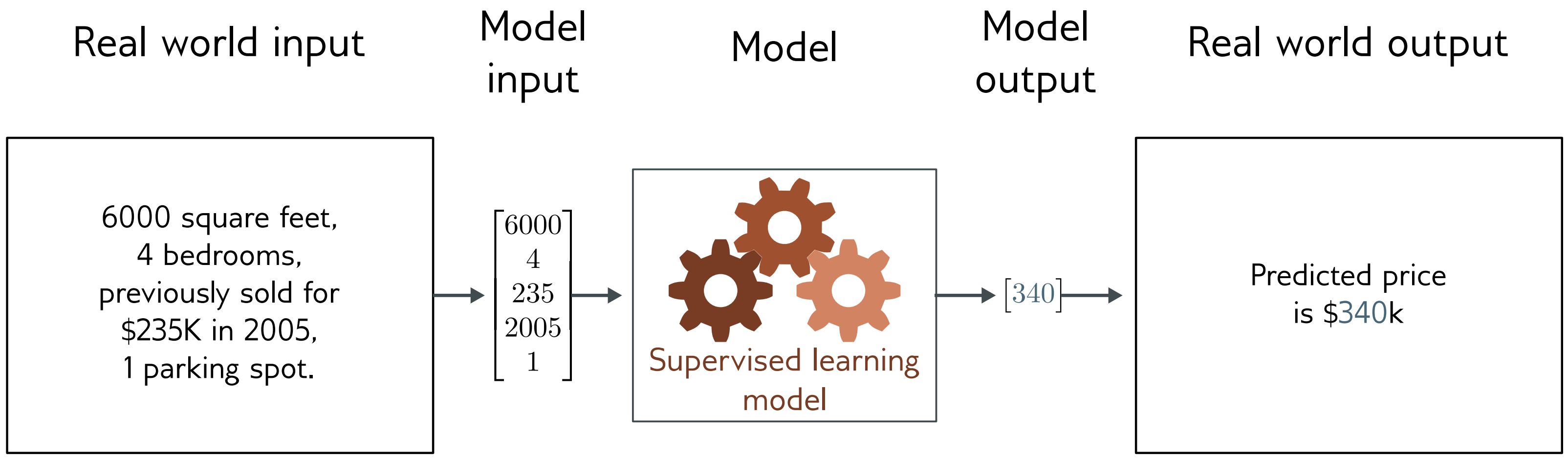
3.3b – 1D shallow network (sigmoid)

3.3c – 1D shallow network (Heaviside/Step)

$$\text{heaviside}[z] = \begin{cases} 0 & z < 0 \\ 1 & z \geq 0 \end{cases}$$

https://udlbook.github.io/udlfigures/

Regression



We have built a model that can:

- take an arbitrary number of inputs
- output an arbitrary number of outputs
- model a function of arbitrary complexity between the two

$$h_d = \mathrm{a}\left[\theta_{d0} + \sum_{i=1}^{D_i} \theta_{di} x_i\right] \qquad y_j = \phi_{j0} + \sum_{d=1}^{D} \phi_{jd} h_d$$