Fundamentals / Foundation

Data Science 9CFU

Computer Science 6CFU

# of Data Science

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From Manual Features to Learned Representations

In traditional machine learning (e.g., SVMs, Logistic Regression), the model's performance depends entirely on the quality of the input features.

Human's Job: A domain expert must manually engineer features from the raw data.

Example (Spam Detection):

- **Raw Data:** "Buy Viagra now for cheap!!!"
- **Manual Features:**
  - contains_word_"viagra" = 1
  - number_of_exclamation_points = 3
  - uses_all_caps = 1
  - contains_word_"cheap" = 1

Problem: This is time-consuming, requires expert knowledge, and is brittle. What if we miss the most important features?

Representation Learning

This is the core paradigm shift.

- **Definition:** Representation Learning is a set of techniques that allows a model to **automatically learn the most useful features (or "representations")** directly from the raw data.
- **Goal:** Instead of a human hand-crafting features, the model *discovers* the optimal way to represent the data to best accomplish the task (e.g., classification or regression).

Deep Learning

Deep Learning is the most powerful and popular method for representation learning.

- **Definition:** Deep learning uses a **hierarchy of layers** to learn multiple levels of representation at increasing levels of complexity.
- **The Hierarchy:** The model doesn't learn everything at once. It builds complex concepts from simpler ones, layer by layer.

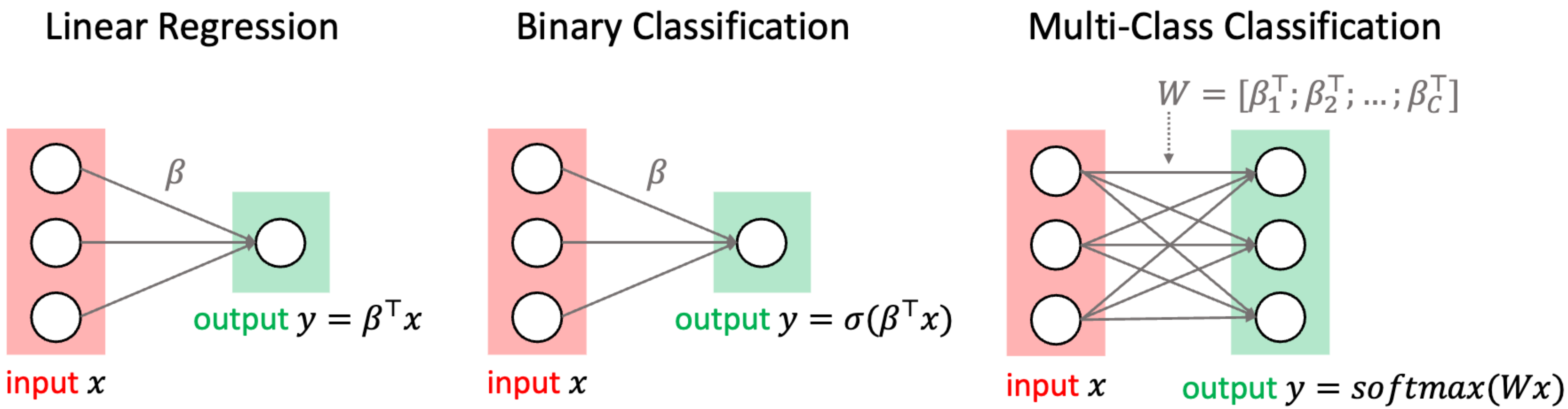
Image Recognition

Imagine a deep neural network learning to recognize a face:

- **Layer 1 (Low-Level):** Learns to "see" simple features like **edges**, **corners**, and **colors** from raw pixels.
- **Layer 2 (Mid-Level):** Learns to **combine edges** to form simple **shapes** and **textures** (e.g., an "oval," a "line," a "patch of skin").
- **Layer 3 (High-Level):** Learns to **combine shapes** to form **"object parts"** (e.g., an "eye," a "nose," a "mouth").
- **Final Layer (Abstract):** Learns to **combine the parts** into the final, abstract concept of a **"face."**

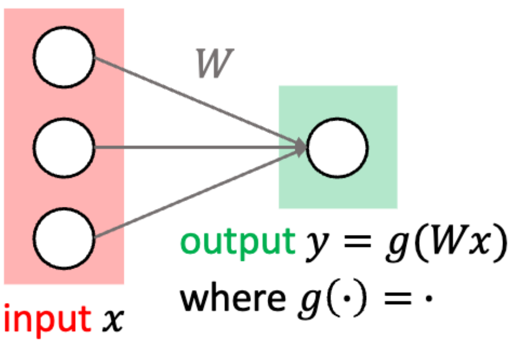
A Unifying View

Linear transformation of input features followed by an activation function

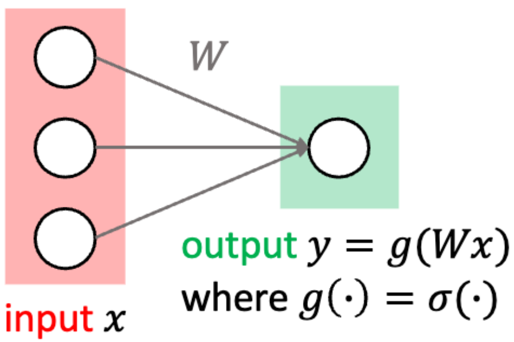


Linear transformation of input features (Wx) followed by an activation function $g(\cdot)$

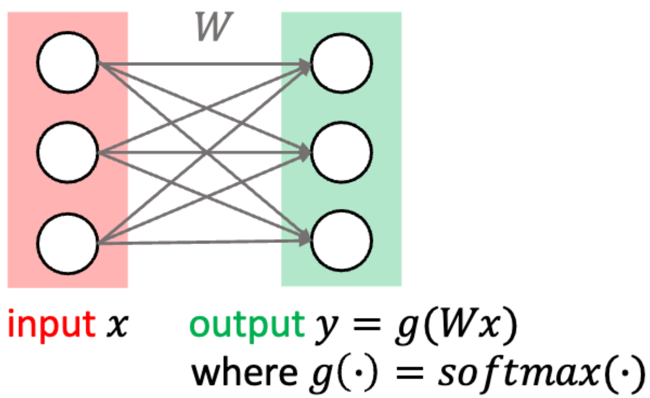
Linear Regression



Binary Classification



Multi-Class Classification



$W \in \mathbb{R}^{C \times D}$ where D is the input dimension and C is the output dimension.

History

1943: Perceptron model (McCulloch & Pitts)

- Intended as theoretical model of biological neurons

1969: Perceptrons cannot learn XOR (Minsky & Papert)

- Highly controversial (may have helped cause “AI winter”)

1997: Long Short-term Memory Networks (Hochreiter, Schmidhuber)

- This breakthrough enabled models to effectively learn from long sequences

1998: Convolutional neural networks for MNIST (Lecun)

- Human-level performance on handwritten digit recognition

Modern History

2012: ImageNet breakthrough (Krizhevsky, Sutskever, & Hinton)
Reduced error on image classification by 50%

2017: Transformer architecture (Vaswani et al.)

2018: Turing award (Bengio, Hinton, & Lecun)

2018:Improving Language Understanding by Generative Pre-Training (OpenAI)

2019: Language Models are Unsupervised Multitask Learners (OpenAI)

2020: Language Models are Few-Shot Learners (OpenAI)

Now and the Future

The Nobel Prize in Chemistry 2024 (Barker, Hassabis, Jumper)

The Nobel Prize in Physics 2024 (Hopfield, Hinton)

Generative AI & LLMs

Why Do We Need Non-Linear Activation Functions?

Deep learning is powerful because it builds **complex, non-linear models**. 👉 The **activation function** is what makes this possible.

Let's build a multi-layer network **using only linear operations**.

3-Layer Linear Network

$$y = W_3\big(W_2(W_1 x)\big) = (W_3 W_2 W_1)x = W_{stacked}x$$

"deep" stack of **linear layers** is **mathematically equivalent** to a single linear layer.

Loss Functions & Capacity

Same principles as in single-layer models

Regression:

- *Mean Squared Error (MSE)*

Classification:

- *Binary Classification:* **Binary Cross-Entropy (BCE)**
- *Multi-Class Classification:* **Cross-Entropy (CE)**

Model Capacity

Capacity of a feed-forward neural network is affected by both:

- Depth: number of hidden layers
- Width: number of neurons in each hidden layer

More neurons = more capacity

Optimization

Backpropagation

The core algorithm for training neural networks.

It's a direct application of the **chain rule** from calculus.

- Computes the error at the final layer.
- Propagates this error signal **backward**, one layer at a time.

- **Modern Practice:** You don't do this by hand!
  - Modern frameworks (PyTorch, Jax) handle it automatically using Automatic Differentiation (Autodiff).

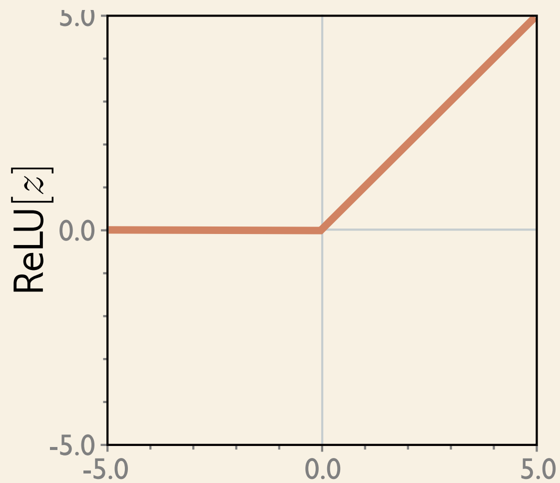
Example shallow network

Activation function

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

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

Rectified Linear Unit



Example shallow network

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

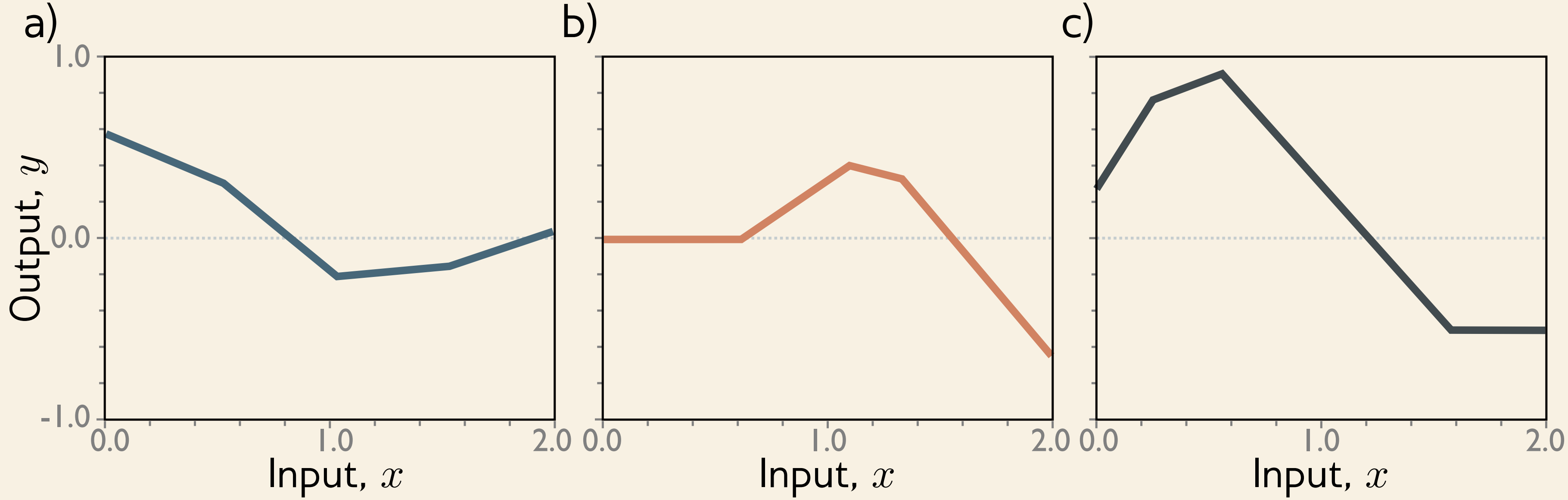
This model has 10 parameters:

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

- Represents a family of functions
- Parameters determine particular function
- Given parameters can perform inference (run 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

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



Piecewise linear functions with three joints

Hidden units

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

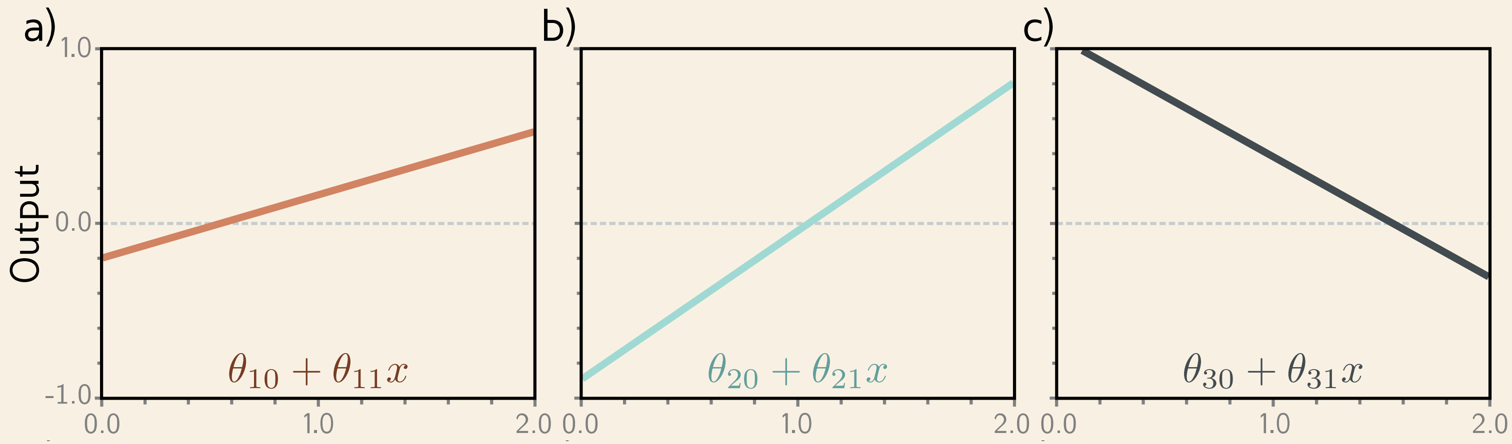
Break down into two parts:

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

where:

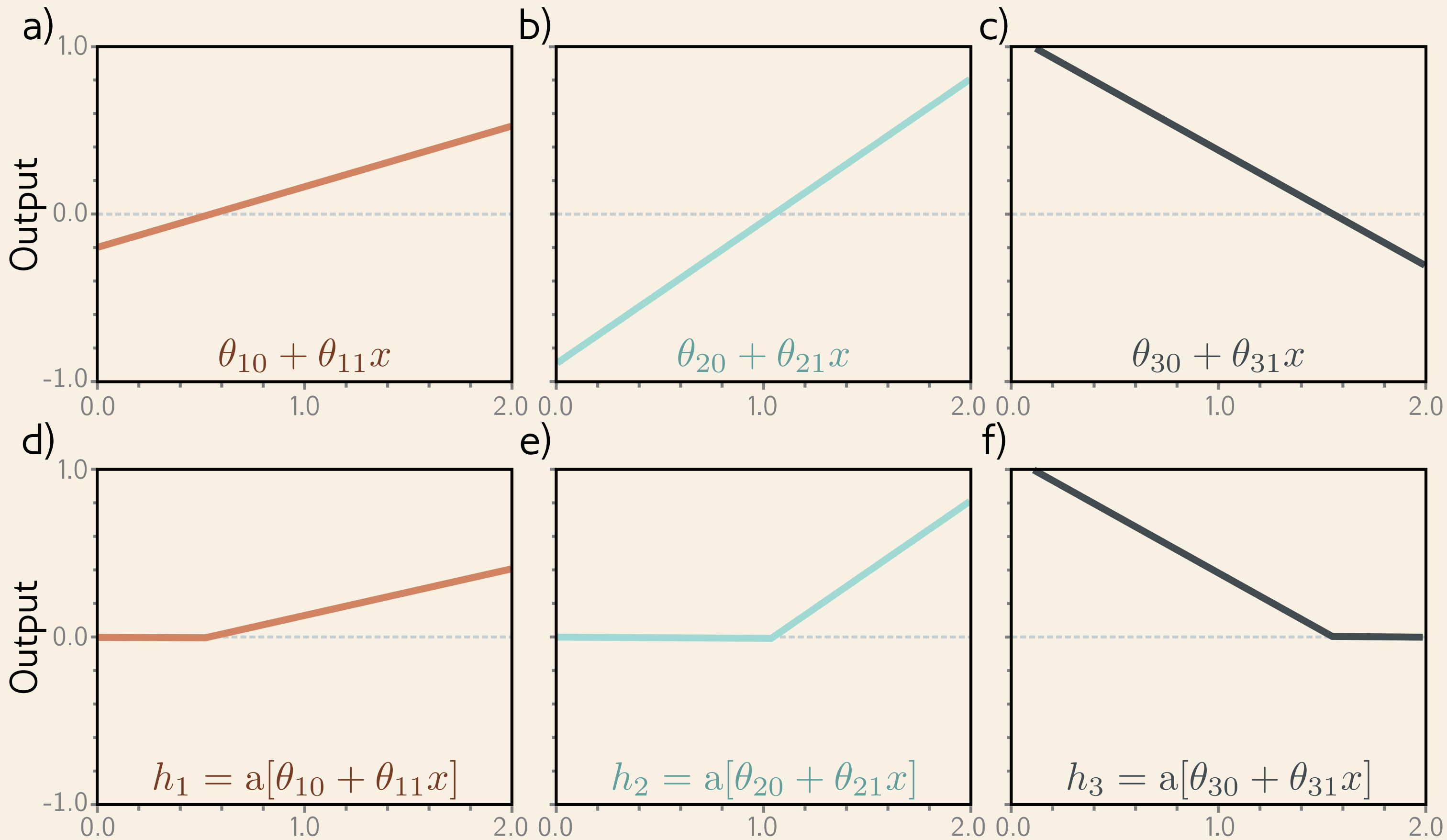
$$\text{Hidden units} \left\{ \begin{aligned} h_1 &= \mathrm{a}[\theta_{10} + \theta_{11}x] \\ h_2 &= \mathrm{a}[\theta_{20} + \theta_{21}x] \\ h_3 &= \mathrm{a}[\theta_{30} + \theta_{31}x] \end{aligned} \right.$$

1. compute three
linear functions

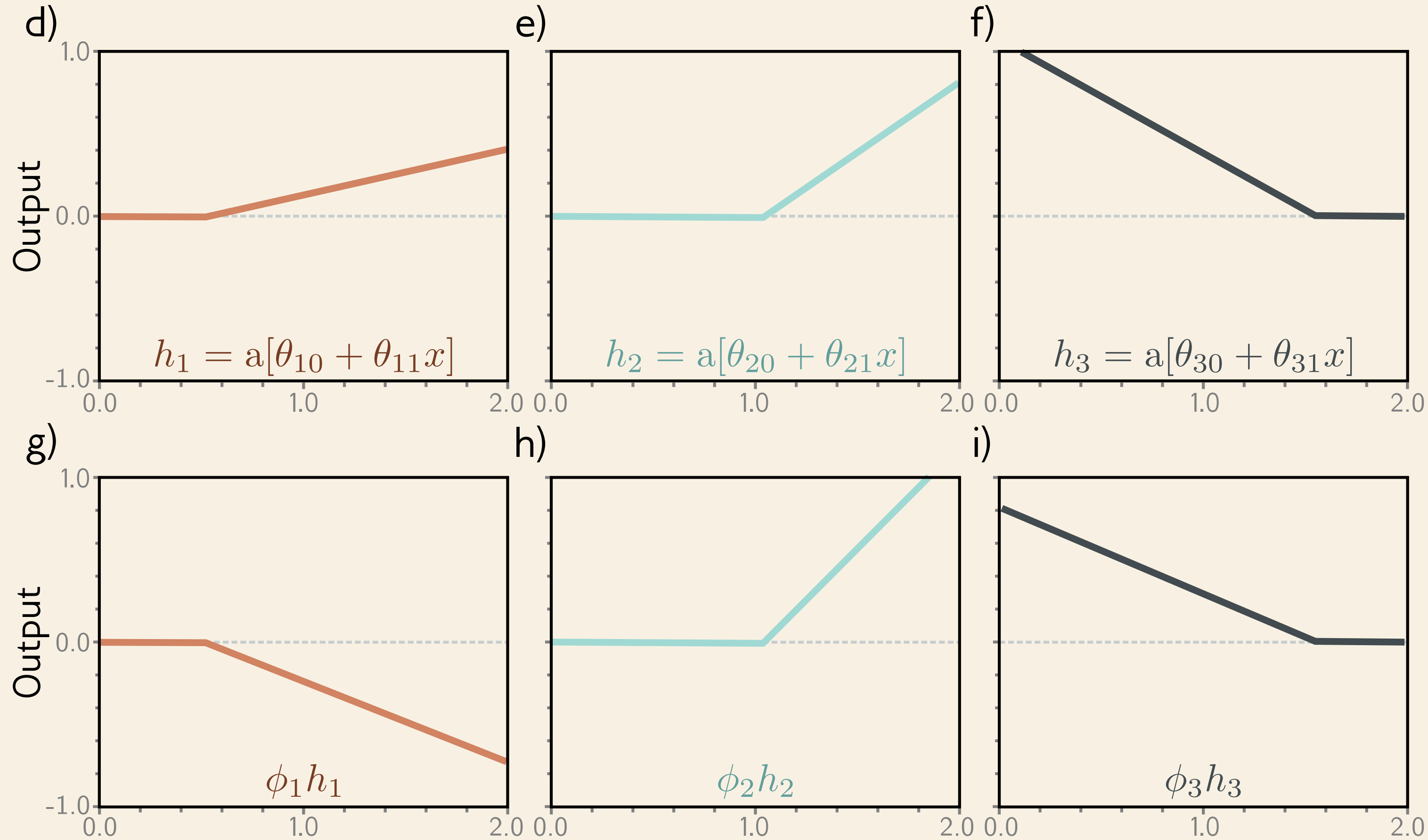


2. Pass through ReLU functions (creates hidden units)

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

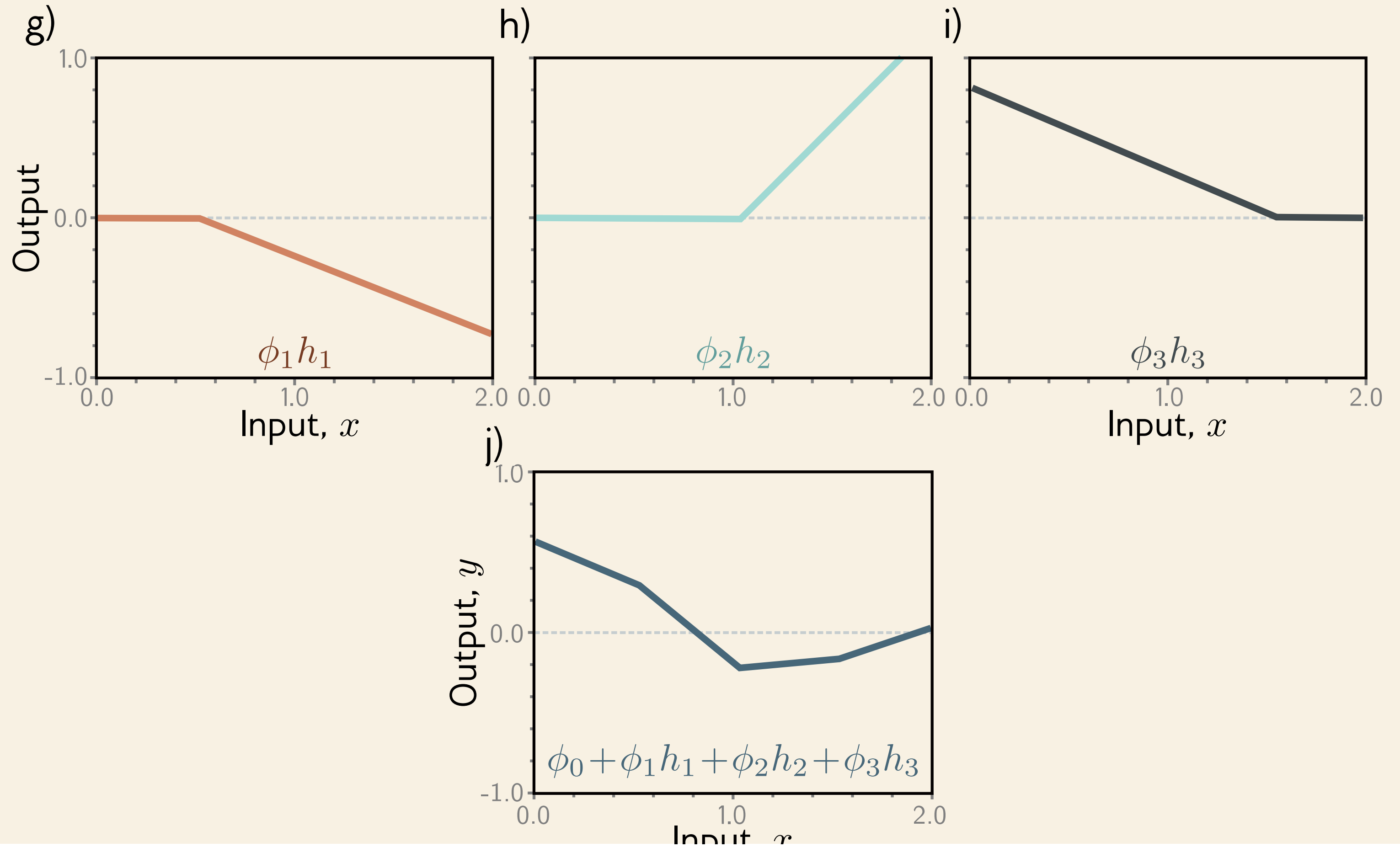


3. Weight the hidden units



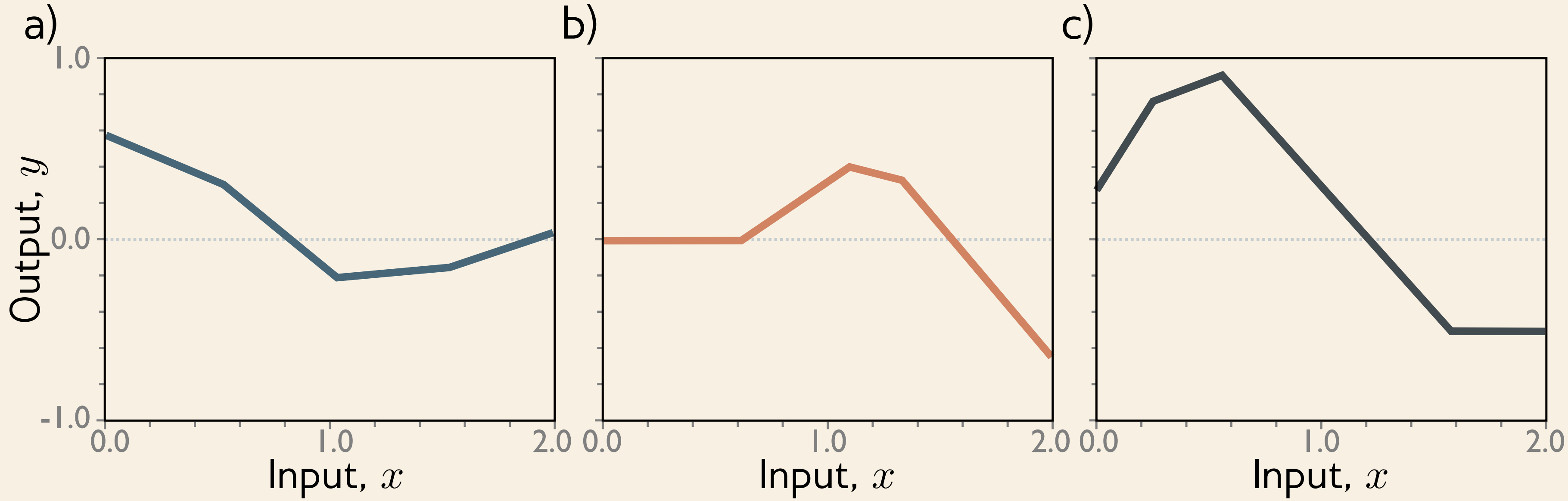
4. Sum the weighted hidden units to create output

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



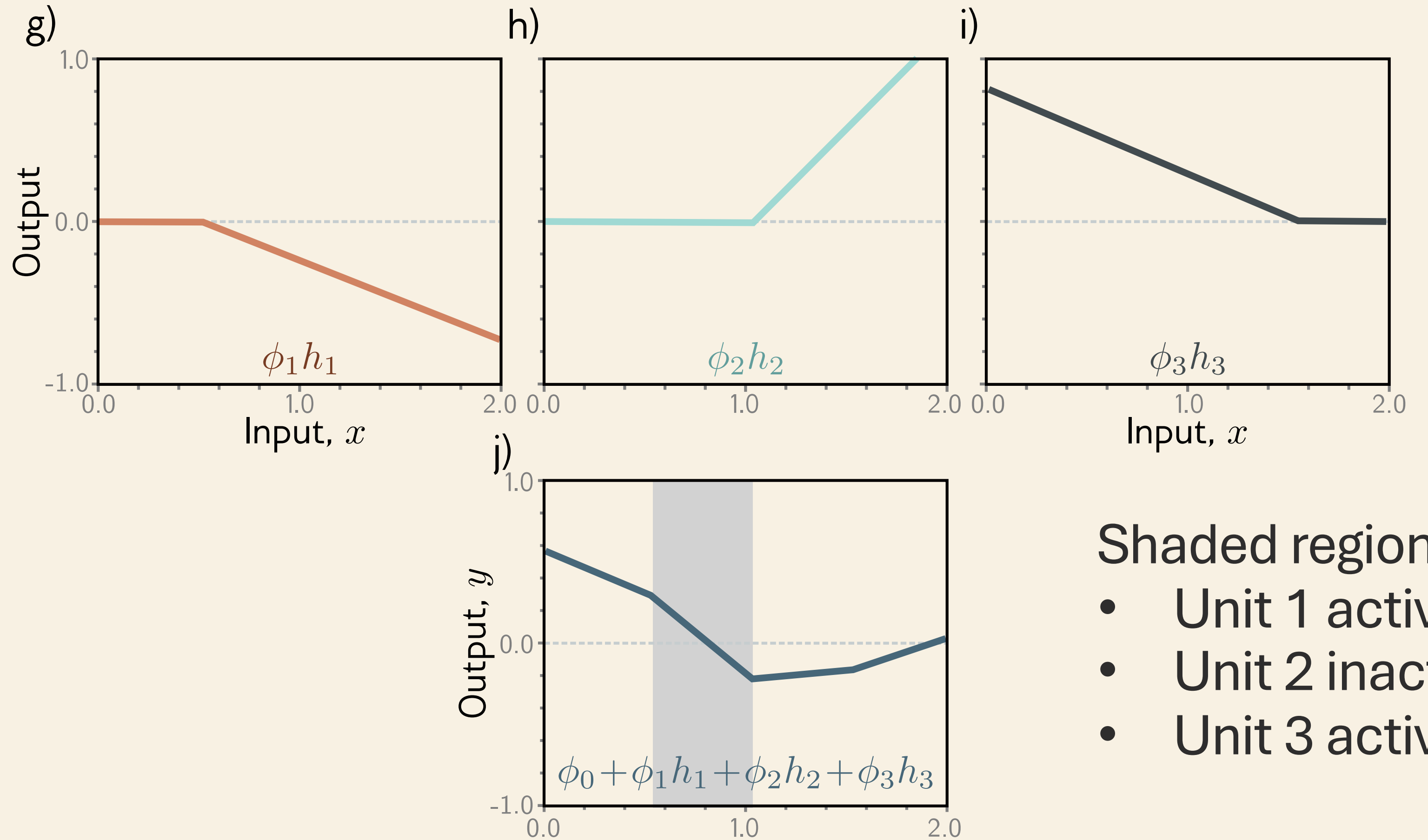
Example shallow network

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



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

Activation pattern = which hidden units are activated



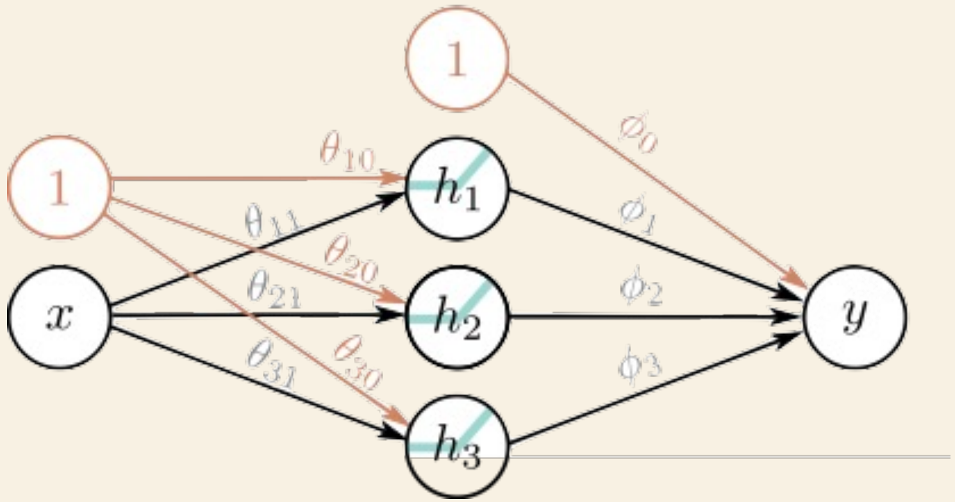
Shaded region:

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

Depicting neural networks

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

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



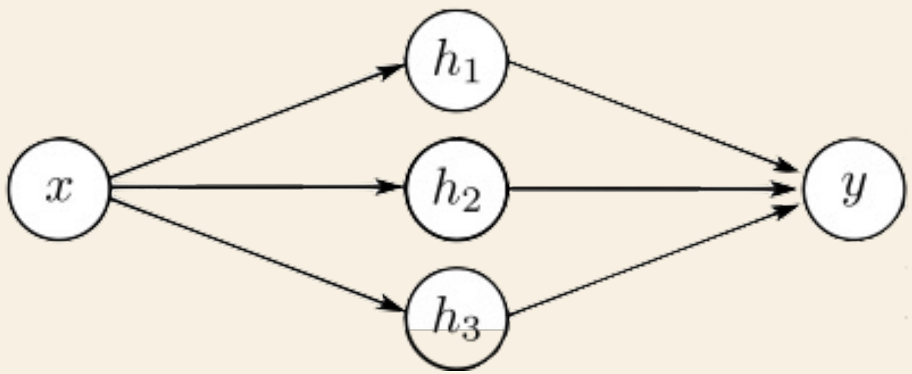
Each parameter multiplies its source and adds to its target

Depicting neural networks

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

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

b)



With 3 hidden units:

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

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

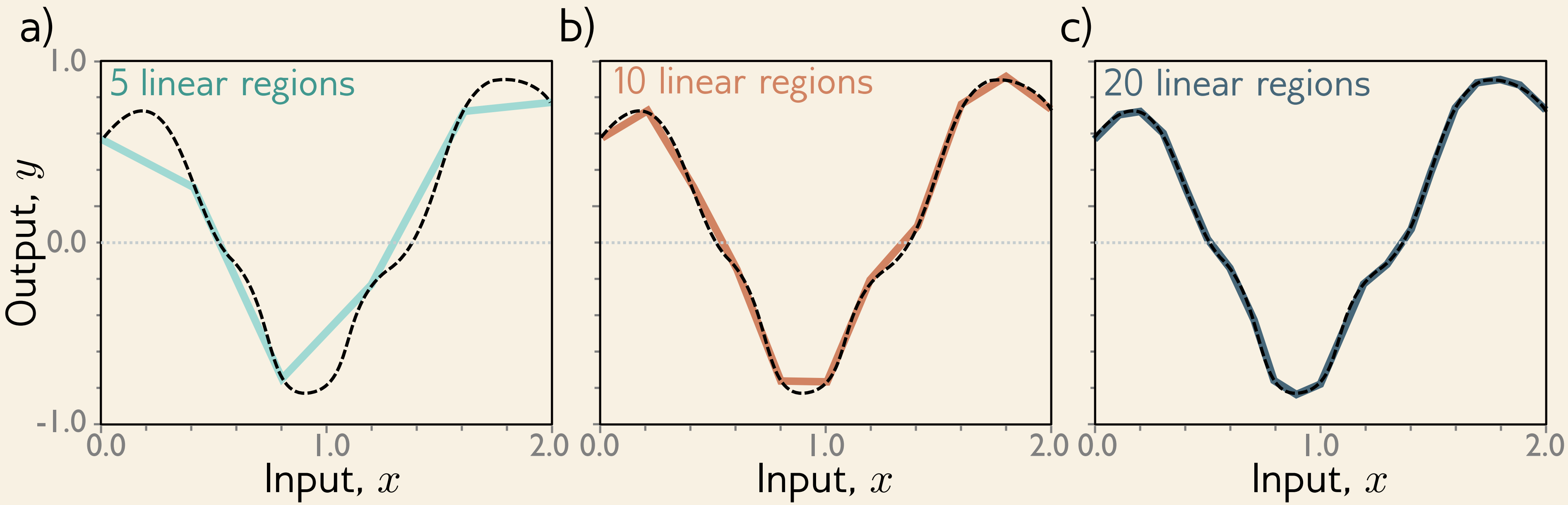
With D hidden units:

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

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

With enough hidden units…

… we can describe any 1D function to arbitrary accuracy



Universal approximation theorem

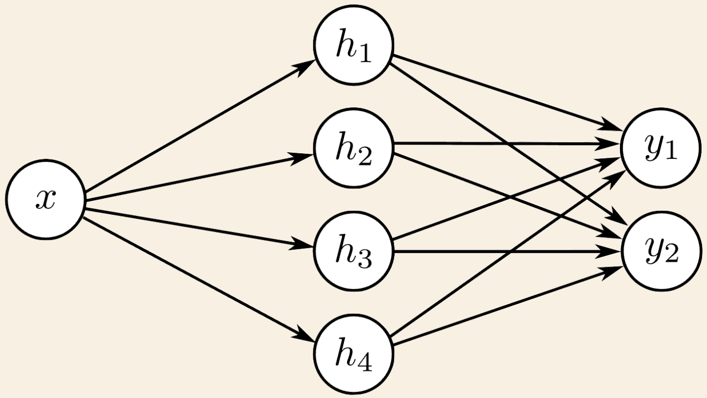
“a formal proof that, with enough hidden units, a shallow neural network can describe any continuous function on a compact subset of $\mathbb{R}^D$ to arbitrary precision”

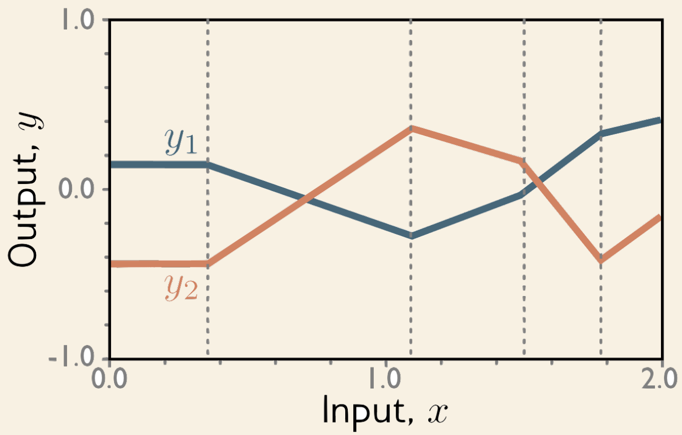
Two outputs

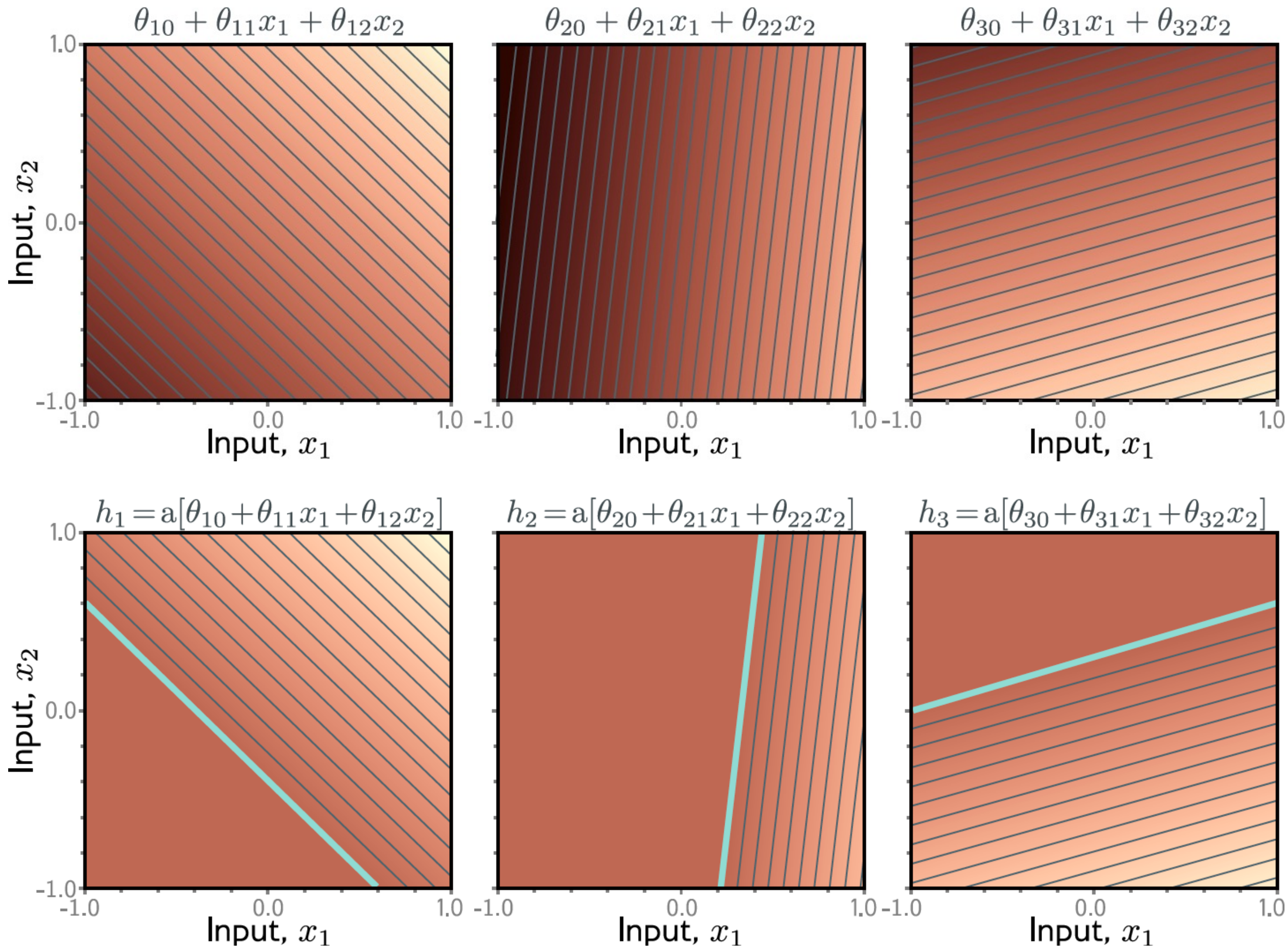
- 1 input, 4 hidden units, 2 outputs

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

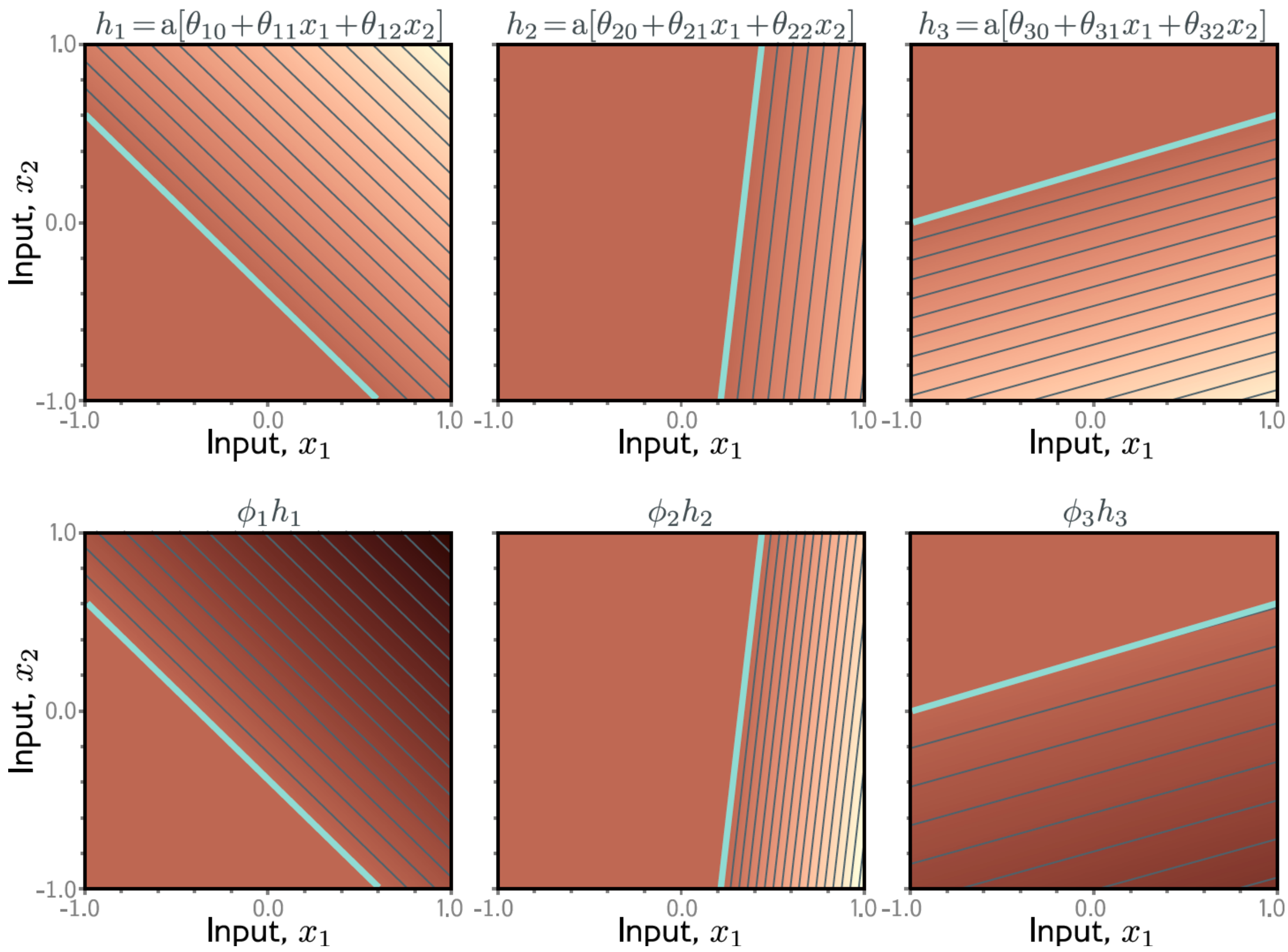
$$
\begin{aligned}
y_1 &= \phi_{10} + \phi_{11}h_1 + \phi_{12}h_2 + \phi_{13}h_3 + \phi_{14}h_4 \\
y_2 &= \phi_{20} + \phi_{21}h_1 + \phi_{22}h_2 + \phi_{23}h_3 + \phi_{24}h_4
\end{aligned}
$$



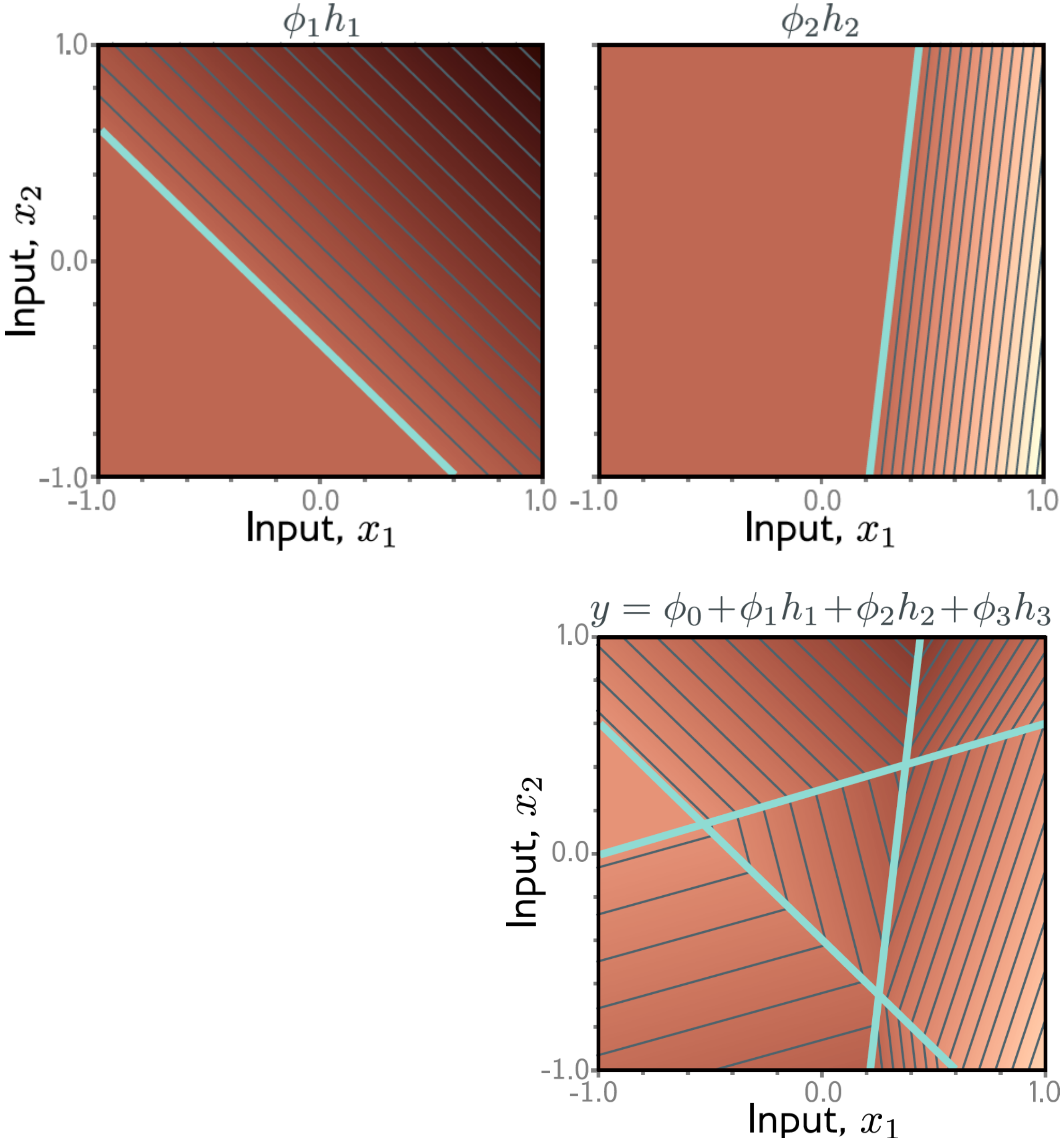




$\theta_{10} + \theta_{11}x_1 + \theta_{12}x_2$
$\theta_{20} + \theta_{21}x_1 + \theta_{22}x_2$
$\theta_{30} + \theta_{31}x_1 + \theta_{32}x_2$
$h_1 = \mathrm{a}[\theta_{10}+\theta_{11}x_1+\theta_{12}x_2]$
$h_2 = \mathrm{a}[\theta_{20}+\theta_{21}x_1+\theta_{22}x_2]$
$h_3 = \mathrm{a}[\theta_{30}+\theta_{31}x_1+\theta_{32}x_2]$
Input, x_1
Input, x_2
1.0
0.0
-1.0

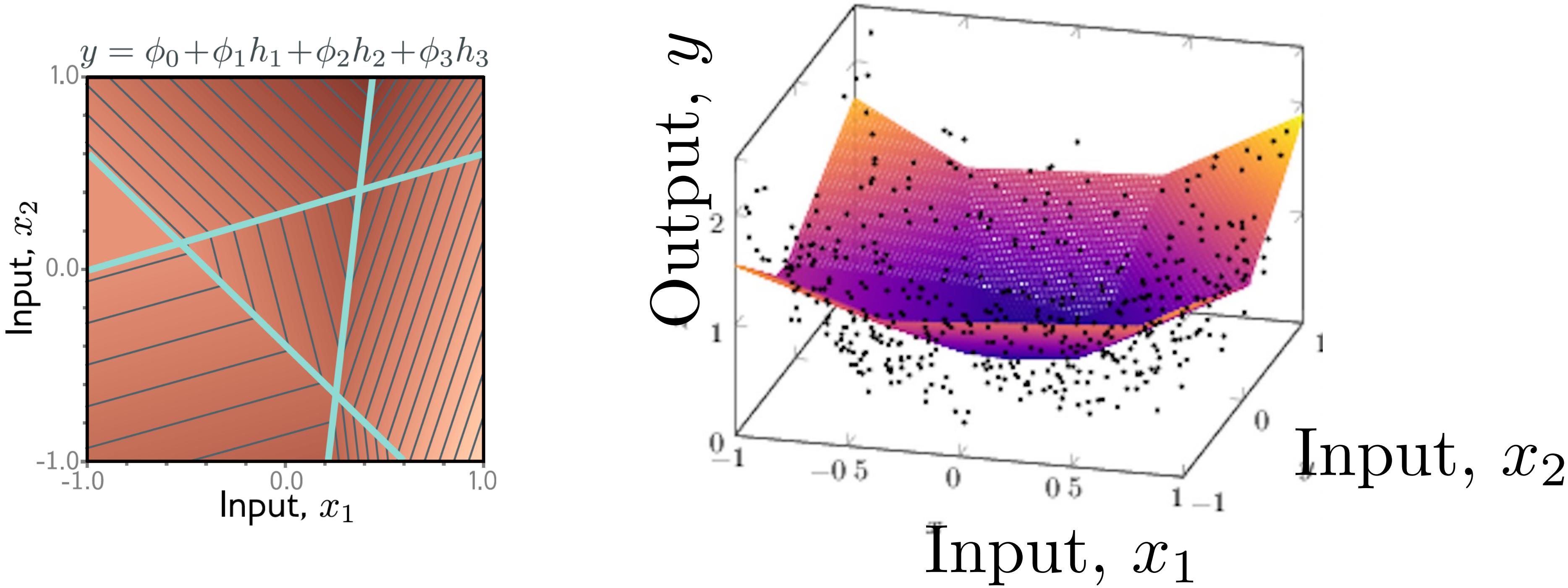


$h_1 = \mathrm{a}[\theta_{10} + \theta_{11}x_1 + \theta_{12}x_2]$
$h_2 = \mathrm{a}[\theta_{20} + \theta_{21}x_1 + \theta_{22}x_2]$
$h_3 = \mathrm{a}[\theta_{30} + \theta_{31}x_1 + \theta_{32}x_2]$
$\phi_1 h_1$
$\phi_2 h_2$
$\phi_3 h_3$
Input, x_1
Input, x_2
-1.0
0.0
1.0



Convex polygons

Fitting



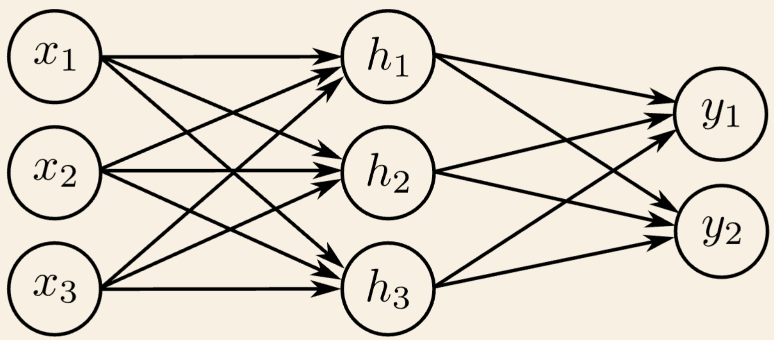
$y = \phi_0 + \phi_1 h_1 + \phi_2 h_2 + \phi_3 h_3$
1.0
0.0
-1.0
Input, x_2
-1.0
0.0
1.0
Input, x_1
Output, y
0
1
2
−1
−0.5
0
0.5
1
−1
0
1
Input, x_2
Input, x_1

Arbitrary inputs, hidden units, outputs

- D_o Outputs, *D* hidden units, and D_i inputs

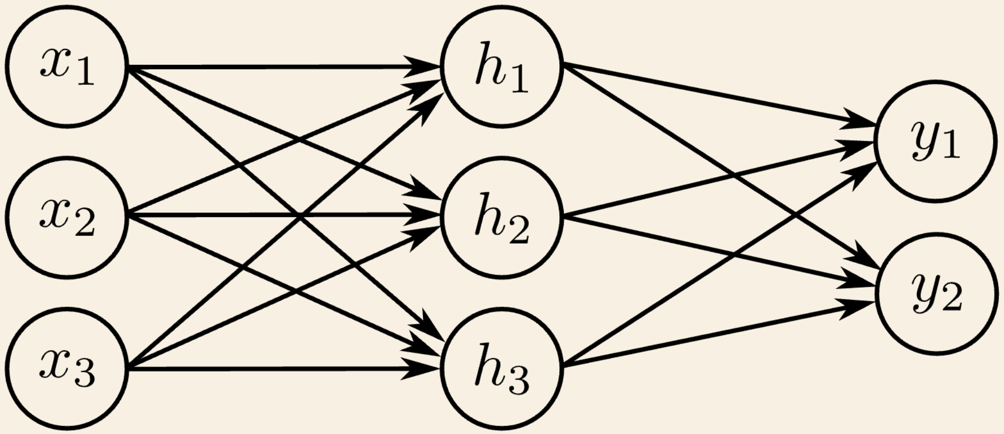
$$h_d = \mathrm{a}\left[\theta_{d0} + \sum_{i=1}^{D_i} \theta_{di} x_i\right] \qquad y_j = \phi_{j0} + \sum_{d=1}^{D} \phi_{jd} h_d$$

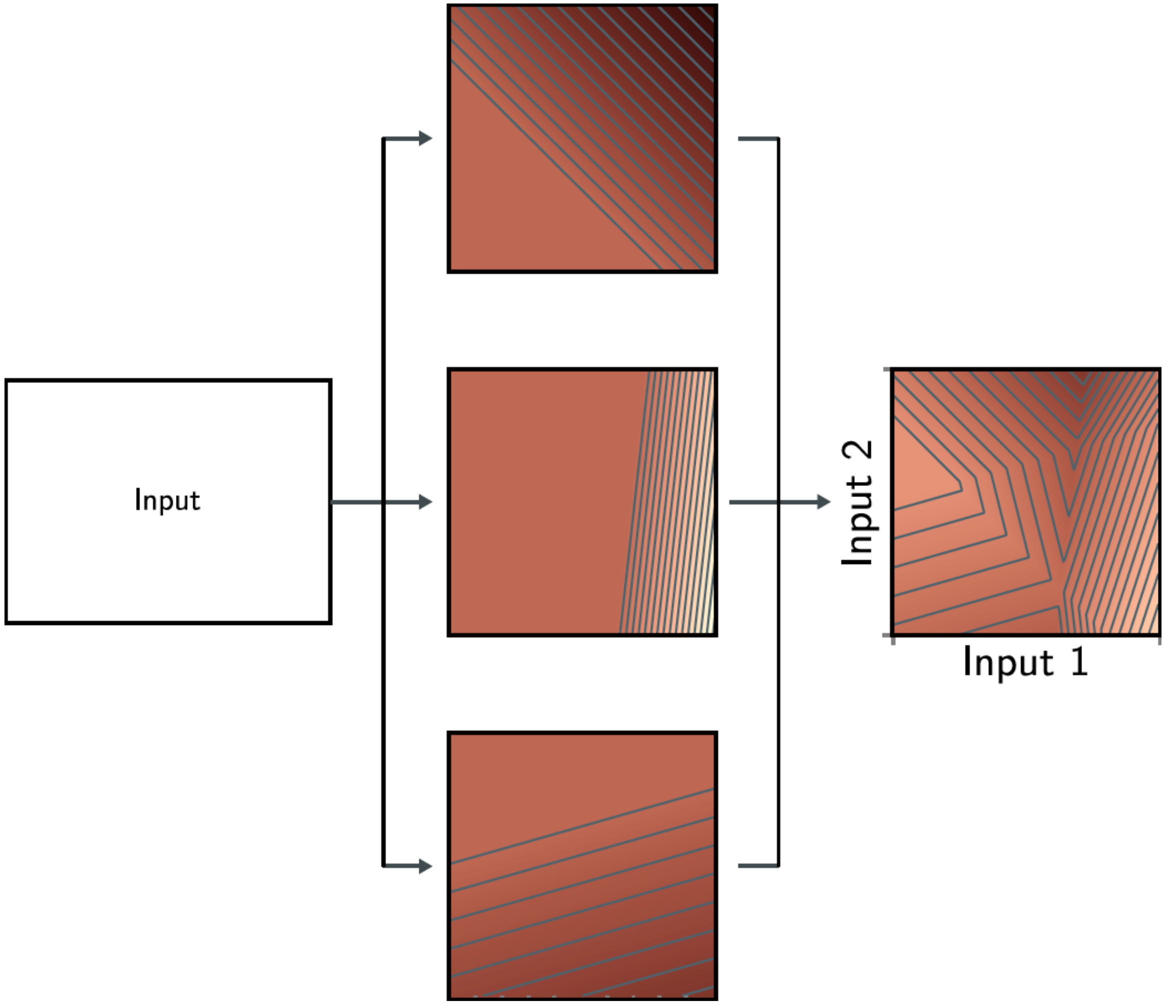
- e.g., Three inputs, three hidden units, two outputs

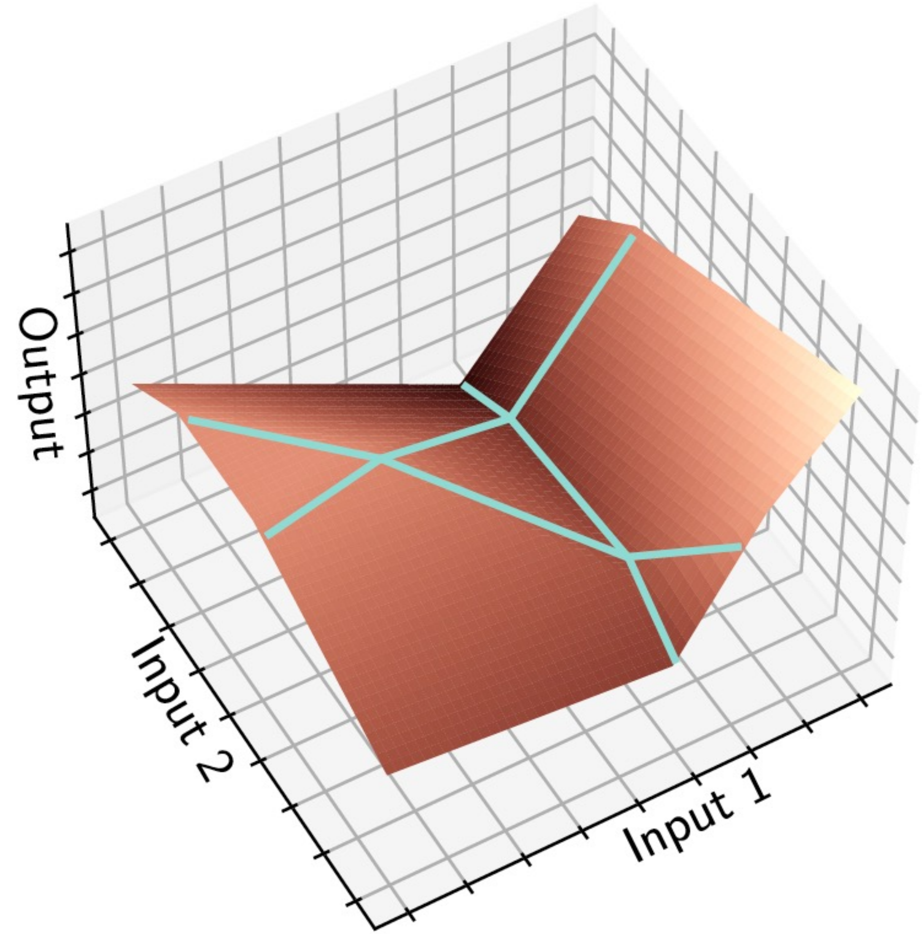


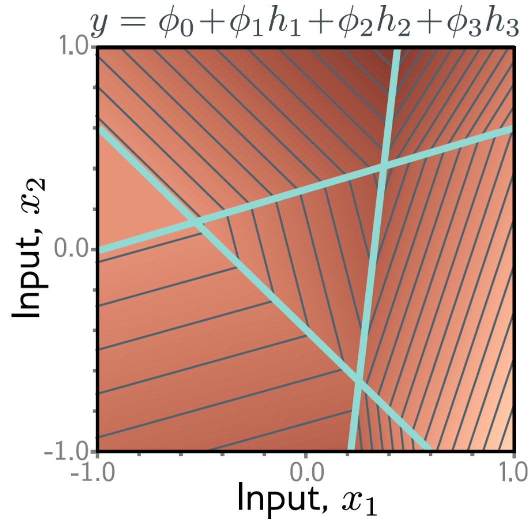
Question:

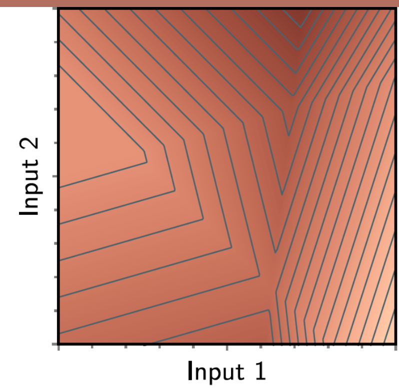
- How many parameters does this model have?

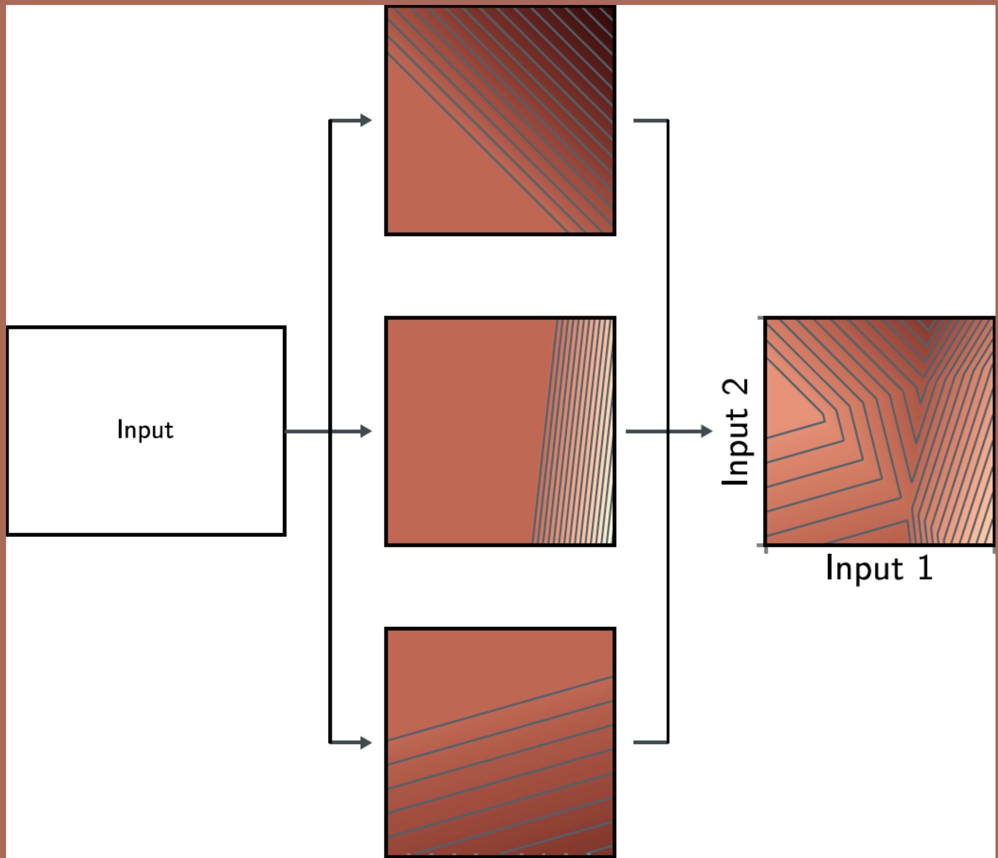


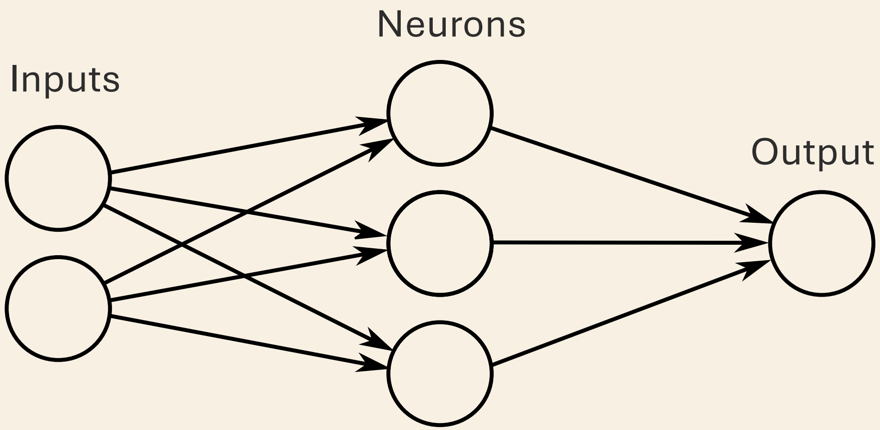

Input
Input 2
Input 1


Output
Input 2
Input 1


$y = \phi_0 + \phi_1 h_1 + \phi_2 h_2 + \phi_3 h_3$
1.0
0.0
-1.0
-1.0
0.0
1.0
Input, x_2
Input, x_1


Input 2
Input 1

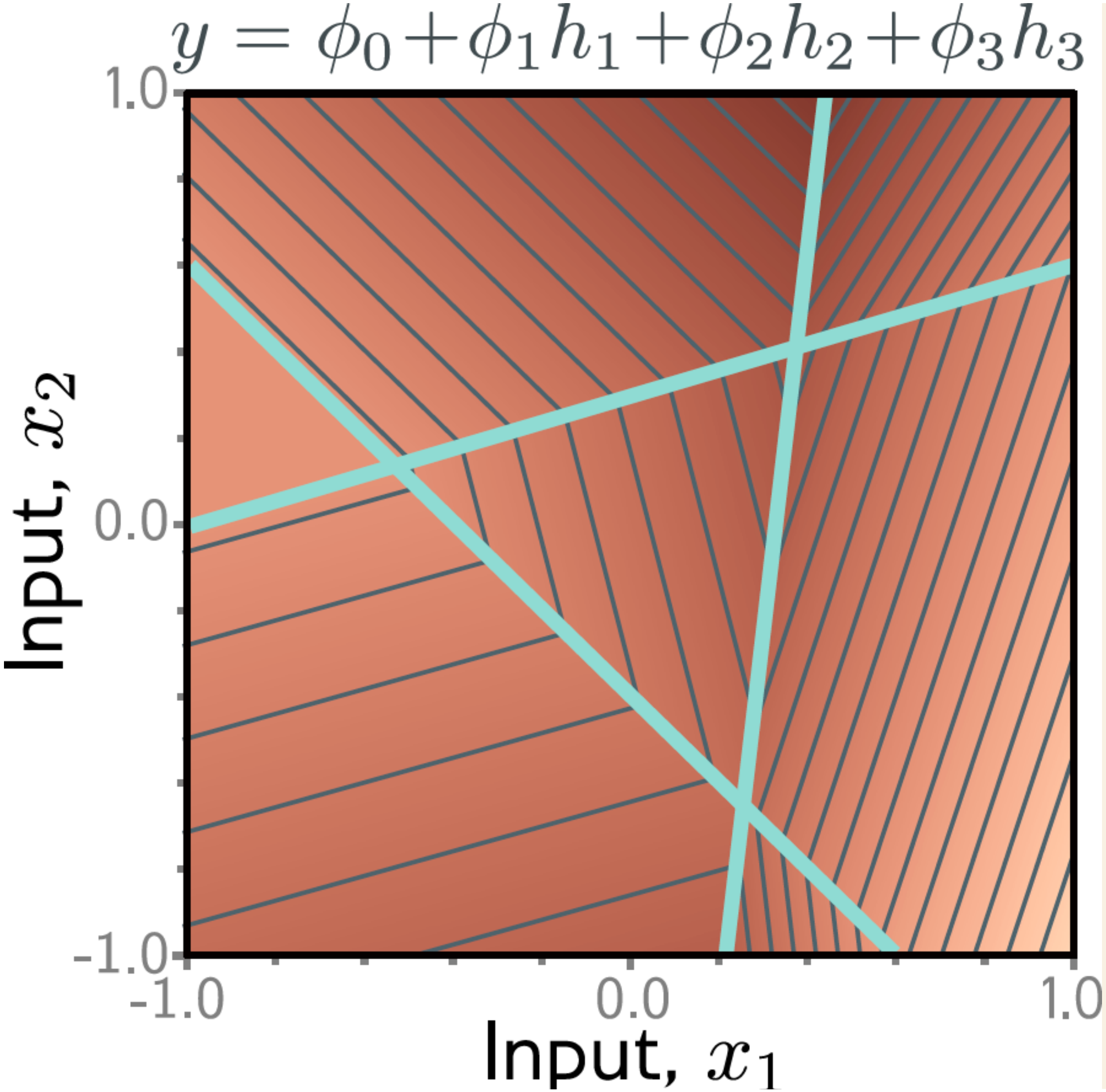




"neural network"

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

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

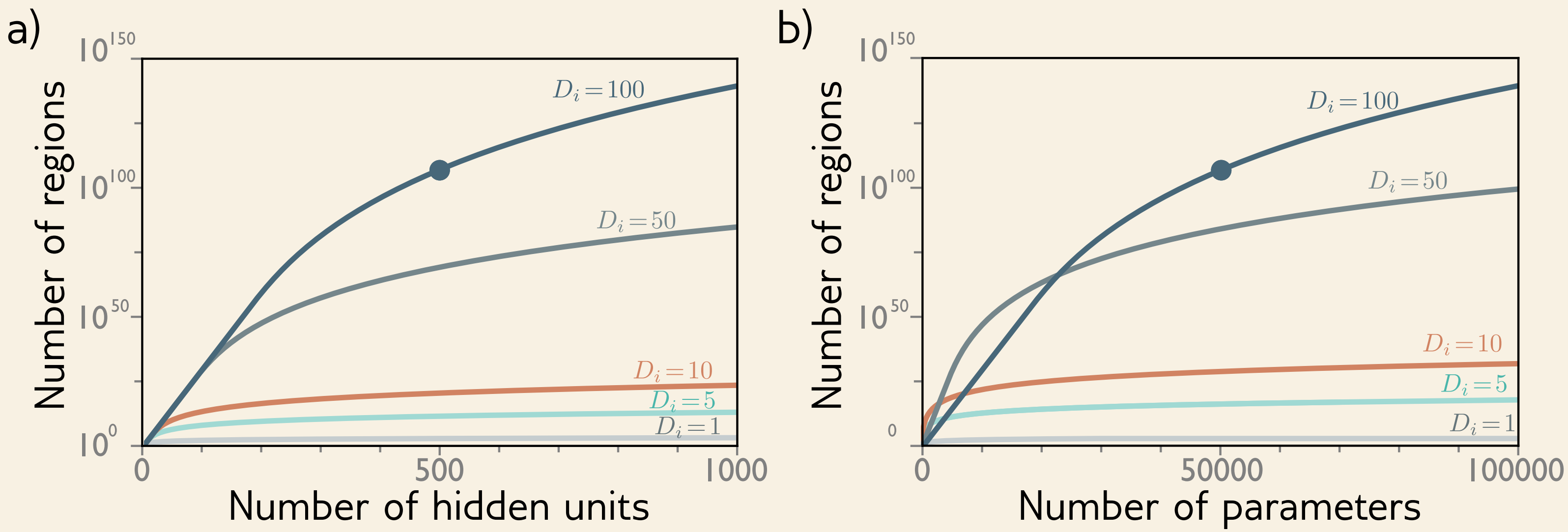


Number of output regions

- In general, each output consists of D dimensional convex polytopes
- With two inputs, and three outputs, we saw there were seven polygons.

Number of output regions

In general, each output consists of D dimensional convex polytopes



Highlighted point = 500 hidden units or 51,001 parameters

Number of regions:

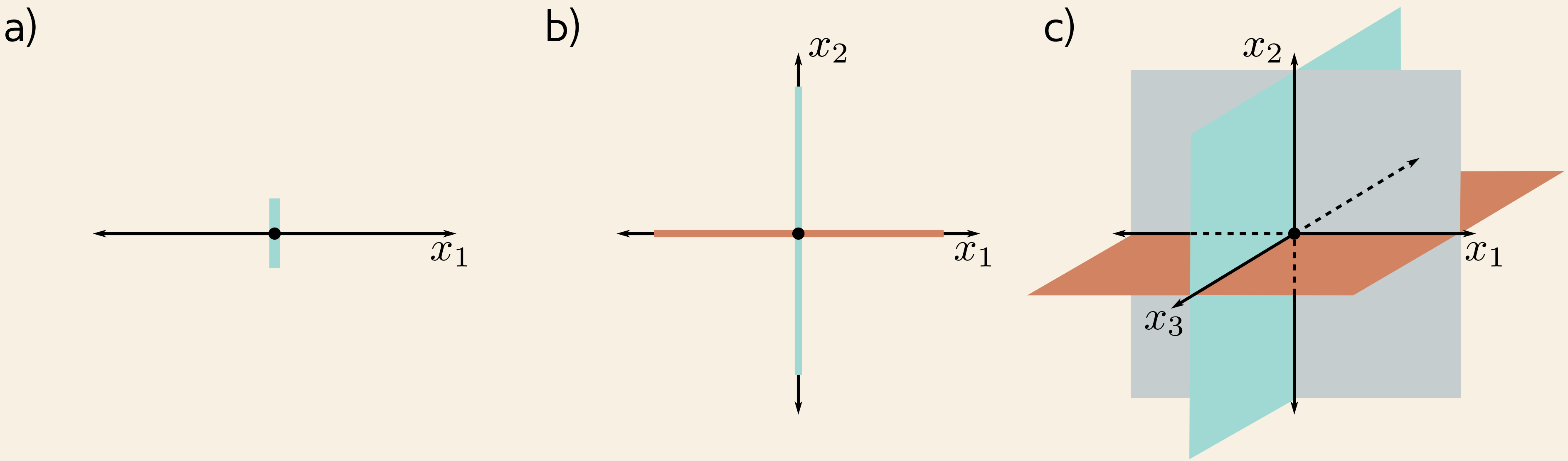
- Number of regions created by $D > D_i$ planes in D_i dimensions was proved by Zaslavsky (1975) to be:

$$\sum_{j=0}^{D_i} \binom{D}{j}$$

Binomial coefficients!

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

Proof that more regions than 2^{Di}

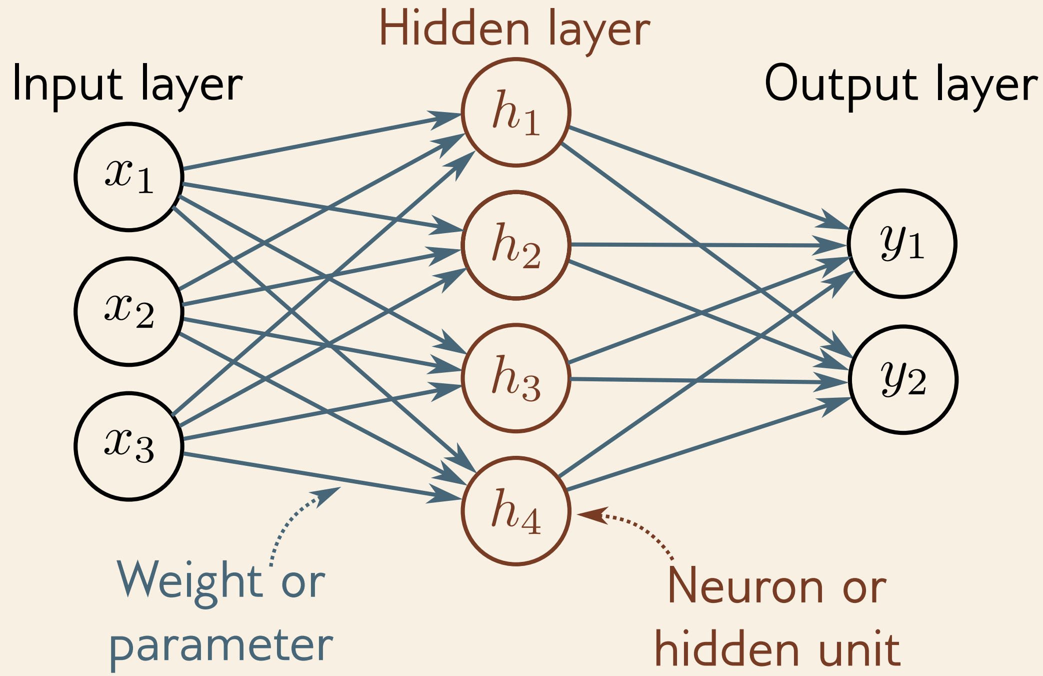


1D input with 1 hidden unit creates two regions (one joint)

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

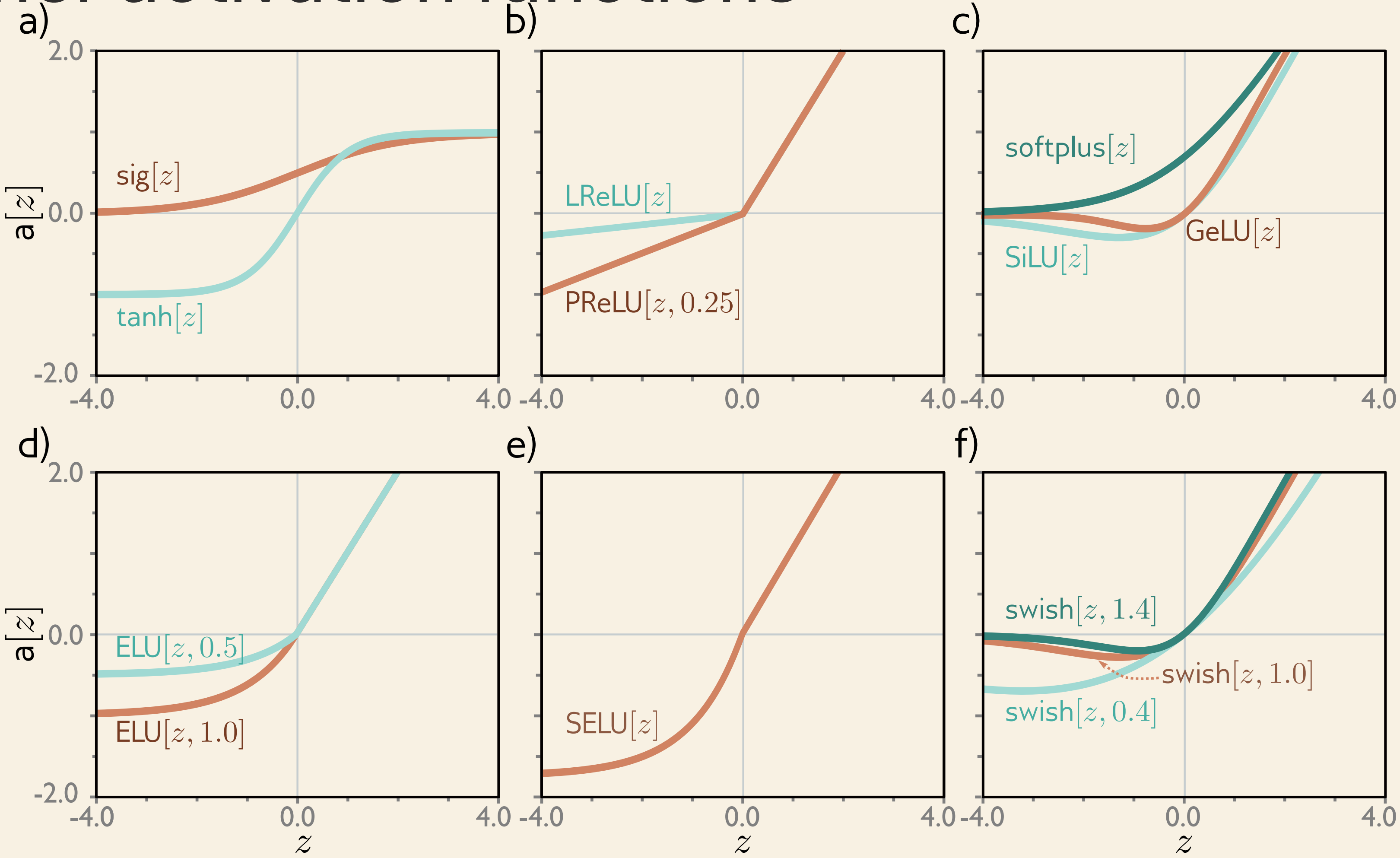
3D input with 3 hidden units creates eight regions (three planes)

Nomenclature



- Y-offsets = biases
- Slopes = weights
- Everything in one layer connected to everything in the next = fully connected network
- 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



A Simple Neural Network for Binary Classification

We’ll explore a minimal neural network that predicts whether an input belongs to **class 0 or 1**

Data

- (X, y): dataset and corresponding labels $X \in \mathbb{R}^{N\times 2}, \quad y \in \{01\}^{N},$

Model

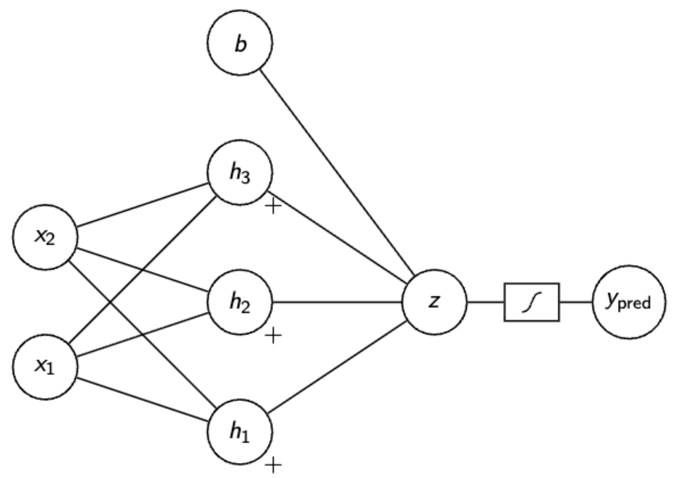
- $f_\theta(x): \mathbb{R}^2 \to [0, 1]$ outputs the **probability** that x belongs to class 1
- θ: all **learnable parameters** (weights and biases)

Activation Functions

- **ReLU:** +(x) = max(0, x). **Sigmoid:** $\sigma(x) = \frac{1}{1+e^{-x}}$

Binary Cross-Entropy (BCE) Loss

- Average over all samples: $\mathcal{L}(p, y) = \frac{1}{N}\sum_{i=1}^{N} \ell_i\,(p_i, y_i)$



$$f_\theta(\mathbf{x}) = \sigma\big(\underbrace{\max(0, \mathbf{x}\mathbf{w}_1)\mathbf{w}_2 + b}_{\mathbf{z}}\big)$$

Computing Gradients

We want to calculate the **gradient of the Binary Cross-Entropy (BCE) loss** with respect to the network parameters w_1, w_2,and b.

- **Binary Cross-Entropy Loss**
- $\mathcal{L} = \frac{1}{N}\sum_{i=1}^{N} \ell_i \, \mathrm{f(x)}$
- Where our objective:
- $\nabla_{w_1,w_2,b} \, \mathcal{L}(f_{\theta}, (X) y)$

Chain Rule

Output layer

$$\frac{\partial \ell}{\partial w_2} = \frac{\partial \ell}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial z} \cdot \frac{\partial z}{\partial w_2}. \qquad \frac{\partial \ell}{\partial b} = \frac{\partial \ell}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial z} \cdot \frac{\partial z}{\partial b}$$

Hidden Layer

$$\frac{\partial \ell}{\partial w_1} = \frac{\partial \ell}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial z} \cdot \frac{\partial z}{\partial h} \cdot \frac{\partial h}{\partial (x w_1)} \cdot \frac{\partial (x w_1)}{\partial w_1}$$

Where $h=\max(0,xw_1)$

Gradient of the Loss w.r.t. Predictions

The gradient of the scalar loss with respect to the prediction vector is itself a **vector**:

$$\frac{\partial \ell}{\partial \hat{y}} = \begin{bmatrix} \frac{\partial \ell}{\partial \hat{y}_1} \\ \frac{\partial \ell}{\partial \hat{y}_2} \\ \vdots \\ \frac{\partial \ell}{\partial \hat{y}_N} \end{bmatrix}^{\mathrm{T}} = \frac{\hat{y} - y}{\hat{y}(1 - \hat{y})}$$

Each component measures how the loss changes when a single prediction $\hat{y}_i$ changes.

Derivative of Predictions w.r.t. Pre-Activations

Both $\hat{y}$ and z are vectors of size N. Since the output activation is applied **element-wise**: $\hat{y} = \sigma(z)$ then the derivative is also **element-wise**:

$$\frac{\partial \hat{y}}{\partial z} = \sigma(z)\big(1 - \sigma(z)\big) = \hat{y}(1 - \hat{y})$$

Computing $\frac{\partial z}{\partial h}$ and $\frac{\partial \mathrm{h}}{\partial \mathrm{w}_2}$

$z = hw_2 + b$, in matrix form $\begin{bmatrix} z_1 \\ \vdots \\ z_N \end{bmatrix} = \begin{bmatrix} h_{11} & h_{12} & h_{13} \\ \vdots & \vdots & \vdots \\ h_{N1} & h_{N2} & h_{N3} \end{bmatrix} \begin{bmatrix} w_{2,1} \\ w_{2,2} \\ w_{2,3} \end{bmatrix} + b$

where $h \in \mathbb{R}^{N\times 3}$, $w_2 \in \mathbb{R}^{3\times 1}$, and $b \in \mathbb{R}$(broadcasted over all Nsamples).

The gradient of z with respect to a single weight $w_{2,j}$ depends on **all samples**:

$$\frac{\partial z}{\partial w_{2,j}} = \begin{bmatrix} h_{1j} \\ h_{2j} \\ \vdots \\ h_{Nj} \end{bmatrix}.$$

Gradient with respect to the Bias b

In the equation $z = hw_2 + b$, the bias term b is **broadcasted** across all N samples. We can make this explicit as:

$$z = hw_2 + \mathbf{1}^\top b,$$

where $\mathbf{1} \in \mathbb{R}^N$ is a vector of ones.

Derivative $\frac{\partial z}{\partial b} = \mathbf{1}^\top$

Computing $\frac{\partial z}{\partial h}$

$z = hw_2 + b$, in matrix form $\begin{bmatrix} z_1 \\ \vdots \\ z_N \end{bmatrix} = \begin{bmatrix} h_{11} & h_{12} & h_{13} \\ \vdots & \vdots & \vdots \\ h_{N1} & h_{N2} & h_{N3} \end{bmatrix} \begin{bmatrix} w_{2,1} \\ w_{2,2} \\ w_{2,3} \end{bmatrix} + b$

where $h \in \mathbb{R}^{N\times 3}$, $w_2 \in \mathbb{R}^{3\times 1}$, and $b \in \mathbb{R}$ (broadcasted over all N samples).

For each sample i: $z_i = h_{i1}w_{2,1} + h_{i2}w_{2,2} + h_{i3}w_{2,3}$.

The gradient of z_i with respect to the row vector h_i is: $\frac{\partial z_i}{\partial h_i} = w_2^\top$.

Computing the Gradient with respect to w_1

To compute $\frac{\partial \mathcal{L}}{\partial w_1}$, we need two components: $\frac{\partial h}{\partial (xw_1)}$ *and* $\frac{\partial (xw_1)}{\partial w_1}$.

For the ReLU function $h = ReLU(xw_1)$, the derivative is given by:

$$\frac{\partial h_{ij}}{\partial \left(xw_1\right)_{ij}} = \begin{cases} 1, & if \left(x \cdot w_1\right)_{ij} > 0 \\ 0, & otherwise. \end{cases}$$ or equivalently $\frac{\partial h}{\partial (xw_1)} = \mathbf{1}_{xw_1>0}$,

a binary mask that passes gradients only where activations are positive.

Derivative of the linear transformation

The forward pass is: $h = xw_1$ where:

$$x = \begin{bmatrix} x_{11} & x_{12} \\ \vdots & \vdots \\ x_{N1} & x_{N2} \end{bmatrix}, w_1 = \begin{bmatrix} w_{1,11} & w_{1,12} & w_{1,13} \\ w_{1,21} & w_{1,22} & w_{1,23} \end{bmatrix}.$$

Thus, the gradient of xw_1 with respect to w_1 depends directly on the input matrix x:

$$\frac{\partial(xw_1)}{\partial w_1} = x.$$

Each **column** of w_1 interacts with **all input features**, since every output dimension receives contributions from all columns of x.

Solution

$$\frac{\partial \mathcal{L}}{\partial w_2} = \frac{\partial \mathcal{L}}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial z} \cdot \frac{\partial z}{\partial w_2} = \frac{\hat{y} - y}{\hat{y}(1 - \hat{y})} \cdot \big(\hat{y}(1 - \hat{y})\big) \cdot (h)$$

$$\frac{\partial \mathcal{L}}{\partial b} = \frac{\partial \mathcal{L}}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial z} \cdot \frac{\partial z}{\partial b} = \frac{\hat{y} - y}{\hat{y}(1 - \hat{y})} \cdot \big(\hat{y}(1 - \hat{y})\big) \cdot (1^T)$$

$$\frac{\partial \mathcal{L}}{\partial w_1} = \frac{\partial \mathcal{L}}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial z} \cdot \frac{\partial z}{\partial h} \cdot \frac{\partial h}{\partial (x w_1)} \cdot \frac{\partial (x w_1)}{\partial w_1}$$
$$= \frac{\hat{y} - y}{\hat{y}(1 - \hat{y})} \cdot \big(\hat{y}(1 - \hat{y})\big) \cdot (w_2^{\mathsf{T}}) \cdot \big(1_{x w_1 > 0}\big) \cdot (x)$$

Slides from Understanding deep learning S. Prince Chapter 3