COMPSCI 389
Introduction to Machine Learning

Days: Tu/Th. **Time:** 2:30 – 3:45 **Building:** Morrill 2 **Room:** 222

Topic 9.0: Neural Networks

Prof. Philip S. Thomas (pthomas@cs.umass.edu)

Linear Parametric Models (review)

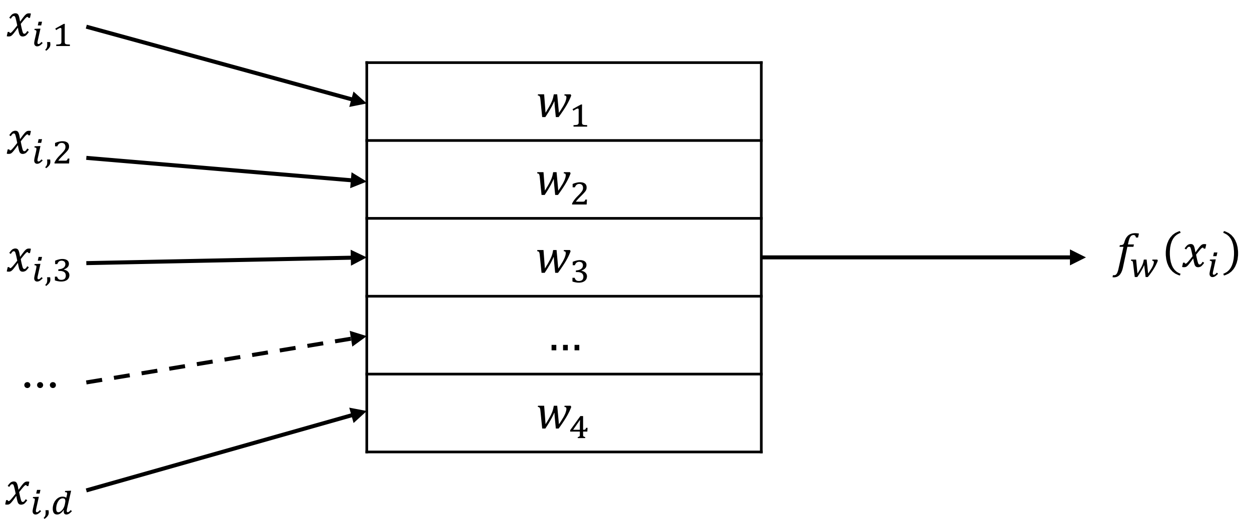
- Linear parametric models f_w are linear with respect to the weights, w, of the model.

$$f_w(x_i) = \sum_{j=1}^{m} w_j \phi_j(x_i)$$

Linear Model (Graphical Representation)

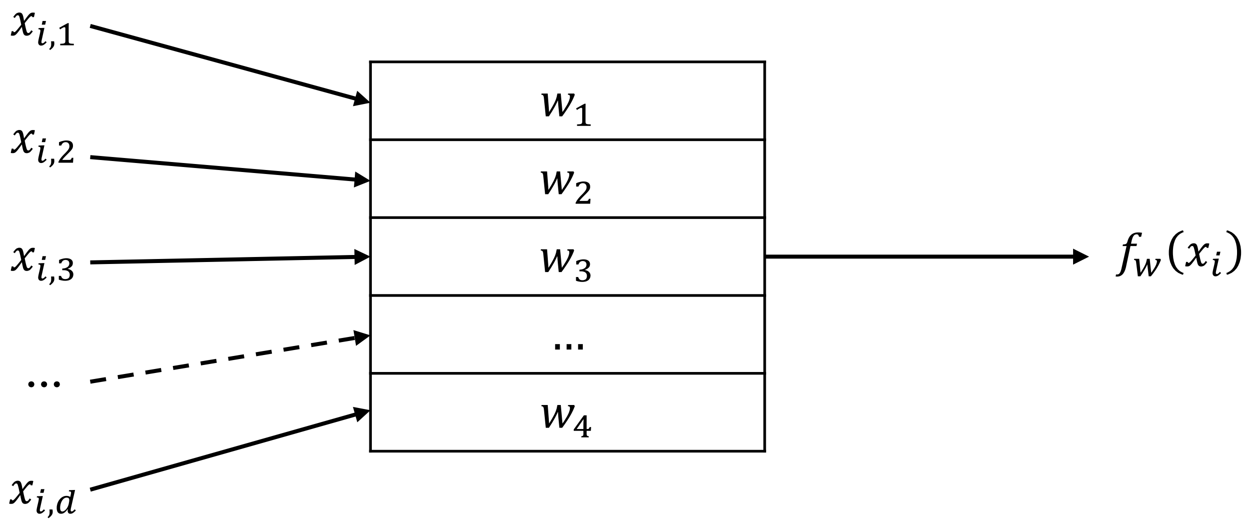
- Consider a linear parametric model **without a basis function** (feature generator, ϕ)

$$f_w(x_i) = \sum_{j=1}^{d} w_j x_{i,j}$$



Question: How can we make this model non-linear w.r.t. the model parameters (weights w)?

$$f_w(x_i) = \sum_{j=1}^{d} w_j x_{i,j}$$

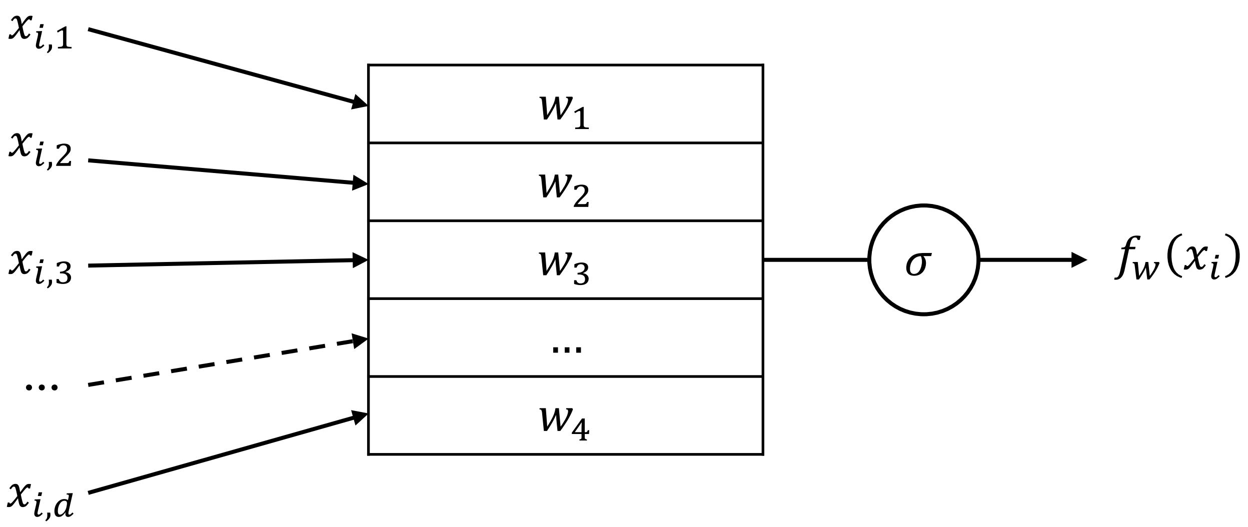


Answer: One way is to apply a non-linear function, σ, to the output.

Question: Would $\sigma(z) = 5z$ work?
Answer: No, this is a linear function. This would be equivalent to multiplying each weight by 5. It doesn't change the functions that can be represented.

Question: Would $\sigma(z) = z^2$ work?
Answer: Yes, this would result in a non-linear parametric model.

$$f_w(x_i) = \sigma\left(\sum_{j=1}^{d} w_j x_{i,j}\right) \qquad f_w(x_i) = \left(\sum_{j=1}^{d} w_j x_{i,j}\right)^2$$

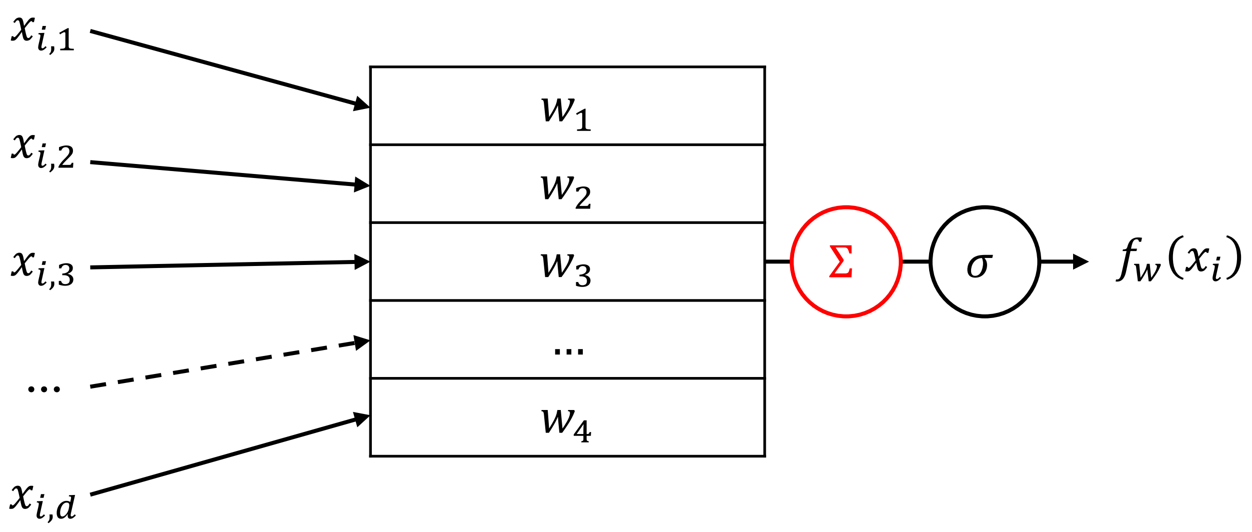


Note: The function σ is often called an **activation function, nonlinearity, threshold function**, or **squashing function**.

Note: This parametric model (with any nonlinear σ) is called a **perceptron**.

Alternative Perceptron Graphics

$$f_w(x_i) = \sigma\left(\sum_{j=1}^{d} w_j x_{i,j}\right)$$



Alternative Perceptron Graphics

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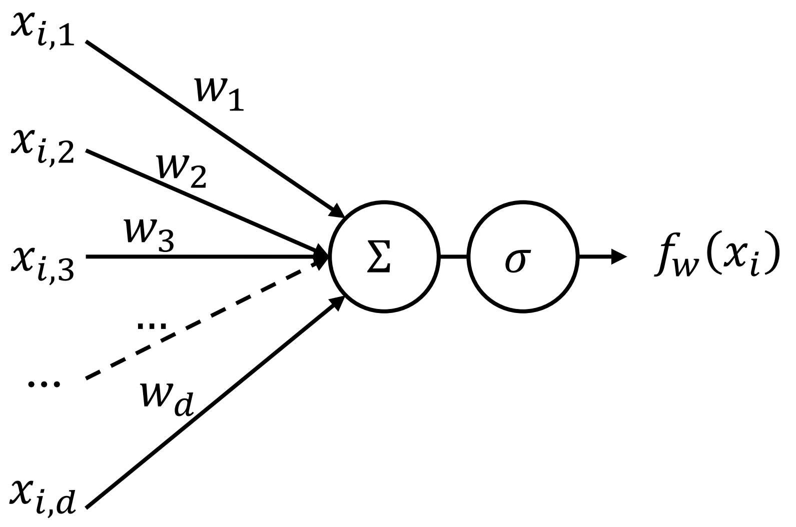

Alternative Perceptron Graphics

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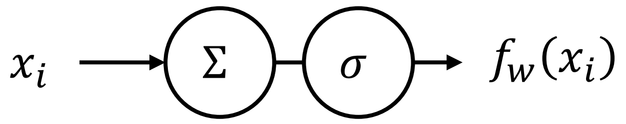
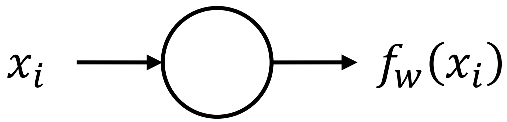


Alternative Perceptron Graphics

$$f_w(x_i) = \sigma\left(\sum_{j=1}^{d} w_j x_{i,j}\right)$$

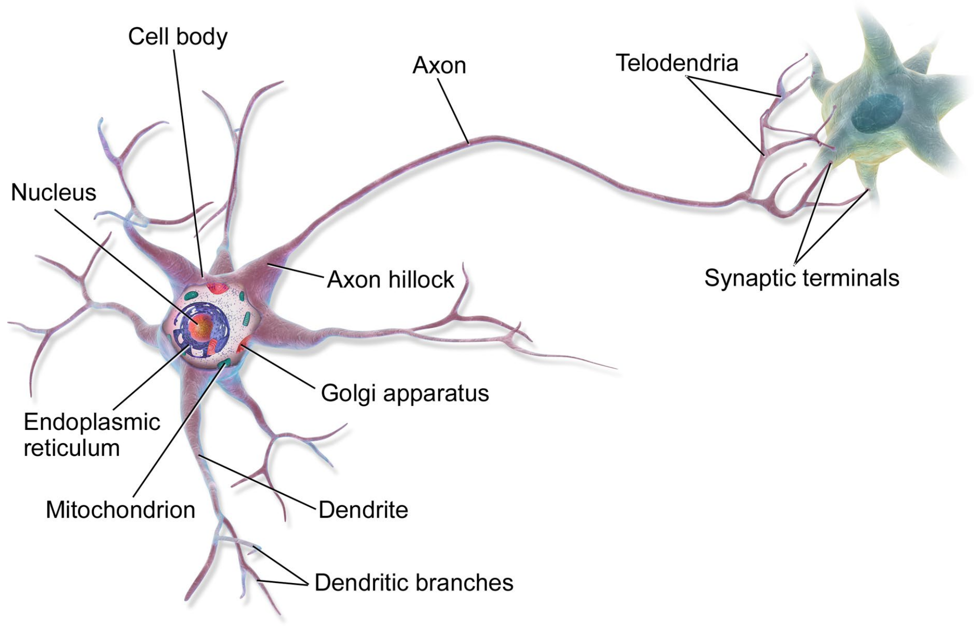


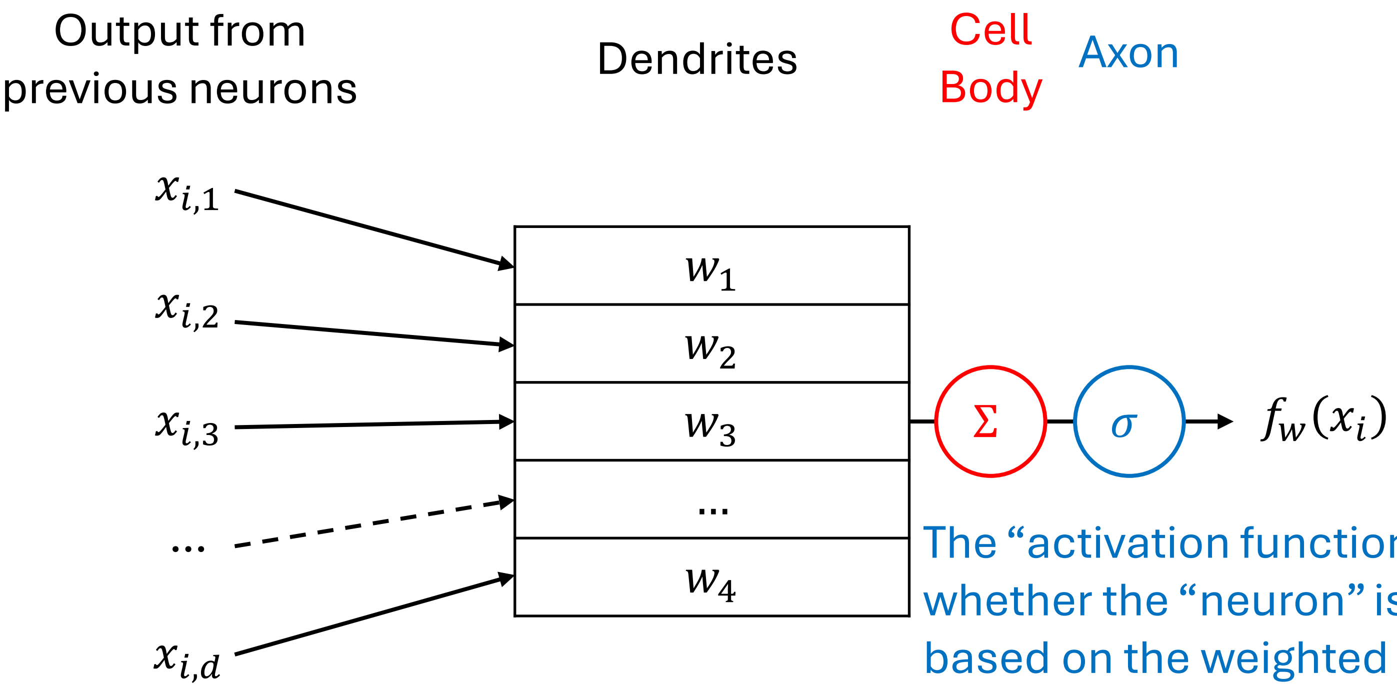
Note: This is most common when working with many perceptrons, connected together in some way.

Perceptron

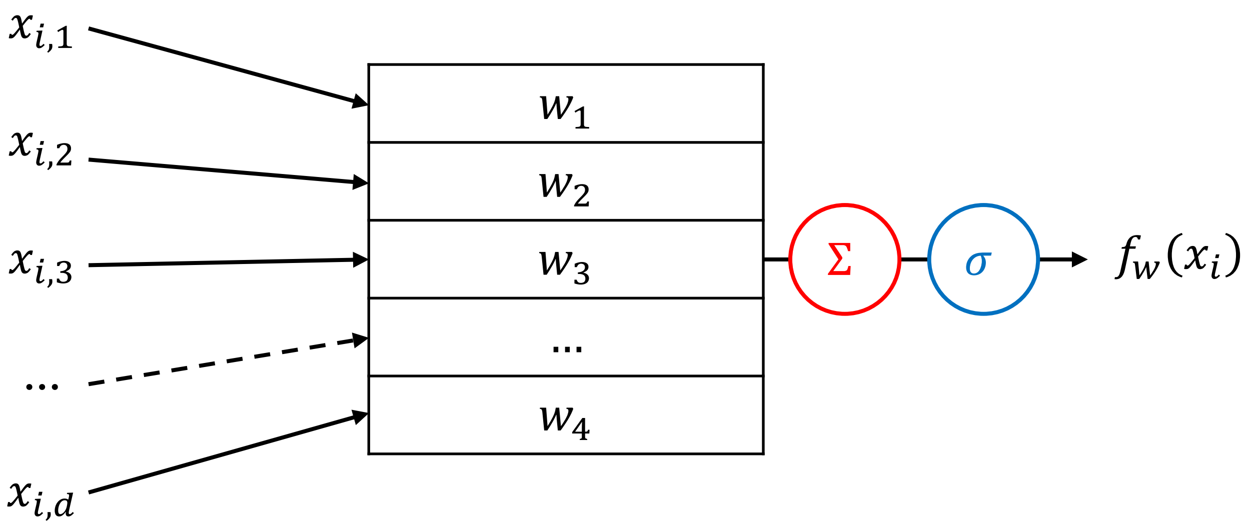
Perceptrons can be viewed as **extremely crude** simulations of neurons.

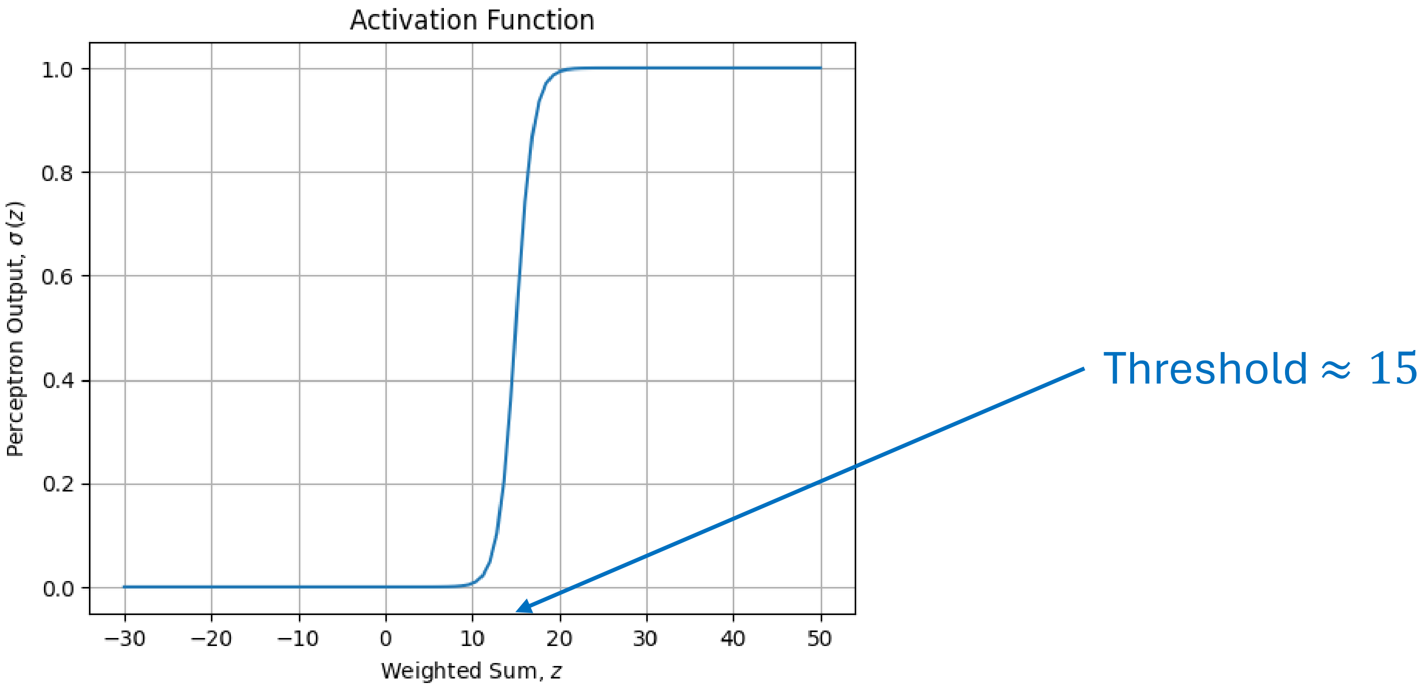
- Roughly speaking (ignoring important aspects of biology and neuroscience), when enough of the inputs to a neuron are activated, the neuron becomes sufficiently stimulated and "fires" (it becomes activated).
- We can select σ to be similar to a threshold function.
  - If the weighted sum is below some threshold for the neuron to be activated, σ outputs 0 (not firing).
  - If the weighted sum is above the threshold, σ outputs 1 (firing).





The "activation function" decides whether the "neuron" is firing based on the weighted sum.





Note: This model typically outputs 0 or 1, which may not be what we want for our parametric model. We will revisit this later.

Note: σ *squashes* the output to the range [0,1], hence the name *squashing function*.

Perceptron vs Neuron

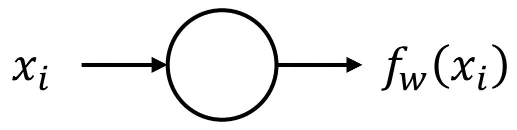
- Perceptrons are **extremely crude** models of real neurons.
- Real neurons do not switch between firing and not firing, but instead change the rate at which they fire.
  - More realistic parametric models of neurons are called “spiking neuron models”
- Real neurons don’t just compute a weighted sum of the inputs.
  - They consider the timing of different inputs arriving.
  - Complex calculations can result from dendritic morphology.
- Neurons experience fatigue.
  - Roughly speaking, when a neuron fires at a high rate for too long, chemical changes force it to fire less frequently.
- And much, much more…

Training Non-Linear Parametric Models

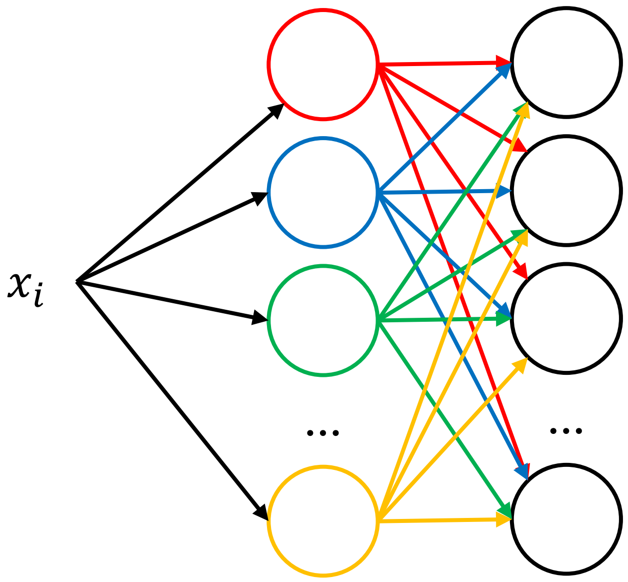
- We train non-linear parametric models using **gradient descent**!
- Later we will discuss how the necessary derivatives can be computed.

Neural Networks: Parametric Models Comprised of Many Perceptrons

- Recall the graphical representation:

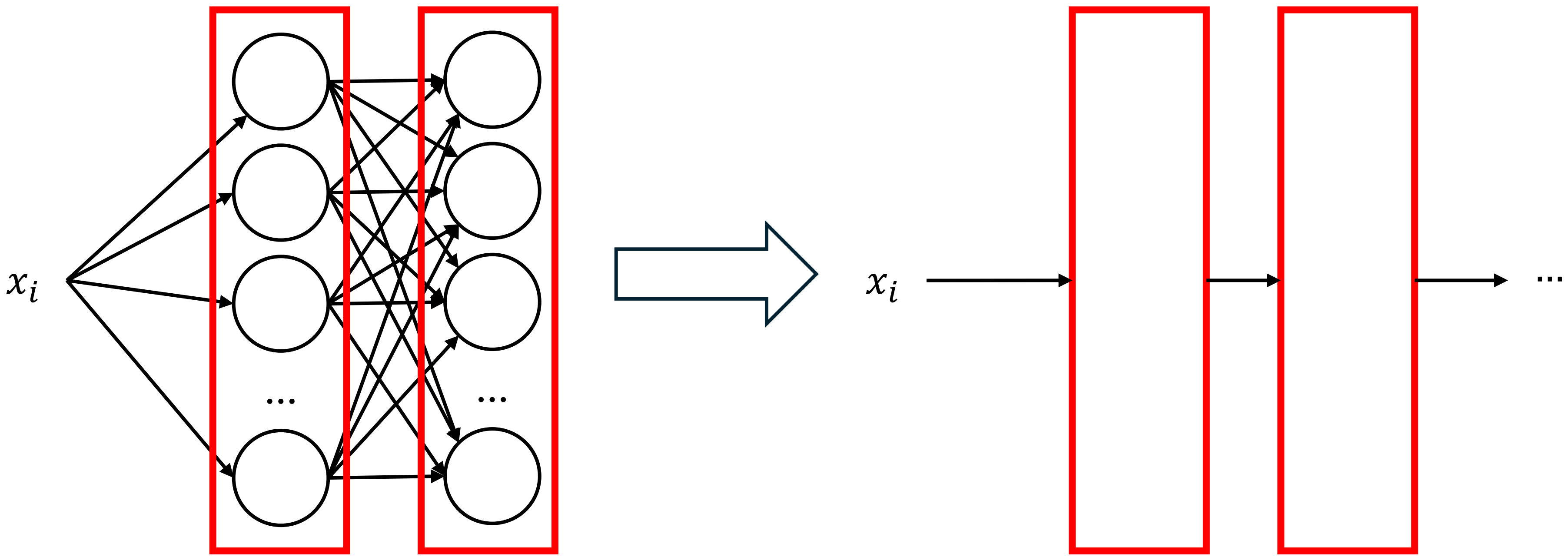


- **Idea**: Connect many perceptrons together.



This is tedious and
too many arrows!

Neural Network Graphical Depiction

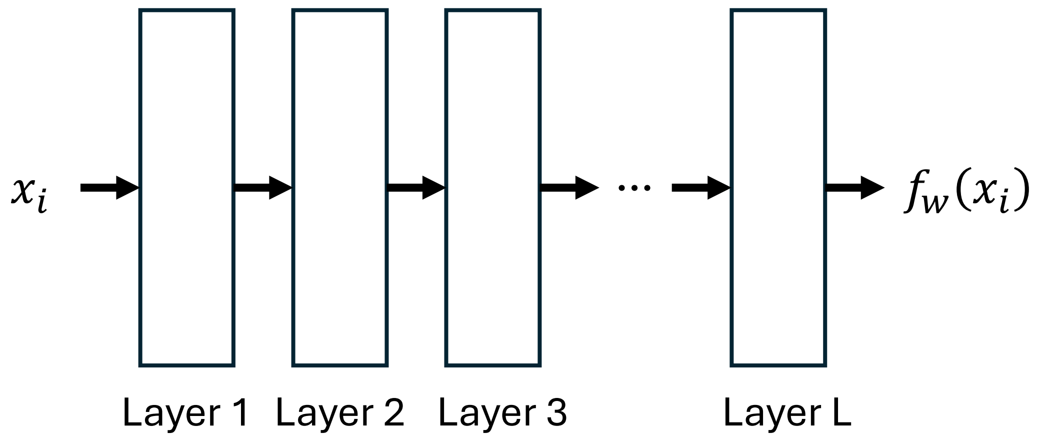


Idea: Use boxes to represent **layers** (columns) of perceptrons.

Here arrows between boxes denote **fully connected layers**.

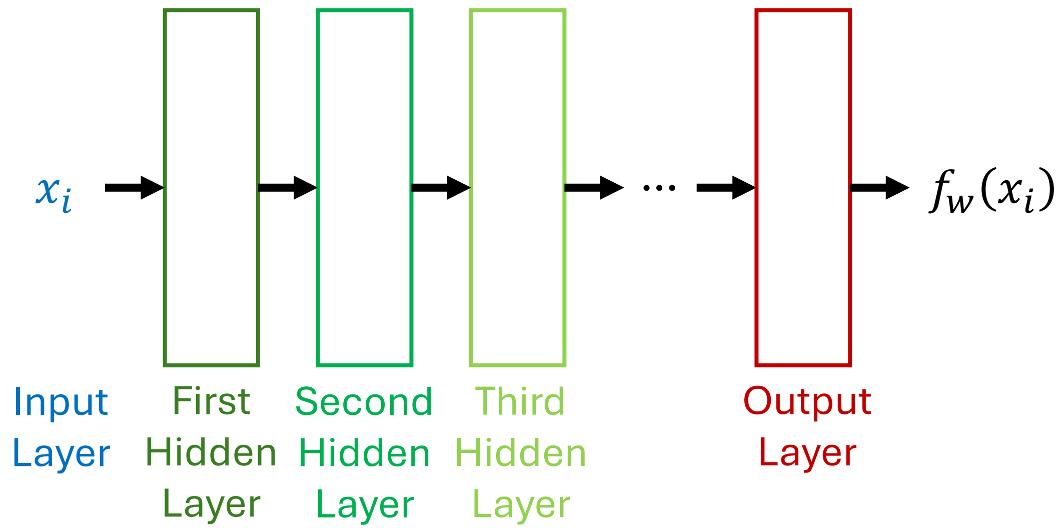
- Each perceptron in the right-layer takes the output of each perceptron in the left-layer as input.

Neural Network (Graphical Depiction)



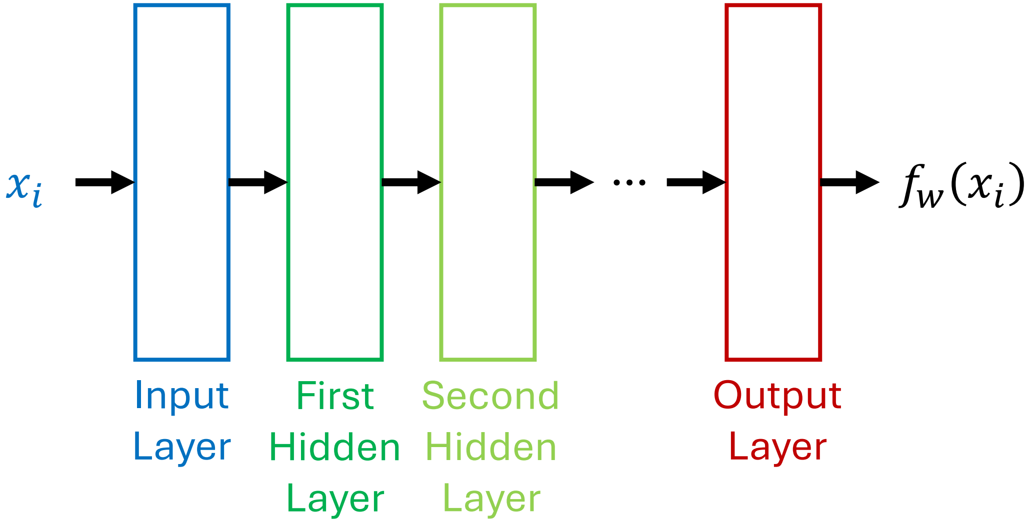
- In the context of neural networks, perceptrons are often called **units**.
- Each layer can have different numbers of units.
  - The number of units in a layer is often called the "size" of the layer.

Neural Network (Graphical Depiction)



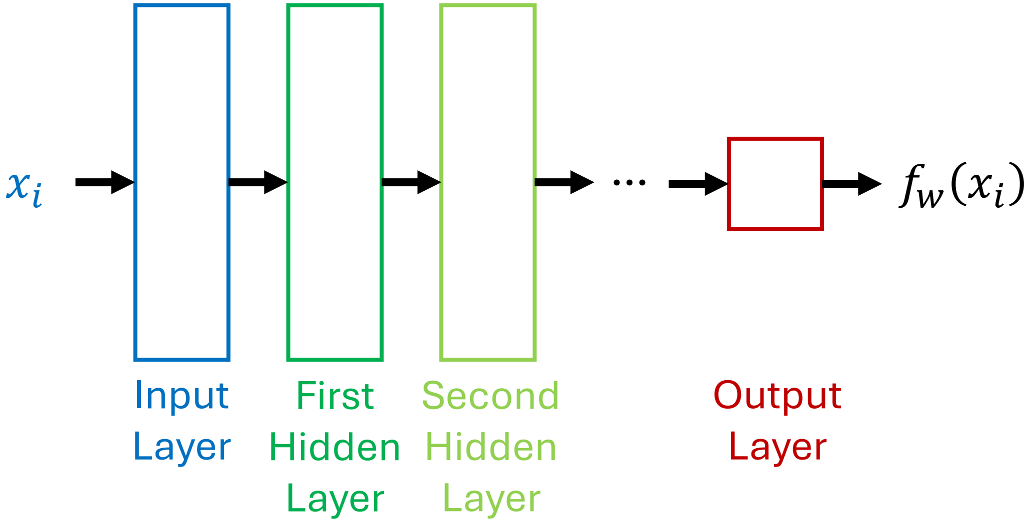
- The input, x_i is called the **input layer**.
- The last layer is called the **output layer**.
- All layers between the input and output layers are called **hidden layers**.

Neural Network (Graphical Depiction)



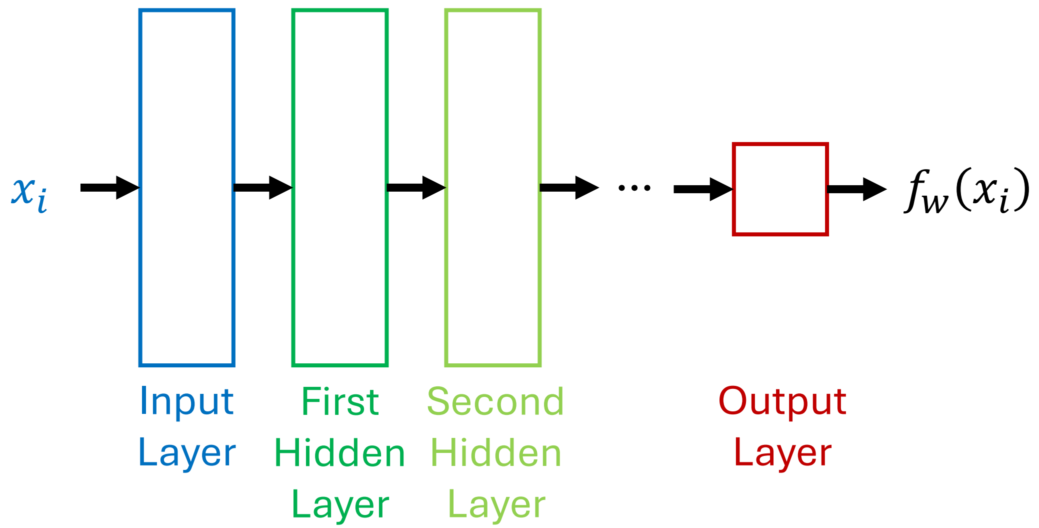
- Sometimes the input layer is represented by its own rectangle.
- This layer simply outputs x_i.

Neural Network (Graphical Depiction)



- The number of units in the output layer should equal the number of outputs of $f_w(x_i)$
  - For the GPA-prediction task, $x_i \in \mathbb{R}^9$ and $y_i \in \mathbb{R}$.
  - So, the output layer should have one unit.

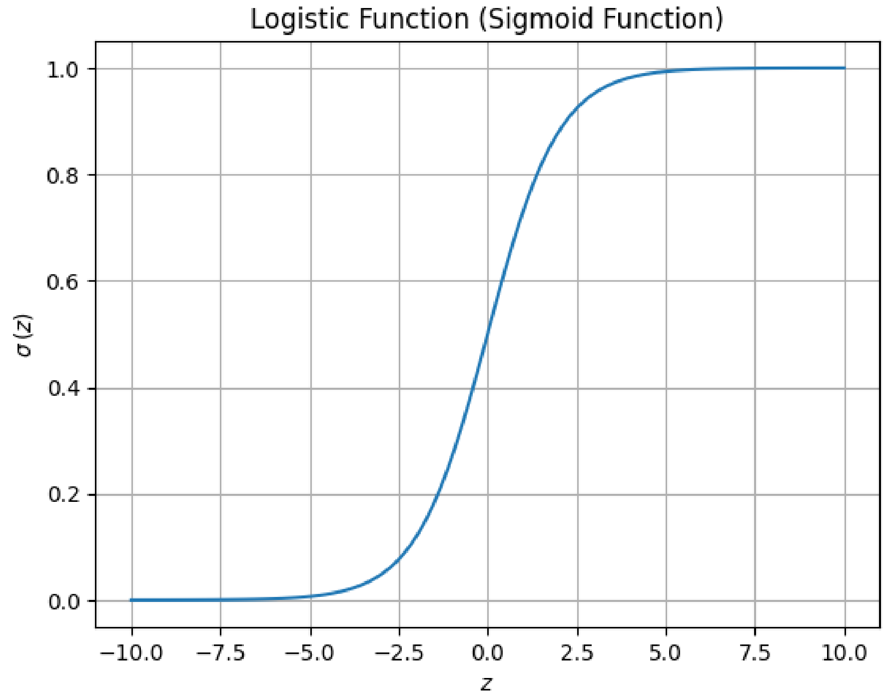
Neural Network (Graphical Depiction)



- If the output of the parametric model should not be "squashed" to [0,1], the squashing function (activation function) can be omitted from the output layer.

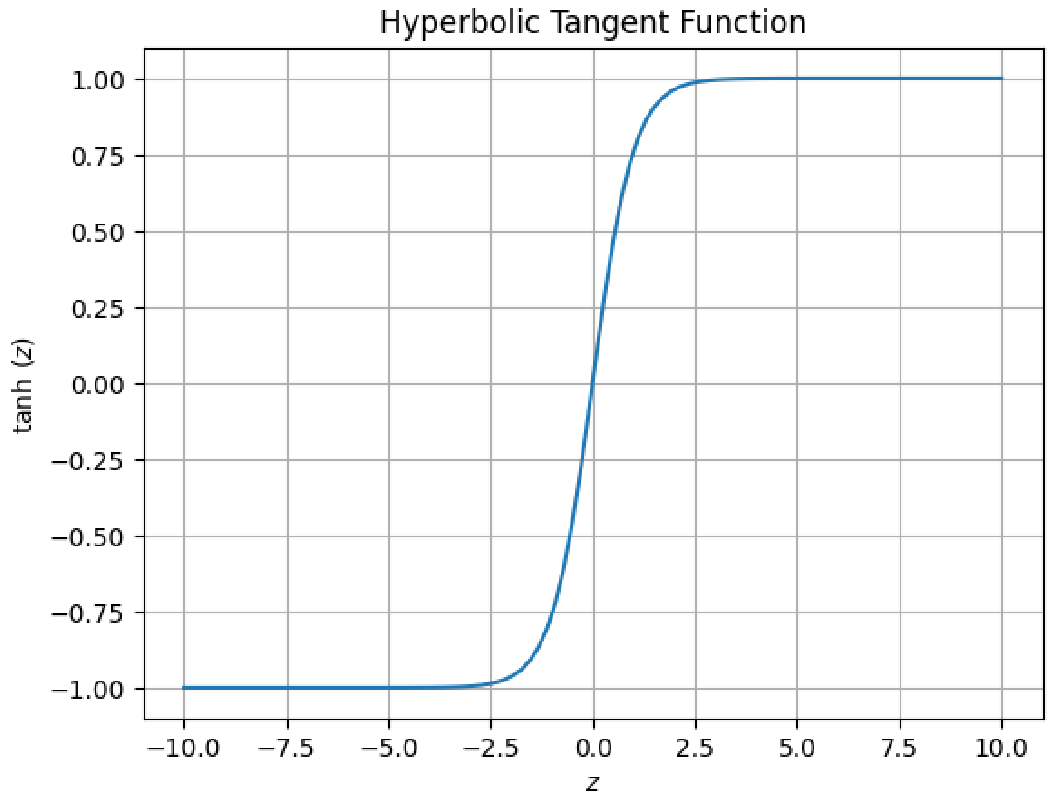
Activation Function: Sigmoid

- **Sigmoid functions** are a class of S-shaped functions.
- The most common one is called the **logistic function.**
  - It is so common that it is often called “the” sigmoid function.
- $\sigma(z) = \frac{1}{1+e^{-z}}$



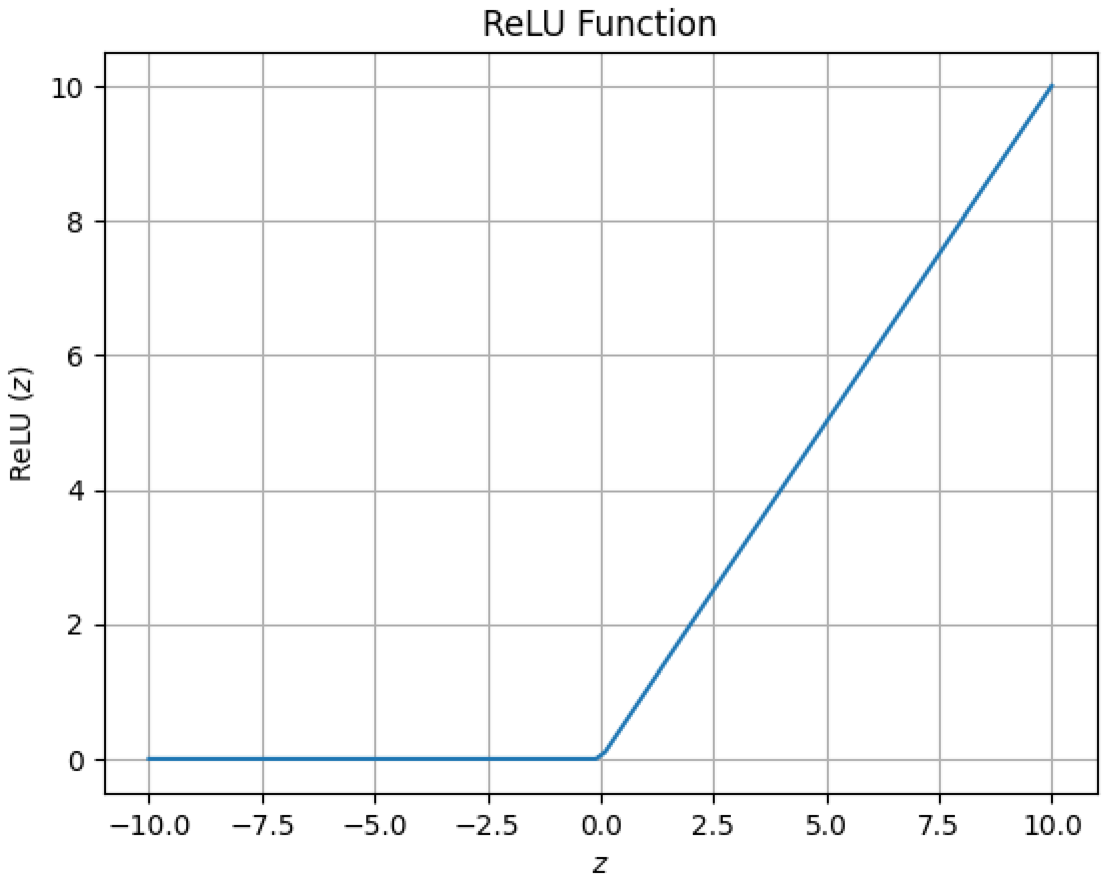
Activation Function: Hyperbolic Tangent Function (tanh)

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



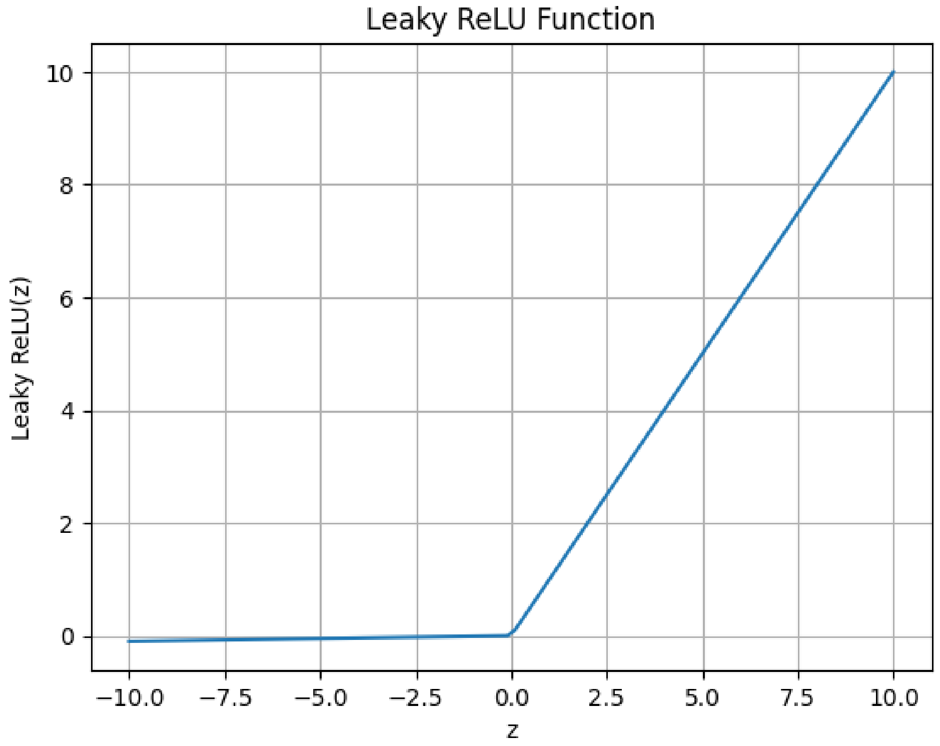
Activation Function: Rectified Linear Unit (ReLU)

- $\mathrm{ReLU}(z) = \max(0, z)$



Activation Function: Leaky ReLU

- Leaky ReLU$(z) = \begin{cases} z & \text{if } z > 0 \\ \alpha z & \text{if } z \leq 0 \end{cases}$
  - Here α is a small constant, typically 0.01.

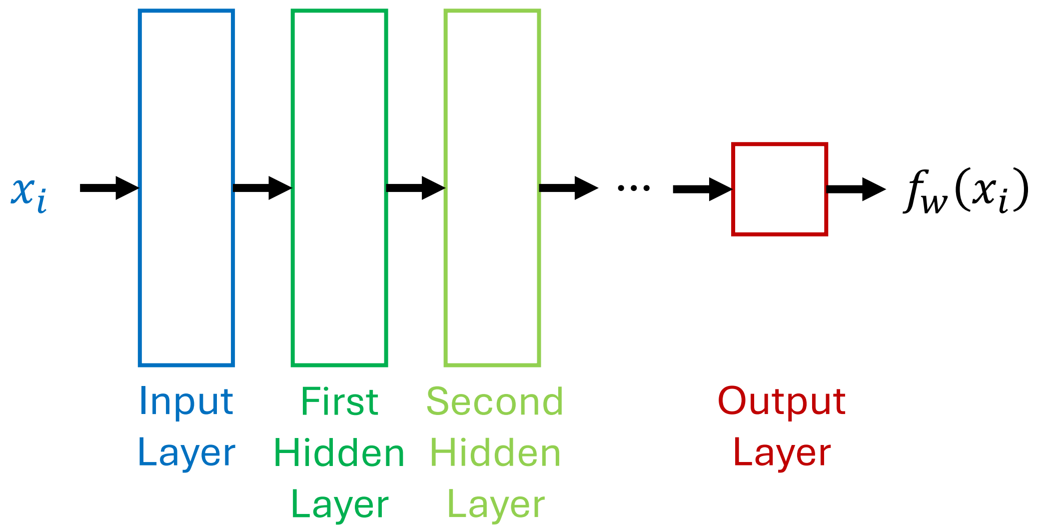


Terminology

- You will see both **neural network** and **artificial neural network** (ANN) used to describe these parametric models.
  - ANN emphasizes that these parametric models are very different from biological neural networks.
  - We will use both phrases, but will use the abbreviation ANN to differentiate from nearest neighbor (NN).

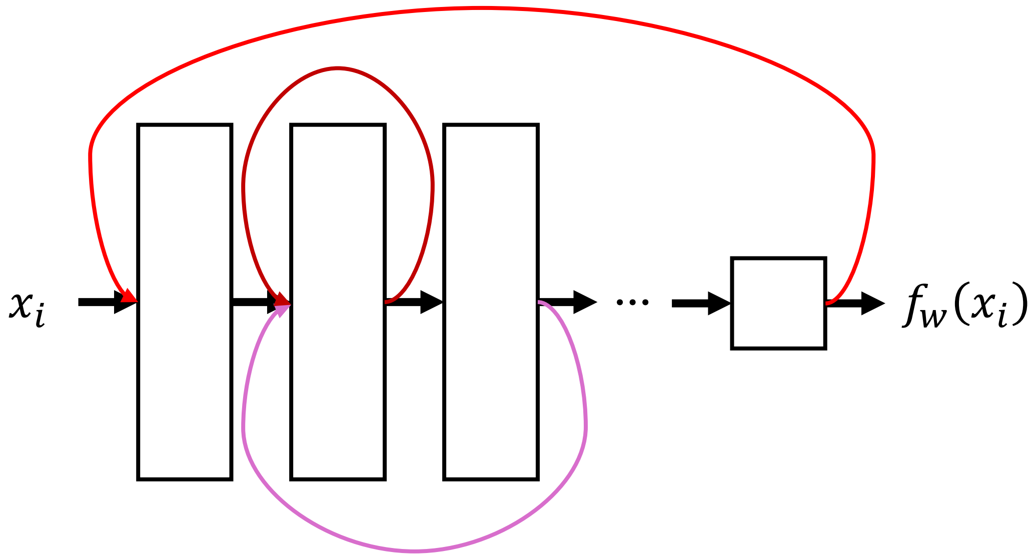
Fully-Connected Feed-Forward Networks

- A fully-connected feed-forward ANN is one where each unit in the i^{th} layer:
  - Takes the output of each unit in the $(i-1)^{\text{th}}$ layer as input.
  - Provides its output to each unit in the $(i+1)^{\text{th}}$ layer.



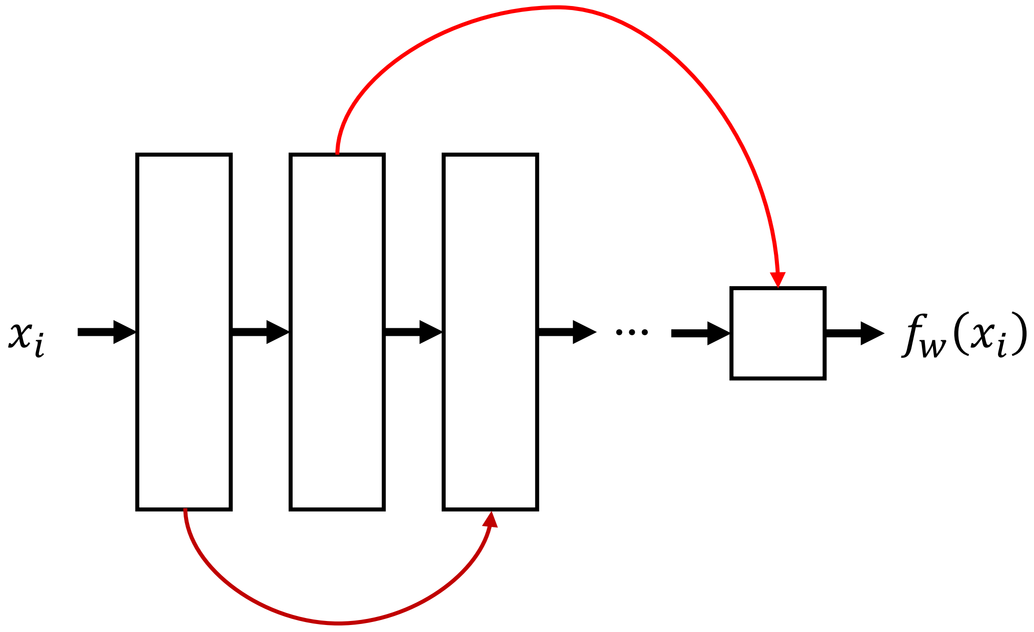
Recurrent Neural Network (RNN)

- Recurrent neural networks can have backwards connections between layers.
- These networks are typically run several times on the same input, and recurrent (backwards) edges provide values from the previous runs.
  - Recurrent connections provide a form of "memory"



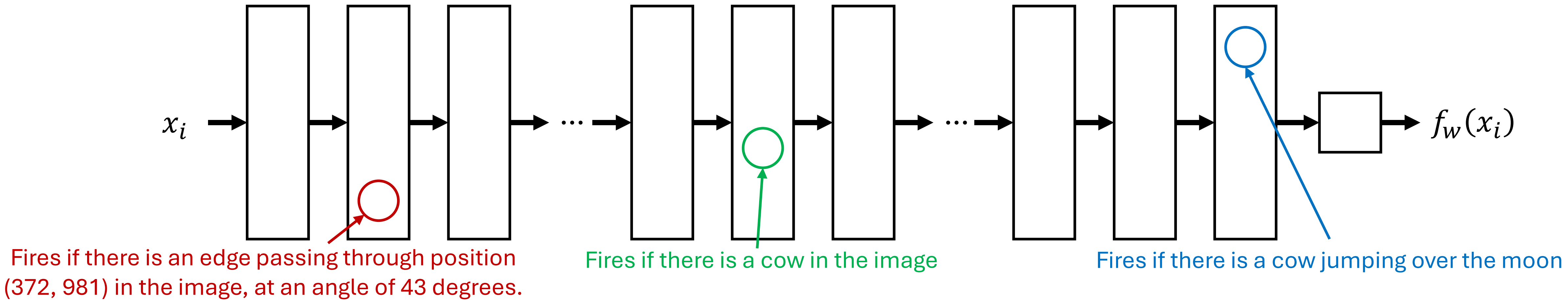
Skip Connections

- Skip connections are connections that skip over one or more layers.



What do different layers learn?

- Consider parametric models that take images as input.
- The layers closer to the input tend to learn low-level visual features.
- Later layers use these low-level features to learn about higher-level features and concepts.

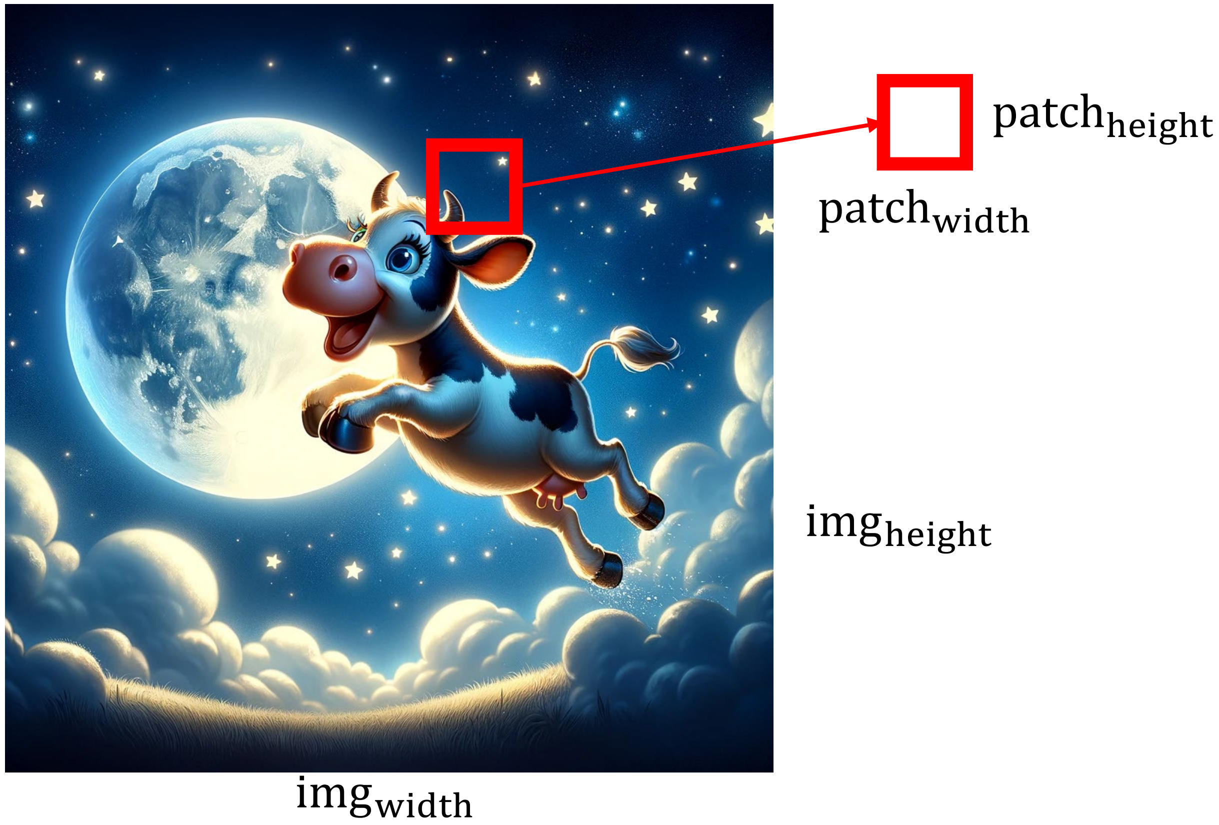


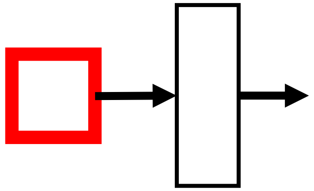
Learning Low-Level Features

- An ANN might use early layers to detect low-level features of an image
  - One unit early in the network might “fire” when there is an edge at position (x,y) in the image, and the edge is vertical.
  - Another unit might fire when there is an edge at position (x,y) at an angle of 80 degrees (nearly vertical).
  - There may be different units for all of these features at each (x,y) coordinate in the image!
- Learning to separately detect the same feature at each location in the image is wasteful.
- **Idea**: Create a parametric model (layer for ANNs) that learns to find and represent features *anywhere* in the image.

Convolutional Layer

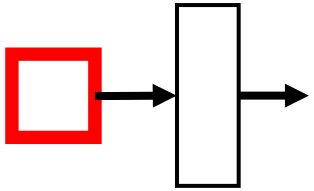
- If an image is of size $\mathrm{img}_{\mathrm{width}} \times \mathrm{img}_{\mathrm{height}}$, create a parametric model, called a **filter,** that takes as input a small subregion of the image, called a **patch**.
- This filter (small parametric model) is run on each patch in the image.
    - The patches can overlap.
    - Each patch is a fixed number of pixels over from the previous patch. This number is called the **stride**.





One number, the “feature” value for this patch.

0.2



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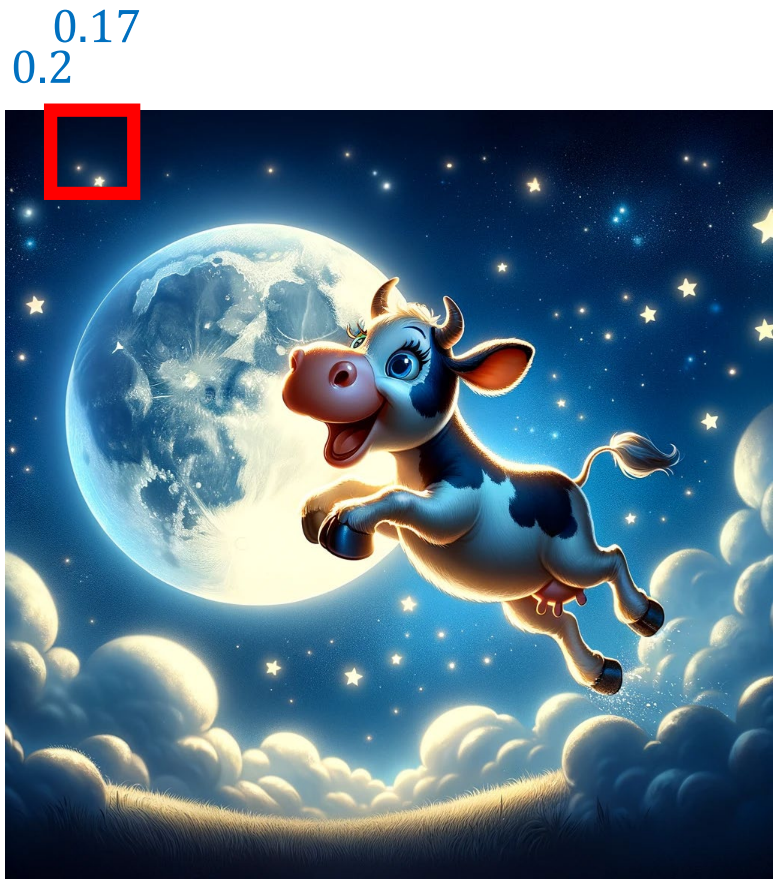

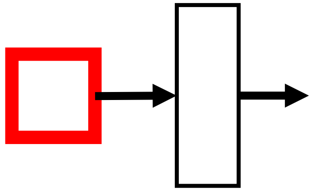

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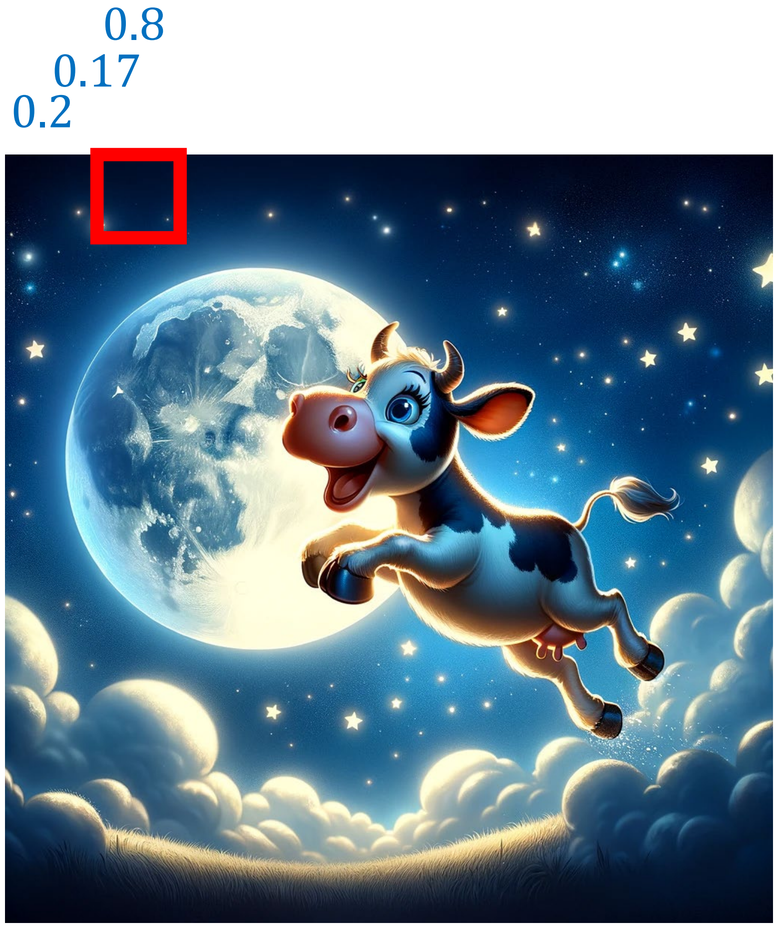
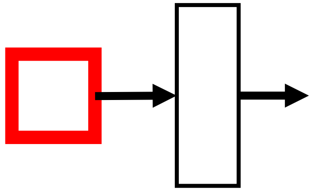
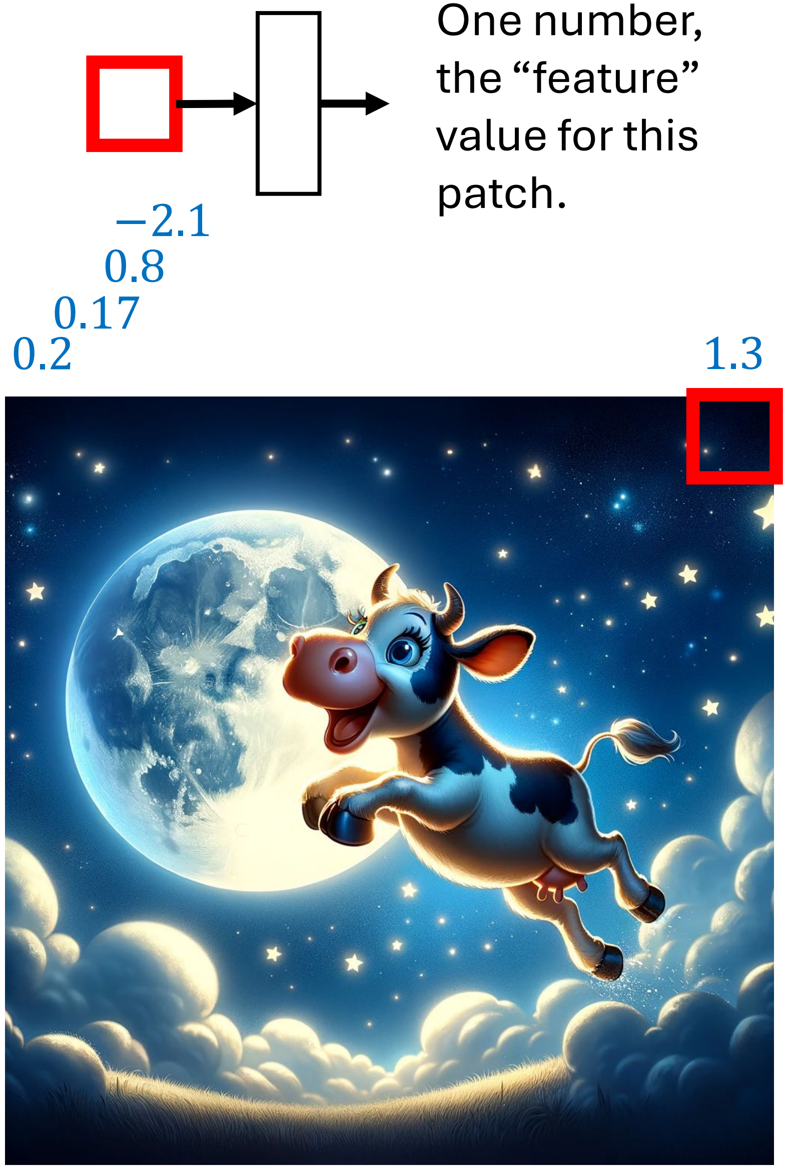




One number, the “feature” value for this patch.

-2.1
0.8
0.17
0.2

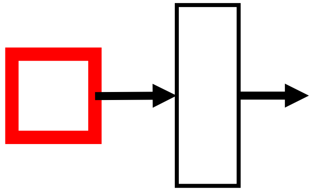
The patch is shifted over by **stride** number of pixels each time.



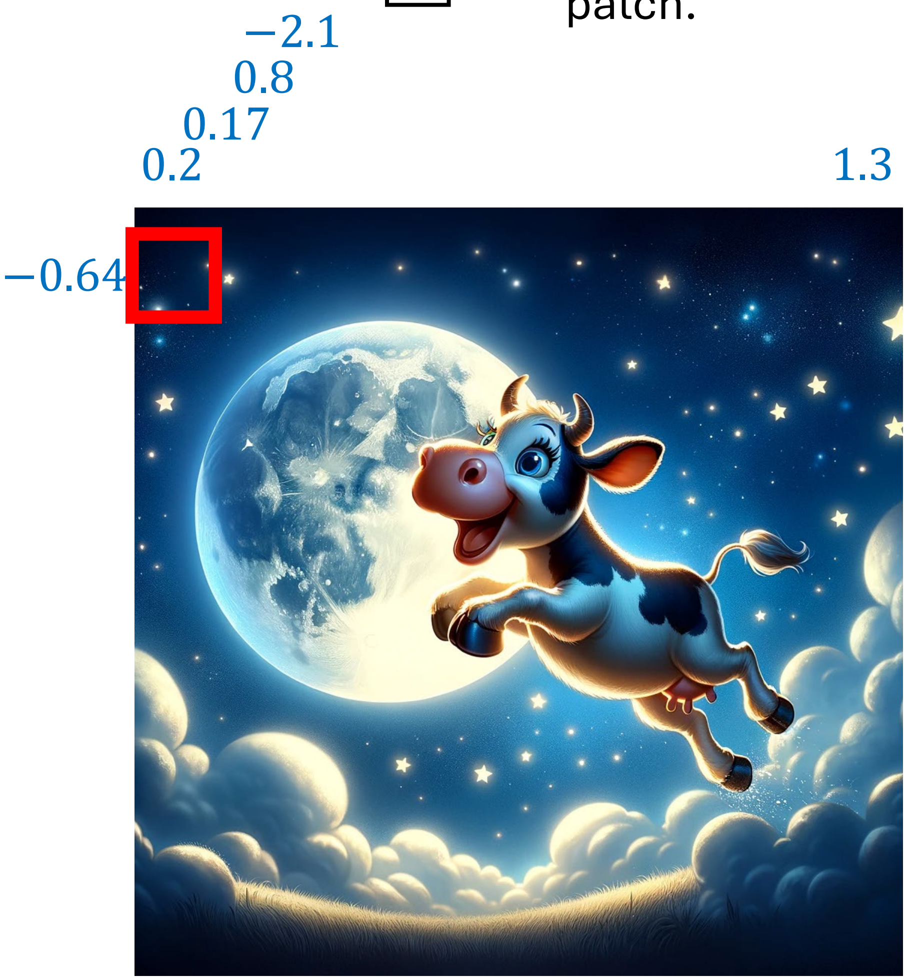
One number, the “feature” value for this patch.

The patch is shifted over by **stride** number of pixels each time.

When the patch reaches the end, it shifts down by **stride** pixels and starts over.



One number, the “feature” value for this patch.



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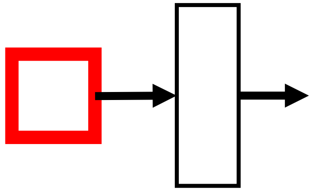


One number, the “feature” value for this patch.

-2.1

0.8

0.17

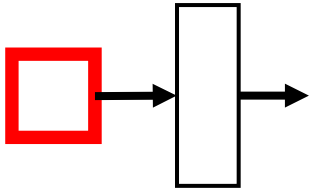
0.2 1.3

-0.64

The patch is shifted over by **stride** number of pixels each time.

When the patch reaches the end, it shifts down by **stride** pixels and starts over.

At the end, the **convolutional layer** outputs all the computed values:
$(0.2, 0.17, 0.8, -2.1, \ldots, 1.3, -0.64, \ldots)$



One number, the “feature” value for this patch.

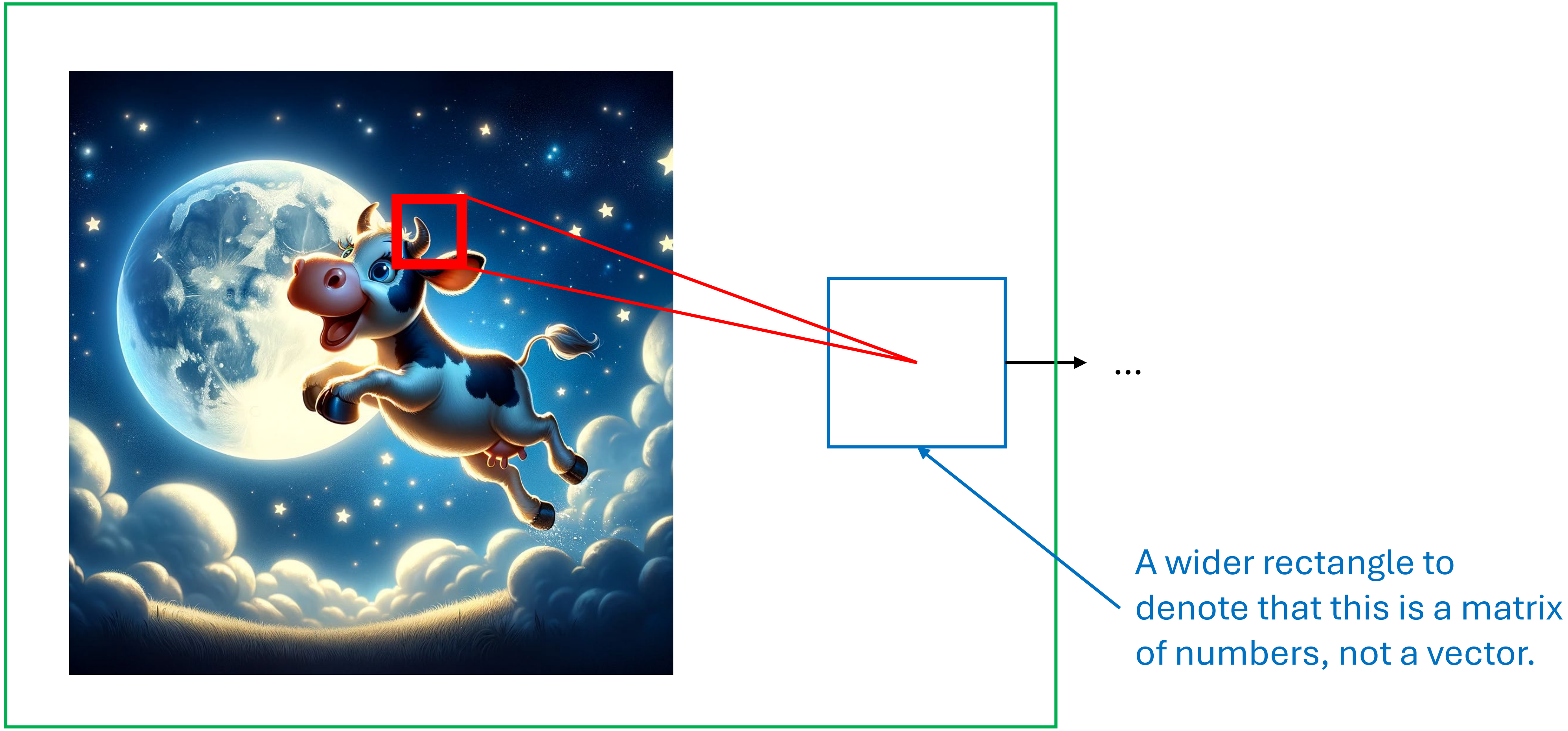
The patch is shifted over by **stride** number of pixels each time.

When the patch reaches the end, it shifts down by **stride** pixels and starts over.

At the end, the **convolutional layer** outputs all the computed values:
$(0.2, 0.17, 0.8, -2.1, \dots, 1.3, -0.64, \dots)$

These values are usually represented as a matrix to track the position of the patch they were computed from.

Convolutional Layer (Graphical Depiction)



This represents a convolutional layer (blue) applied to an image.

Convolutional Layer (summary)

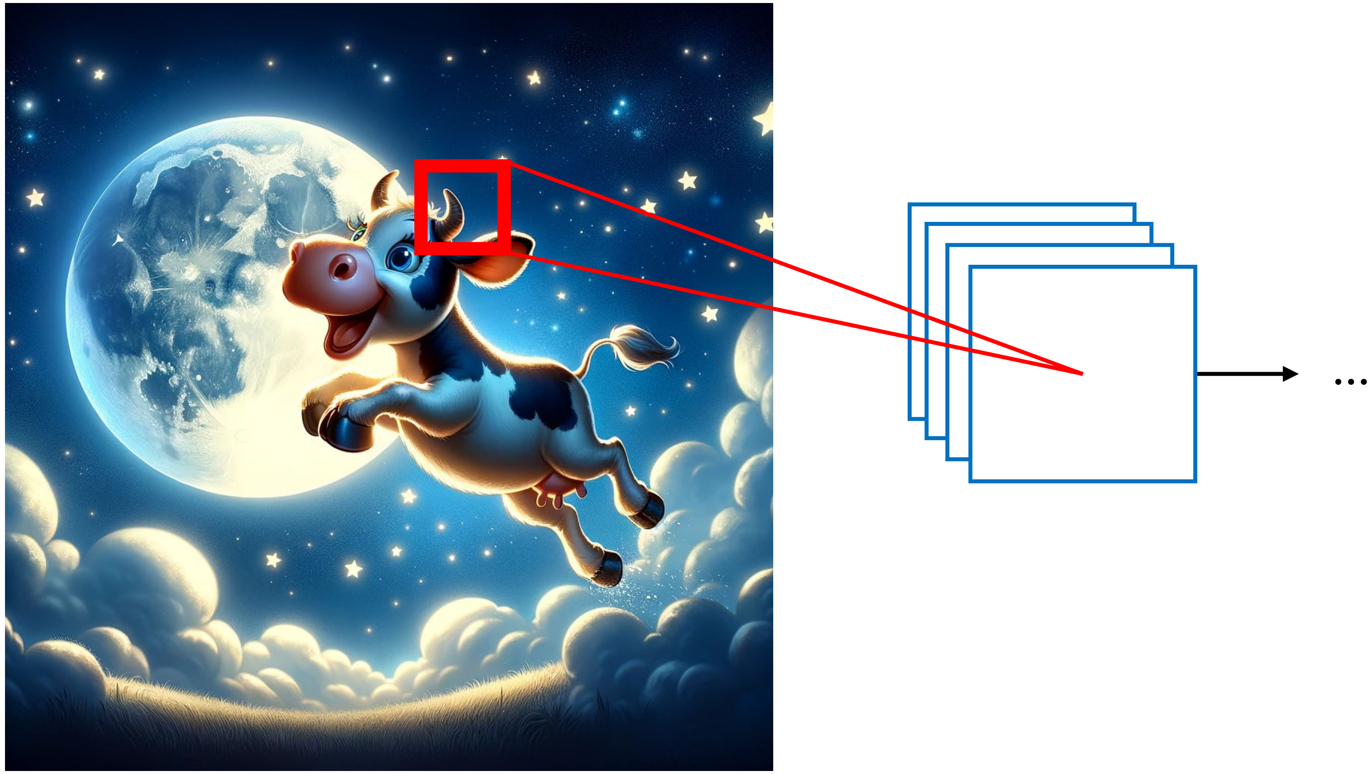
- A convolutional layer can be viewed as a small parametric model (within the main parametric model) that has a relatively small number of parameters.
    - This model is called a **filter**.
- The filter is applied to patches of an image.
- The outputs of the filter, for all patches, is viewed as the output of the convolutional layer.
    - These outputs are represented as a matrix.
    - The position in the matrix represents the position of the patch in the image.
- A single filter can learn features like “do two edges meet to form a corner in this patch?” or “is there a line at a specific angle in this patch?”

Convolutional Layer (Multiple Filters)

- We typically want to learn more than one feature for each patch.
  - For example, line detectors for lines at different angles.
- A convolutional layer, as described so far, learns only one feature.
- Convolutional layers can learn k features by applying k different filters (small parametric models) to each patch.
  - Each filter produces one number for each patch.
  - The outputs for each filter are stored as separate matrices, one per filter.

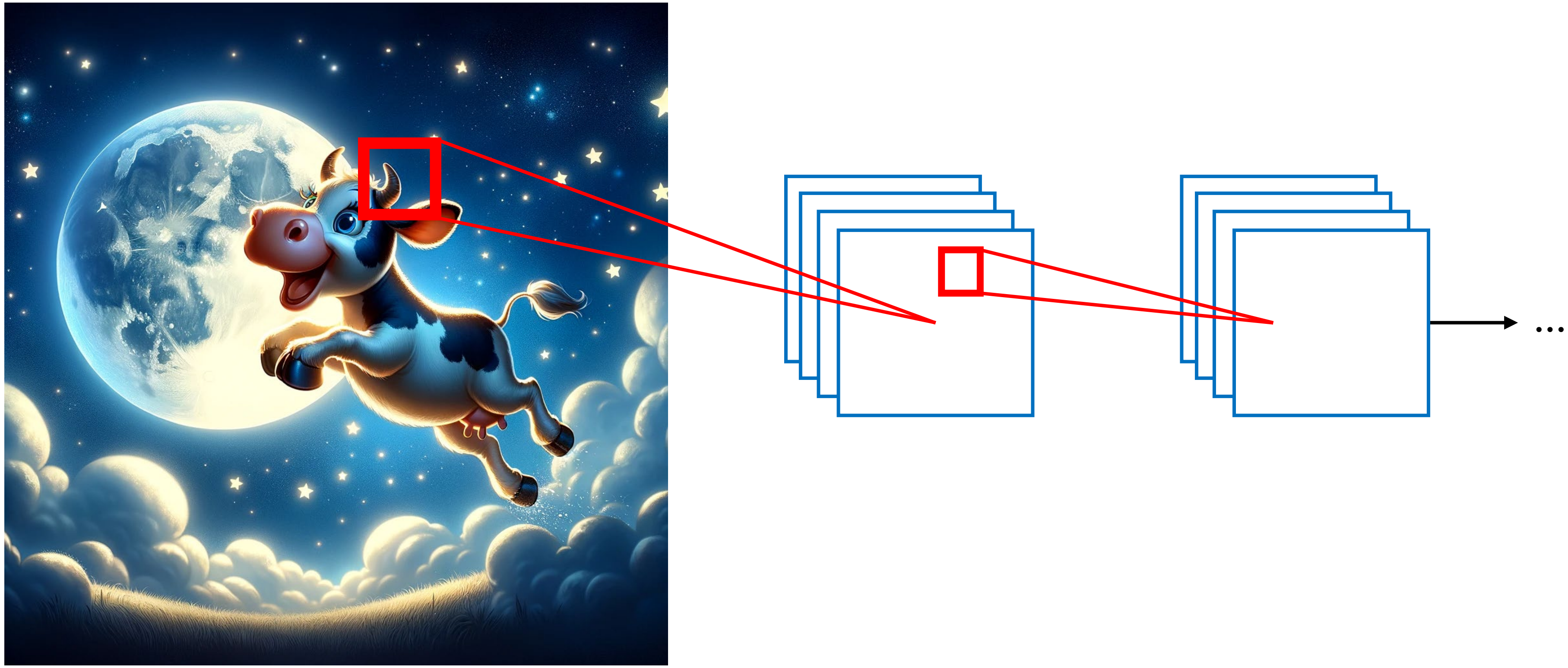
Convolutional Layer

- A convolutional layer with multiple filters is represented using many stacked boxes:



Convolutional Layer

- Convolutional layers can be applied in a sequence!



Max Pooling Layers

- When using convolutional layers with many filters, you can end up with more outputs from the convolutional layer than there were pixels in the original image!
- To make the number of values more manageable, a **max pooling** layer can be used to downsample (reduce) the number of features.
- A max pooling layer acts like a convolutional layer, but without any parameters.
  - For each patch, it returns the maximum value within the patch.
  - Other pooling layers (e.g., average pooling layers) compute other fixed functions of a patch (e.g., the average value in the patch)
  - A max pooling layer typically has a relatively wide stride and/or patch.
    - For example, a 2x2 patch with no overlap between patches quarters the number of values.