Machine Learning (CE 40717)

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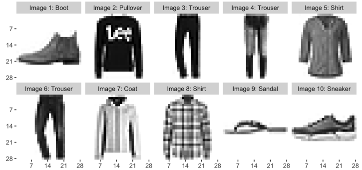
Why Neural Networks?

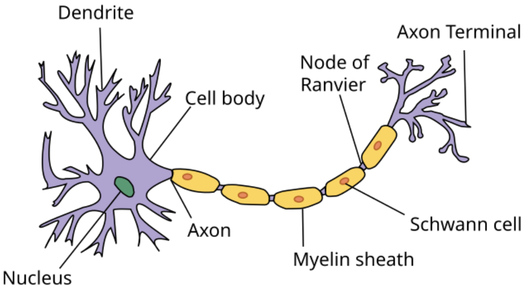
- We can find explicit formulas for some problems (no machine learning)
  - $\Delta x = \frac{1}{2} a \cdot t^2 + v_0 \cdot t$
- We can model some problems by assuming simple relationships (classical machine learning)
  - House price as a linear function of its features
  - $y = a_1 \cdot x_1 + a_2 \cdot x_2 + \ldots + a_p \cdot x_p$
- How can we classify these images?



Why Neural Networks? Cont.

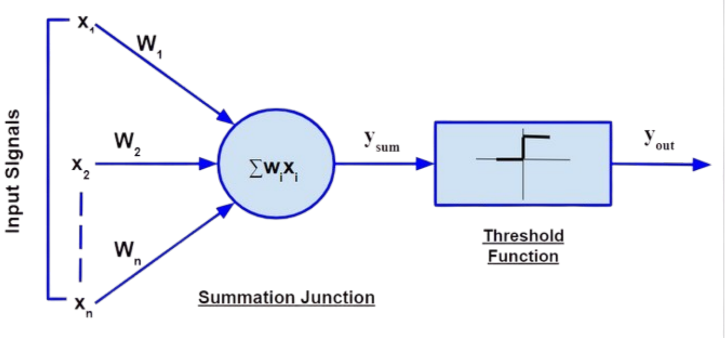
- **No explicit formula** exists to recognize a sneaker
- We intuitively recognize any sneaker
- Our brains use a **complex function** for this recognition
- **Deep neural networks** can learn this complex function

Modelling the Brain



- Building units are neurons.
- **Dendrite:** Receives signals from other neurons neurons.
- **Soma:** Processes the information
- **Axon:** Transmits the output of this neuron
- **Synapse:** Point of connection to other neurons

McCulloch-Pitts Neurons

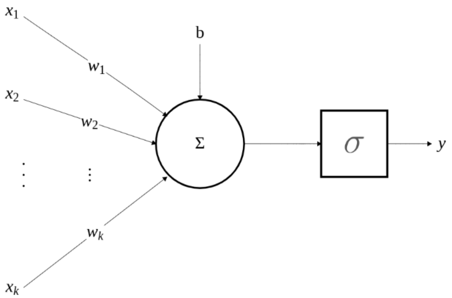


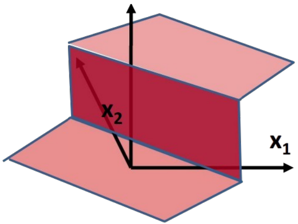
$$y = \begin{cases} 1 & \text{if } \sum_i w_i x_i - T \geq 0 \\ 0 & \text{otherwise.} \end{cases}$$

Perceptron Reminder

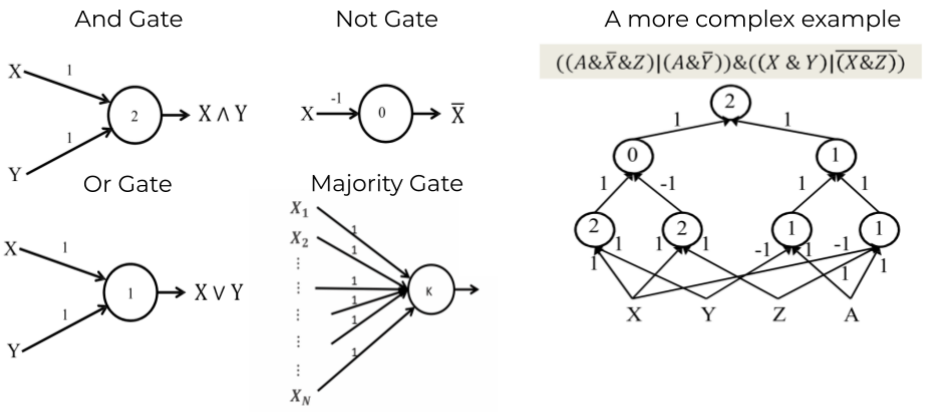
The building block of each neural network is the perceptron:

- $\{x_1, x_2, \ldots, x_k\}$: input features
- $\{w_1, w_2, \ldots, w_k\}$: feature weights
- b : bias term
- $\sigma(\cdot)$: activation function
- y : output of the neuron





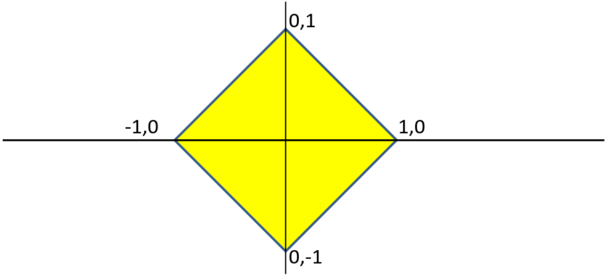
Example: Perceptron as a Boolean Gate



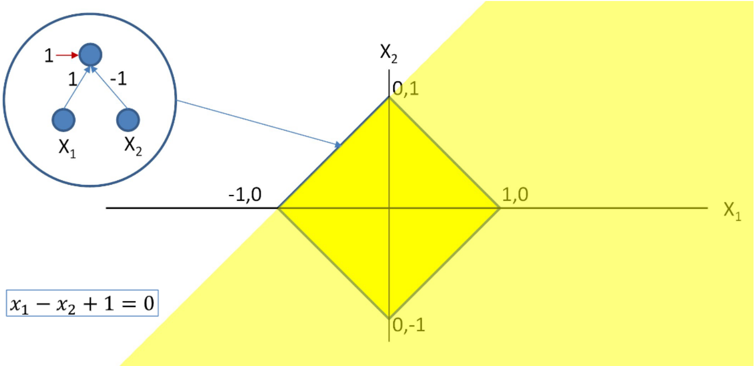
- A perceptron can model any simple binary Boolean gate.
- MLPs are universal Boolean functions.

Example: MLP for Complex Patterns

- What network to learn this area?
- Example is adapted from [1].

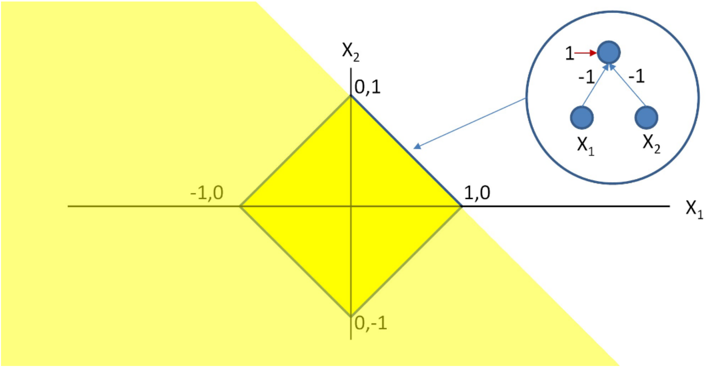


Example: MLP for Complex Patterns Cont.

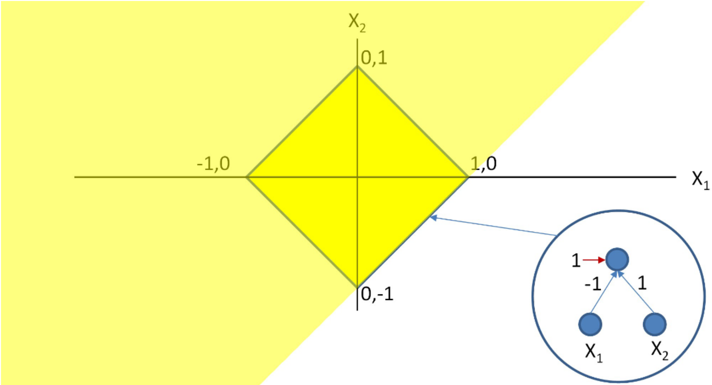


$x_1 - x_2 + 1 = 0$

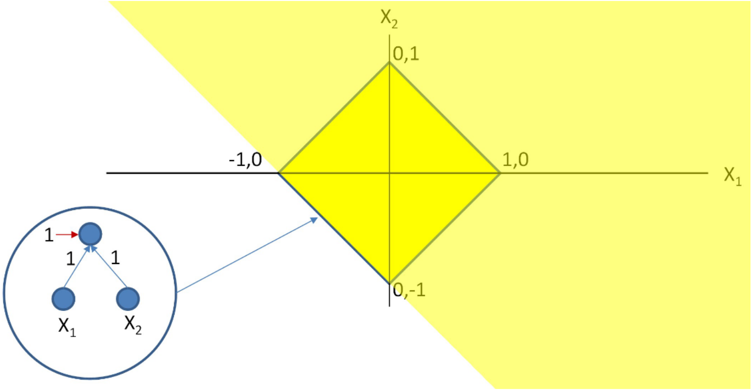
Example: MLP for Complex Patterns Cont.



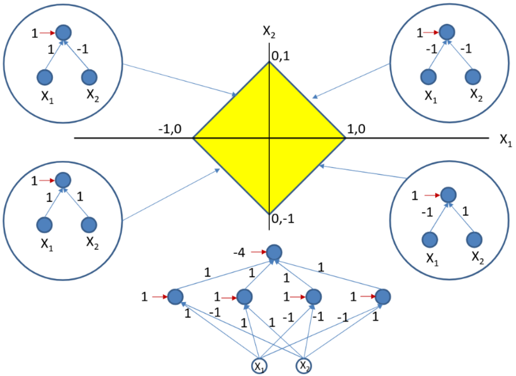
Example: MLP for Complex Patterns Cont.

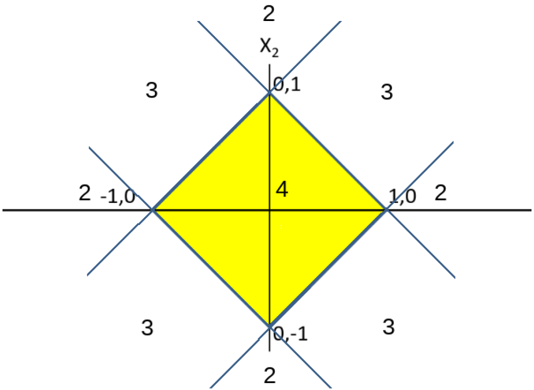


Example: MLP for Complex Patterns Cont.

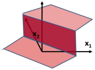
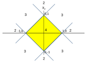


Example: MLP for Complex Patterns Cont.

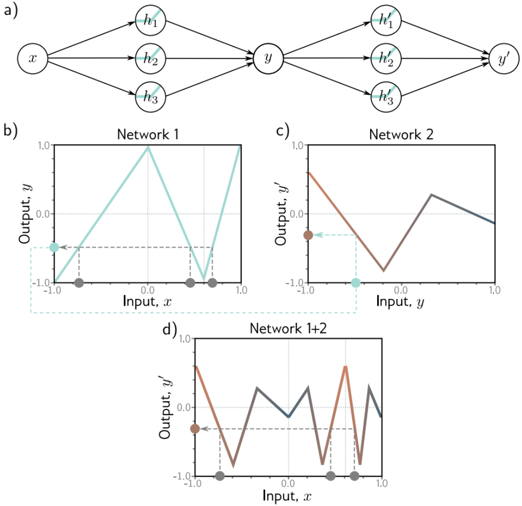


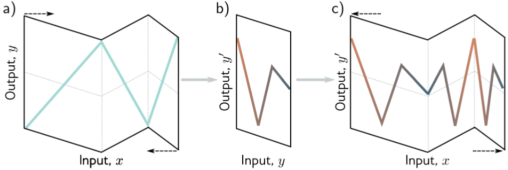


Neural Networks for Region Classification

Layer Type	Decision Region	Interpretation	Visualization
Single layer (perceptron)	Half-space	Linear separator defined by a hyperplane $w^\top x + b = 0$	
Two layers (1 hidden)	Closed, convex regions	Intersections of half-spaces ⇒ convex polytopes	
Three layers (2+ hidden)	Arbitrary (finite unions)	Union of polytopes; universal approximation of regions	

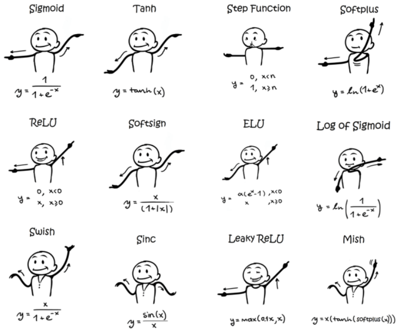
Example: Composing Neural Networks.





MLP Capacity

- Increasing **width and depth** allow us to approximate **complex decision boundaries**
- An **activation function** makes a neuron's output **non-linear**, allowing the network to learn complex pattern
- It is **not limited** to Boolean or step functions
- With appropriate activation functions, neural networks can **approximate any real-valued function** (More details later)



Adapted from Sefiks

Single Hidden Layer Neural Network

- Hidden layer pre-activation:

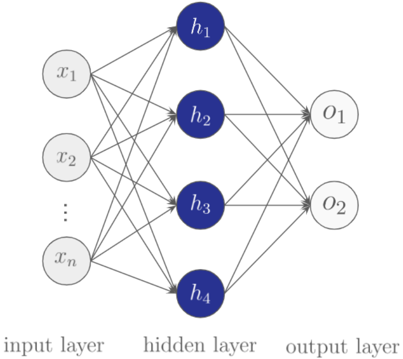
$$a_i(x) = b_i^{(1)} + \sum_j W_{ij}^{(1)} \cdot x_j$$

- Weight between neuron i and j in layer ℓ: $W_{ij}^{(\ell)}$
- Activated hidden layer:

$$h(x) = \sigma^{(1)}(a())$$

- Output layer:

$$o() = \sigma^{(2)}\left(^{(2)} + \mathbb{W}^{(2)} h^{(1)}()\right)$$



Multi-Hidden Layer Neural Network

- Let $h_i^0 = x_i$ for $i \in \{1, 2, \ldots, n\}$
- For $\ell \in \{0, 1, \ldots, L\}$:

$$a_j^{(\ell+1)} = b_j^{(\ell)} + \sum_i W_{ij}^{(\ell)} \cdot h_i^{(\ell)}$$

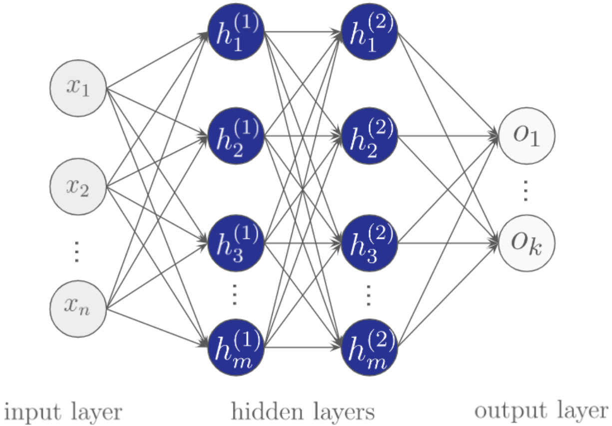
$$h_j^{(\ell+1)} = \sigma^{(\ell+1)}(a_j^{(\ell+1)})$$

- Learnable parameters:

$$b_j^{(\ell)}, W_{ij}^{(\ell)}$$

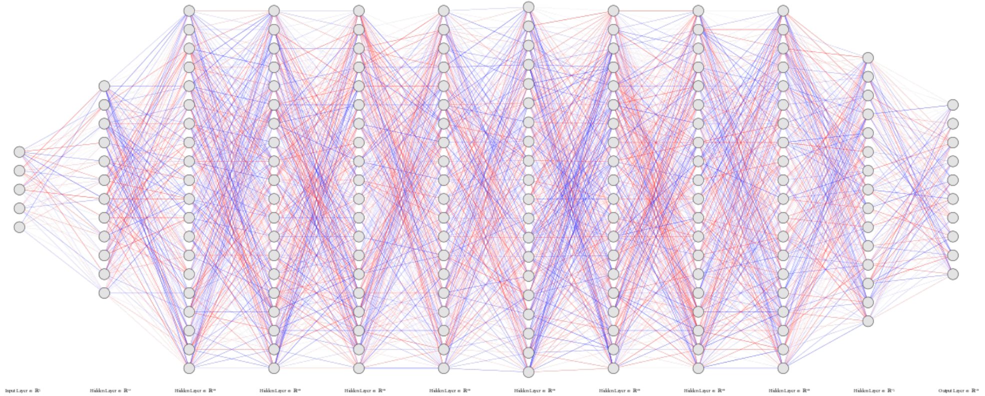
- Number of learnable parameters:

$$(n+1)m_1 + (m_1+1)m_2 + \ldots + (m_L+1)k$$



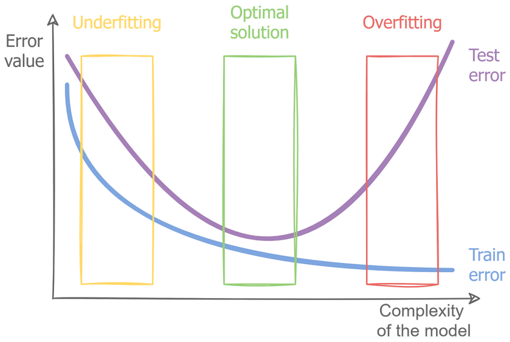
Deep Neural Network Architecture

- More than a few hidden layers: **Deep Neural Network (DNN)**
- Designing neural network architecture is **more of an art than a science**.



Network Width and Depth

- **Width:** More neurons, more complexity
- **Depth:** More layers, more abstraction
- **Balance:**
  - Too narrow/shallow: risk of underfitting
  - Too wide/deep: risk of overfitting



Adapted from Towards Data Science

Universal Approximation Theorem

Key Concept

- The Universal Approximation Theorem states that a feedforward neural network with:
  - A single hidden layer
  - Sufficient number of hidden neurons
  - Appropriate activation functions (e.g., sigmoid)

  Can approximate any continuous function on a **compact subset** of $\mathbb{R}^n$ to any desired accuracy.

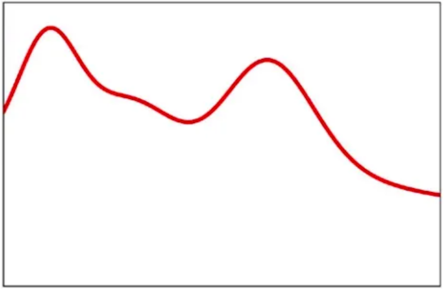
Understanding Compact Sets

What is a Compact Set?

- In the context of the Universal Approximation Theorem, approximation is guaranteed on a **compact subset** of $\mathbb{R}^n$.
- A set is compact if it is both:
  - **Bounded**: Enclosed within a finite space.
  - **Closed**: Contains all its boundary points.
- Compact sets ensure certain mathematical properties that enable reliable function approximation by the MLP within that region.

Breaking Down Complex Functions

- Idea: Complex functions can be decomposed into multiple smaller parts, each represented by a simpler function.
- By combining a series of simpler functions (like square pulses), the target function can be closely approximated.



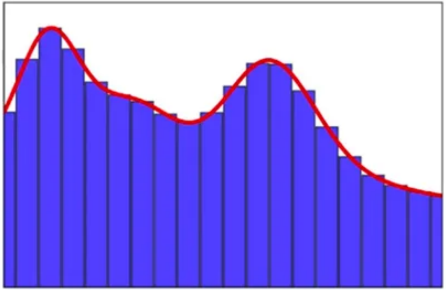


Figure adapted from Niranjan Kumar, Illustrative Proof of Universal Approximation Theorem

MLPs as Universal Approximators

- By constructing a series of these `Square Pulse` functions, we can approximate any continuous function mapping from input to output.
- A simple 3-unit MLP with a summing output unit can generate a square pulse.
- Therefore, an MLP with enough units and the right configuration is a universal approximator!

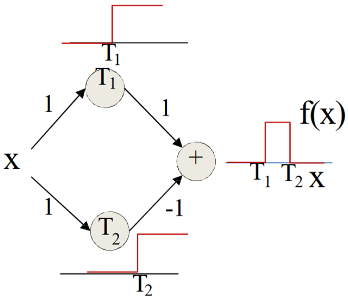
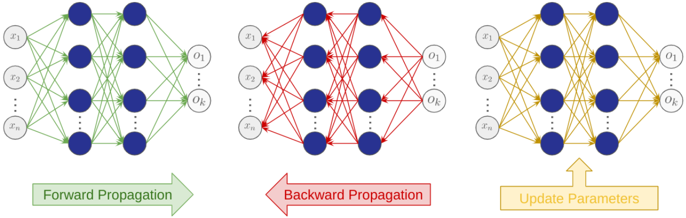


Figure adapted from Dr. Mahdieh Soleymani Baghshah, Deep Learning Course

Training Phases

- **Initialize weights and biases**: These values control how the network initially processes information (more details later)
- **Forward pass**: Pass the input through the network to get an output
- **Calculate the error**: Compare the network's output to the correct answer to measure the difference (called the 'loss' – more details later)
- **Backpropagation**: Use the loss value to adjust the weights and biases to improve the network's accuracy

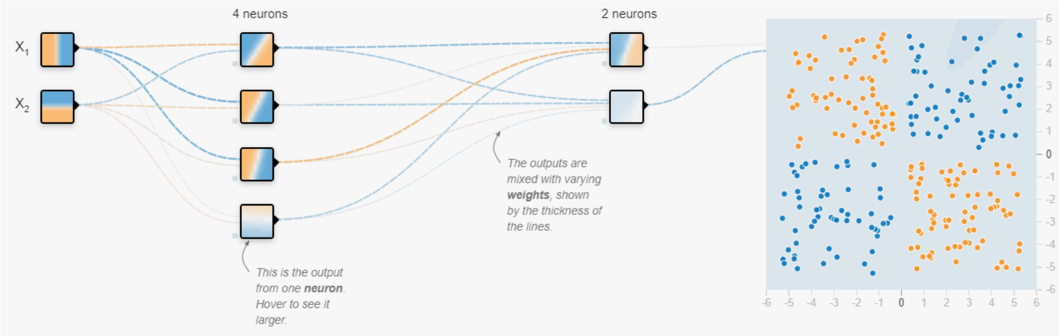


Forward Propagation

- This is the pass where we send input data through the network to make a prediction (likely inaccurate at first).
- The prediction is made by calculating weighted sums and applying an activation function in each layer

$$o(x) = a^{(L)} = \sigma^{(L)}\left(b^{(L)} + W^{(L)}\sigma^{(L-1)}\left(\ldots\sigma^{(1)}(b^{(1)} + W^{(1)}x)\ldots\right)\right)$$

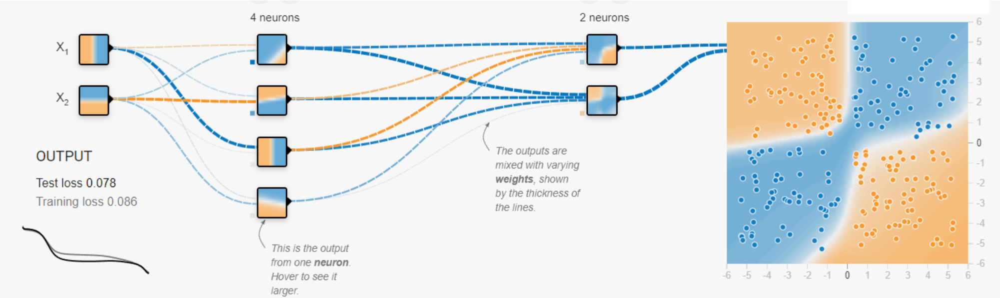
Forward Propagation Cont.



Before making predictions. Adapted from TensorFlow playground: Daniel Smilkov and Shan Carter.

Forward Propagation Cont.

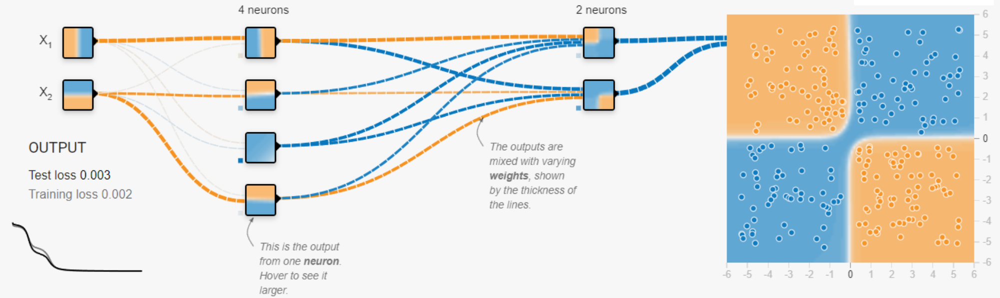
- The goal is to adjust the network's parameters to improve the predictions
- The loss is calculated after the forward pass, indicating how far off our predictions are from the true values



Loss values for predictions. Adapted from TensorFlow playground: Daniel Smilkov and Shan Carter.

BackPropagation and Parameter Update

- The network uses the **loss** to adjust its **weights and biases** through a process known as **backpropagation**
- Backpropagation calculates how much weights should change to reduce the error
- This will be explained in more detail in the following lecture



Predictions improve as the weights get updated. Adapted from TensorFlow playground: Daniel Smilkov and Shan Carter.

Contributions

These slides are authored by:

- Sogand Salehi
- Erfan Sobhaei

[1] R. Ramakrishnan, "Deep learning course at carnegie mellon university." `https://deeplearning.cs.cmu.edu/F23/index.html`, 2023. Accessed: 2024–09-04.

[2] E. Mousavi and K. Alishahi, "Deep learning course at sharif university of technology." `https://https://dnncourse.github.io/lectures`, 2023. Accessed: 2024–09-04.

[3] D. Smilkov and S. Carter, "A neural network playground." `playground.tensorflow.org`, 2022. Accessed: 2024-10-14.

[4] I. Goodfellow, Y. Bengio, and A. Courville, *Deep Learning*. MIT Press, 2016.

[5] A. Géron, *Hands-On Machine Learning with Scikit-Learn, Keras, and TensorFlow: Concepts, Tools, and Techniques for Building Intelligent Systems*. O'Reilly Media, 2019.