Neural Networks and Function Approximation

Krishna Kumar

University of Texas at Austin

krishnak@utexas.edu

Overview

Outline

The 1D Poisson Equation: Our Benchmark Problem

Consider the one-dimensional Poisson equation on $[0, 1]$:

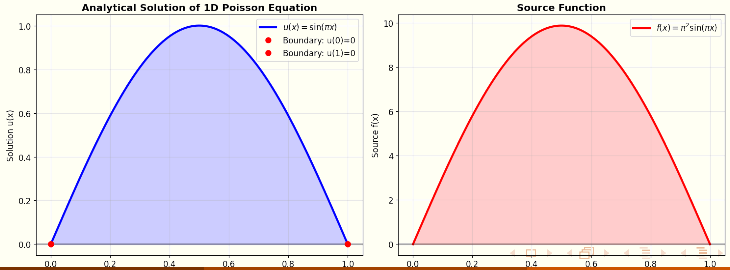
$$-\frac{d^2u}{dx^2} = f(x), \quad x \in [0, 1]$$

with boundary conditions:

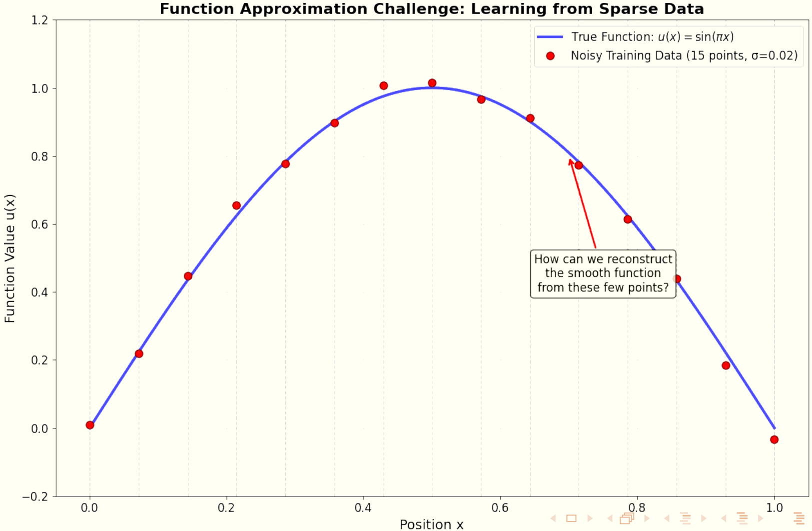
$$u(0) = 0, \quad u(1) = 0$$

For $f(x) = \pi^2 \sin(\pi x)$, the analytical solution is:

$$u(x) = \sin(\pi x)$$



Key Question: Can we learn to approximate $u(x) = \sin(\pi x)$ from sparse data?



Traditional vs Neural Network Approaches

Traditional Methods (Finite Difference):

- Discretize domain into grid points
- Solve for values at specific locations
- Result: Discrete representation

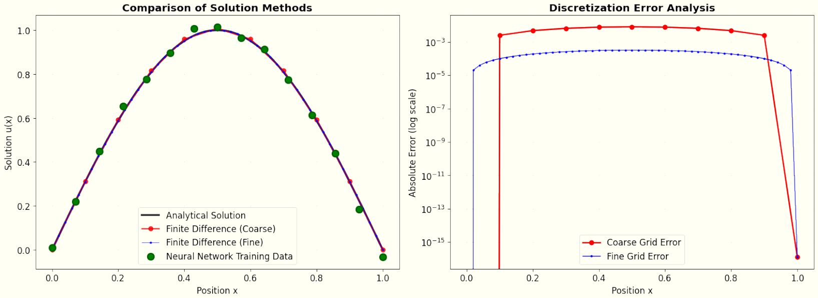
Finite difference approximation:

$$\frac{d^2u}{dx^2} \approx \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2}$$

Neural Network Approach:

- Learn continuous function $u_{NN}(x; \theta)$
- Approximate solution over entire domain
- Parameters θ trained from sparse data

Finite Difference vs Neural Networks



Comparison of solution methods and discretization errors

Key Insight: Neural networks learn continuous functions, not just discrete values.

Outline

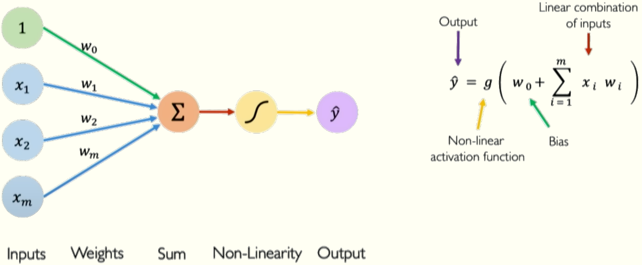
The Perceptron: Basic Building Block

A perceptron computes:

$$z = \mathbf{w}^T \mathbf{x} + b = \sum_{i=1}^{n} w_i x_i + b$$

$$\hat{y} = g(z)$$

where g is the activation function.



Perceptron architecture

Key components: Input vector, weights, bias, activation function, output.

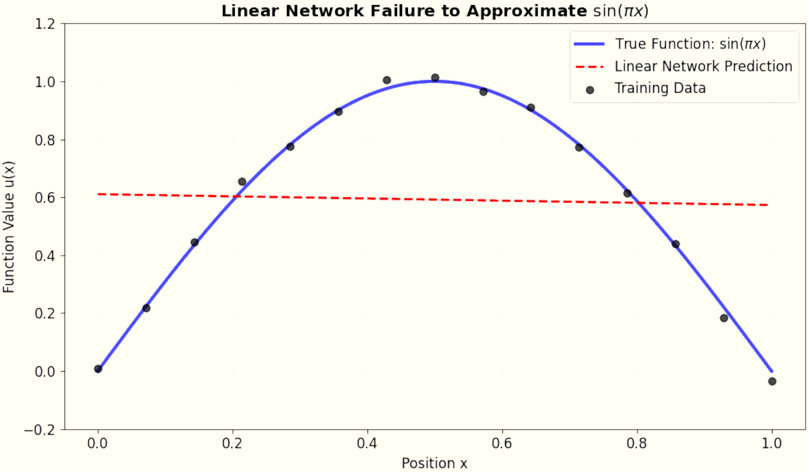
The Critical Role of Nonlinearity

Without activation functions: Multiple linear layers collapse to single linear transformation.
Consider two linear layers:

$$
\begin{aligned}
h_1 &= W_1 x + b_1 \\
h_2 &= W_2 h_1 + b_2 = W_2(W_1 x + b_1) + b_2 \\
&= (W_2 W_1)x + (W_2 b_1 + b_2)
\end{aligned}
$$

This is equivalent to: $h_2 = W_{eq}x + b_{eq}$ (still linear!)
Problem: Linear networks can only learn $y = mx + b$, but $\sin(\pi x)$ is curved!

Demonstrating Linear Network Failure



Linear network cannot approximate $\sin(\pi x)$

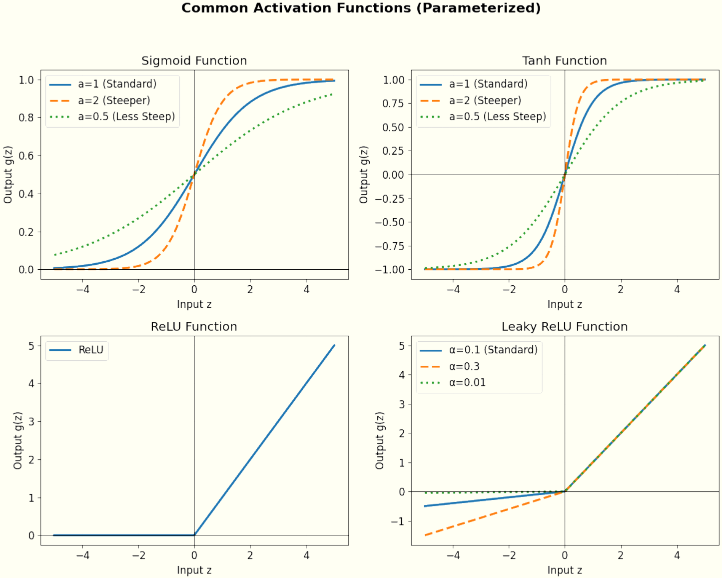
Conclusion: Nonlinearity is essential for complex function approximation.

Common Activation Functions

Sigmoid: $\sigma(x) = \frac{1}{1+e^{-x}}$ (squashes to (0,1))
Tanh: $\tanh(x) = \frac{e^{x}-e^{-x}}{e^{x}+e^{-x}}$ (squashes to (-1,1))
ReLU: $f(x) = \max(0, x)$ (efficient, prevents vanishing gradients)
Leaky ReLU: $f(x) = \max(\alpha x, x)$ (prevents dead neurons)

ReLU Demo

Common Activation Functions



Outline

Universal Approximation Theorem

Theorem (Cybenko, 1989): A single hidden layer network with sufficient neurons can approximate any continuous function to arbitrary accuracy.

$$F(x) = \sum_{i=1}^{N} w_i \sigma(v_i x + b_i) + w_0$$

Mathematical statement: For any continuous $f : [0,1] \to \mathbb{R}$ and $\epsilon > 0$, there exists N and parameters such that $|F(x) - f(x)| < \epsilon$ for all $x \in [0,1]$.
Key Questions:

- How many neurons N do we need?
- Is this practical?
- Can we verify experimentally?

Single Hidden Layer Architecture

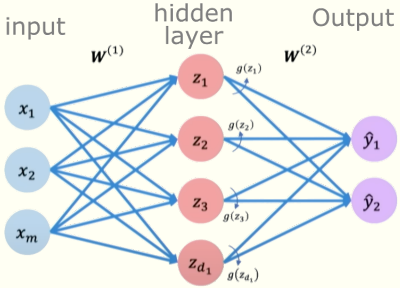
For 1D input x, a single-layer network with N_h hidden neurons:

$$\mathbf{z}^{(1)} = W^{(1)}x + \mathbf{b}^{(1)} \quad \text{(pre-activation)}$$

$$\mathbf{h} = g(\mathbf{z}^{(1)}) \quad \text{(hidden layer output)}$$

$$z^{(2)} = W^{(2)}\mathbf{h} + b^{(2)} \quad \text{(output layer)}$$

$$\hat{y} = z^{(2)} \quad \text{(final prediction)}$$



Single hidden layer neural network

Outline

Training Process

Goal: Find optimal parameters θ^* that minimize loss function.
Loss function (MSE):

$$\mathcal{L}(\theta) = \frac{1}{N} \sum_{i=1}^{N} (u_{NN}(x_i; \theta) - u_i)^2$$

Optimization problem:

$$\theta^* = \arg\min_{\theta} \mathcal{L}(\theta)$$

Training Steps:

1. Forward pass: compute predictions
2. Calculate loss
3. Backward pass: compute gradients
4. Update parameters
5. Repeat until convergence

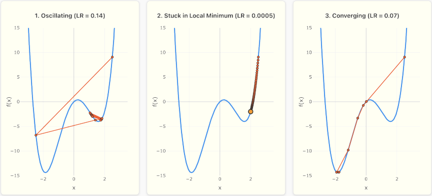
Gradient Descent Algorithm

Basic Algorithm:

1. Initialize weights randomly
2. Loop until convergence:
3. Compute gradient $\frac{\partial \mathcal{L}}{\partial \theta}$
4. Update weights: $\theta \leftarrow \theta - \eta \frac{\partial \mathcal{L}}{\partial \theta}$
5. Return weights

$$\theta_{new} = \theta_{old} - \eta \nabla \mathcal{L}(\theta)$$

where η is the learning rate.



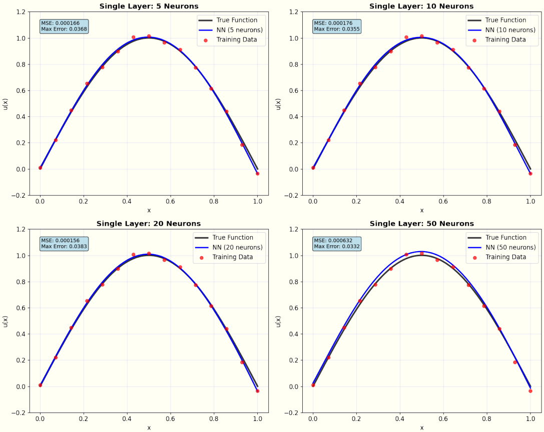
Gradient descent optimization

▸ SGD Demo

Width vs Approximation Quality

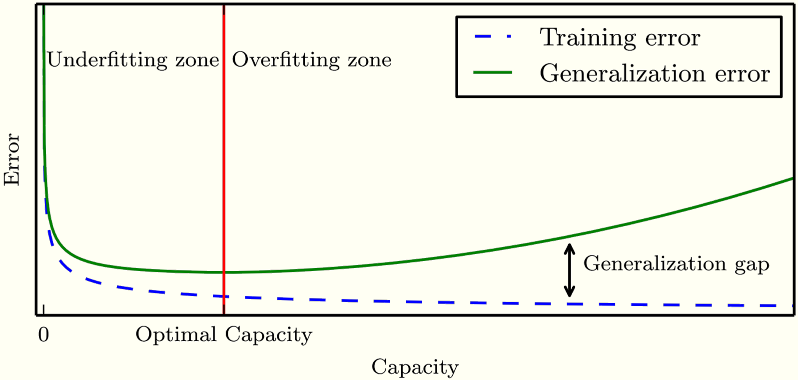
Hypothesis: More neurons → better approximation

Experiment: Train networks with 5, 10, 20, 50 neurons



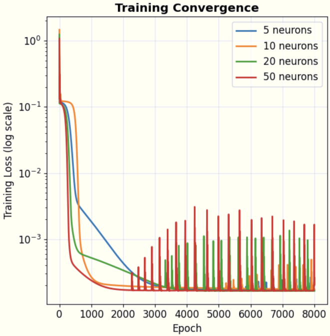
Approximation quality vs network width

Training/Validation



Training and validation convergence

Training Convergence Analysis



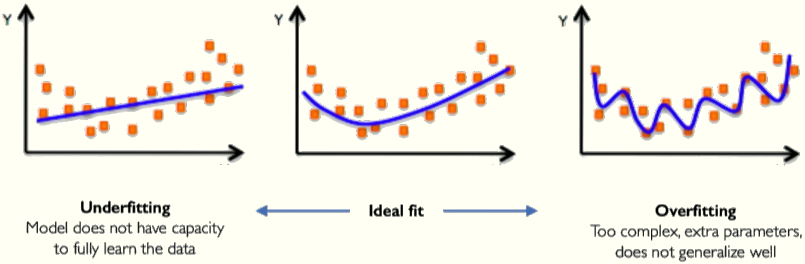
Training convergence and final loss vs width

Key Findings:

- 50 neurons: $\sim$10x better than 5 neurons
- Logarithmic improvement with width
- Convergence rate similar across widths

Overfitting and Model Capacity

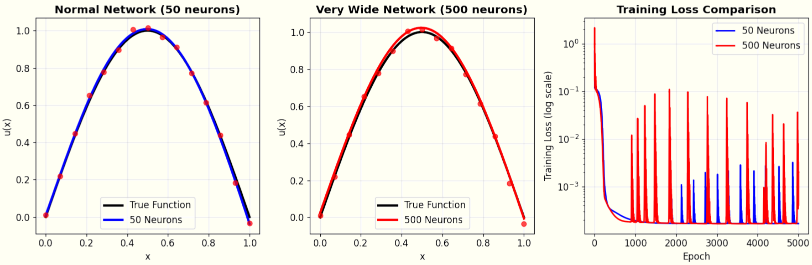
Problem: High-capacity networks can memorize training data.



Under and overfitting illustration

Detection: Monitor validation loss during training.
Solutions: More data, regularization, early stopping, simpler architectures.

Demonstrating Overfitting



Normal (50 neurons) vs very wide (500 neurons) network

Observation: Very wide networks may generalize worse despite lower training loss.

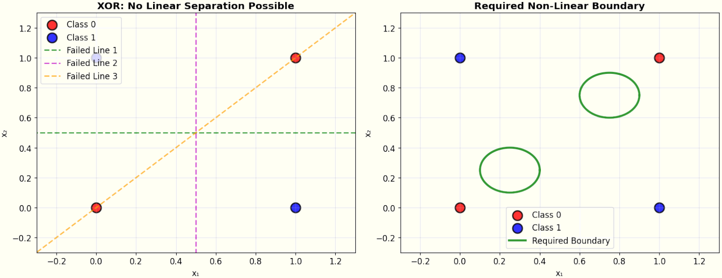
Outline

The XOR Problem: Historical Crisis

XOR Truth Table:

x_1	x_2	y
0	0	0
0	1	1
1	0	1
1	1	0

The Crisis: No single line can separate these classes!



XOR is not linearly separable

True Single-Layer vs Multi-Layer

Critical Distinction:

- **True Single-Layer:** Input → Output (NO hidden layers)
- **Multi-Layer:** Input → Hidden → Output (1+ hidden layers)

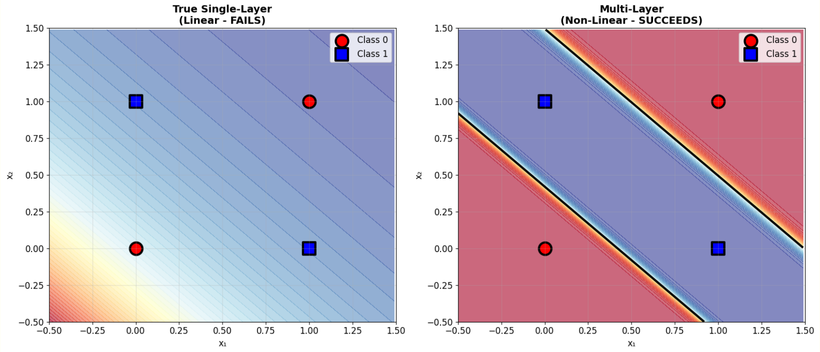
True Single-Layer (fails):

$$y = \sigma(w_1 x_1 + w_2 x_2 + b)$$

Multi-Layer (succeeds):

$$h_1 = \sigma(w_{11} x_1 + w_{12} x_2 + b_1)$$
$$h_2 = \sigma(w_{21} x_1 + w_{22} x_2 + b_2)$$
$$y = \sigma(v_1 h_1 + v_2 h_2 + b_3)$$

XOR Solution: Decision Boundaries



Linear (fails) vs Non-linear (succeeds) decision boundaries

Key Insight: Hidden layers enable curved boundaries through non-linear transformations.

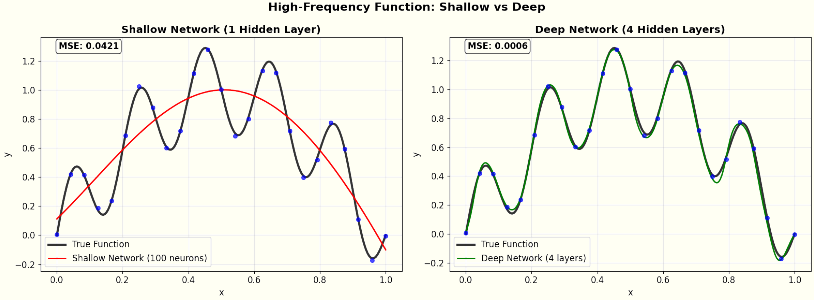
XOR Decomposition:

$$
\begin{aligned}
h_1 &= \sigma(\text{weights}) \quad (\approxeq \text{OR gate}) \\
h_2 &= \sigma(\text{weights}) \quad (\approxeq \text{AND gate}) \\
y &= \sigma(v_1 h_1 + v_2 h_2 + b_3) \quad (\approxeq \text{OR AND NOT})
\end{aligned}
$$

Result: XOR = (OR) AND (NOT AND) = compositional solution!
General Principle: Complex functions = composition of simple functions.

Beyond XOR: High-Frequency Functions

Test Case: $f(x) = \sin(\pi x) + 0.3\sin(10\pi x)$



Shallow (100 neurons) vs Deep (4 layers, 25 each) networks

Result: Deep networks achieve better performance with fewer parameters.

Historical Timeline: From Crisis to Revolution

Year	**Event**	**Impact**
1943	McCulloch-Pitts neuron	Foundation laid
1957	Rosenblatt's Perceptron	First learning success
1969	**Minsky & Papert: XOR**	**Showed limits**
1970s-80s	"AI Winter"	Funding dried up
1986	Backpropagation	Enabled multi-layer training
1989	Universal Approximation	Theoretical foundation
2006+	Deep Learning Revolution	Depth proves essential

Lesson: XOR taught us that depth is necessity, not luxury.

Four Key Insights on Depth

1. **Representation Efficiency**
   - Shallow: May need exponentially many neurons
   - Deep: Hierarchical composition is exponentially more efficient
2. **Feature Hierarchy**
   - Layer 1: Simple features (edges, patterns)
   - Layer 2: Feature combinations (corners, textures)
   - Layer 3+: Complex abstractions (objects, concepts)
3. **Geometric Transformation**
   - Each layer performs coordinate transformation
   - Deep networks "unfold" complex data manifolds
4. **Compositional Learning**
   - Complex functions = composition of simple functions
   - Build complexity incrementally

Summary and Conclusions

Key Takeaways:

- Neural networks learn continuous functions from sparse data
- Nonlinearity is essential for complex function approximation
- Universal Approximation Theorem provides theoretical foundation
- Width increases capacity but depth is more efficient
- Historical XOR problem revealed importance of hidden layers
- Deep networks enable hierarchical feature learning

Applications:

- Scientific computing and PDE solving
- Function approximation and regression
- Pattern recognition and classification
- Physics-informed neural networks (PINNs)

Questions?

Thank you!

Contact:
Krishna Kumar
krishnak@utexas.edu
University of Texas at Austin