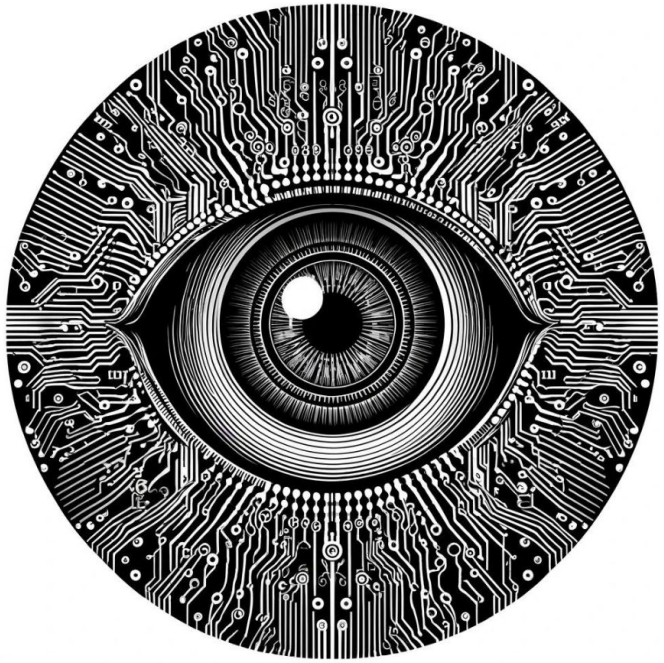
Matrix Multiplication, Non-linear Activations, and Network Shape



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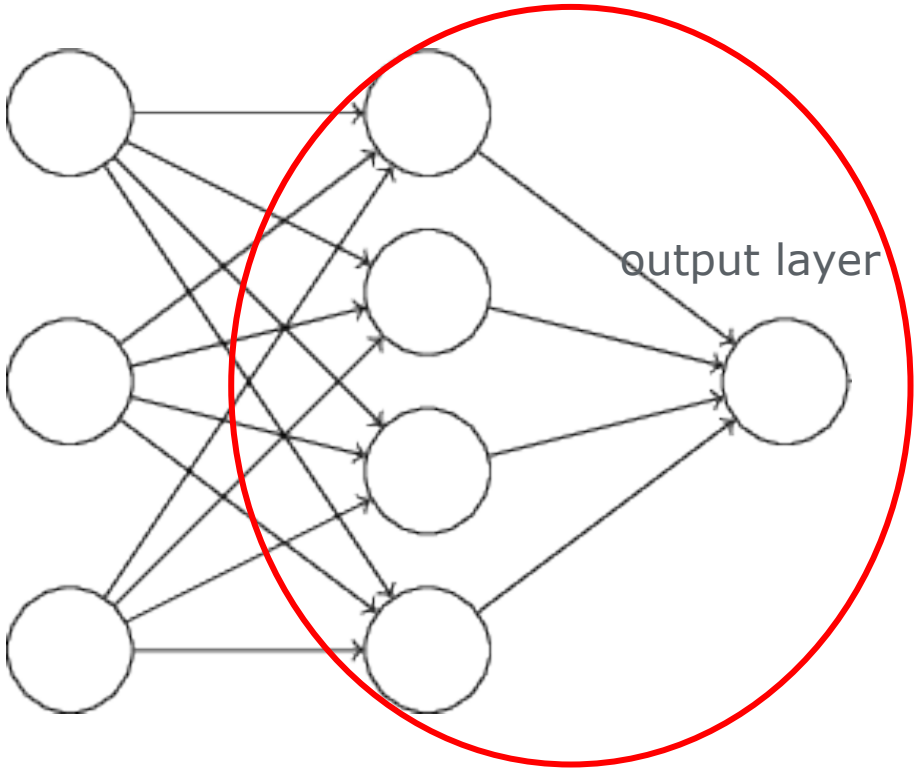
Learning goals

- Understand the correspondence between the matrix multiplication dimensions and the network’s architecture
- Recognize the importance of passing the output of matrix multiplication operations to non-linear activation functions

The feedforward pass - output layer



To compute the **output Z** with **1 unit**:

Explicitly:

$$Z = XW$$

$$Z = \begin{bmatrix} X_1 & X_2 & X_3 & X_4 \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ w_3 \\ w_4 \end{bmatrix}$$

Resulting in a **scalar output**

$$Z = X_1 w_1 + X_2 w_2 + X_3 w_3 + X_4 w_4$$

Matrix multiplication and network shape - output layer

```python
import torch

# Create input with batch_size = 1
batch_size = 1
input_features = 4  # X1, X2, X3, X4 as shown in the image
output_features = 1  # Scalar output Z as shown

# Create input tensor X = [X1, X2, X3, X4]
X = torch.randn(batch_size, input_features)  # Shape: (1, 4)
print(f"Input X: {X[0]}")  # Print without batch dimension for clarity

# Create weights w = [w1, w2, w3, w4]
weights = torch.randn(input_features, output_features)  # Shape: (4, 1)
print(f"Weights w: {weights.squeeze()}")  # Print without extra dimensions

# Approach 1: Direct matrix multiplication (Z = XW)
output_matmul = torch.matmul(X, weights)  # Shape: (1, 1)
print(f"Output using matrix multiplication: {output_matmul.item():.4f}")

# Approach 2: Using nn.Linear
layer = torch.nn.Linear(in_features=input_features,
                        out_features=output_features,
                        bias=False)
```

$$Z = XW$$

$$Z = \begin{bmatrix} X_1 & X_2 & X_3 & X_4 \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ w_3 \\ w_4 \end{bmatrix}$$

$$Z = X_1 w_1 + X_2 w_2 + X_3 w_3 + X_4 w_4$$

Common errors with tensor dimensions

```python
import torch

# Create input with batch_size = 1
batch_size = 1
input_features = 4  # X1, X2, X3, X4 as shown in the image
output_features = 1  # Scalar output Z as shown

# Wrong: Missing batch dimension
X = torch.randn(input_features)  # Shape: (4,) instead of (1,4)
# Error: Expected 2D input, got 1D

# Wrong: Reversed multiplication order
output_matmul = torch.matmul(weights, X)  # Wrong order
# Error: size mismatch, got [4,1] x [1,4]

# Wrong: Inconsistent dimensions
layer = torch.nn.Linear(in_features=3,  # Wrong input size
                        out_features=output_features, bias=False)
# Error: size mismatch, expected input of size [*,3], got [*,4]
```

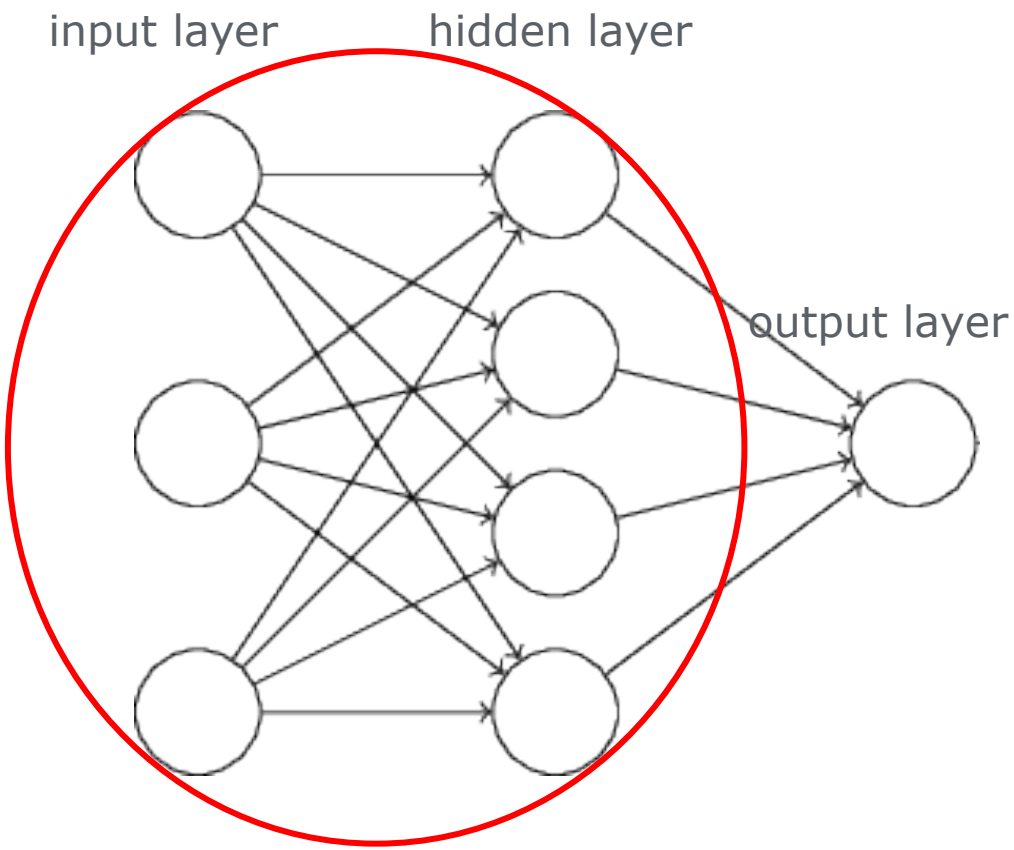
Tip:
always check the shape of tensors with a_tensor.shape or a_tensor.size()

$$Z = XW$$

$$Z = \begin{bmatrix} X_1 & X_2 & X_3 & X_4 \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ w_3 \\ w_4 \end{bmatrix}$$

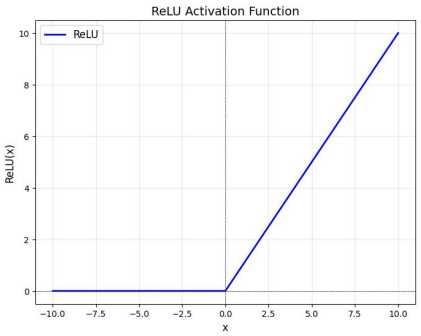
$$Z = X_1 w_1 + X_2 w_2 + X_3 w_3 + X_4 w_4$$

Adding non-linearity between layers



$$Z = ReLU(XW)$$

$$Z = \text{ReLU}\left(\begin{bmatrix} X_1 & X_2 & X_3 \end{bmatrix} \begin{bmatrix} w_{11} & w_{12} & w_{13} & w_{14} \\ w_{21} & w_{22} & w_{23} & w_{24} \\ w_{31} & w_{32} & w_{33} & w_{34} \end{bmatrix} \right)$$

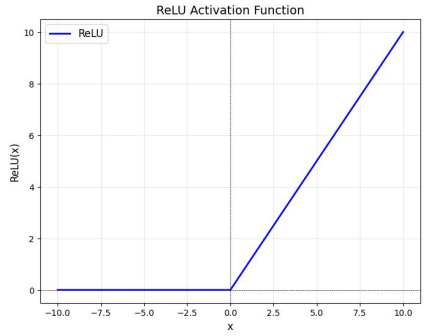


Adding non-linearity between layers

```python
import torch
from torch.nn.parameter import Parameter

X = torch.randn(batch_size, 3)

# Create weight matrix as Parameter
weights = Parameter(torch.randn(3, 4))  # Shape: (3, 4)

# Approach 1: Direct matrix multiplication with ReLU
output_matmul = torch.relu(torch.matmul(X, weights))

# Approach 2: Using nn.Linear with ReLU
layer = torch.nn.Sequential(
    torch.nn.Linear(in_features=input_features,
                    out_features=output_features,
                    bias=False),
    torch.nn.ReLU()
)
```

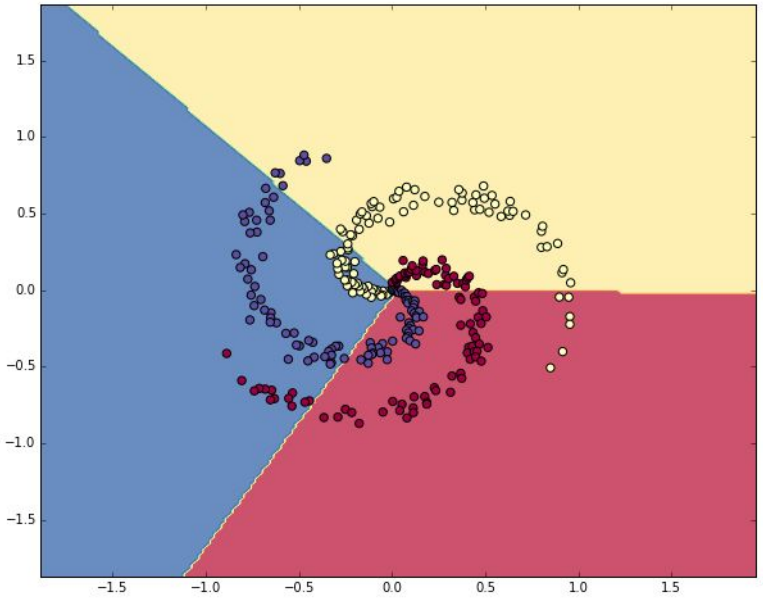
$$Z = ReLU(XW)$$

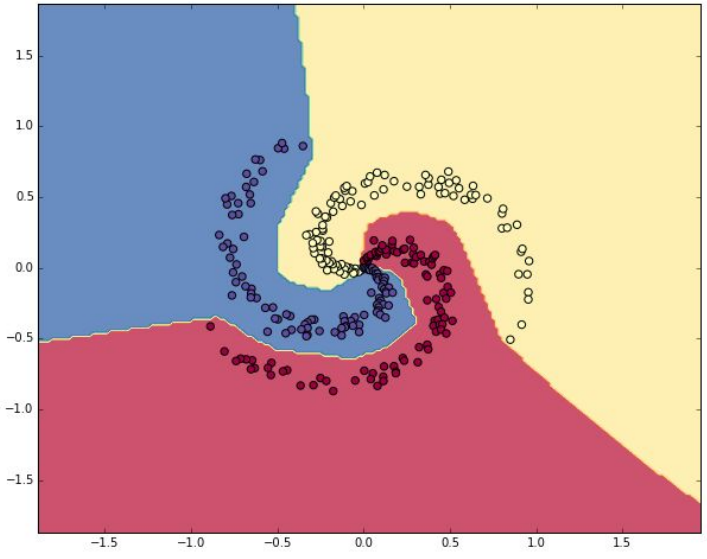
$$Z = \text{ReLU}\left(\begin{bmatrix} X_1 & X_2 & X_3 \end{bmatrix} \begin{bmatrix} w_{11} & w_{12} & w_{13} & w_{14} \\ w_{21} & w_{22} & w_{23} & w_{24} \\ w_{31} & w_{32} & w_{33} & w_{34} \end{bmatrix} \right)$$



Deep learning is the art of making squiggly functions

- Squiggly function = ‘sophisticated decision boundary’
- More weights and non linear activations ~ more squiggly boundaries
-
-





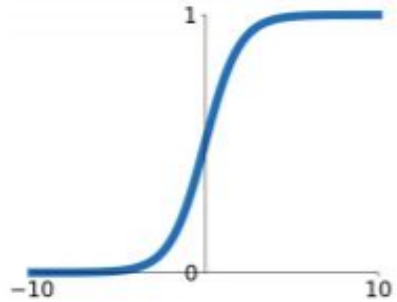
https://cs231n.github.io/neural-networks-case-study
Experiment notebook

Activation functions

ReLU is a good default choice for most problems

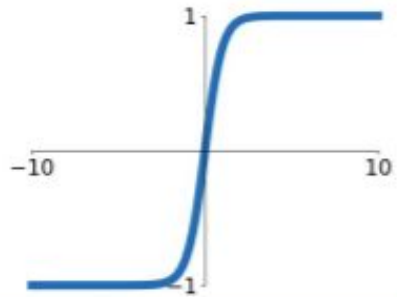
Sigmoid

$$\sigma(x) = \frac{1}{1+e^{-x}}$$



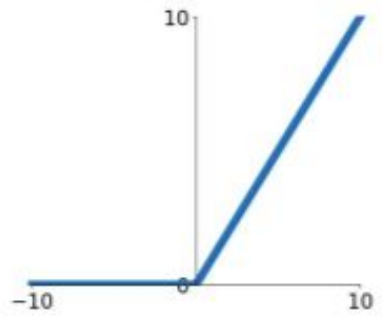
tanh

$$\tanh(x)$$



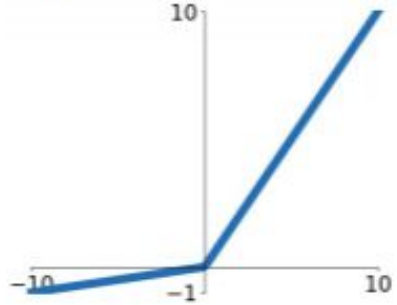
ReLU

$$\max(0, x)$$



Leaky ReLU

$$\max(0.1x, x)$$

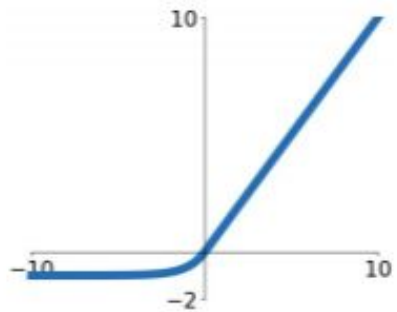


Maxout

$$\max(w_1^T x + b_1, w_2^T x + b_2)$$

ELU

$$\begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$$



Practicing matrix multiplication

$$\begin{bmatrix} 0.1 & 0.2 & 0.3 & 0.4 \end{bmatrix} \times \begin{bmatrix} 0.11 & 0.12 & 0.13 & 0.14 \\ 0.21 & 0.22 & 0.23 & 0.24 \\ 0.31 & 0.32 & 0.33 & 0.34 \\ 0.41 & 0.42 & 0.43 & 0.44 \end{bmatrix} = \begin{bmatrix} 0.31 & 0.32 & 0.33 & 0.34 \end{bmatrix}$$

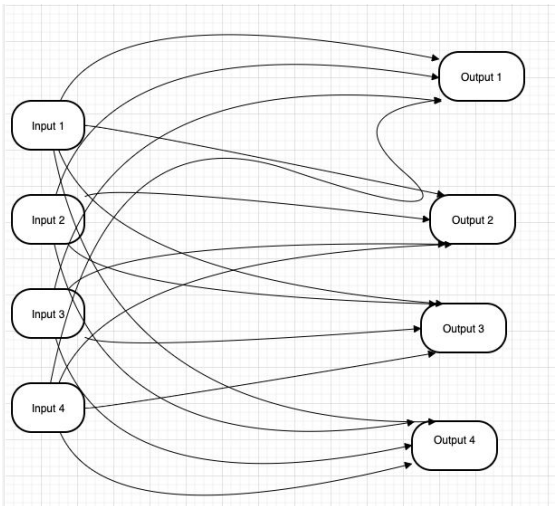
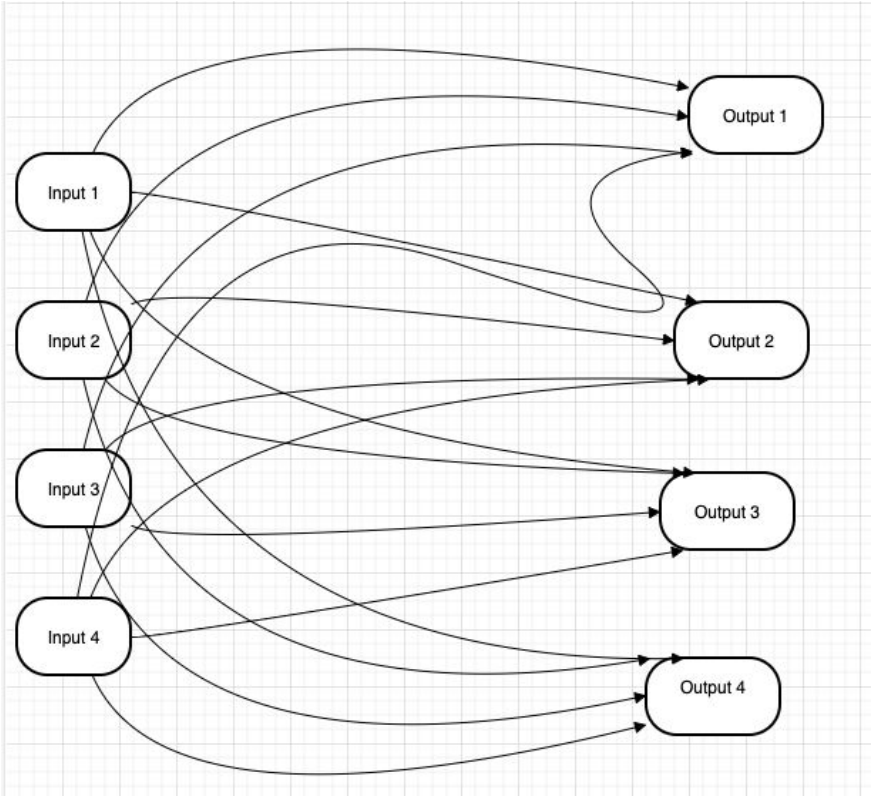


Image from http://matrixmultiplication.xyz/

Practicing matrix multiplication

```python
import torch

# Create the input matrices with exact values from the example
X = torch.tensor([[0.1, 0.2, 0.3, 0.4]], dtype=torch.float32)  # Shape: (1, 4)

W = Parameter(torch.tensor([
   [0.11, 0.12, 0.13, 0.14],
   [0.21, 0.22, 0.23, 0.24],
   [0.31, 0.32, 0.33, 0.34],
   [0.41, 0.42, 0.43, 0.44]
], dtype=torch.float32))  # Shape: (4, 4)

# Perform matrix multiplication
result = torch.matmul(X, W)

# Print results with clear formatting
print("Matrix multiplication verification:")
print(f"Input shape: {X.shape}")
print(f"Weight shape: {W.shape}")
print(f"Output shape: {result.shape}")
```



Summary

Matrix multiplication fundamentals

- Matrix shapes determine network architecture
- Input dimension (n,m) maps to weight matrix (m,p) producing output of (n, p)

Implementation in PyTorch

- `torch.matmul` provides direct matrix multiplication
- `nn.Linear` layer add structure for neural networks
- Shape verification prevents common errors (e.g. `tensor_name.shape`)

Beyond linear operations

- Non-linear functions like ReLU enable the learning of complex patterns and must be added to the output of matrix multiplication operations

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Further reading and references

torch.matmul

- https://pytorch.org/docs/main/generated/torch.matmul.html

A case study on neural network training

- https://cs231n.github.io/neural-networks-case-study/

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