Imperial College London

THE THOMAS YOUNG CENTRE TyC

Machine Learning for Materials

6. Artificial Neural Networks

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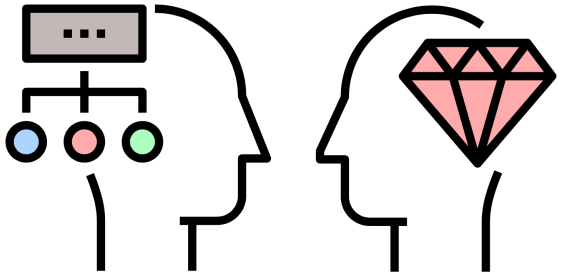


Course Contents

1. Course Introduction
2. Materials Modelling
3. Machine Learning Basics
4. Materials Data and Representations
5. Classical Learning
6. **Artificial Neural Networks**
7. Building a Model from Scratch
8. Recent Advances in AI
9. and 10. Research Challenge

Class Outline

Artificial Neural Networks

A. From neuron to perceptron

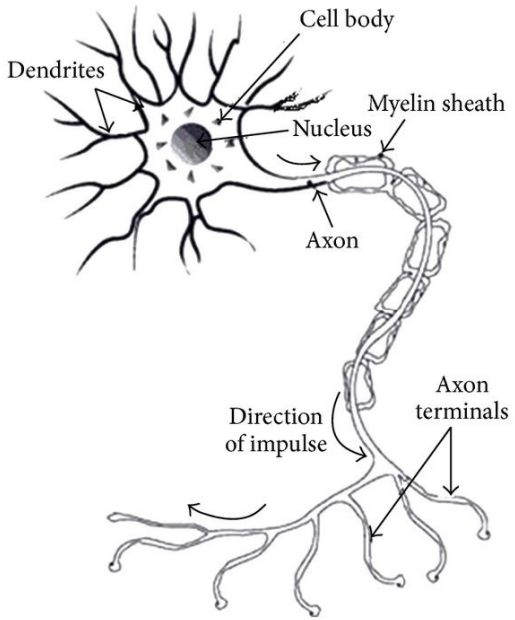
B. Network architecture and training

C. Convolutional neural networks

Artificial Neuron

Neurons transmit chemical and electrical signals in the brain. Artificial neurons mimics this behaviour using mathematical functions

Biological neuron	Artificial neuron
Cell nucleus	Node
Dendrites	Input
Synapse	Weights (Interconnects)
Axon	Output



The human brain has ~ 10^{11} neurons and 10^{15} synapses (~10^{15} FLOPS)

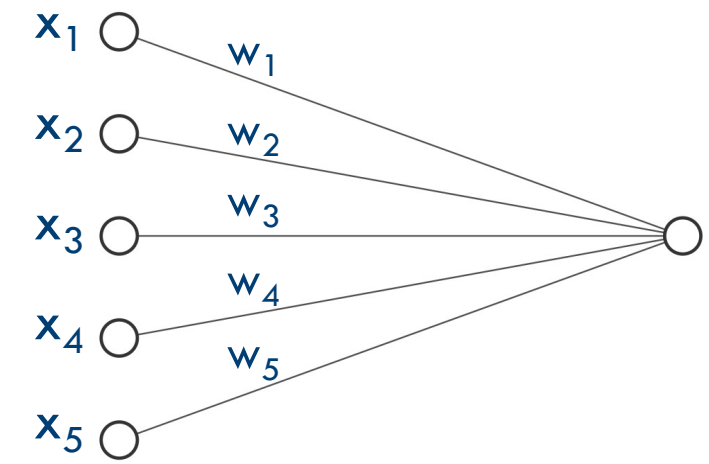
Image: BioMed Research International

Artificial Neuron

The perceptron is a binary neural network classifier: weighted inputs produce an output of 0 or 1

Output: y = Weighted input: $f(\mathbf{w}\cdot\mathbf{x}+b)$

Activation function: f — Bias (constant): b



if $\sum x_i w_i + b >$ **threshold:**

output = 1

else

output = 0

Weights are adjusted to minimise the model error

F. Rosenblatt, Cornell Aeronautical Laboratory, Report 85-460-1 (1957)

```python
def perceptron(x, w, b):
    """
    Computes the output of a perceptron given inputs x, weights w, and bias b.

    Args:
    x: a list or numpy array of input features
    w: a list or numpy array of weights
    b: a scalar bias term

    Returns:
    The output of the perceptron, computed from a binary step function.
    """
    z = sum([x_i * w_i for x_i, w_i in zip(x, w)]) + b
    return 1 if z >= 0 else 0
```

Note the function “zip” pairs the elements of **x** and **w** together in tuples

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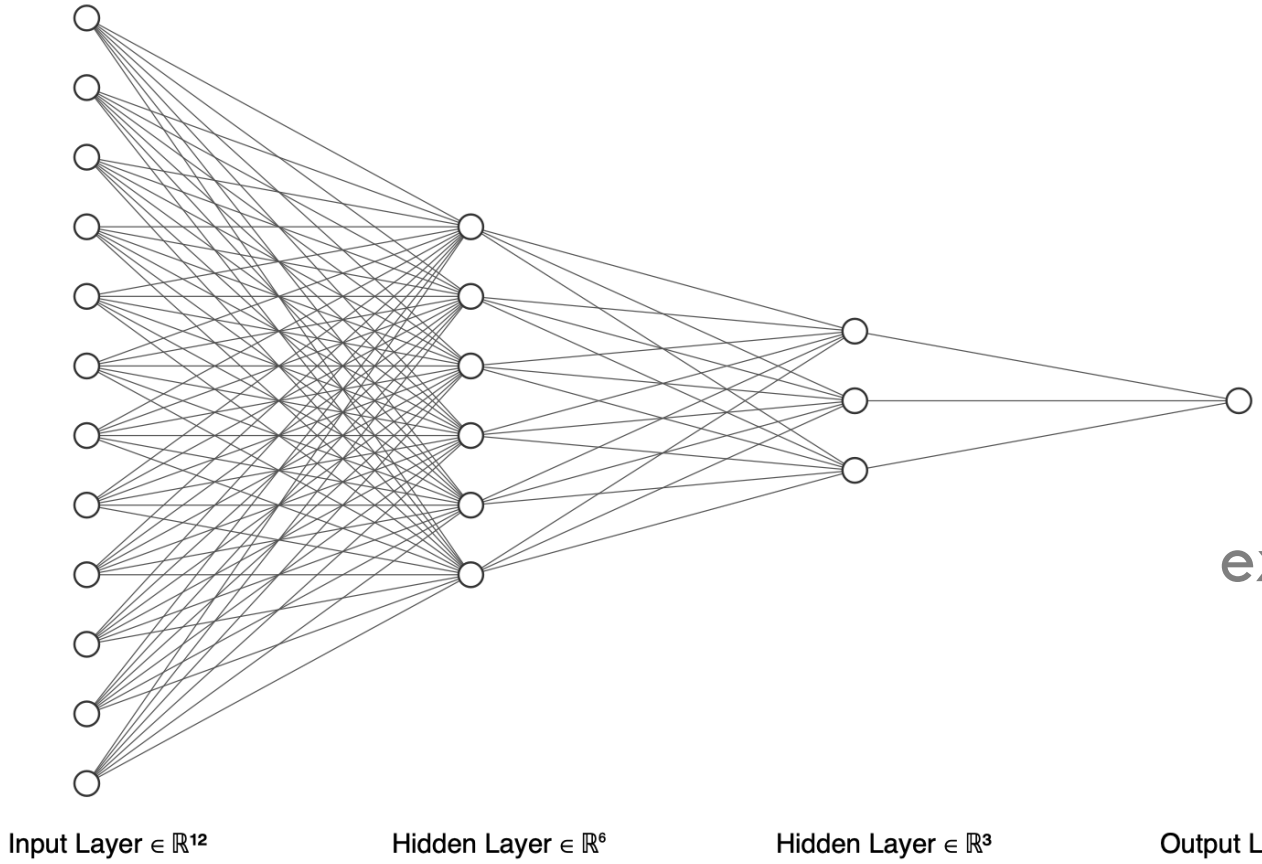
Neural Network Architecture

Basic neural network: One or two layers

Deep neural network: Three or more layers



Three layer model

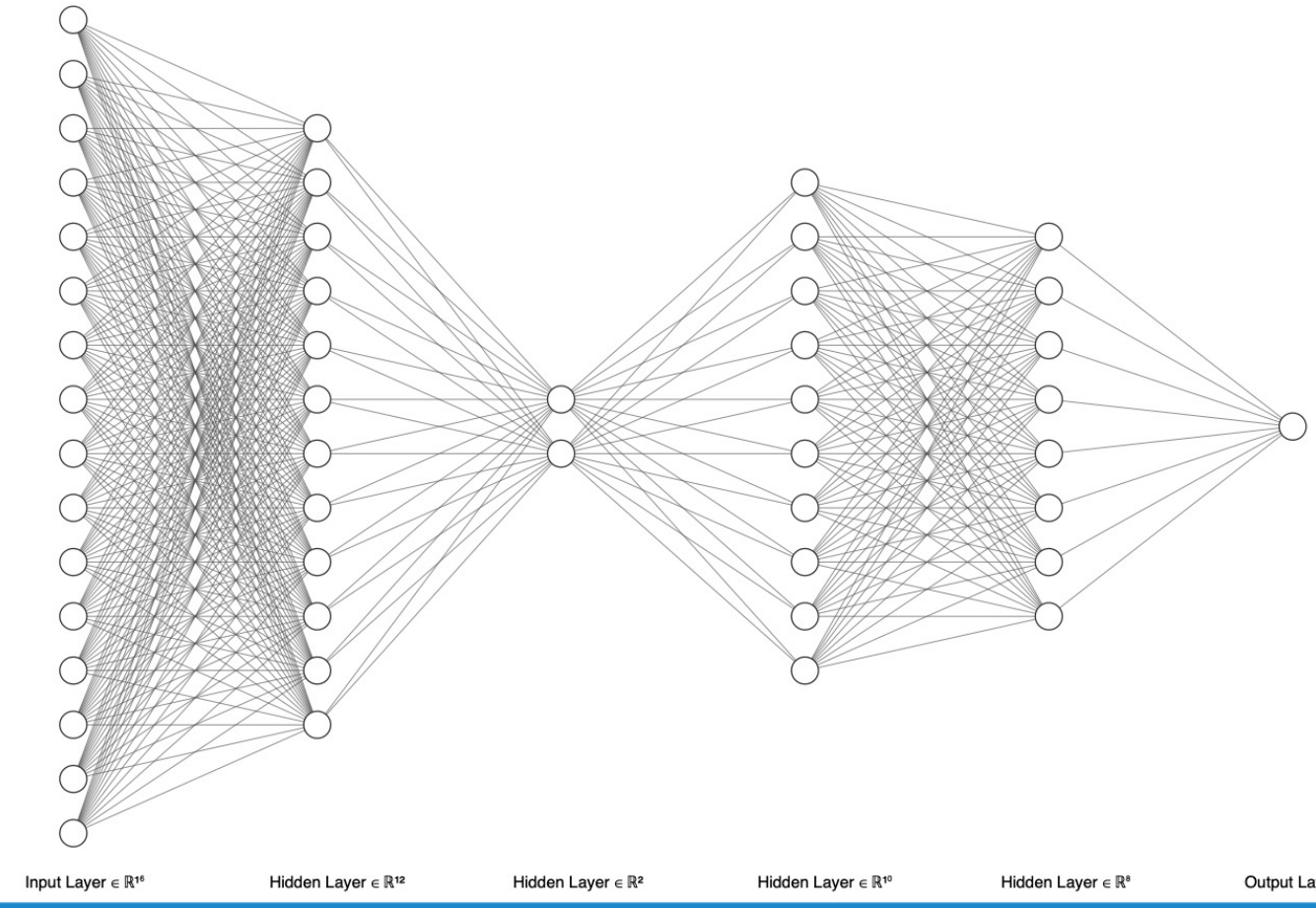
(input layer is excluded in counting)

Image generator: https://alexlenail.me/NN-SVG

Neural Network Architecture

Basic neural network: One or two layers

Deep neural network: Three or more layers



Five layer model

Note the layer 2 bottleneck

Why? Compressed representation

Image generator: https://alexlenail.me/NN-SVG

Activation Function

w·x+b is simply a linear combination.

Activation function ***f*(w·x+b)** introduces non-linearity

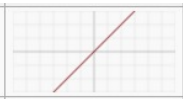
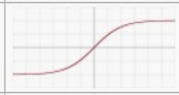
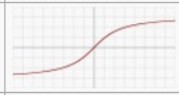
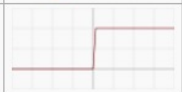
		Activation function	Derivative	
Identity		$f(x) = x$	$f'(x) = 1$	
Binary step		$f(x) = \begin{cases} 0 & \text{for } x < 0 \\ 1 & \text{for } x \geq 0 \end{cases}$	$f'(x) = \begin{cases} 0 & \text{for } x \neq 0 \\ ? & \text{for } x = 0 \end{cases}$	Perceptron model
Logistic (a.k.a Soft step)		$f(x) = \frac{1}{1+e^{-x}}$	$f'(x) = f(x)(1-f(x))$	Popular in early models
TanH		$f(x) = \tanh(x) = \frac{2}{1+e^{-2x}} - 1$	$f'(x) = 1 - f(x)^2$	
ArcTan		$f(x) = \tan^{-1}(x)$	$f'(x) = \frac{1}{x^2+1}$	
Rectified Linear Unit (ReLU)		$f(x) = \begin{cases} 0 & \text{for } x < 0 \\ x & \text{for } x \geq 0 \end{cases}$	$f'(x) = \begin{cases} 0 & \text{for } x < 0 \\ 1 & \text{for } x \geq 0 \end{cases}$	Common for deep learning
Parameteric Rectified Linear Unit (PReLU) [2]		$f(x) = \begin{cases} \alpha x & \text{for } x < 0 \\ x & \text{for } x \geq 0 \end{cases}$	$f'(x) = \begin{cases} \alpha & \text{for } x < 0 \\ 1 & \text{for } x \geq 0 \end{cases}$	
Exponential Linear Unit (ELU) [3]		$f(x) = \begin{cases} \alpha(e^x - 1) & \text{for } x < 0 \\ x & \text{for } x \geq 0 \end{cases}$	$f'(x) = \begin{cases} f(x) + \alpha & \text{for } x < 0 \\ 1 & \text{for } x \geq 0 \end{cases}$	
SoftPlus		$f(x) = \log_e(1 + e^x)$	$f'(x) = \frac{1}{1+e^{-x}}$	Common for deep learning

Image from https://towardsdatascience.com

Activation Function

Corresponding weights and thresholds are learned (fit) during model training

		Activation function	Derivative	
Identity		$f(x) = x$	$f'(x) = 1$	
Binary step		$f(x) = \begin{cases} 0 & \text{for } x < 0 \\ 1 & \text{for } x \geq 0 \end{cases}$	$f'(x) = \begin{cases} 0 & \text{for } x \neq 0 \\ ? & \text{for } x = 0 \end{cases}$	Perceptron model
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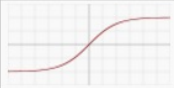
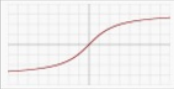
TanH		$f(x) = \tanh(x) = \frac{2}{1+e^{-2x}} - 1$	$f'(x) = 1 - f(x)^2$	
ArcTan		$f(x) = \tan^{-1}(x)$	$f'(x) = \frac{1}{x^2+1}$	
Rectified Linear Unit (ReLU)		$f(x) = \begin{cases} 0 & \text{for } x < 0 \\ x & \text{for } x \geq 0 \end{cases}$	$f'(x) = \begin{cases} 0 & \text{for } x < 0 \\ 1 & \text{for } x \geq 0 \end{cases}$	Common for deep learning
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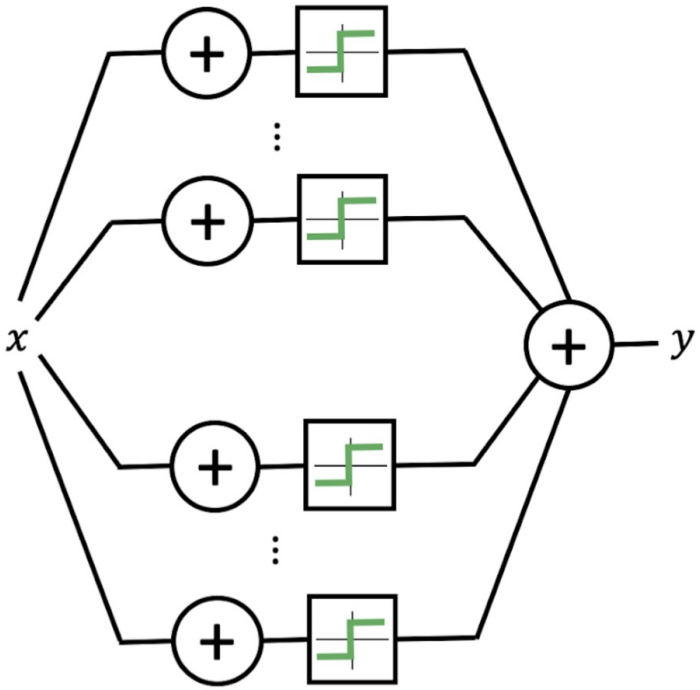
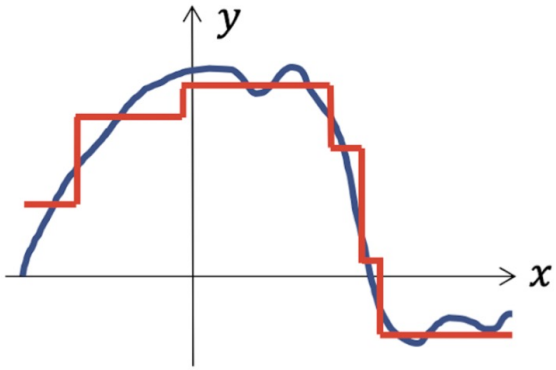
Image from https://towardsdatascience.com

Universal Function Approximators

Multilayer neural networks can approximate any continuous function to any desired accuracy





Practical performance will depend on the number of hidden layers, choice of activation function, and training data available

K. Hurt, M. Stinchcombe and H. White, Neural Networks 2, 359 (1989)

Universal Function Approximators

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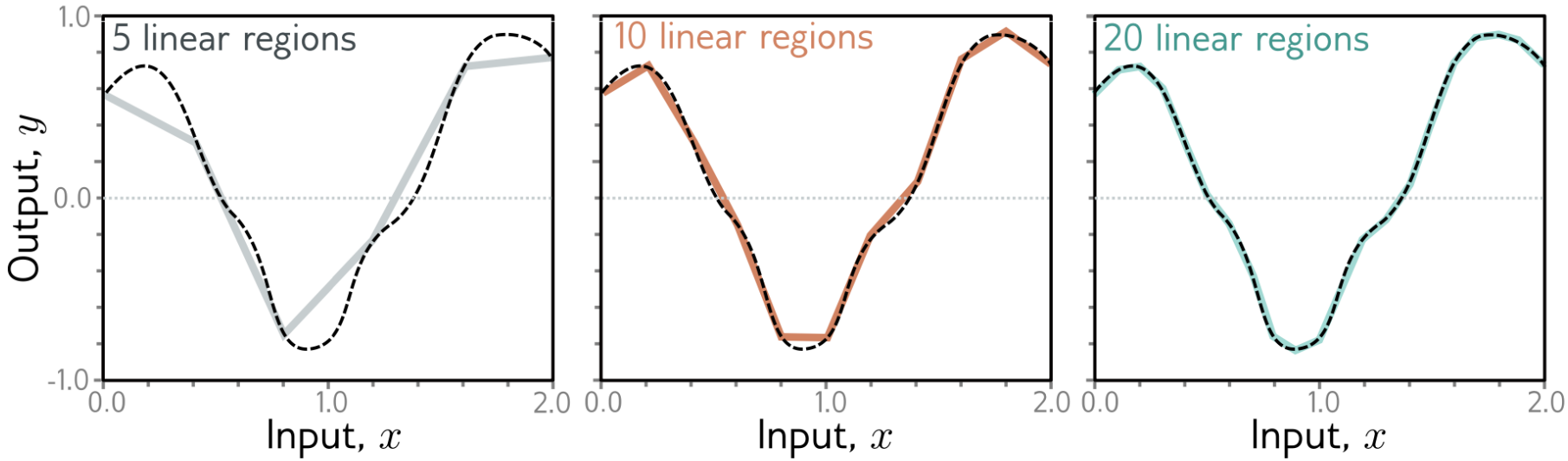
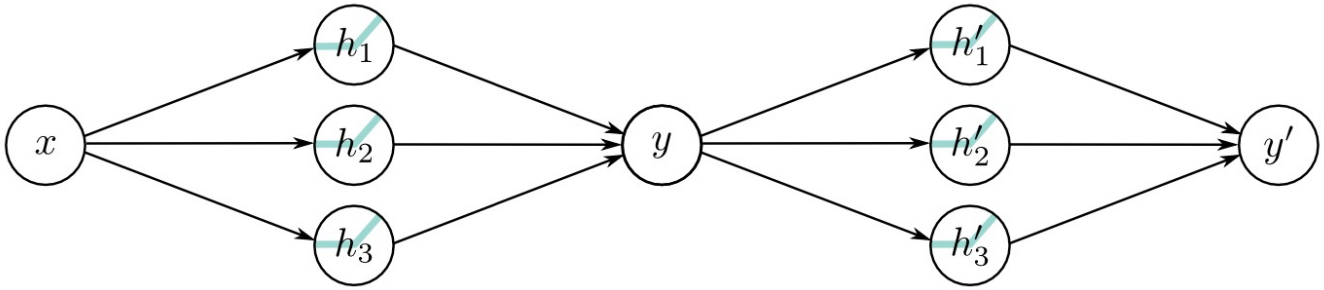
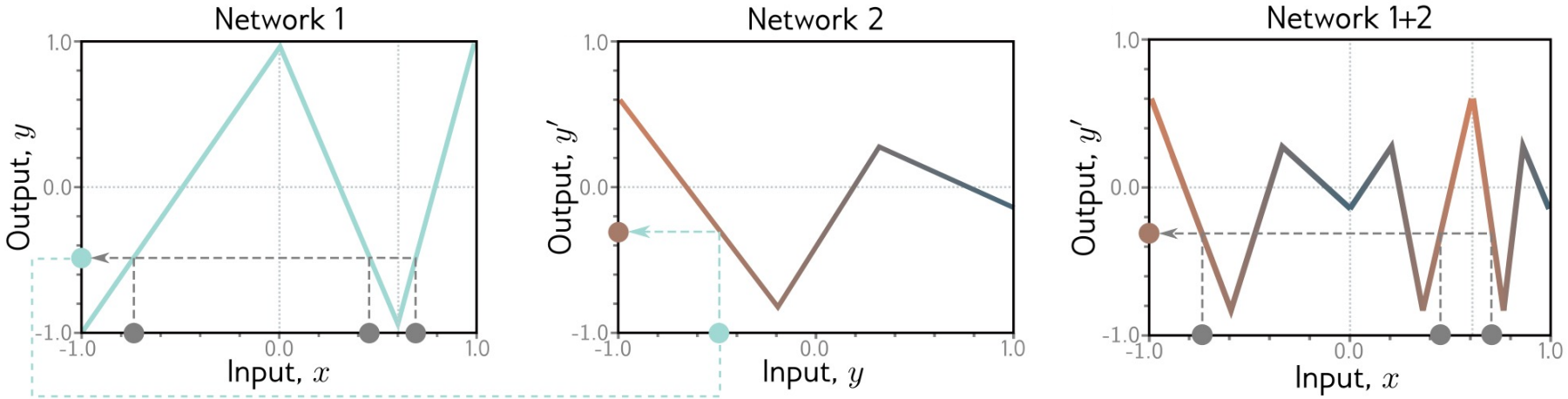


Approximation of a 1D function (dashed line) by a piecewise linear model

Universal Function Approximators



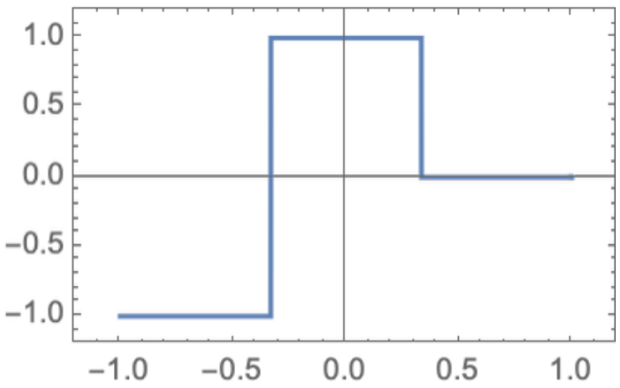


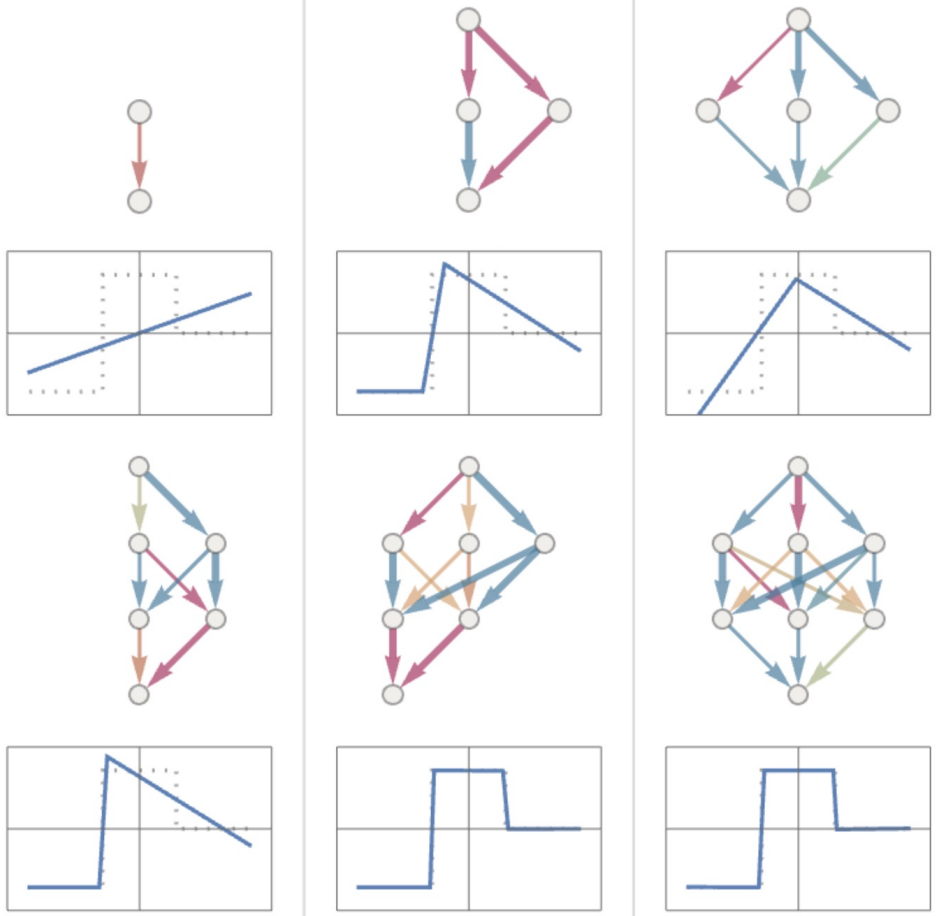
The combination of two single-layer networks with three hidden units each

Universal Function Approximators

Performance depends on model architecture

Target function





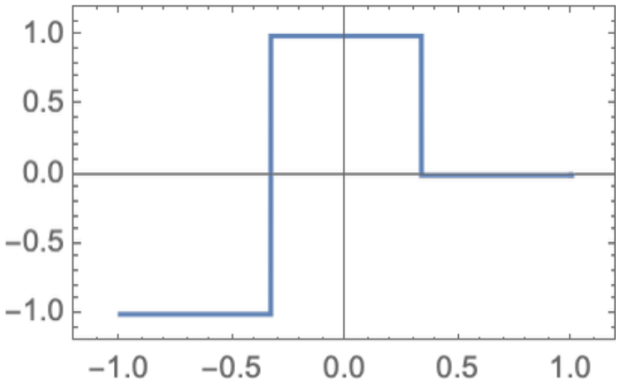
Optimal trained model for each network

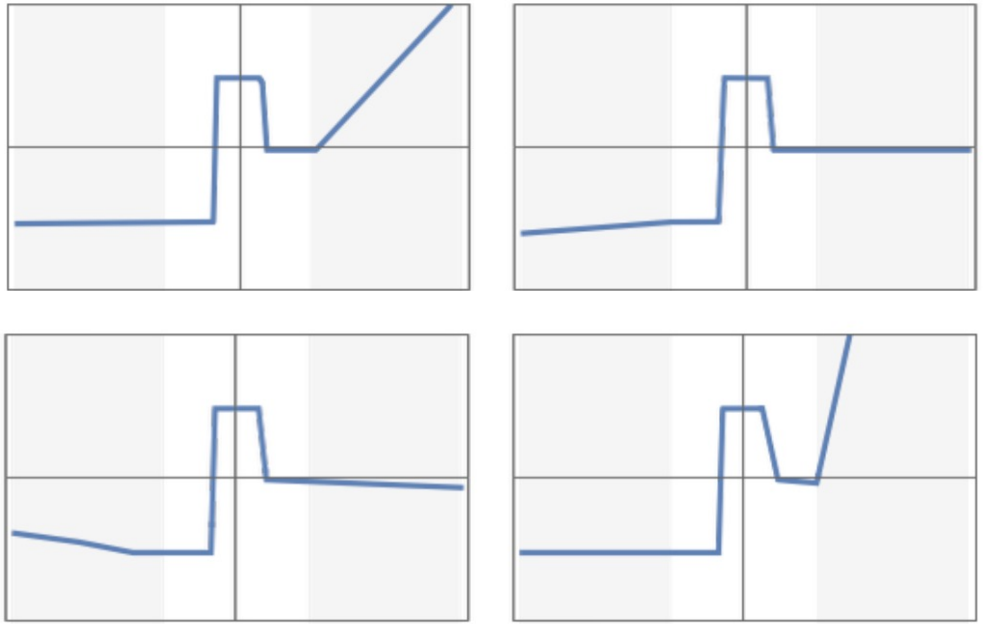
Example from https://writings.stephenwolfram.com

Universal Function Approximators

Extrapolation outside training region is not guaranteed (no fixed functional form)

Target function





Four models with similar training accuracy (in the white region)

Types of Layer in Deep Learning

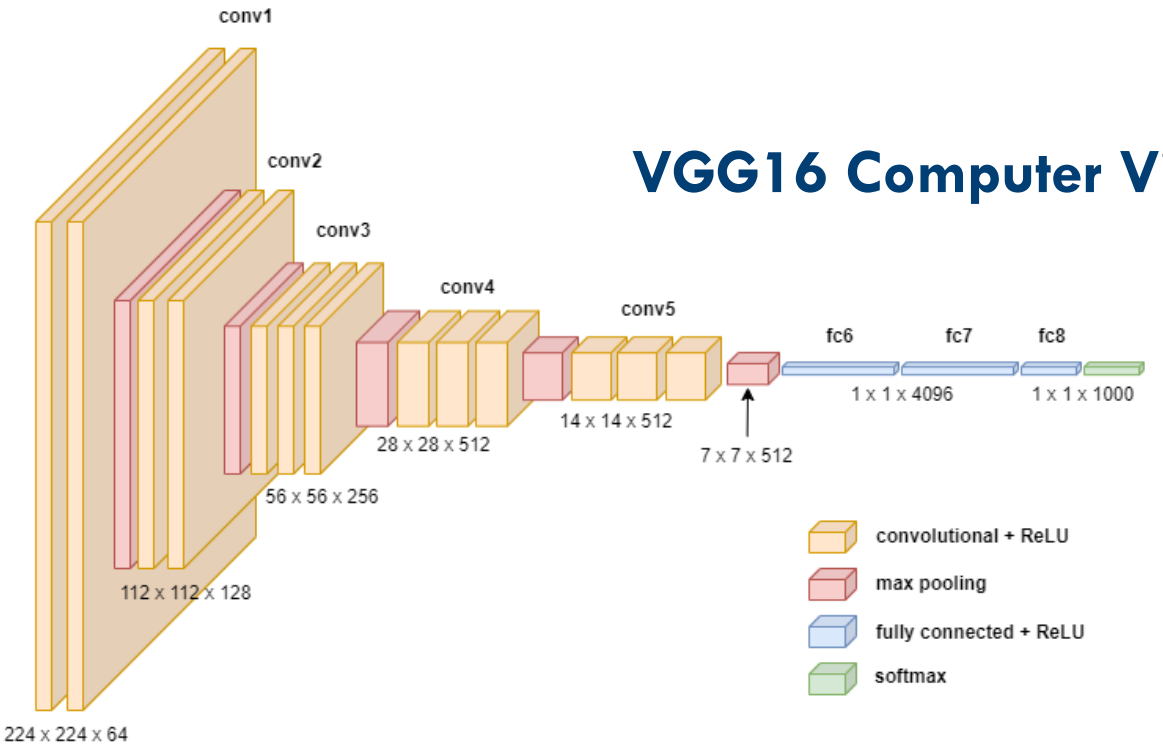
Layers are combined to learn representations and capture data patterns effectively

- **Dense (fully connected):** neurons connected to every other neuron
- **Convolutional:** filter applied to grid-like input, extracting features
- **Pooling:** reduce spatial dimensions, retaining key information
- **Recurrent:** incorporate feedback loops for sequential data flow
- **Dropout:** randomly zero out inputs to mitigate overfitting in training
- **Embedding:** map categorical variables into continuous vectors
- **Upscaling:** increase spatial resolution of feature maps

Self-study is needed if you want to get deeper into these (beyond our scope)

Towards State of the Art (SOTA)

Modern deep learning models combine many layer types with 10^3-10^{12} parameters



VGG16 Computer Vision Model

Softmax is an activation function common in the output layer of a neural network for classification tasks

Example from https://towardsdatascience.com

Towards State of the Art (SOTA)

Modern deep learning models combine many layer types with 10^3-10^{12} parameters

Input vector

$$\begin{bmatrix} 3 \\ 6 \\ 7 \\ 11 \\ 4 \end{bmatrix}$$

Softmax

$$\sigma(z_i) = \frac{e^{z_i}}{\sum_{j=1}^{n} e^{z_j}}$$

Partition function

Class probability

$$\begin{bmatrix} 0.00 \\ 0.03 \\ 0.04 \\ 0.92 \\ 0.01 \end{bmatrix}$$

Appearance of the Boltzmann distribution

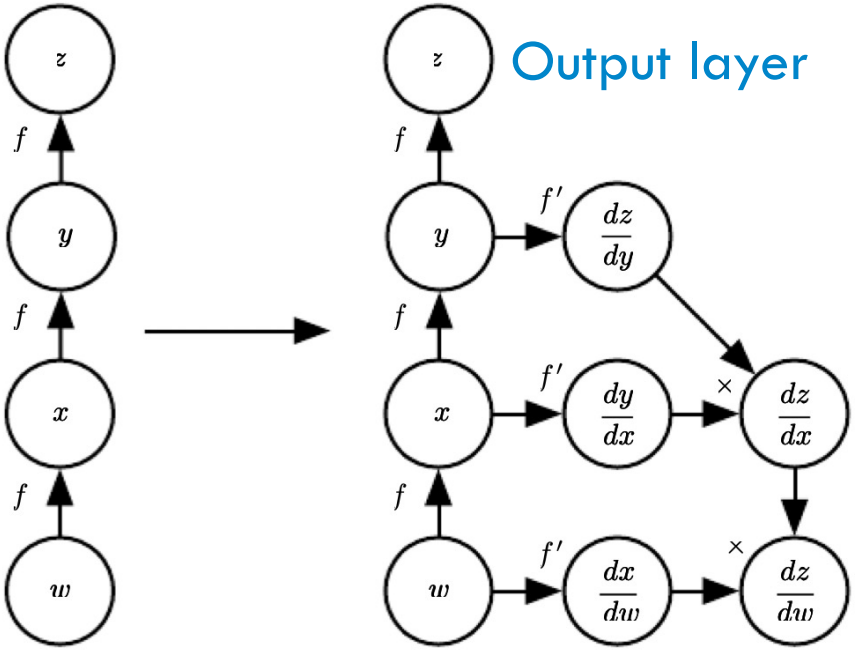
(recall your thermodynamics lectures)

Example from https://towardsdatascience.com

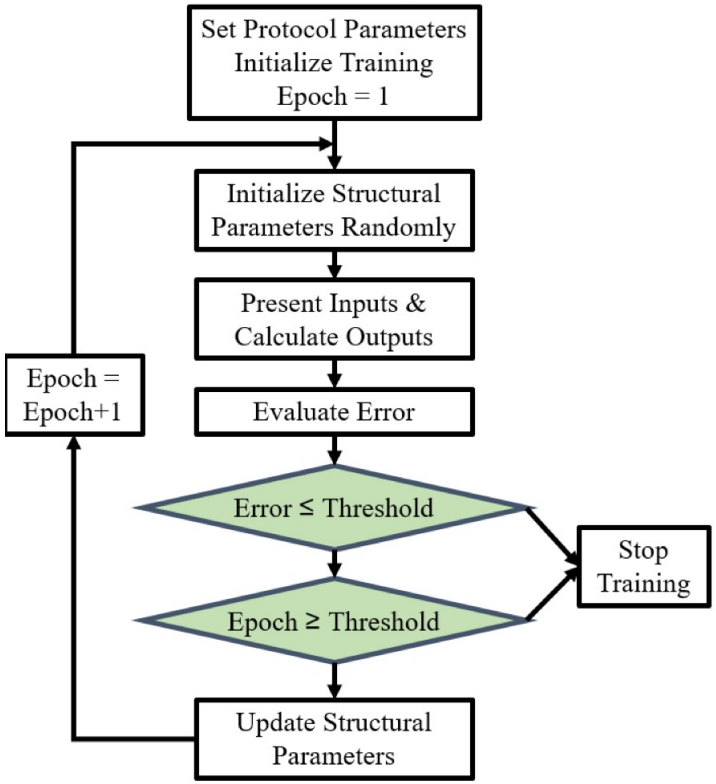
Backpropogation (Backprop)

An algorithm used to adjust the weights of a neural network using gradient descent (from the output layer)

Application of the chain rule



Training iteration



I. Goodfellow, Y Bengio, A. Courville, "Deep Learning"

Backpropogation (Backprop)

Backprop efficiently computes gradients, enabling networks to learn parameters by error minimisation

Limitations

- Slow training
- Failure to converge
- Local minima

Improvements

- Stochastic gradient descent (use random subset of data)
- Batch normalisation (avoid vanishing gradients)
- Adaptive learning rates (more robust convergence)

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Quiz

What features could you use to separately cluster dogs and cats?

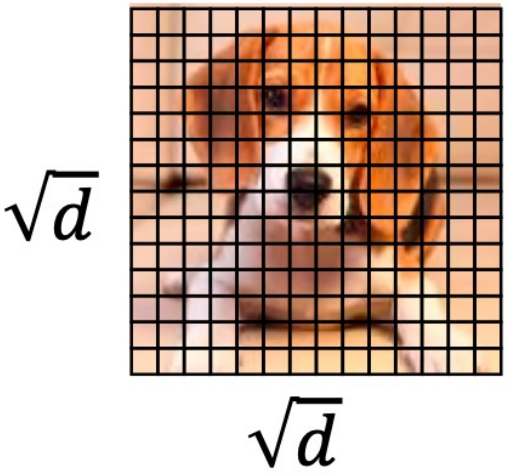
Image from https://www.halifaxhumanesociety.org

Images as Arrays

Pixels are a convenient representation, but inefficient, e.g. 1 MP image = 1,000,000 pixels

Image

Array of pixels



Feature vector

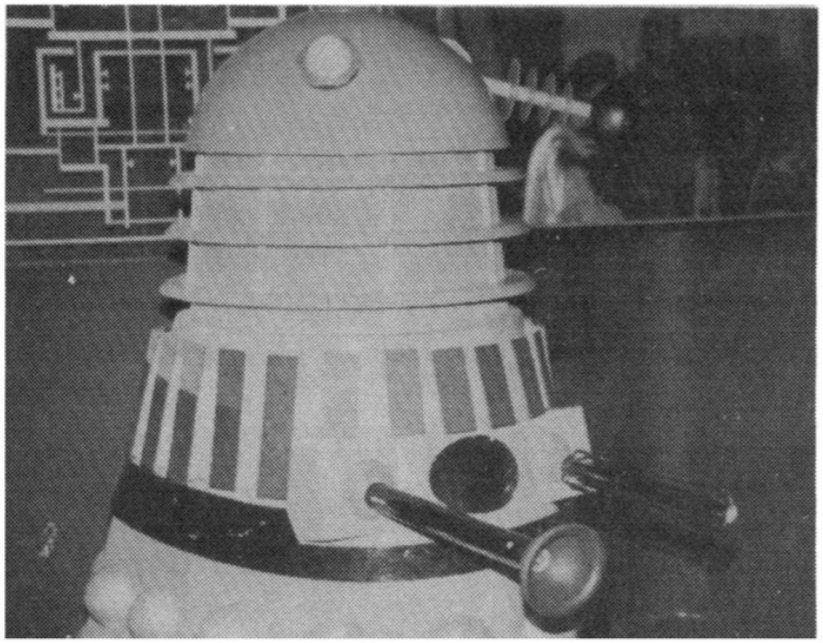
Decision boundaries are difficult to define, e.g. to distinguish between animals based on pixels alone

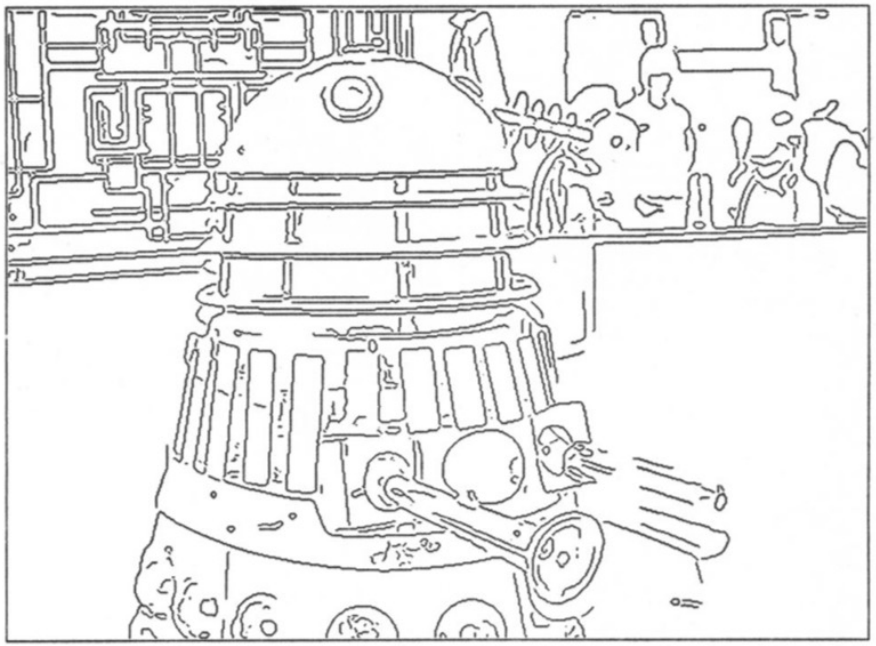
Image: Eric Eaton and Dinesh Jayaraman (Penn Engineering)

Feature Identification

Significant progress has been made for image processing in the field of computer vision

Algorithmic edge detection (e.g. intensity gradients)





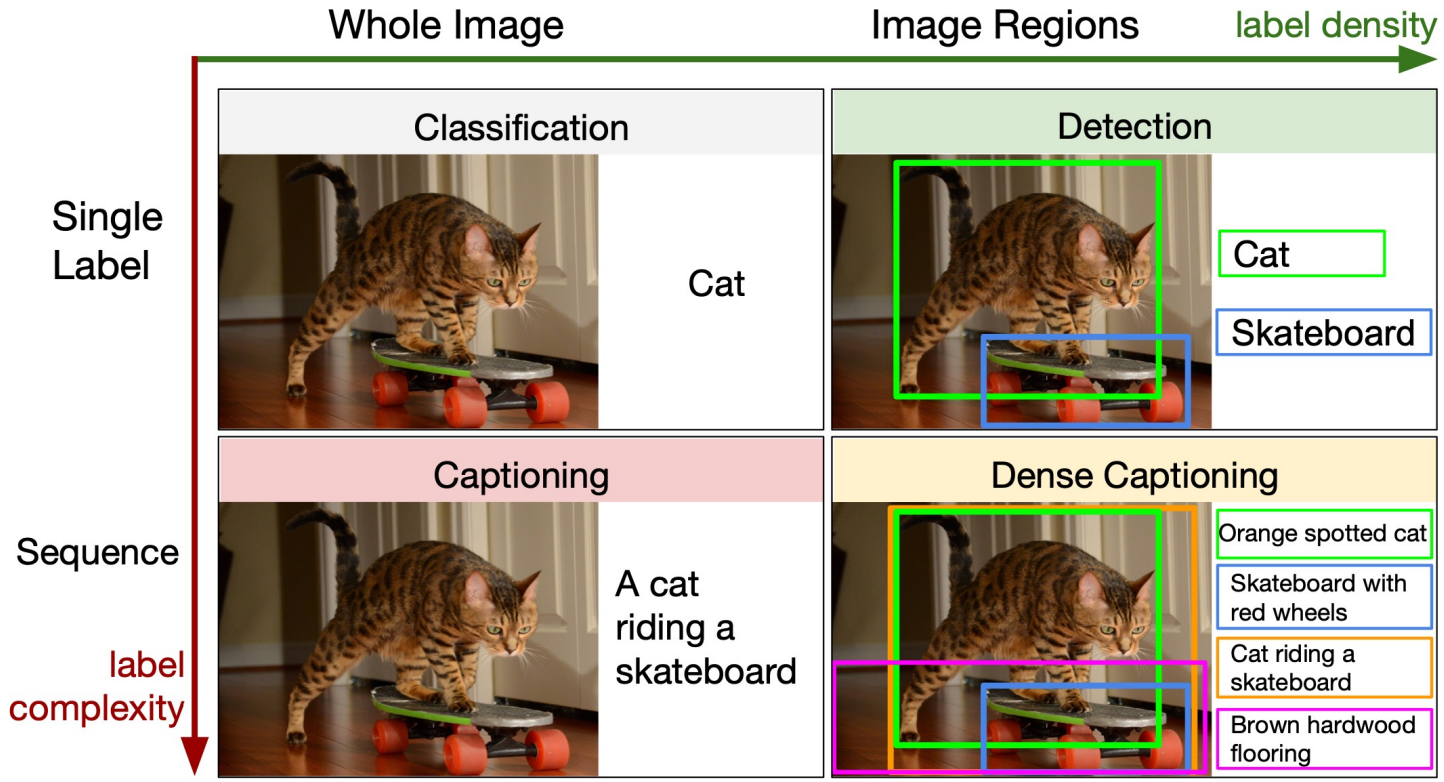
Popular packages for classical filters include imagej and scikit-image

J. Canny, IEEE Trans. Pat. Anal. Mach. Intell. 6, 679 (1986)

Feature Identification

Significant progress has been made in the field of computer vision

Deep learning image and language model (e.g. DenseCap)

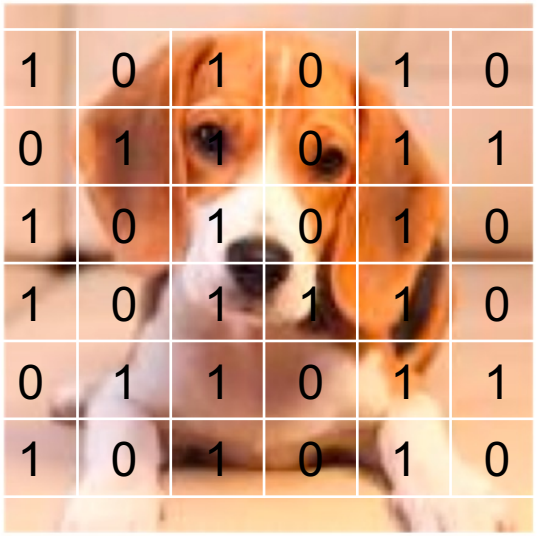


J. Johnson, A. Karpathy, L. Fei-Fei, arXiv:1511.07571 (2015)

Feature Identification

Each layer in a deep neural network can improve the representation of the preceding layer

Image



Classification model

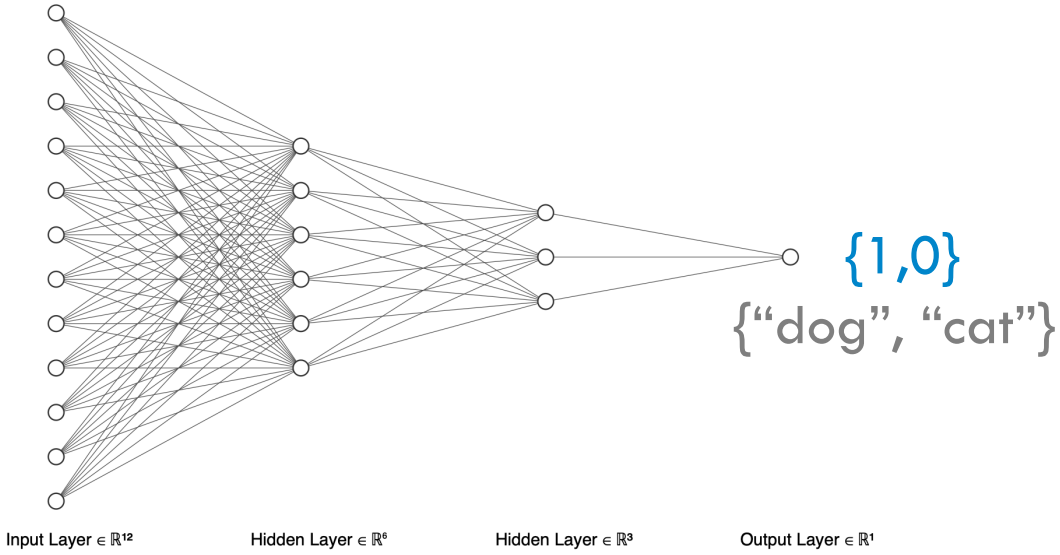


Image: Eric Eaton and Dinesh Jayaraman (Penn Engineering)

Convolutional Filters

Small matrices (kernels) to extract features from data by performing localised operations

2D input data

1	0	1	0	1	0
0	1	1	0	1	1
1	0	1	0	1	0
1	0	1	1	1	0
0	1	1	0	1	1
1	0	1	0	1	0

*

Kernel (filter)

1	2	3
4	5	6
7	8	9

learned weights

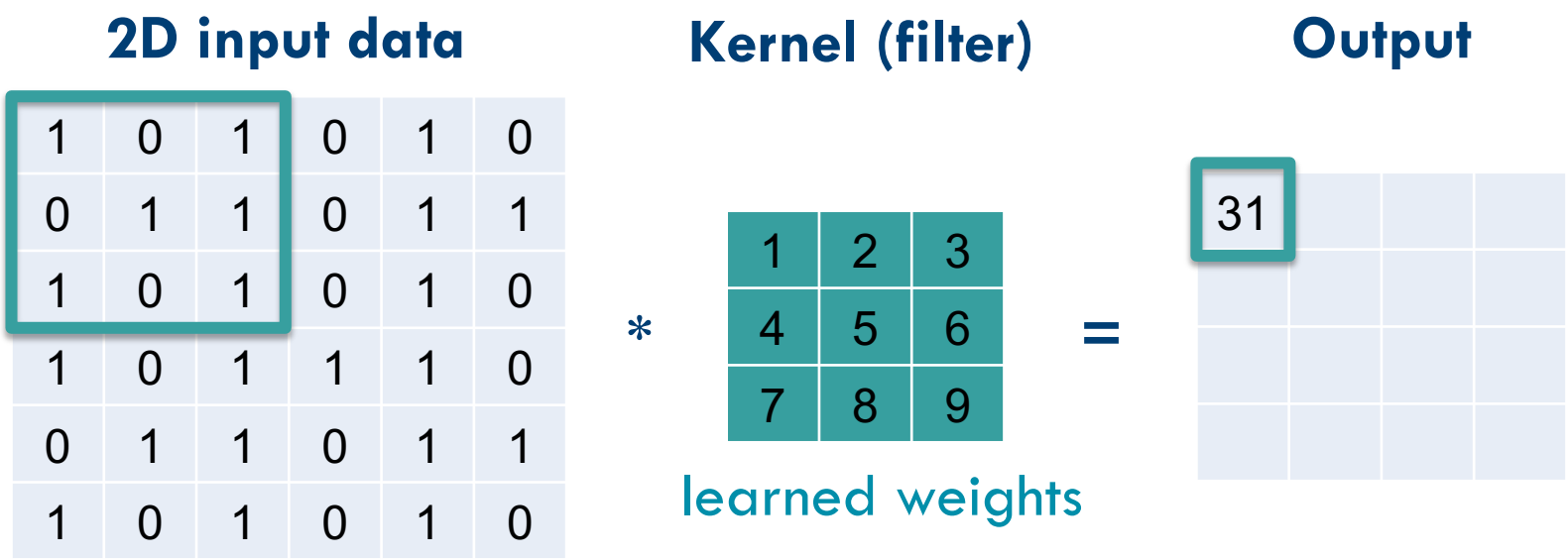
=

Output

Kernel passes over the input data, capturing patterns at different locations, enabling the network to learn and detect specific features

Convolutional Filters

Small matrices (kernels) to extract features from data by performing localised operations



Sum of element-wise products:

1*1+0*2+1*3+0*4+1*5+1*6+1*7+0*8+1*9 = 31

Filters can be made translation and rotational invariant (equivariant deep learning)

Convolutional Filters

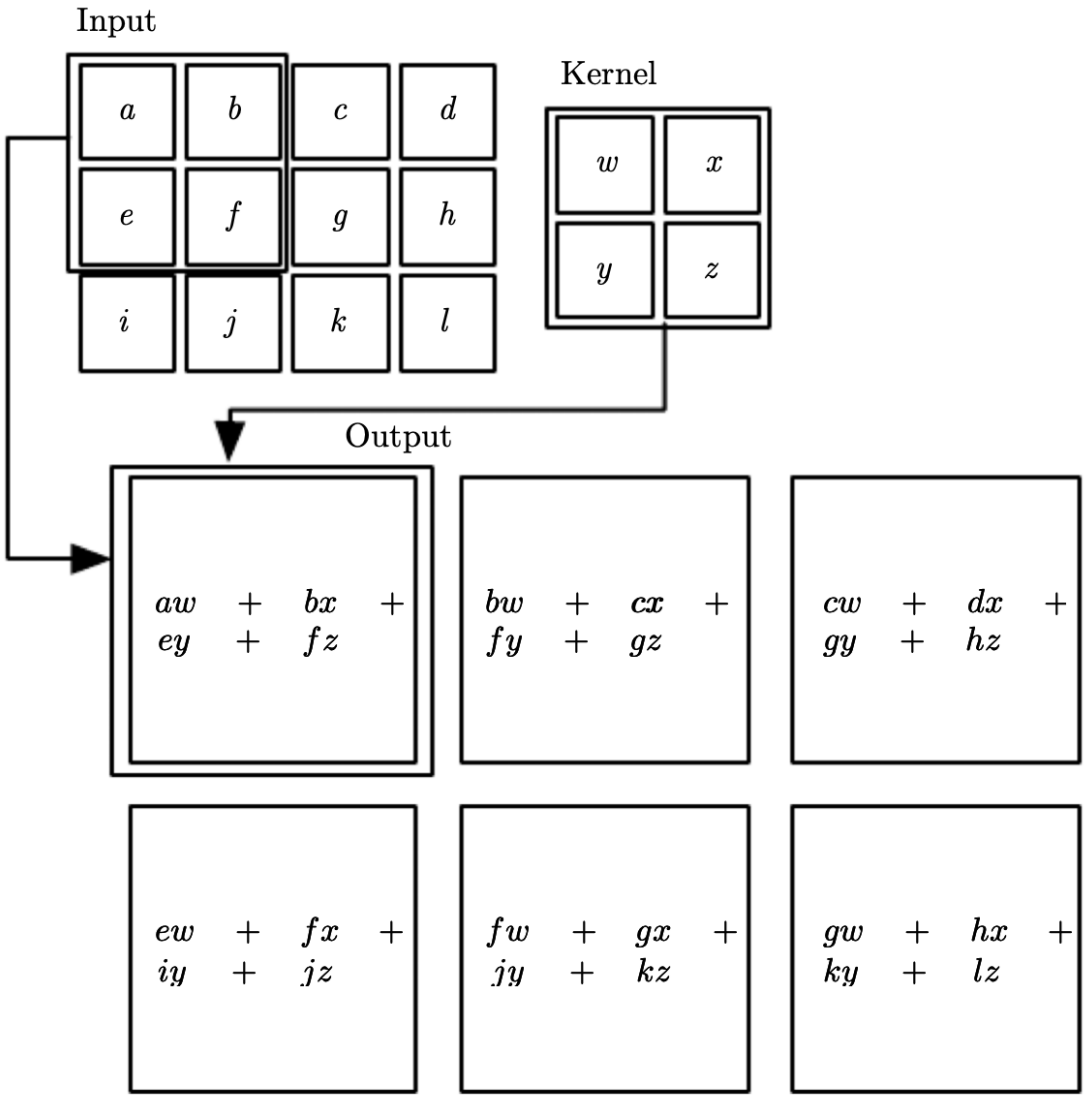


Image: I. Goodfellow, Y Bengio, A. Courville, "Deep Learning"

Quiz

What would these kernels do to an image?

Kernel A

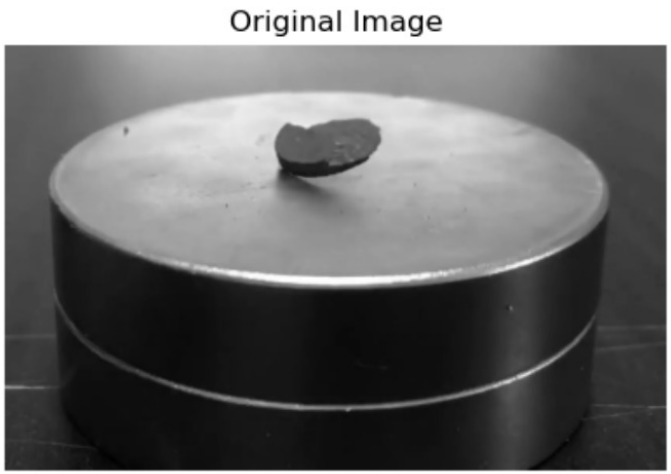
1/9	1/9	1/9
1/9	1/9	1/9
1/9	1/9	1/9

Kernel B

-1	-1	-1
2	2	2
-1	-1	-1

Kernel C

-1	-1	-1
-1	8	-1
-1	-1	-1



An image of the proposed room-temperature superconductor LK-99

Quiz

What would these kernels do to an image?

Kernel A

1/9	1/9	1/9
1/9	1/9	1/9
1/9	1/9	1/9

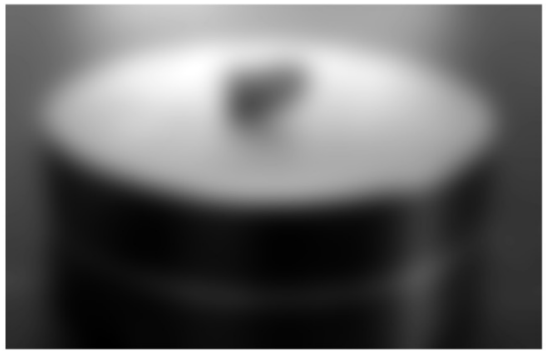
Kernel B

-1	-1	-1
2	2	2
-1	-1	-1

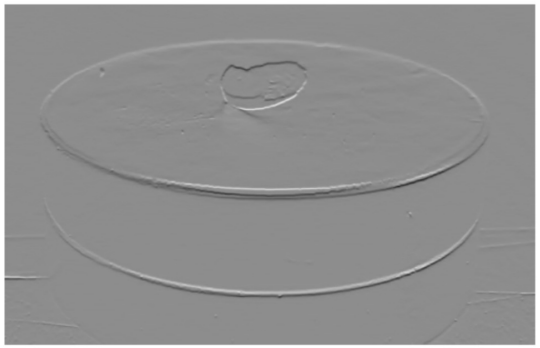
Kernel C

-1	-1	-1
-1	8	-1
-1	-1	-1

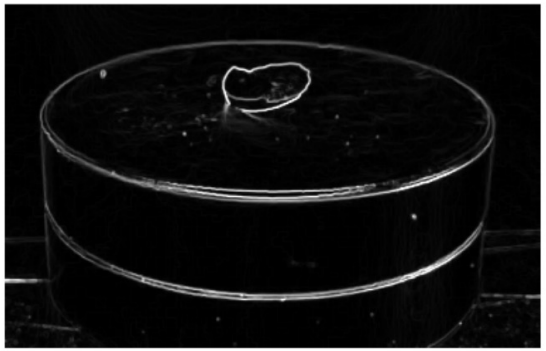
Blur



Horizontal lines



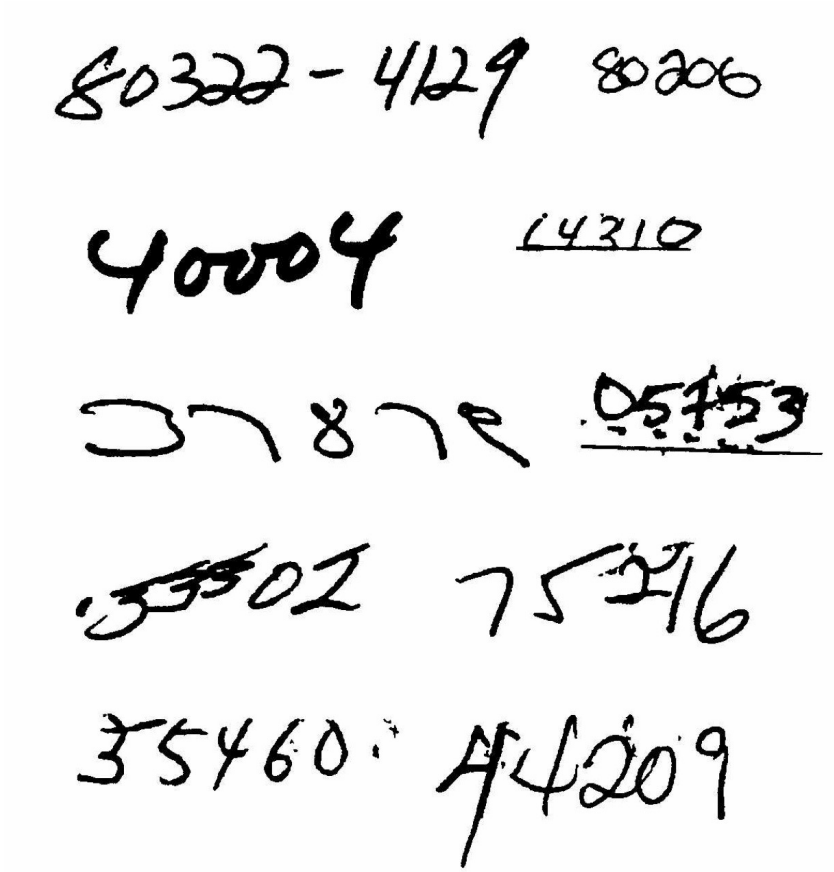
Edge detection



An image of the proposed room-temperature superconductor LK-99

Convolutional Neural Networks (CNN)

A type of neural network used for processing data with a grid-like topology (images, time series…)



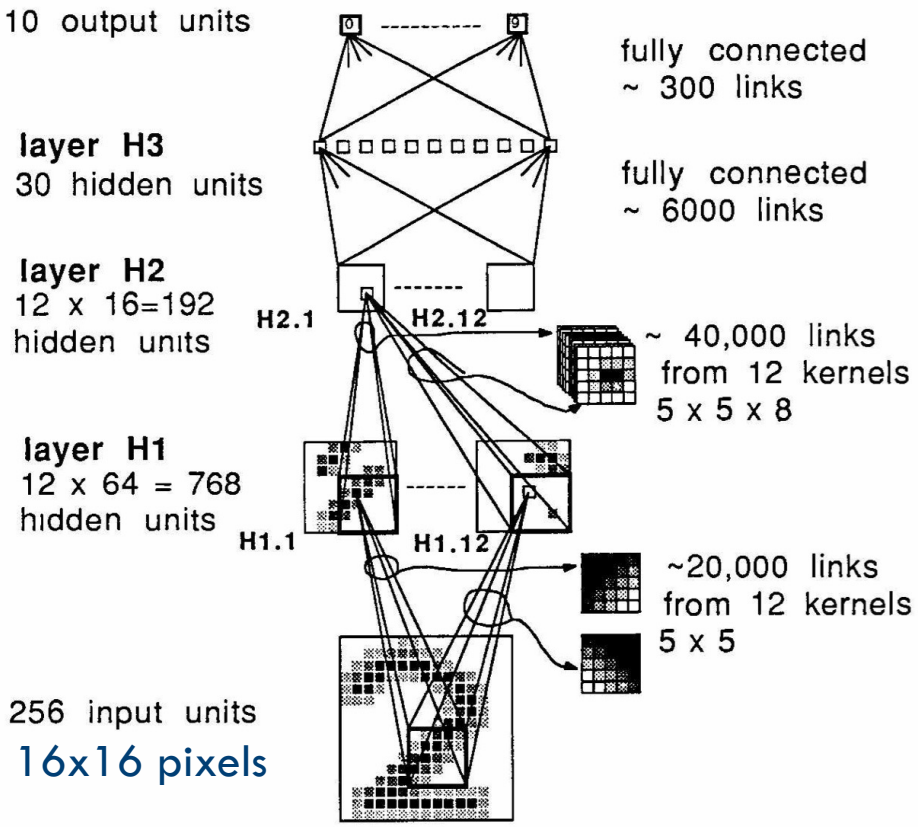
US Postal Service Challenge

Computer recognition of handwritten zip codes

Y. LeCun et al, Neural Computation 1, 541 (1989)

Convolutional Neural Networks (CNN)

A type of neural network used for processing data with a grid-like topology (images, time series…)



Output

{0,1,2,3,4,5,6,7,8,9}

Model

1000 neurons

9760 parameters

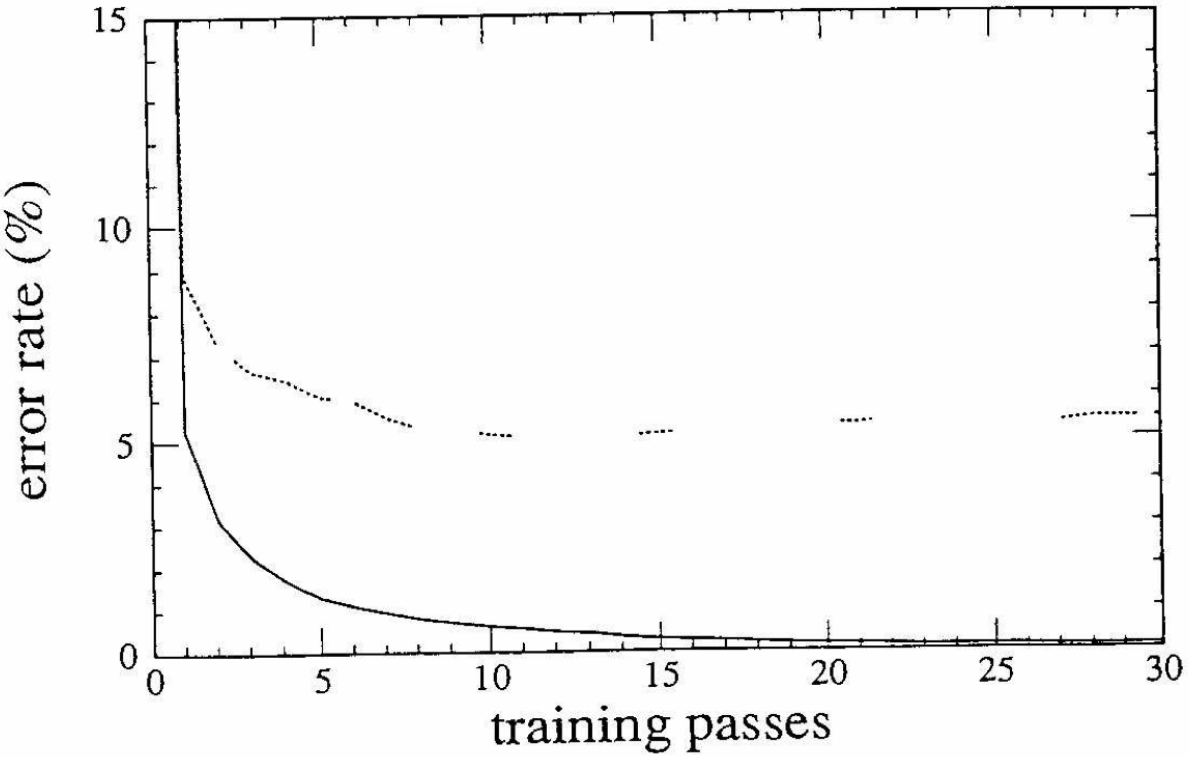
Input

Direct images rather than feature vectors

Y. LeCun et al, Neural Computation 1, 541 (1989)

Convolutional Neural Networks (CNN)

A type of neural network used for processing data with a grid-like topology (images, time series…)



Training

7291 examples

Testing

2007 examples

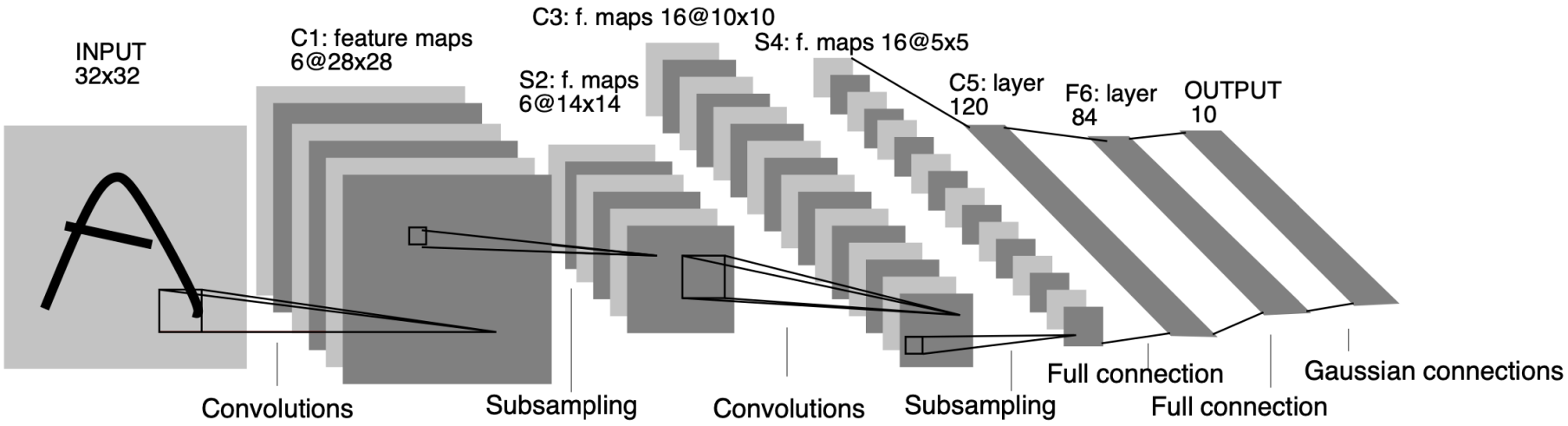
(included hand-chosen ambiguous or unclassifiable samples)

Y. LeCun et al, Neural Computation 1, 541 (1989)

Convolutional Neural Networks (CNN)

LeNet-5 was the fifth evolution of this network and became a standard in the field

Higher resolution input (MNIST dataset)



C*n* = convolutional layer *n* *(extract features)*

S*n* = sub-sampling layer *n* *(reduce spatial dimensions)*

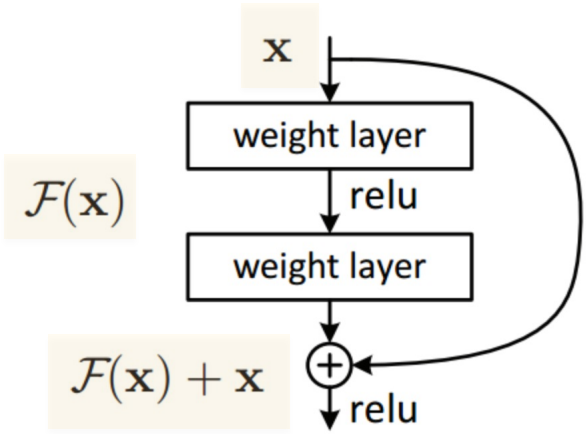
Y. LeCun et al, Proc. IEEE 1 (1998)

```python
import torch.nn as nn

class LeNet5(nn.Module):
    def __init__(self):
        super(LeNet5, self).__init__()
        self.conv1 = nn.Conv2d(in_channels=1, out_channels=6, kernel_size=5)
        self.conv2 = nn.Conv2d(in_channels=6, out_channels=16, kernel_size=5)
        self.fc1 = nn.Linear(in_features=16*5*5, out_features=120)
        self.fc2 = nn.Linear(in_features=120, out_features=84)
        self.fc3 = nn.Linear(in_features=84, out_features=10)  # Assuming 10 classes

    def forward(self, x):
        x = nn.functional.relu(self.conv1(x))
        x = nn.functional.max_pool2d(x, kernel_size=2)
        x = nn.functional.relu(self.conv2(x))
        x = nn.functional.max_pool2d(x, kernel_size=2)
        x = x.view(-1, 16*5*5)
        x = nn.functional.relu(self.fc1(x))
        x = nn.functional.relu(self.fc2(x))
        x = self.fc3(x)
        return x

# Create an instance of the LeNet-5 model
lenet5_model = LeNet5()
```

Advanced Architecture: ResNet

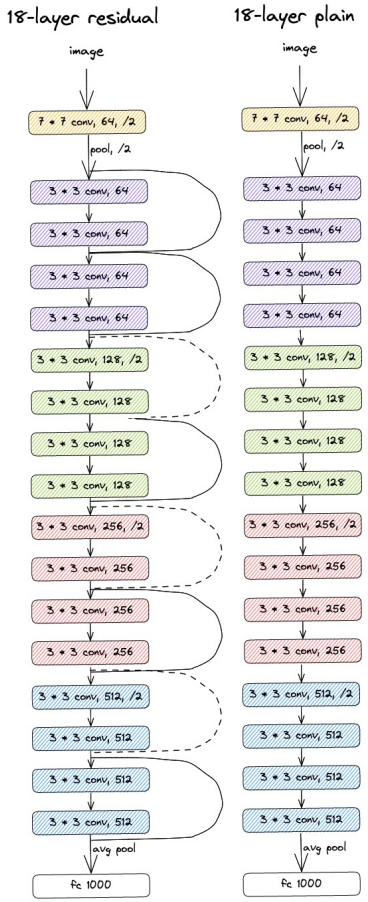
ResNet (Residual Network) is a deep neural network with "skip" connections for effective training

Residual Block



skip connection for *x*

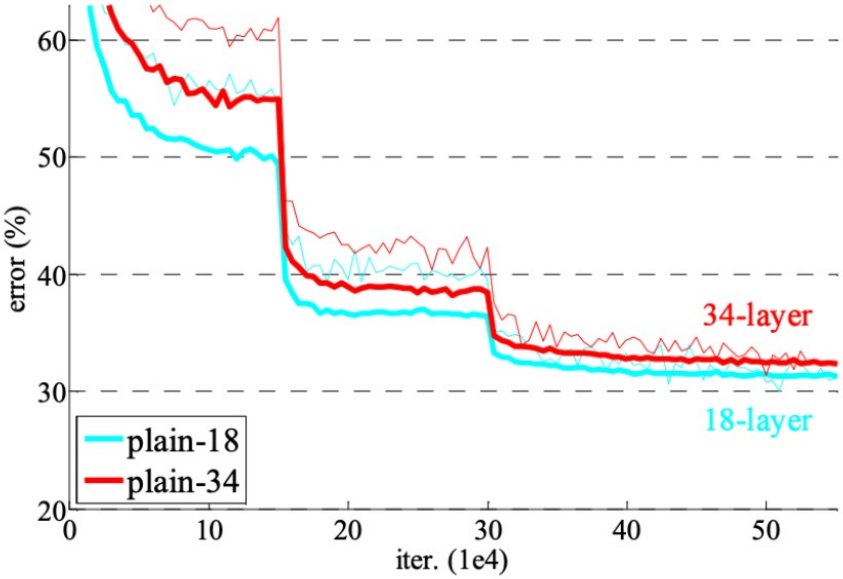
Approach avoids vanishing gradient problem for training of deep networks

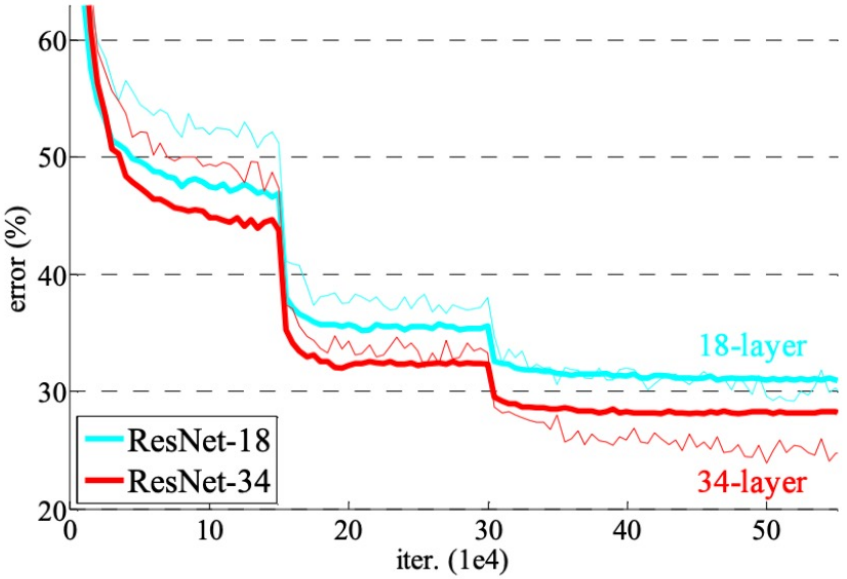


Images from https://www.baeldung.com/cs/residual-networks

Advanced Architecture: ResNet

ResNet (Residual Network) is a deep neural network with "skip" connections for effective training



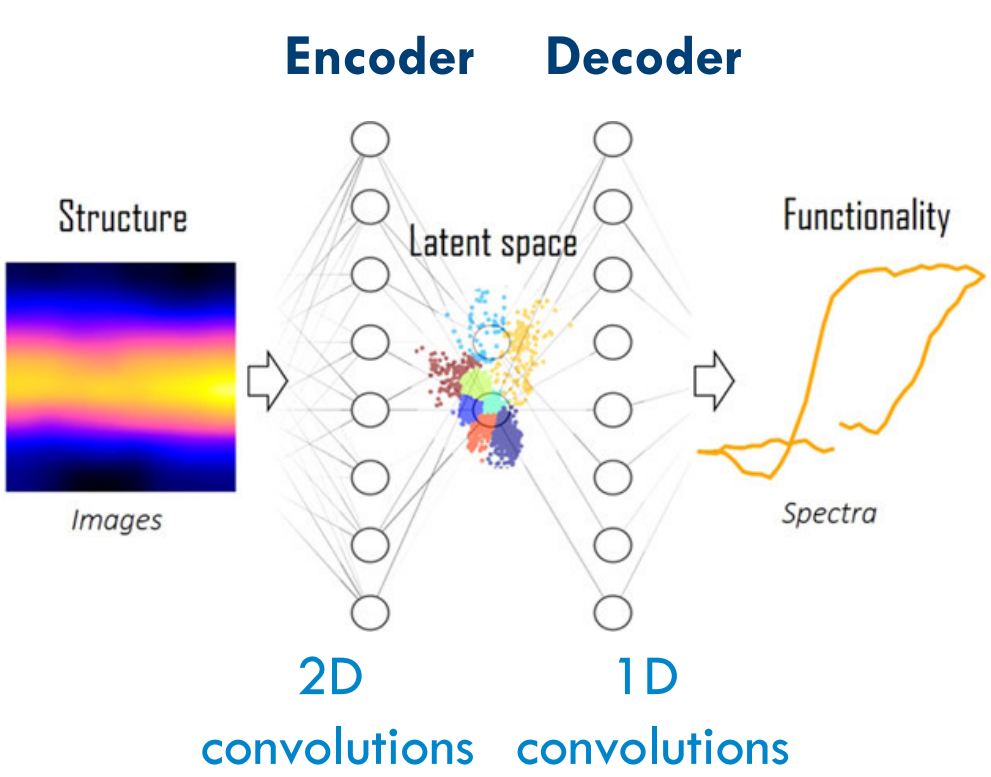


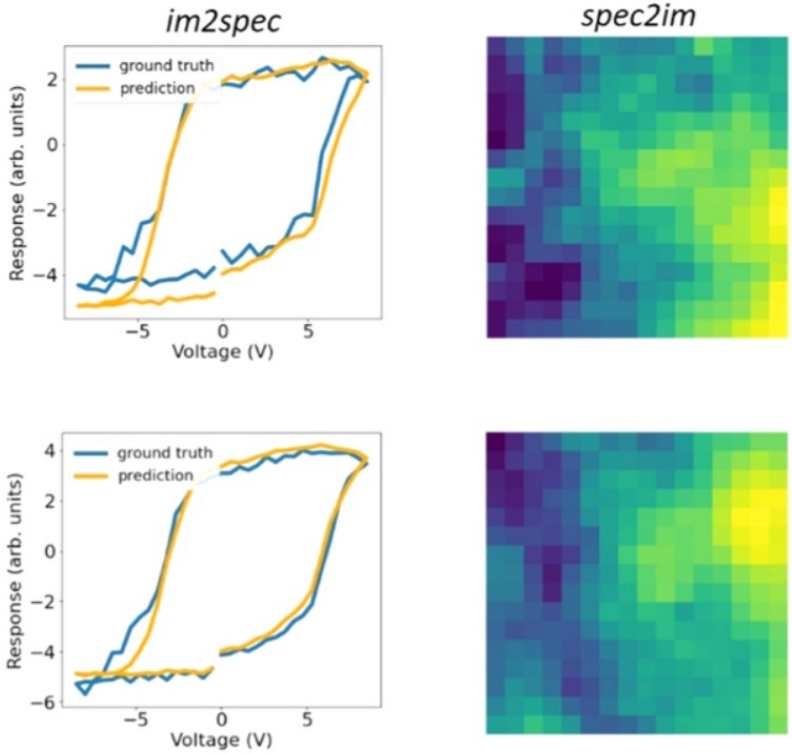
Access higher performance deep models

Images from https://www.baeldung.com/cs/residual-networks

CNN for Ferroelectrics

Convolutional network to map between local domain structures and switching behaviour



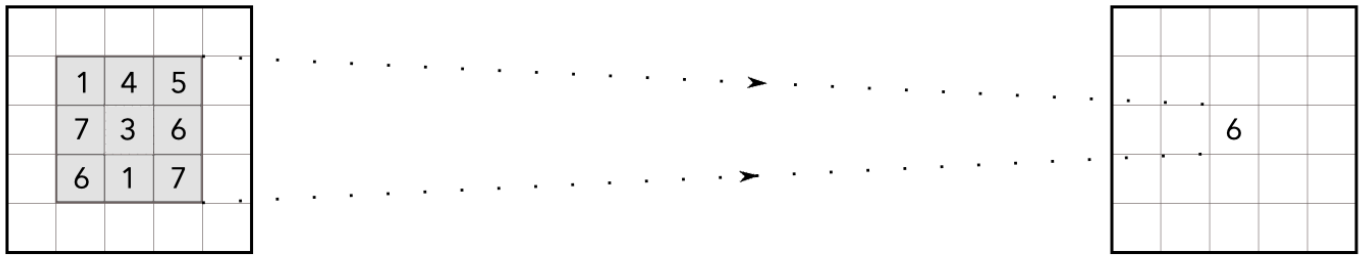


S. V. Kalinin et al, ACS Appl. Mater. Inter. 13. 1693 (2021)

Application to Materials

Graph Convolutional Neural Networks (GCNN) are designed for graph-structured data

Pixel-based convolutions



Graph-based convolutions

Information is stored on each piece of the graph,
i.e. vectors associated with the nodes, edges and global attributes

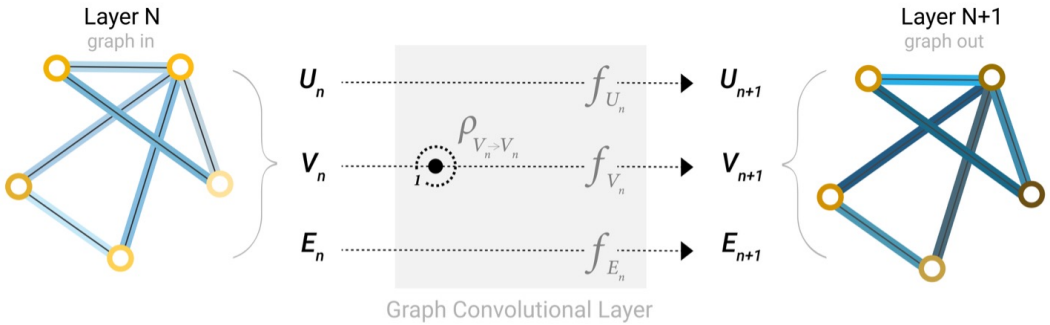
Images from: https://distill.pub/2021/understanding-gnns

Application to Materials

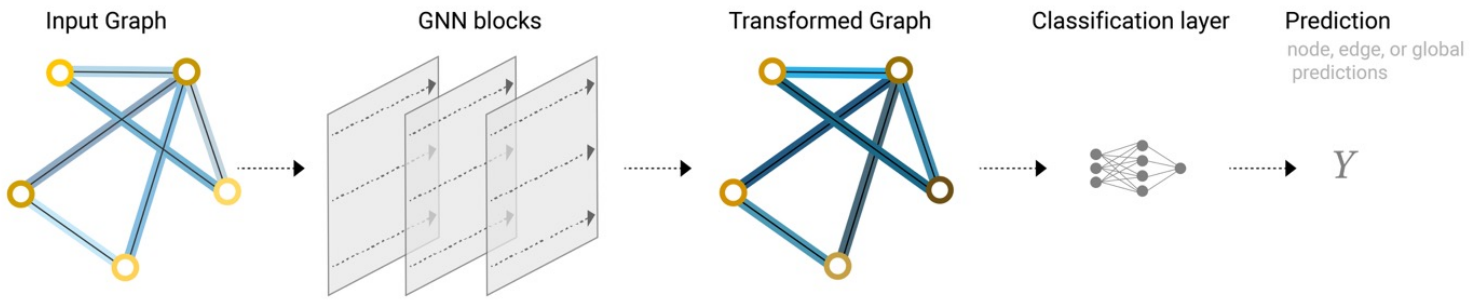
Input graphs can be transformed and tailored for regression or classification tasks

(V = vertex; E = edge, U = global attribute)

Graph update



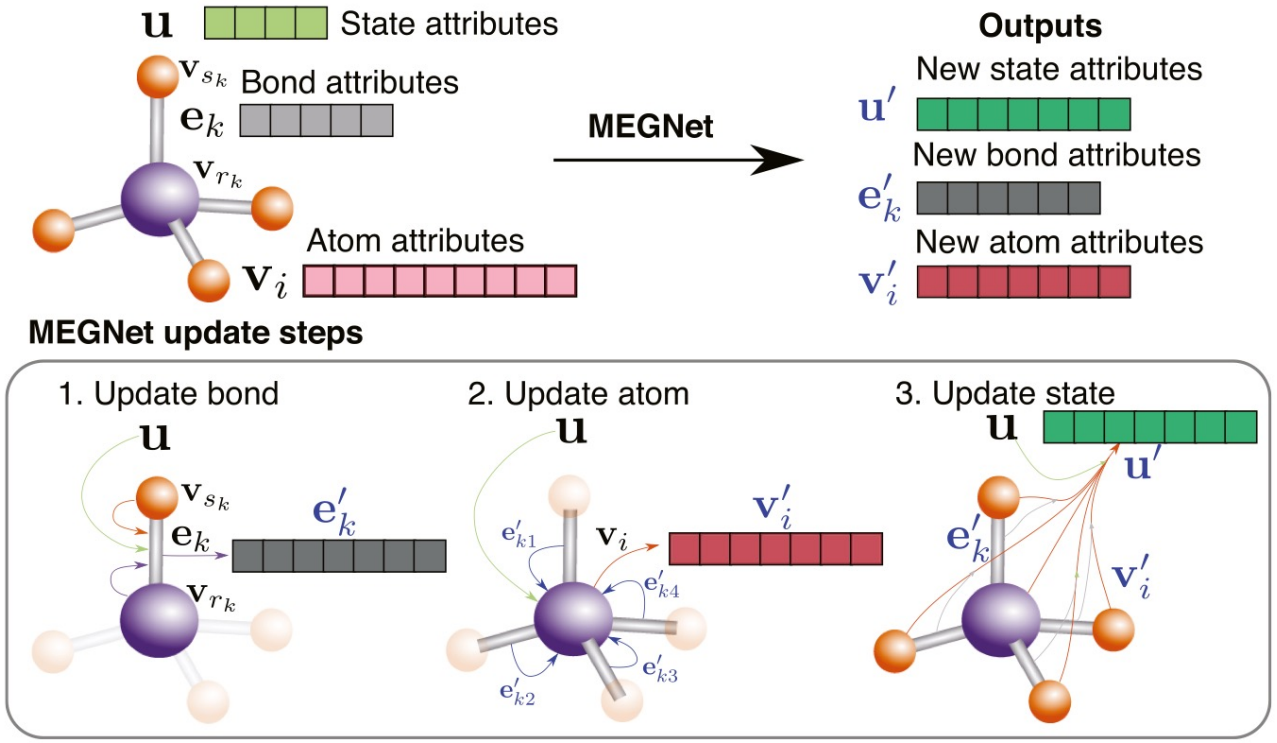
End-to-end prediction



Images from: https://distill.pub/2021/understanding-gnns

Application to Materials

Crystal Graph Convolutional Neural Networks (CGCNN) are being used for materials modelling



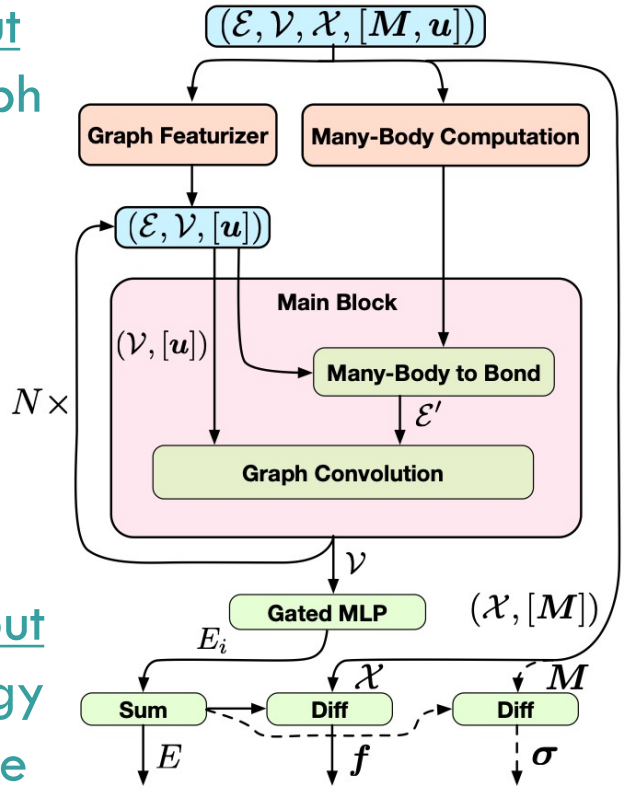
MEGNet (two-body connections); https://github.com/materialsvirtuallab/matgl

C. Chen et al, Chem. Mater. 31, 3564 (2019)

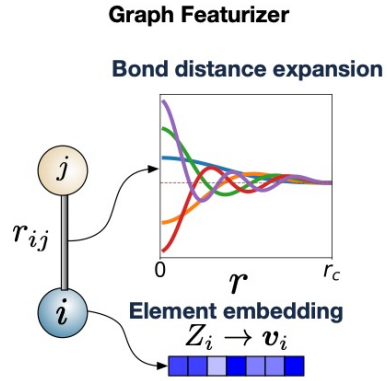
Application to Materials

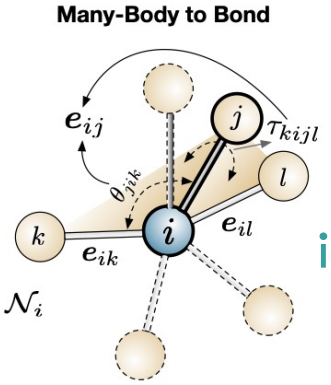
A new generation of universal force fields that can predict energies and forces for any material

Input Graph

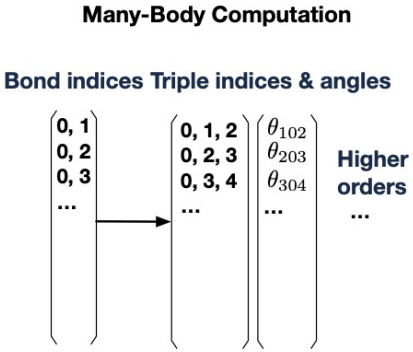


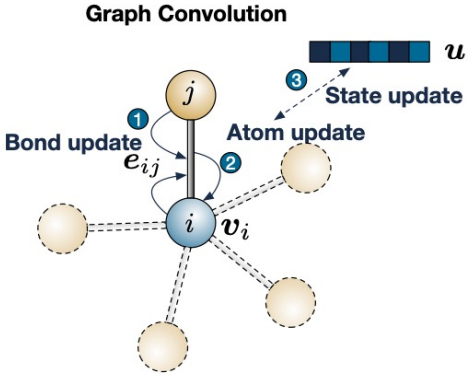
Output Energy Force Stress





Beyond pairwise interactions

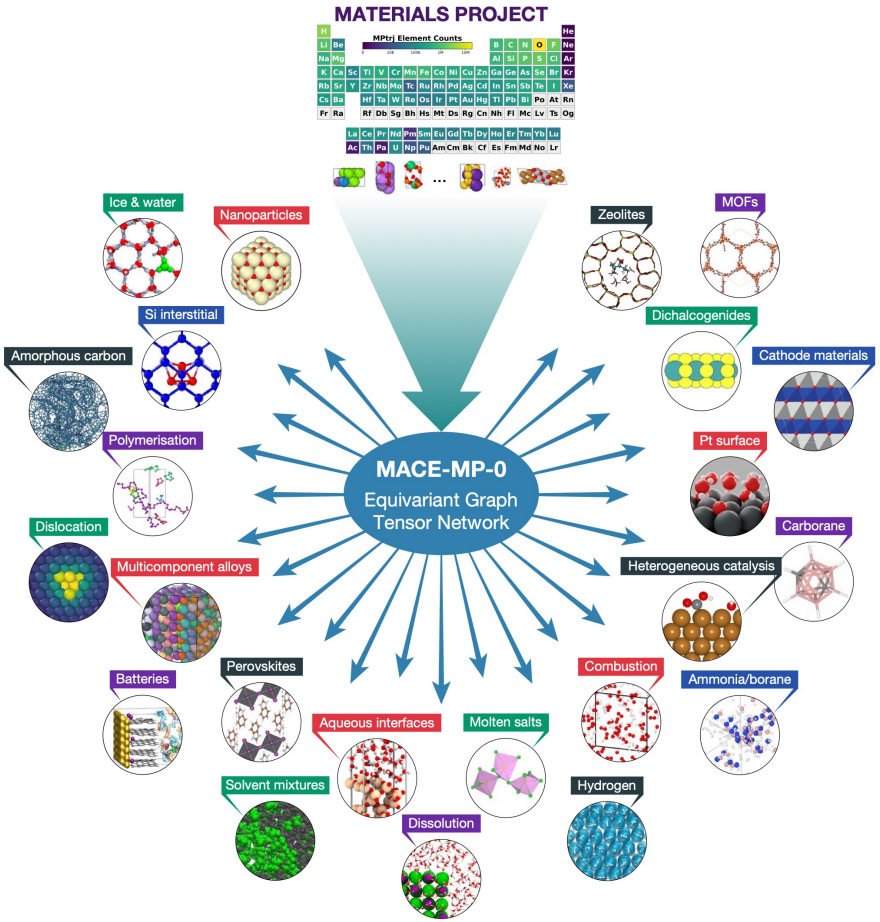




M3GNet; https://github.com/materialsvirtuallab/matgl

Application to Materials

A new generation of universal force fields that can predict energies and forces for any material




```python
from ase.io import read, write
from mace.calculators import mace_mp

calc = mace_mp(model="medium")

# Initial energy and structure parameters
material = read('./data/Sn5S4Cl2.cif')
material.calc=calc
print(material.get_potential_energy())

print("Initial Energy:", material.get_potential_energy())

print("Initial Cell Parameters:")
print(material.cell)
```

I. Batatia et al, arXiv:2401.00096 (2023); pip install mace-torch

Class Outcomes

1. Describe how a perceptron works
2. Distinguish between different types of deep learning architectures
3. Specify how convolutional neural networks work and can be applied to materials problems

Activity:

Microscopy