

Deep Learning: From Theory to Practice

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(Responsible AI) Entrepreneurship & Innovation, Rotkreuz, 13th March 2023

Organisational Matters

Schedule:

18:30 - 19:20	Lecture
19:30 - 20:50	Lab Exercise

Material:

- Slides for the theoretical and practical part.
- Lab assignment (Jupyter Notebook, Google Colab).
- You are not allowed to distribute or use the material without consent.

#1 Introduction

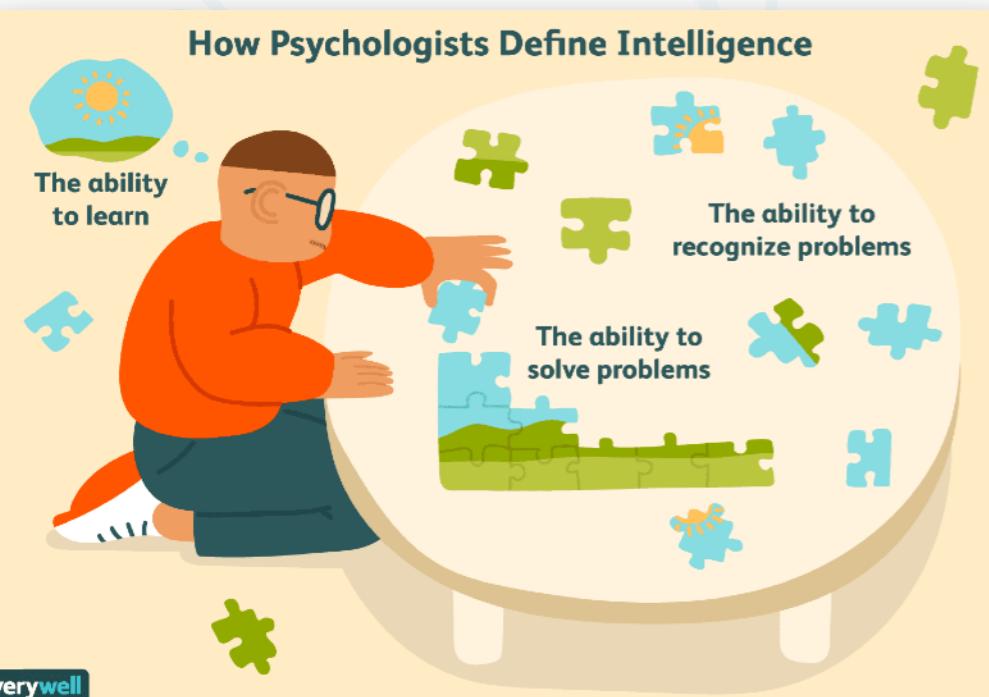
What is Artificial Intelligence?

Intelligence → *intelligere* (*latin*) → to comprehend or perceive. [Wikipedia]

Intelligence: general mental capacity that involves:

- Capability to reason and to plan
- Solve problems and think abstractly
- Comprehend complex ideas
- Learn from experience and apply knowledge to manipulate one's environment

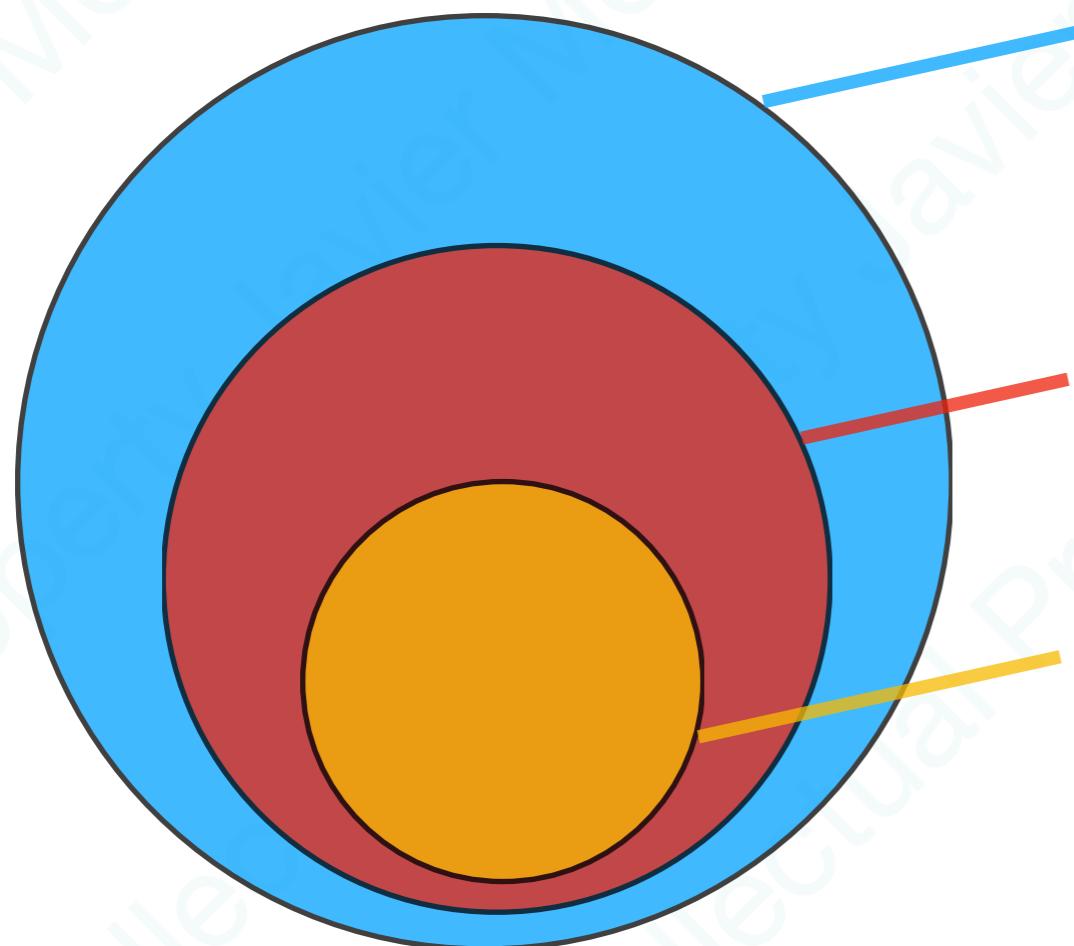
[Gottfredson, Mainstream science on intelligence]



- **Learn from experience:** The acquisition, retention, and use of knowledge is an important component of intelligence.
- **Recognise problems:** To put knowledge to use, people must be able to identify possible problems in the environment that need to be addressed.
- **Solve problems:** People must then be able to take what they have learned to come up with a useful solution to a problem they have noticed in the world around them.

[Verywellmind]

What is Artificial Intelligence?



Artificial Intelligence

- Techniques that enables machines to imitate intelligent human behaviour.
- Goal: solve tasks humans are good at, e.g sensing, reasoning, acting, adapting.

Machine Learning

- Subset of algorithms based on statistical models that enables machine: (i) to learn, (ii) improve from experience, and (iii) make accurate predictions.

Deep Learning

- Methods inspired by the information processing patterns in the **brain**.

What is Artificial Intelligence?



“Machine Learning is the field of study that gives computers the ability to learn without being explicitly programmed”.

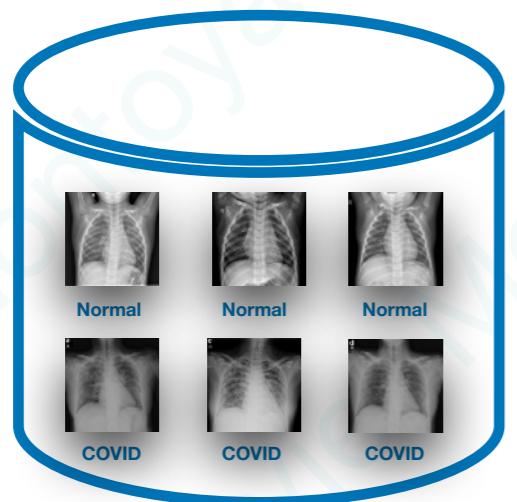
Arthur L. Samuel, AI Pioneer, 1959

#2 Machine Learning: Basic Concepts

The Neural Network Pipeline

TRAINING PHASE

Training Dataset



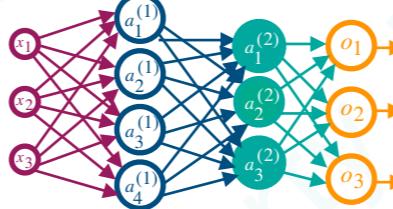
$$\mathbb{D} = \{x_i \in \mathbb{R}^d, y_i \in \mathbb{R}\}_{i=1}^n$$

③ Compute Error via Loss Function $\hat{y} \neq y$

1 Train

Learned Model
 $f()$

2 Predict



\hat{y} Predictions

y Labels

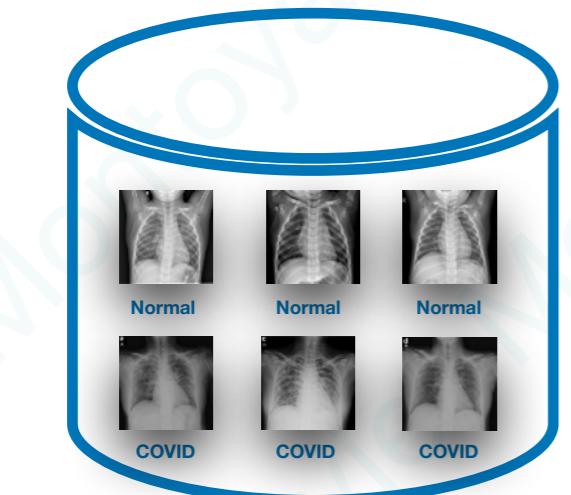
		VII	I
		I	XII

Confusion Matrix

The Neural Network Pipeline

TRAINING PHASE

Training Dataset

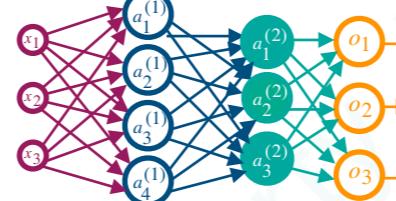


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2 Predict

\hat{y}

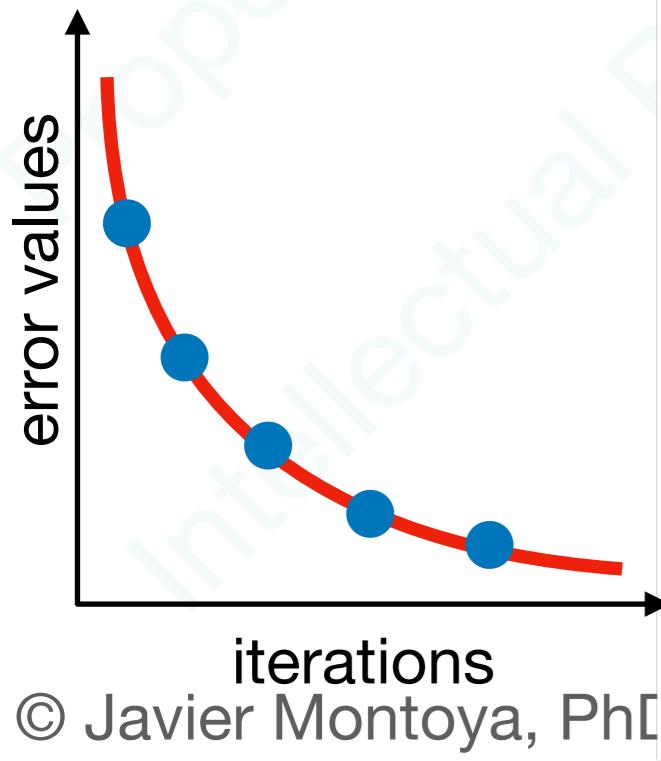
y Labels

\hat{y} Predictions

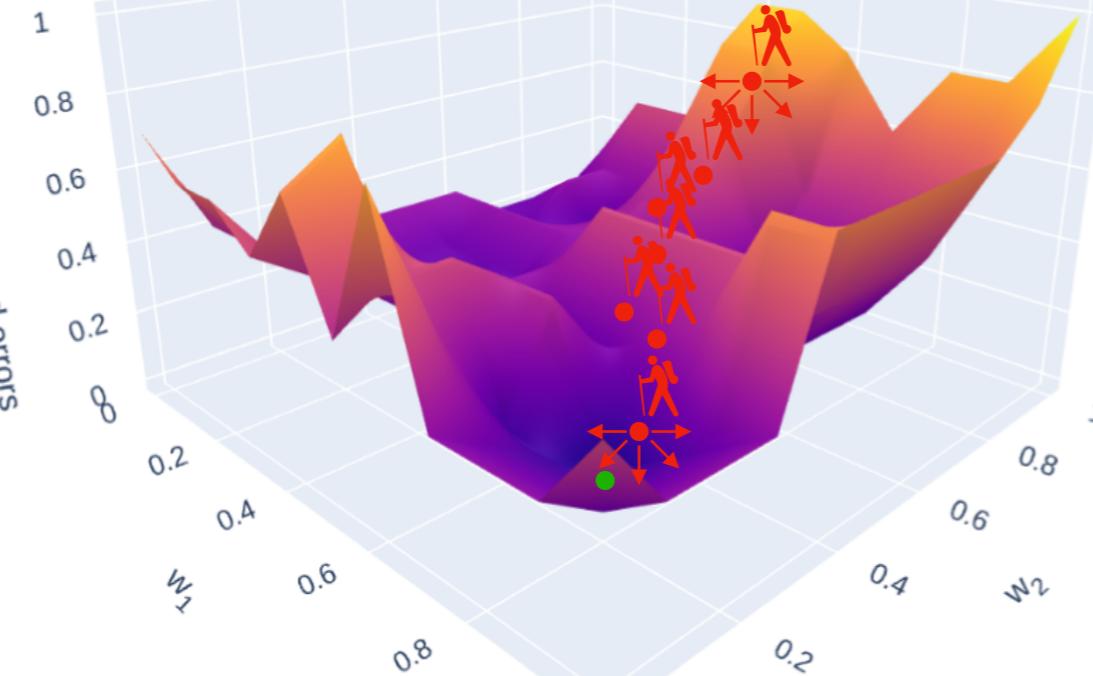
	VII	I	
	I	XII	

Confusion Matrix

Error Surface



mean of squared errors



new values old values learning rate Loss derivates

$$w_1 = w_1 - \eta \frac{\partial \mathbb{L}}{\partial w_1}$$

$$w_2 = w_2 - \eta \frac{\partial \mathbb{L}}{\partial w_2}$$

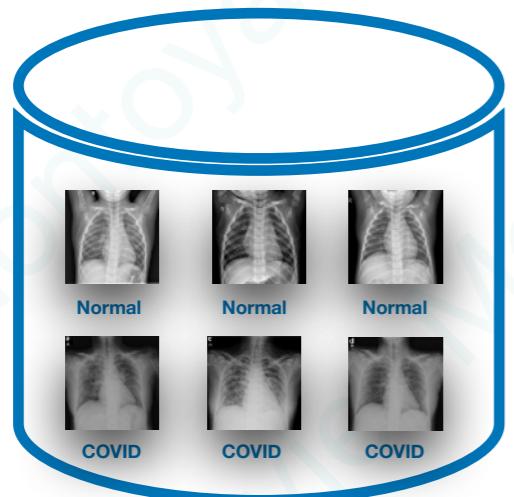
$$\vdots$$

$$w_M = w_M - \eta \frac{\partial \mathbb{L}}{\partial w_M}$$

The Neural Network Pipeline

TRAINING PHASE

Training Dataset

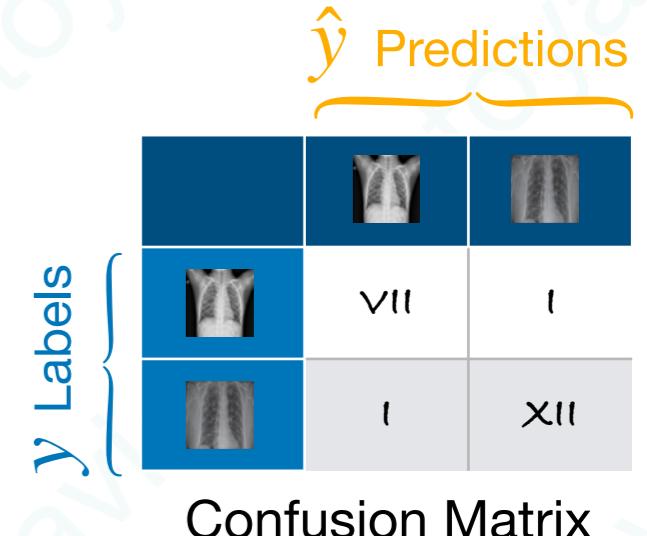
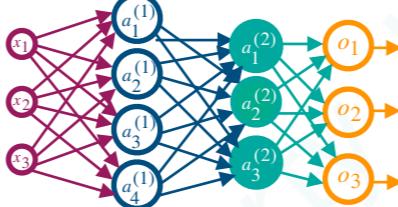


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③ Compute Error via Loss Function $\hat{y} \neq y$

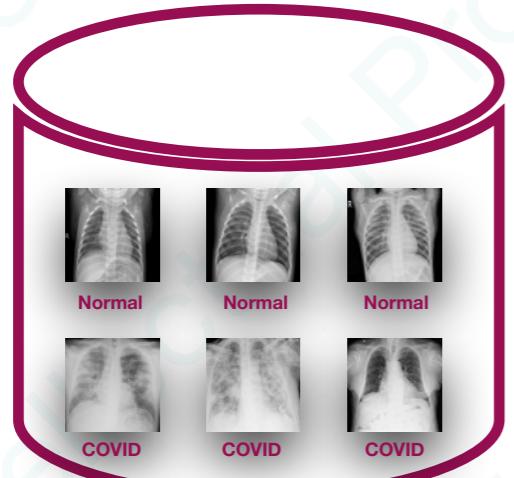
① Train
Learned Model $f()$

② Predict
 \hat{y}



TESTING PHASE

Unseen Dataset



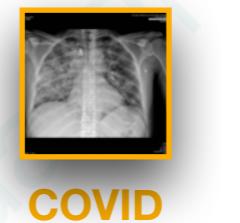
$$\mathbb{D} = \{x_i \in \mathbb{R}^d, y_i \in \mathbb{R}\}_{i=1}^n$$

⑤ Evaluate

⑥ Prediction
Learned Model $f()$

Output
 \hat{y}

$$\hat{y} = f(x)$$

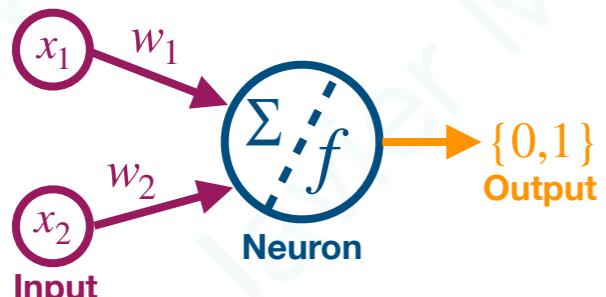


#3 Milestones of AI

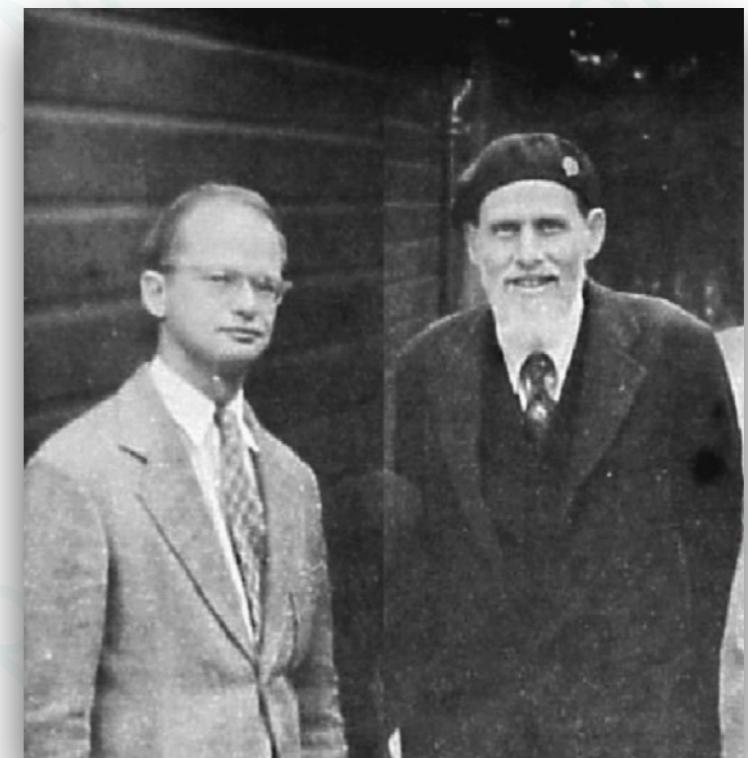
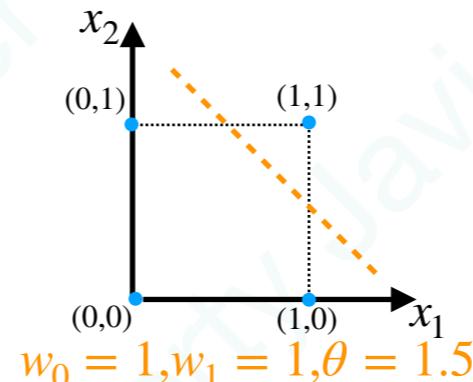
A Brief History of A.I

1943: McCulloch and Pitts (Artificial Neuron)

- Early model of artificial neuron:



Truth Table for AND Function		
x_1	x_2	Output
0	0	0
0	1	0
1	0	0
1	1	1



- Linear neural activation:

$$f_w(x) = \begin{cases} 1, & \text{if } w^T x \geq \theta \\ 0, & \text{if } w^T x < \theta \end{cases}$$

- Mainly used for AND/OR logic gates.
- No learning procedure.

A LOGICAL CALCULUS OF THE IDEAS IMMANENT IN NERVOUS ACTIVITY*

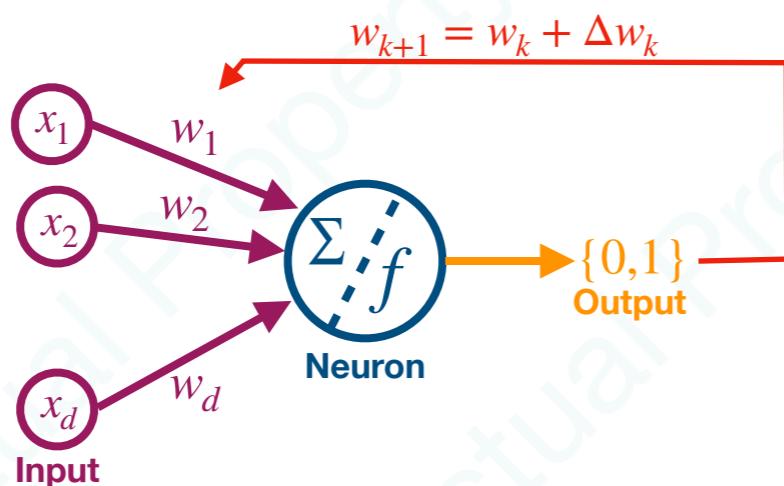
■ WARREN S. McCULLOCH AND WALTER PITTS
University of Illinois, College of Medicine,
Department of Psychiatry at the Illinois Neuropsychiatric Institute,
University of Chicago, Chicago, U.S.A.

A Brief History of A.I

1958-1962: Rosenblatt (Perceptron)

- First model to train an artificial neuron.
- Optimisation of perceptron:

$$w_{k+1} = w_k + \Delta w_k$$



Psychological Review
Vol. 65, No. 6, 1958

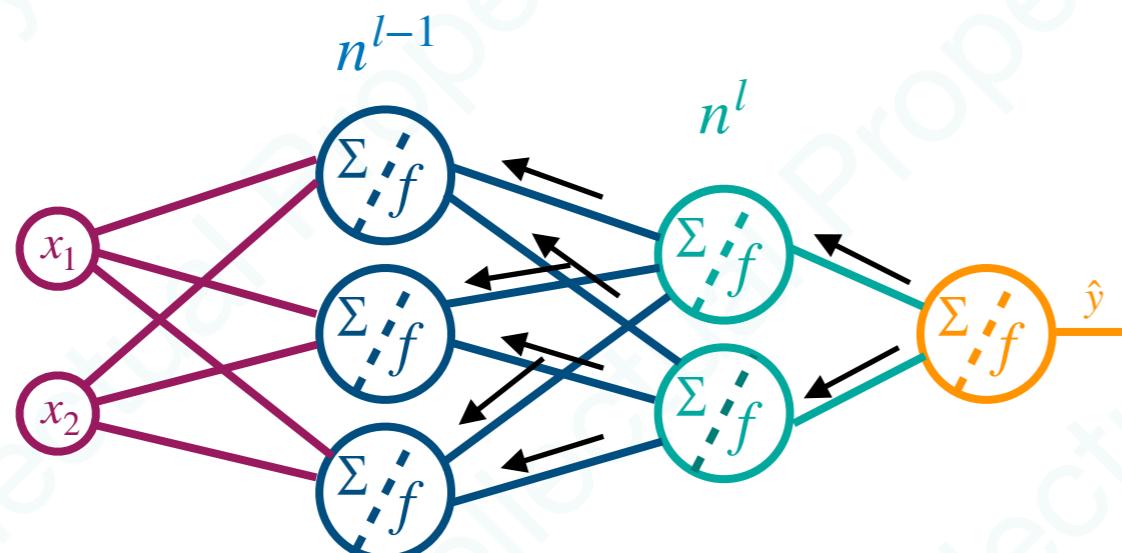
THE PERCEPTRON: A PROBABILISTIC MODEL FOR
INFORMATION STORAGE AND ORGANIZATION
IN THE BRAIN¹

F. ROSENBLATT
Cornell Aeronautical Laboratory

A Brief History of A.I

1986: Backpropagation Algorithm

- Main training procedure for actual deep networks based on gradients.
- Enables the automatic learning of model parameters.



Learning representations by back-propagating errors

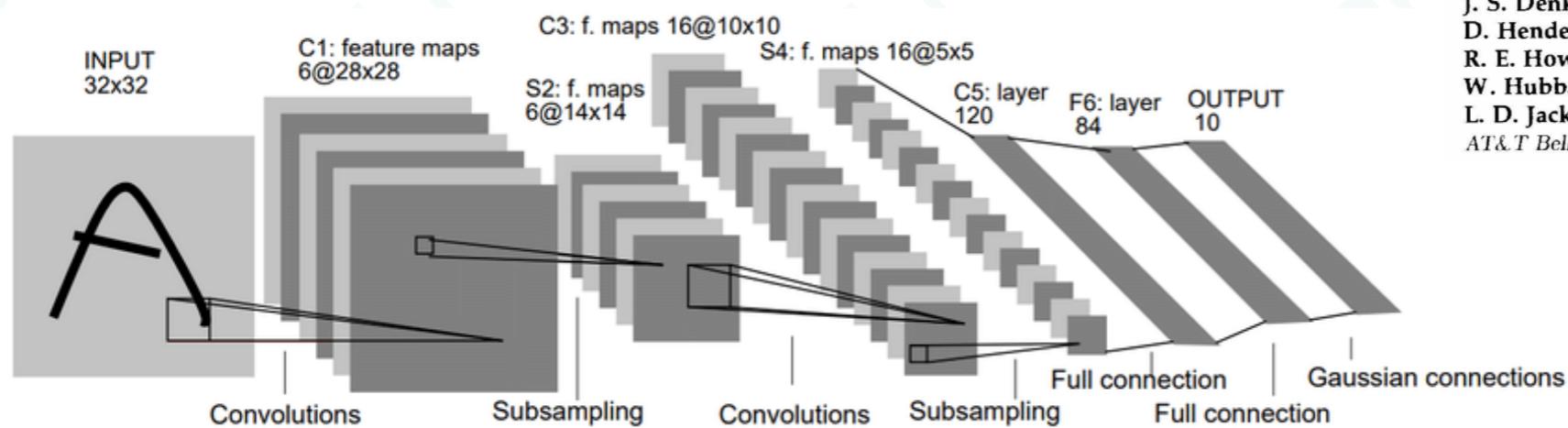
[David E. Rumelhart, Geoffrey E. Hinton & Ronald J. Williams](#)

[Nature](#) 323, 533–536 (1986) | [Cite this article](#)

A Brief History of A.I

1998: Convolutional Neural Networks

- Neural architecture intended for visual analysis tasks.
- Local features: feature sharing and pooling.
- Promising results on digit recognition.



Backpropagation Applied to Handwritten Zip Code Recognition

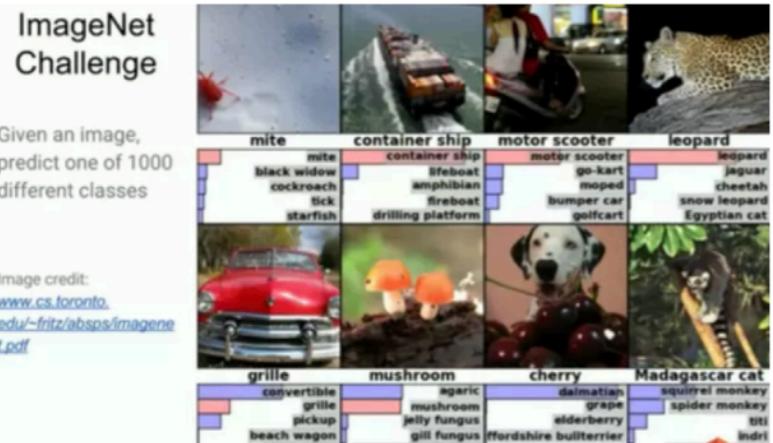
Y. LeCun
B. Boser
J. S. Denker
D. Henderson
R. E. Howard
W. Hubbard
L. D. Jackel

AT&T Bell Laboratories Holmdel, NJ 07733 USA

A Brief History of A.I

2010: Benchmark datasets

- **Imagenet:**
 - Largest image recognition challenge.



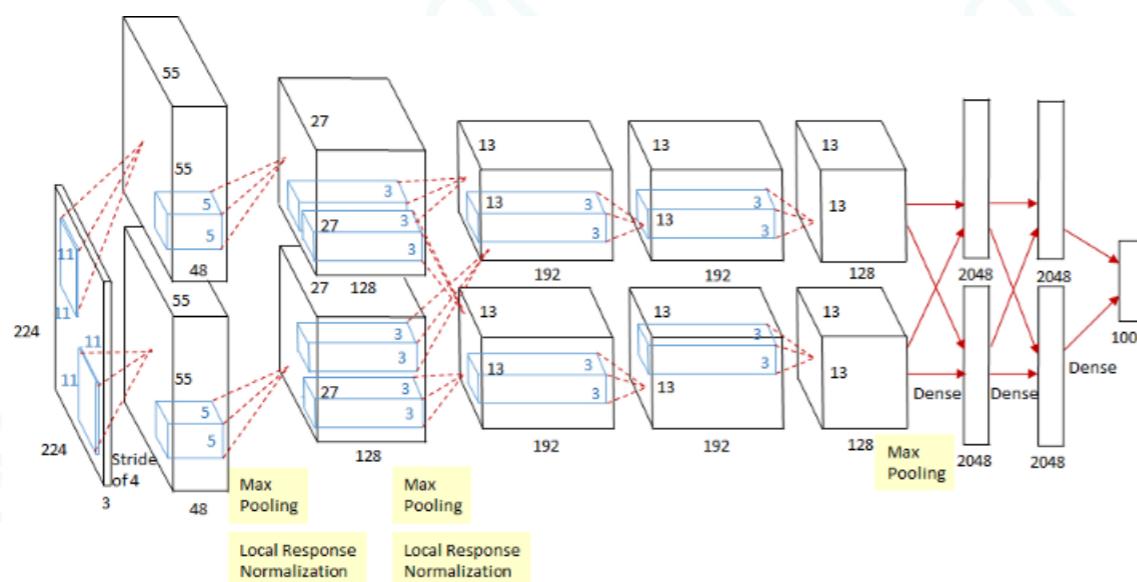
IMAGENET (2010):

- ~1.5 Million of Images, 1000 classes.
- Image Dimensions: full resolution.
- Largest Dimension: 4288x2848x3.
- Smallest Dimension: 75x56x3.
- <http://www.image-net.org>

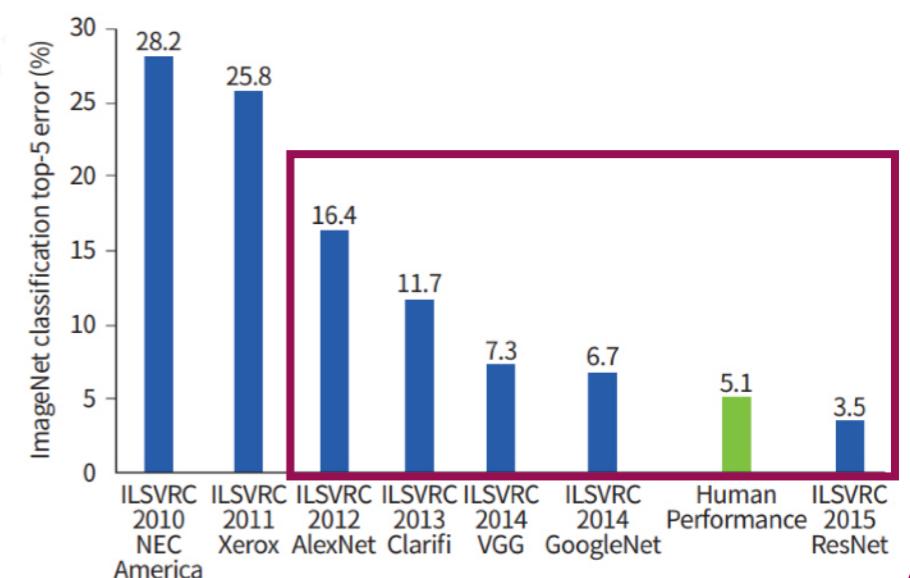
A Brief History of A.I

2012: Deep Learning Models

- **AlexNet:**
 - First deep learning model to win ImageNet competition.
 - Significant improvements over SOTA.



ImageNet Classification with Deep Convolutional Neural Networks



A Brief History of A.I

Why now?

1. Large Data

- Easier acquisition.
- Bigger numbers.



2. Hardware

- New optimised HW.
- Larger storage.



Graphic Processing Unit (GPU)

3. Software

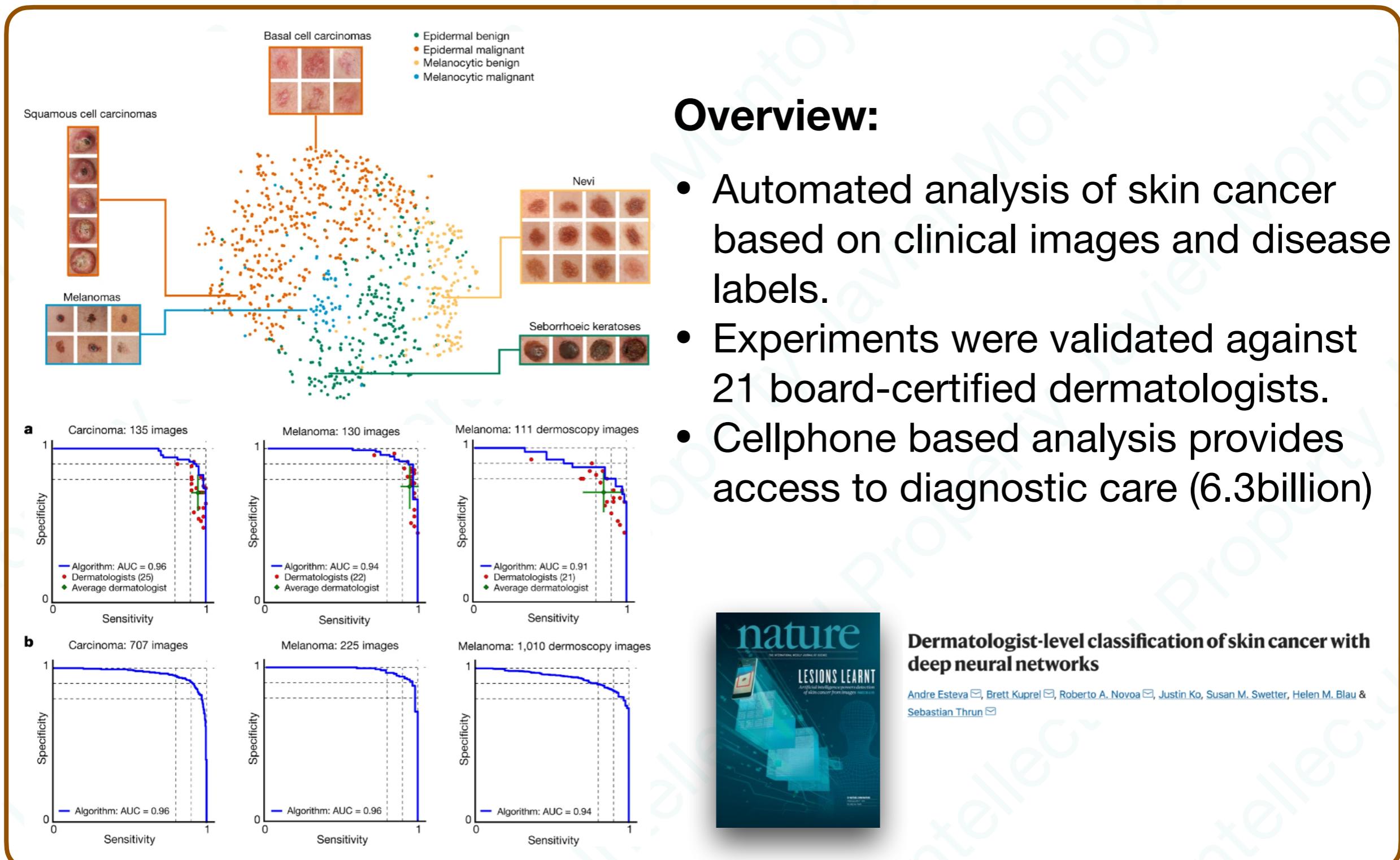
- New Models
- New Toolboxes



#4 AI as Business Disruptor

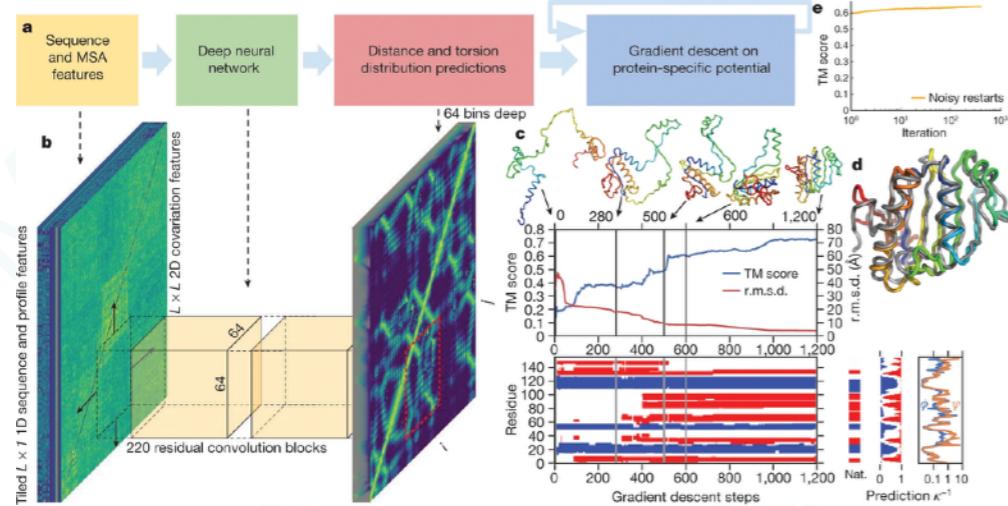
AI as Business Disruptor

Digital Health



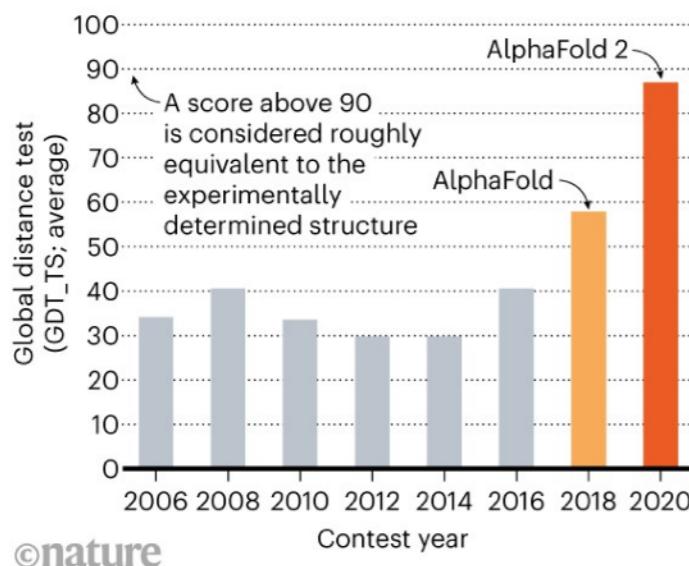
AI as Business Disruptor

Biology



STRUCTURE SOLVER

DeepMind's AlphaFold 2 algorithm significantly outperformed other teams at the CASP14 protein-folding contest — and its previous version's performance at the last CASP.



Overview:

- Prediction of protein structure to predict the 3D shape of a protein.
- AlphaFold achieves a new SOTA.
- It provides new insights into the function and malfunction of proteins.



Improved protein structure prediction using potentials from deep learning

Andrew W. Senior [✉](#), Richard Evans, John Jumper, James Kirkpatrick, Laurent Sifre, Tim Green, Chongli Qin, Augustin Žídek, Alexander W. R. Nelson, Alex Bridgland, Hugo Penedones, Stig Petersen, Karen Simonyan, Steve Crossan, Pushmeet Kohli, David T. Jones, David Silver, Koray Kavukcuoglu & Demis Hassabis

Nature 577, 706–710 (2020) | [Cite this article](#)

Highly accurate protein structure prediction with AlphaFold

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Nature 596, 583–589 (2021) | [Cite this article](#)

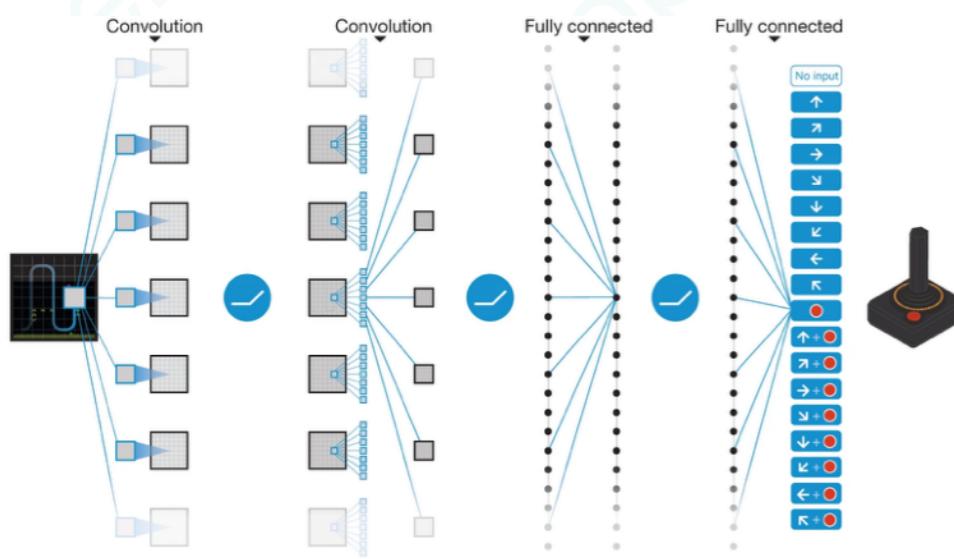
AI as Business Disruptor

Gaming



Overview:

- Deep Q-Network: Novel AI agent that learns policies from high-dimensional sensory inputs.
- The Agent achieves professional human scores.
- It relies only on pixel information and game scores as inputs.



Self-taught system



Human-level control through deep reinforcement learning

Volodymyr Mnih, Koray Kavukcuoglu, David Silver, Andrei A. Rusu, Joel Veness, Marc G. Bellemare, Alex Graves, Martin Riedmiller, Andreas K. Fidjeland, Georg Ostrovski, Stig Petersen, Charles Beattie, Amir Sadik, Ioannis Antonoglou, Helen King, Dharshan Kumaran, Daan Wierstra, Shane Legg & Demis Hassabis

Nature 518, 529–533 (2015) | Cite this article

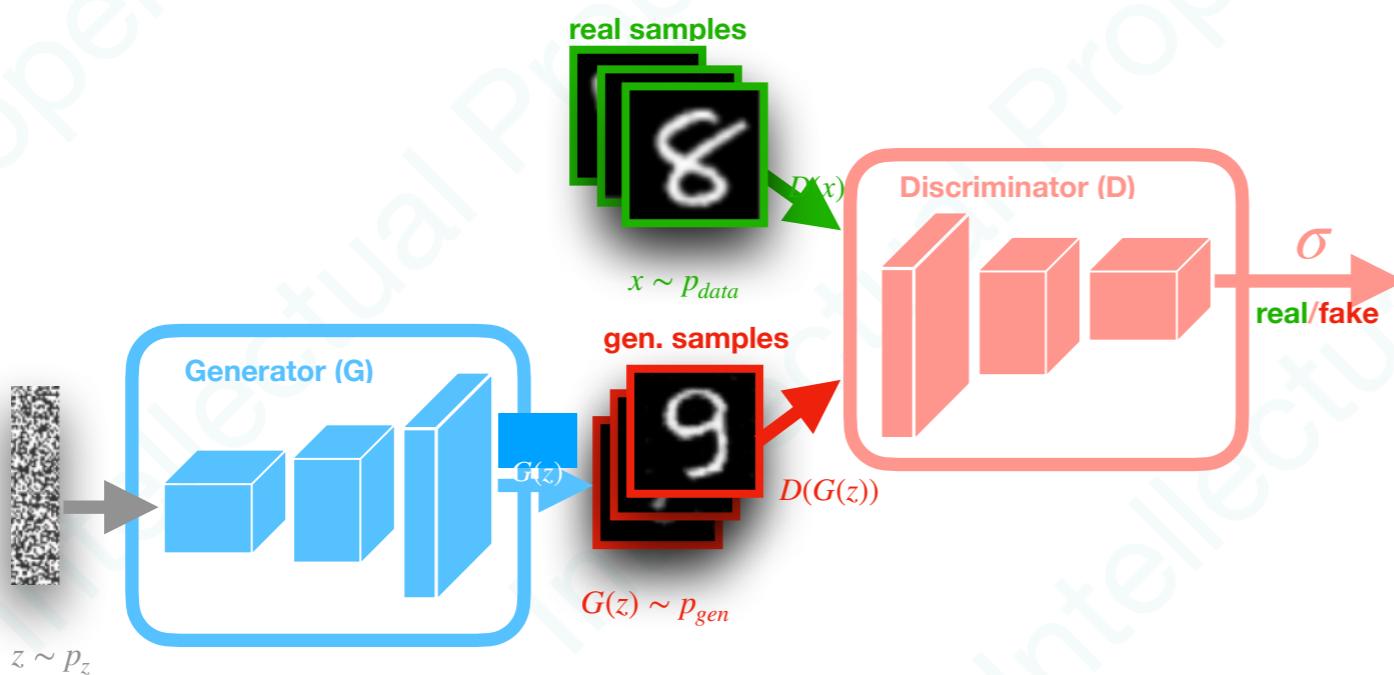
AI as Business Disruptor

Data Synthesis



Overview:

- Enables the generation of real-looking images based on existing data.
- Applications can include: gaming, film industry, clothing industry, architecture, photography, etc.



Generative Adversarial Nets

Ian J. Goodfellow, Jean Pouget-Abadie,^{*} Mehdi Mirza, Bing Xu, David Warde-Farley,
Sherjil Ozair,[†] Aaron Courville, Yoshua Bengio[‡]
Département d'informatique et de recherche opérationnelle
Université de Montréal
Montréal, QC H3C 3J7

#5 Artificial Neural Networks

Artificial Neural Networks

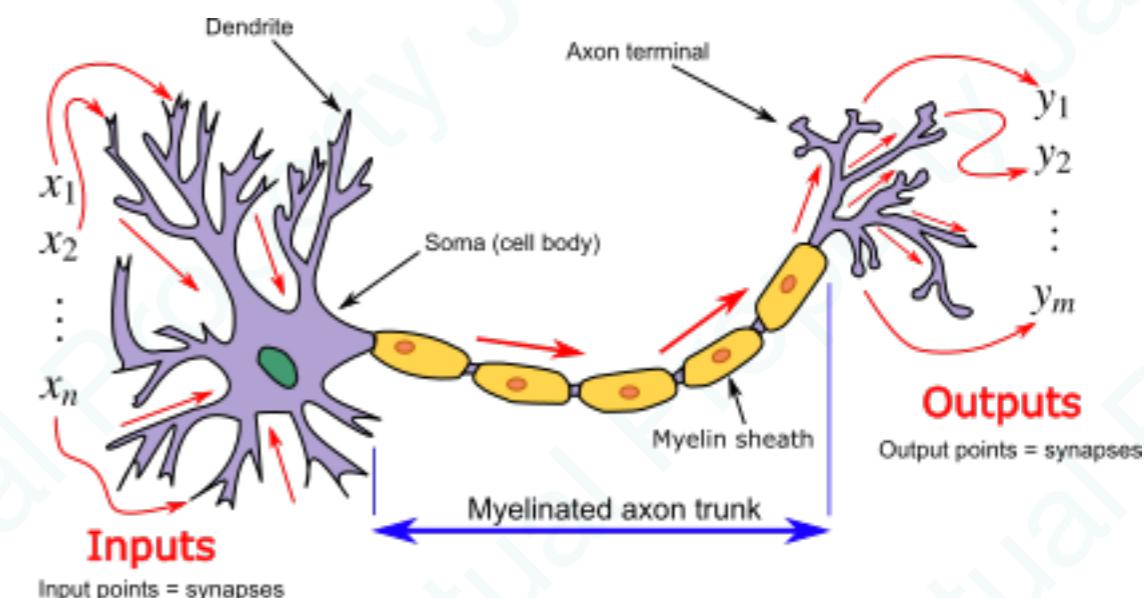
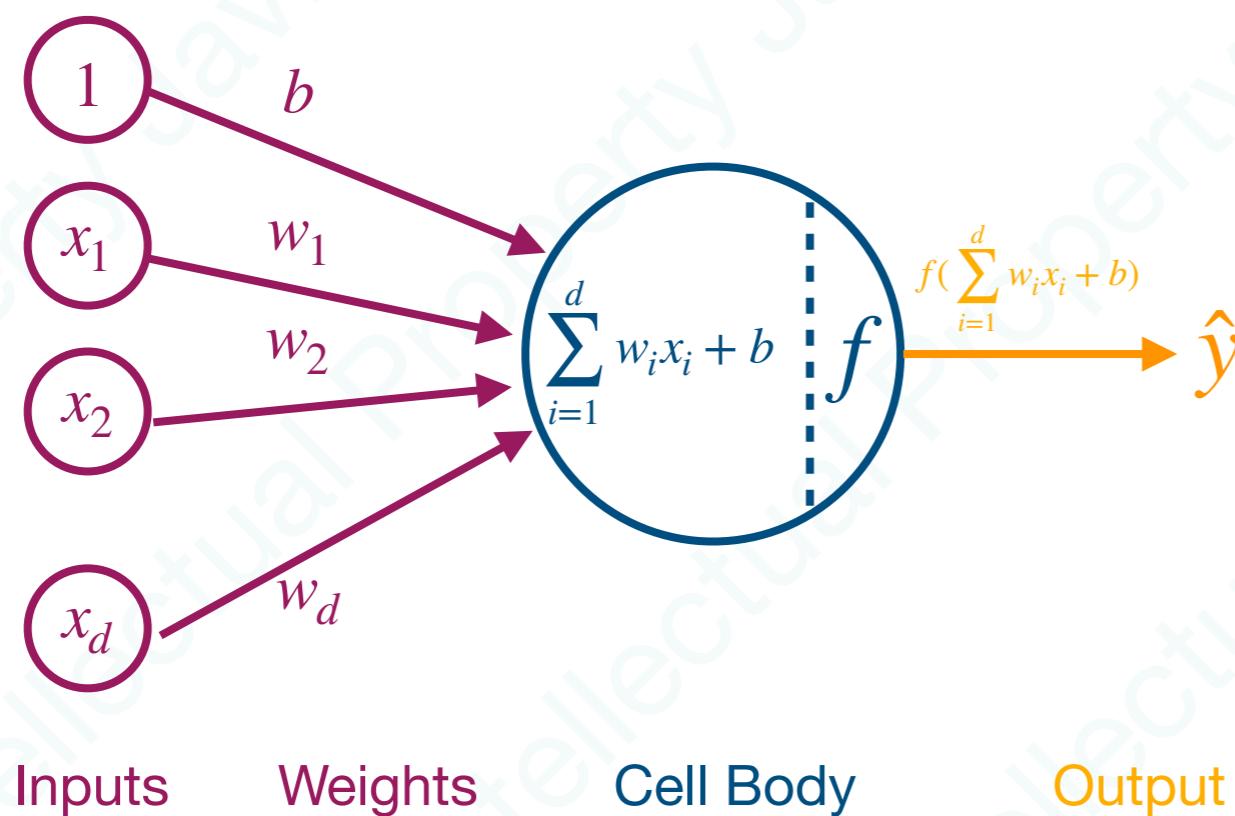
The Neuron Metaphor

Biological Neurons:

- They accept information from multiple inputs.
- They activate and transmit information to other neurons.

Artificial Neurons:

- They multiple inputs by weights (edges).
- Apply some function to define their activation.

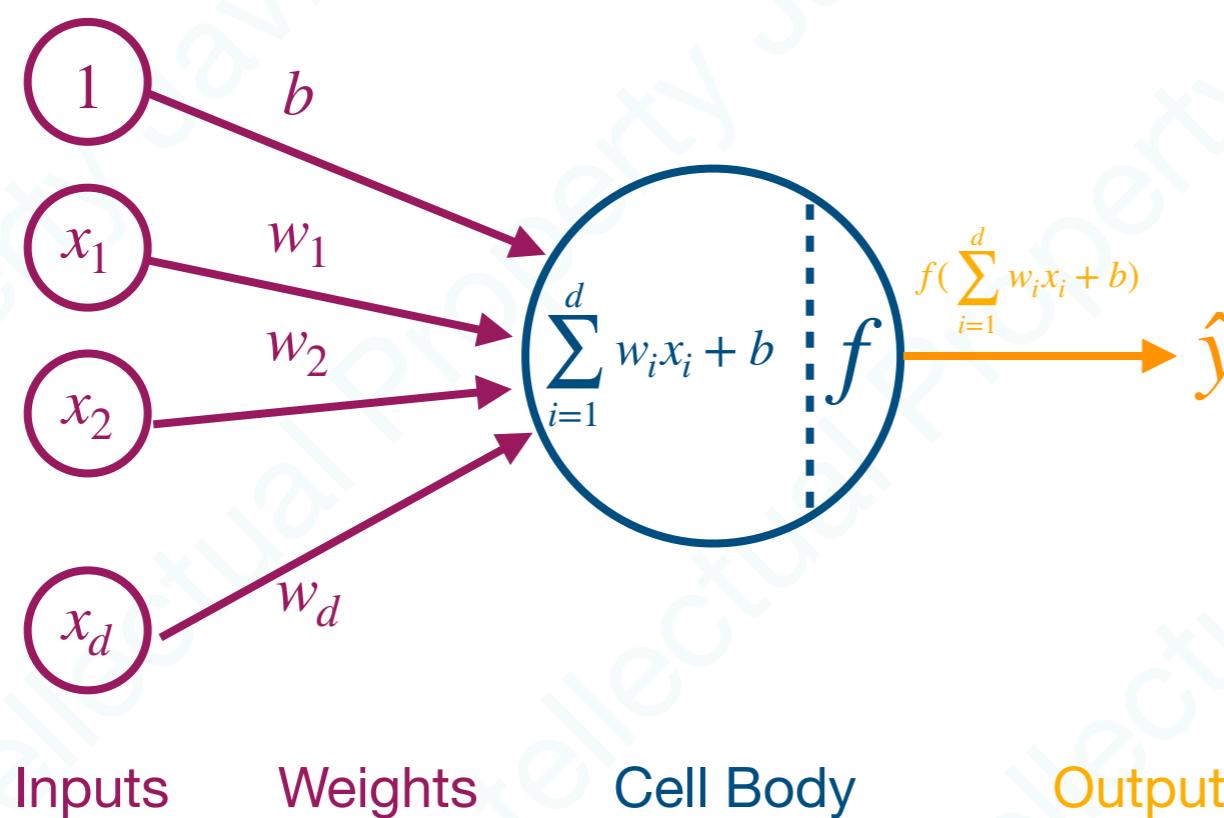


Artificial Neural Networks

The Perceptron Model

One of the earliest models based on the fundamental properties of the nervous system at that time. It comprises:

- A linear function that aggregates the input signals.
- A threshold function that determines whether the neuron fires or no.
- A learning mechanism to adjust the connection weights (error-correction).



Activation Function
Output ↓
$$\hat{y} = f\left(\sum_{i=1}^d w_i x_i + b\right)$$
$$= f(w^T x + b)$$

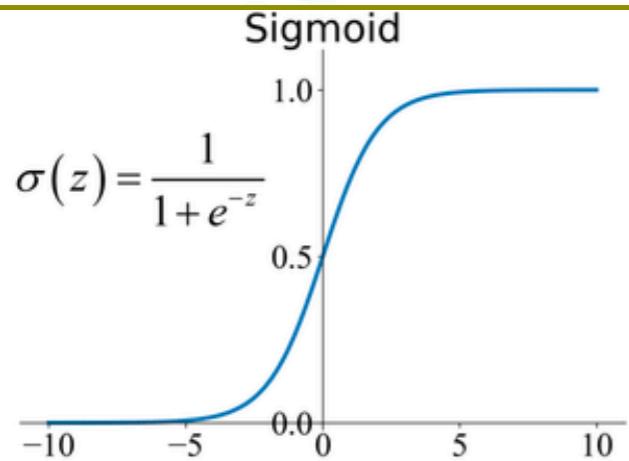
with:

$$x = \begin{bmatrix} x_1 \\ \vdots \\ x_d \end{bmatrix}; W = \begin{bmatrix} w_1 \\ \vdots \\ w_d \end{bmatrix}; b \in \mathbb{R}$$

Artificial Neural Networks

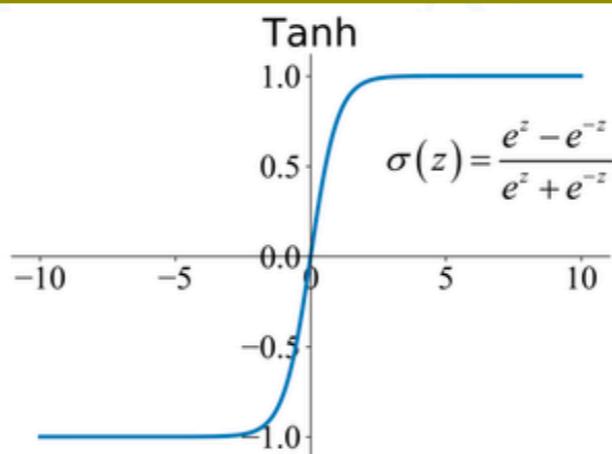
Activation Functions: Types

Sigmoid Function



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

Hyperbolic Tangent



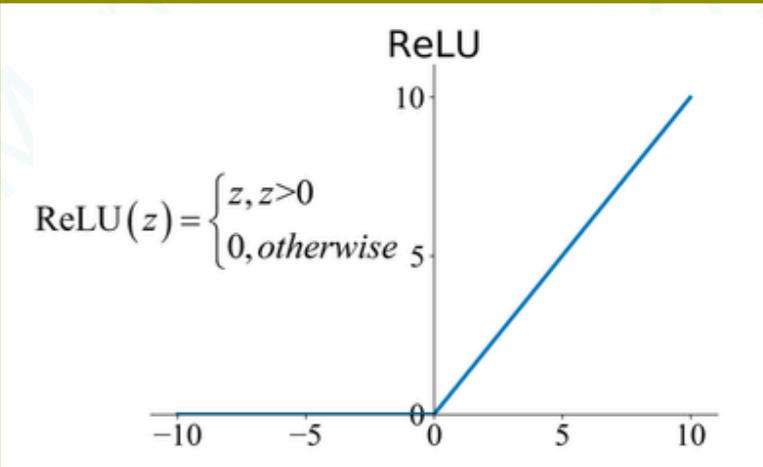
$$\tanh(z) = \frac{e^z - e^{-z}}{e^z + e^{-z}}$$

Overview:

- Normalises its input to the range [-1,1].
- It is mainly used for binary classification tasks

```
>>> m = nn.Sigmoid()  
>>> input = torch.randn(2)  
>>> output = m(input)
```

Rectified Linear Unit



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

Overview:

- Normalises its input to the range [0,inf[
- All the negative values become zero.

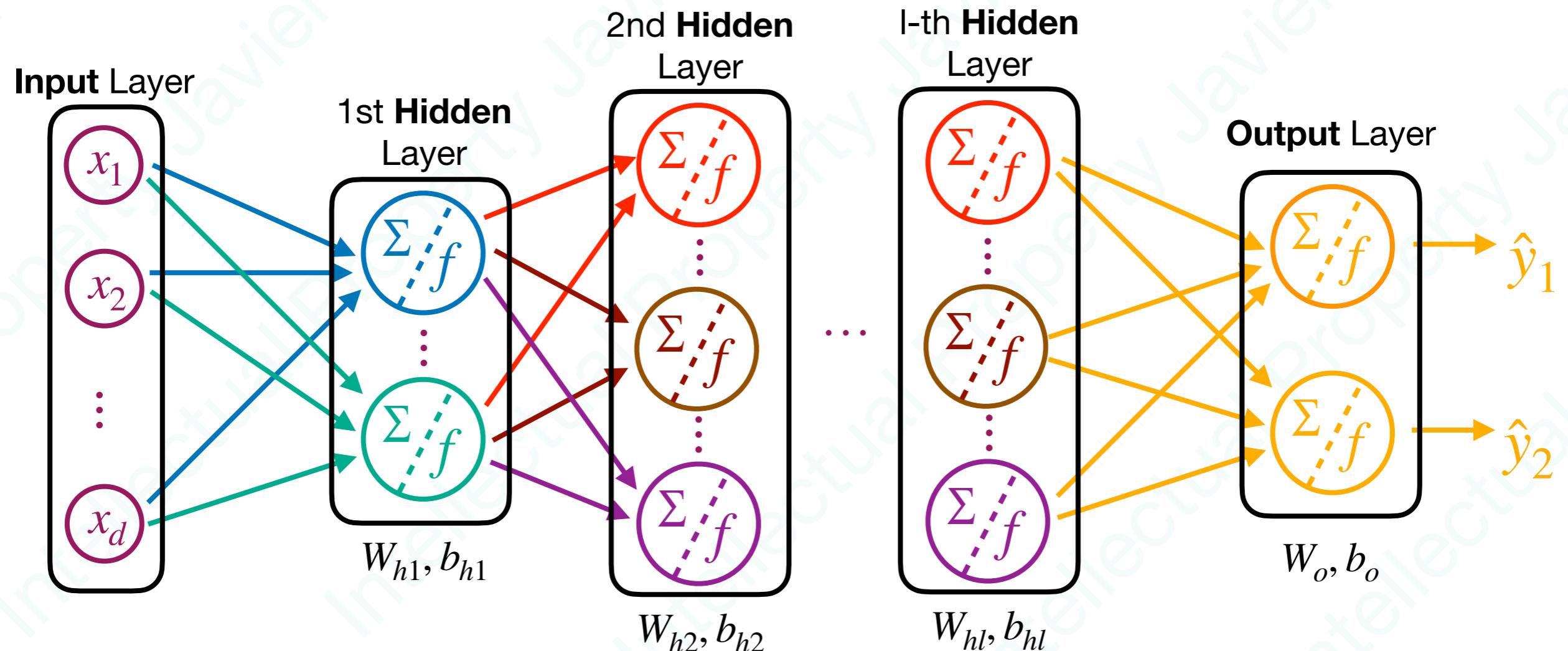
```
>>> m = nn.ReLU()  
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```

Artificial Neural Networks

Multi-layer Perceptron

A **MLP** is a supervised learning approach that learns a function $f() : \mathbb{R}^d \rightarrow \mathbb{R}^o$ by training on a dataset \mathbb{D} .

- A MLP learns a non-linear function approximation for classification or regression.
- It consists of a set of layers: {input, hidden, output} containing a set of neurons.
- Different hyper parameters need to be tuned.

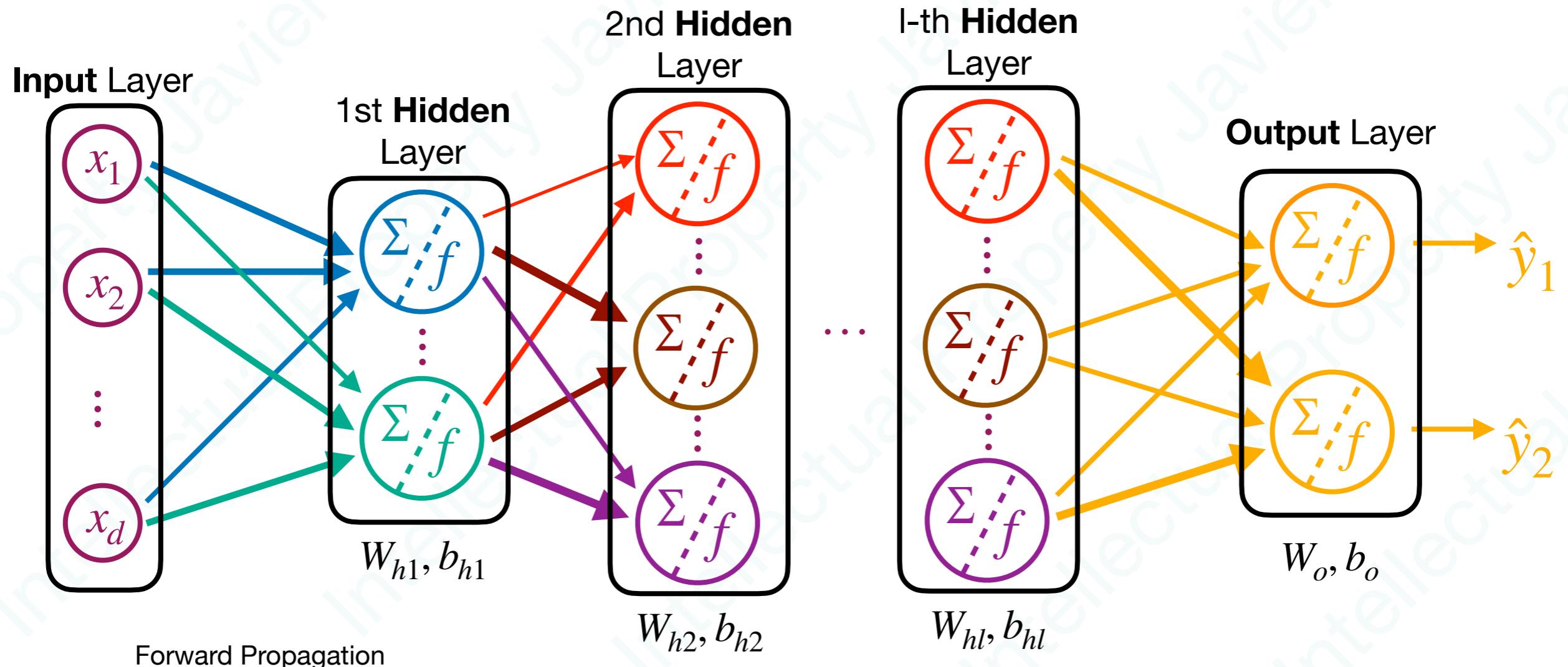


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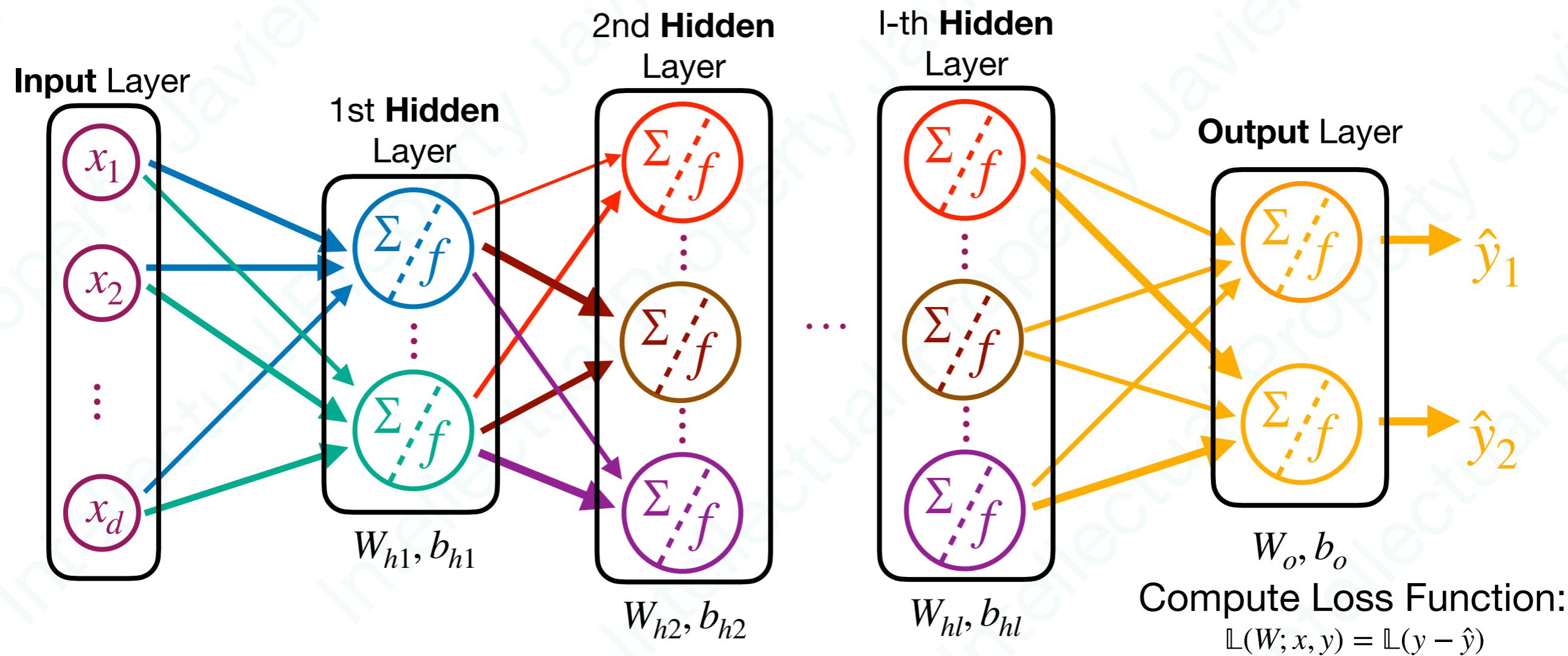


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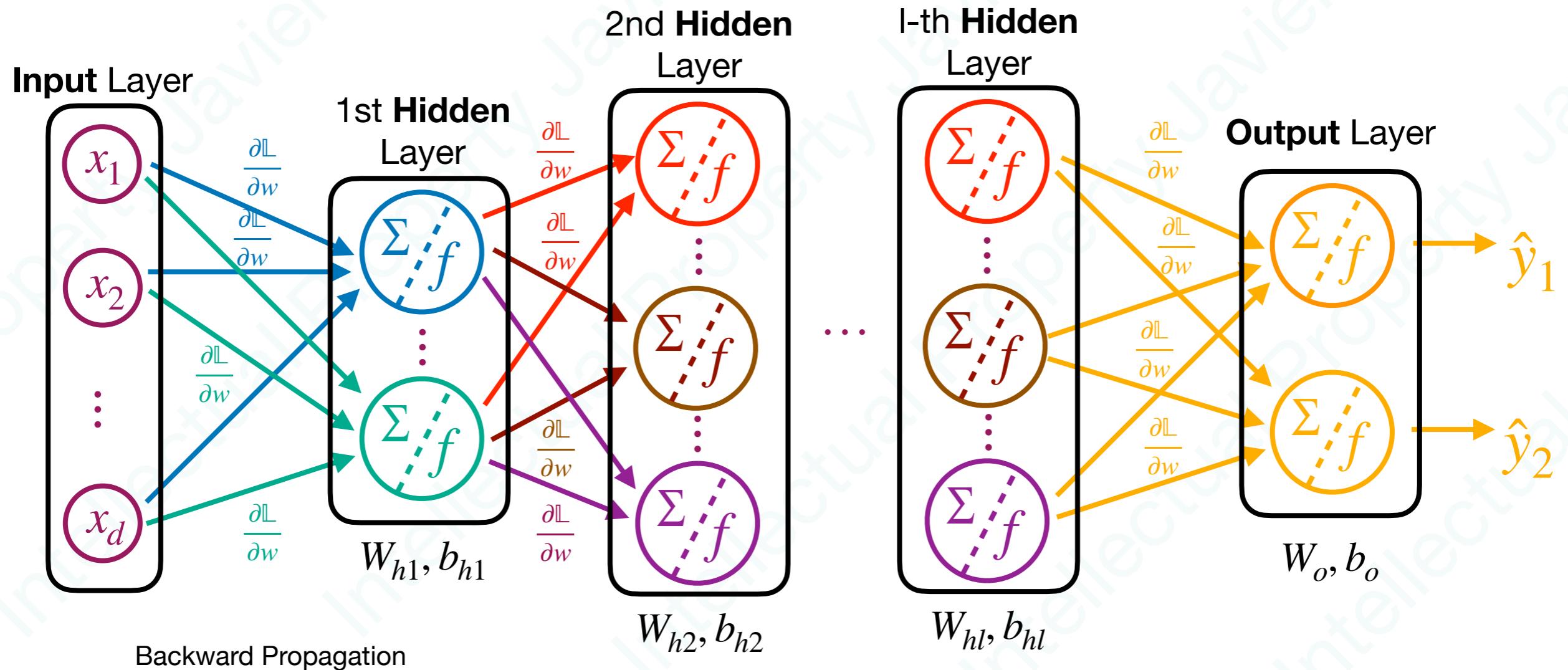


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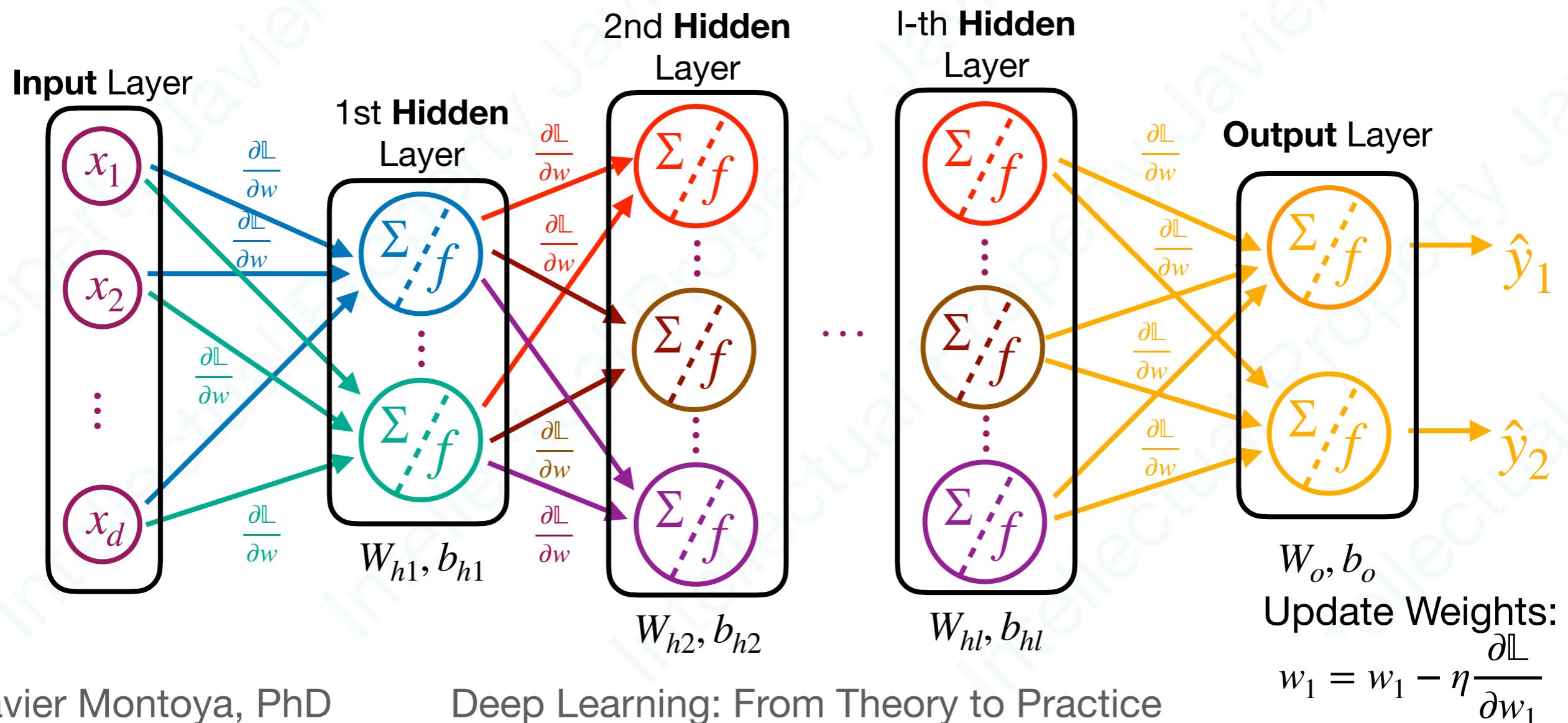


Artificial Neural Networks

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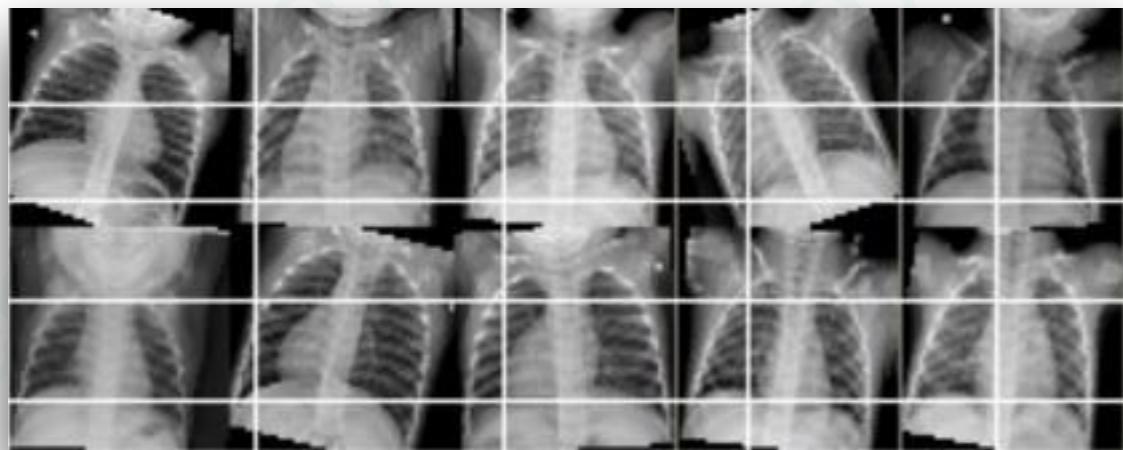
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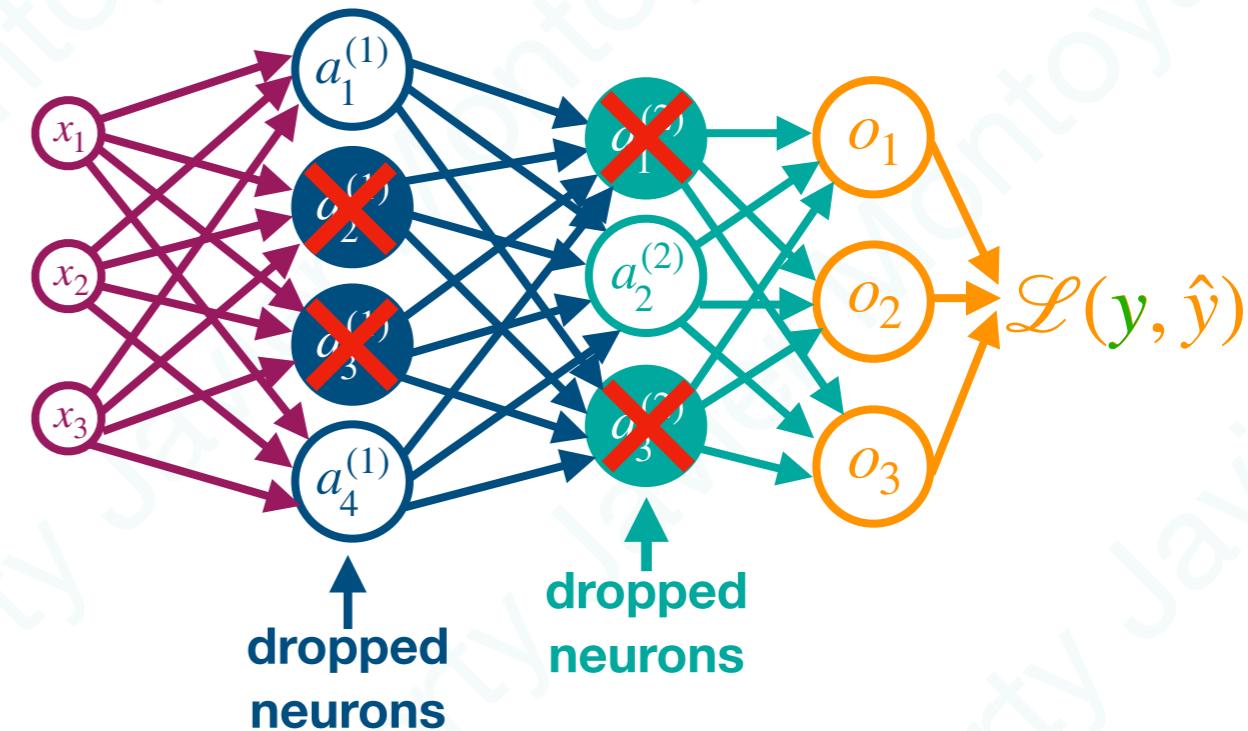
Artificial Neural Networks

Improving model generalisation

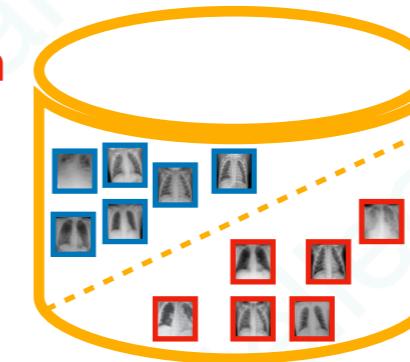
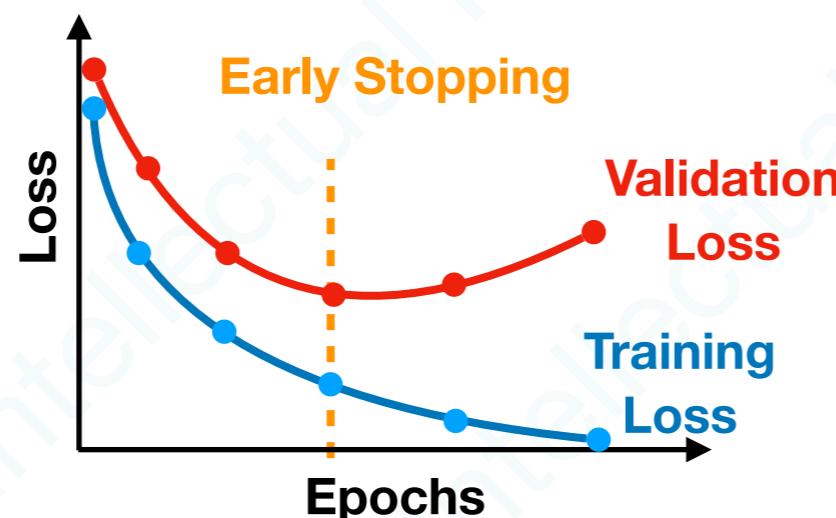
Data Augmentation:



Dropout:



Early Stopping:



Artificial Neural Networks: PyTorch

```
class MultilayerPerceptron(torch.nn.Module):
    def __init__(self, num_features, num_classes, drop_proba,
                 num_hidden_1, num_hidden_2):
        super(MultilayerPerceptron, self).__init__()

        self.my_network = torch.nn.Sequential(
            torch.nn.Linear(num_features, num_hidden_1),
            torch.nn.ReLU(),
            torch.nn.Dropout(drop_proba),
            torch.nn.Linear(num_hidden_1, num_hidden_2),
            torch.nn.ReLU(),
            torch.nn.Dropout(drop_proba),
            torch.nn.Linear(num_hidden_2, num_classes)
        )

    def forward(self, x):
        logits = self.my_network(x)
        probas = F.softmax(logits, dim=1)
        return logits, probas
```

Class inheritance: nn.Module
General building block for NNs

Class Constructor:
Initialise model parameters

Architecture Definition

Forward Propagation:
The forward() method must be overwritten for any subclass of nn.Module

Artificial Neural Networks: PyTorch

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Class inheritance: nn.Module
General building block for NNs

torch.nn.Module



def __init__():



def forward():



Architecture Definition

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            torch.nn.ReLU(),
            torch.nn.Dropout(drop_proba),
            torch.nn.Linear(num_hidden_2, num_classes))

    def forward(self, x):
        logits = self.my_network(x)
        probas = F.softmax(logits, dim=1)
        return logits, probas
```

The diagram illustrates a Multilayer Perceptron (MLP) architecture and its corresponding PyTorch code definition. The architecture consists of three layers: an input layer with four nodes (x_1, x_2, x_3, x_4), a hidden layer 1 with three nodes ($a_1^{(1)}, a_2^{(1)}, a_3^{(1)}$), and a hidden layer 2 with two nodes ($a_1^{(2)}, a_2^{(2)}$). The output layer has three nodes (o_1, o_2, o_3) from which the predicted output \hat{y} is derived. The connections between layers are represented by arrows labeled W_1 , W_2 , and W_3 . A ReLU activation function is shown with its mathematical definition: $\text{ReLU}(z) = \begin{cases} z, & z \geq 0 \\ 0, & \text{otherwise} \end{cases}$. The PyTorch code defines the network structure using the `Sequential` container and various layers from the `torch.nn` module, including Linear, ReLU, and Dropout layers. The forward pass method performs the computation from input x through the network to produce logits and probas.

Architecture Definition

Artificial Neural Networks: PyTorch

Training Procedure

```
for epoch in range(EPOCHS):
    print('EPOCH {}'.format(epoch_number + 1))

    # Make sure gradient tracking is on, and do a pass over the data
    model.train(True)
    avg_loss = train_one_epoch(epoch_number, writer)

    # We don't need gradients on to do reporting
    model.train(False)

    running_vloss = 0.0
    for i, vdata in enumerate(validation_loader):
        vinputs, vlabels = vdata
        voutputs = model(vinputs)
        vloss = loss_fn(voutputs, vlabels)
        running_vloss += vloss

    avg_vloss = running_vloss / (i + 1)
    print('LOSS train {} valid {}'.format(avg_loss, avg_vloss))

    # Log the running loss averaged per batch
    # for both training and validation
    writer.add_scalars('Training vs. Validation Loss',
                      { 'Training' : avg_loss, 'Validation' : avg_vloss },
                      epoch_number + 1)

    writer.flush()

    # Track best performance, and save the model's state
    if avg_vloss < best_vloss:
        best_vloss = avg_vloss
        model_path = 'model_{}_{}'.format(timestamp, epoch_number)
        torch.save(model.state_dict(), model_path)

    epoch_number += 1
```

The diagram illustrates the training procedure as a sequence of nested loops and conditional blocks, each highlighted with a dashed border of a specific color:

- Red dashed border:** Training over different epochs.
- Blue dashed border:** Set the model on training status.
- Purple dashed border:** Set the model on evaluation phase.
- Green dashed border:** Set the model on evaluation status.
- Orange dashed border:** Evaluate the model on the validation set.
- Brown dashed border:** Record and show training and validation statistics after 1x epoch.
- Brown dashed border:** Track and save best model on the validation set.

Artificial Neural Networks: PyTorch

Training Procedure

```
def train_one_epoch(epoch_index, tb_writer):
    running_loss = 0.
    last_loss = 0.

    # Here, we use enumerate(training_loader) instead of
    # iter(training_loader) so that we can track the batch
    # index and do some intra-epoch reporting
    for i, data in enumerate(training_loader):
        # Every data instance is an input + label pair
        inputs, labels = data

        # Zero your gradients for every batch!
        optimizer.zero_grad()

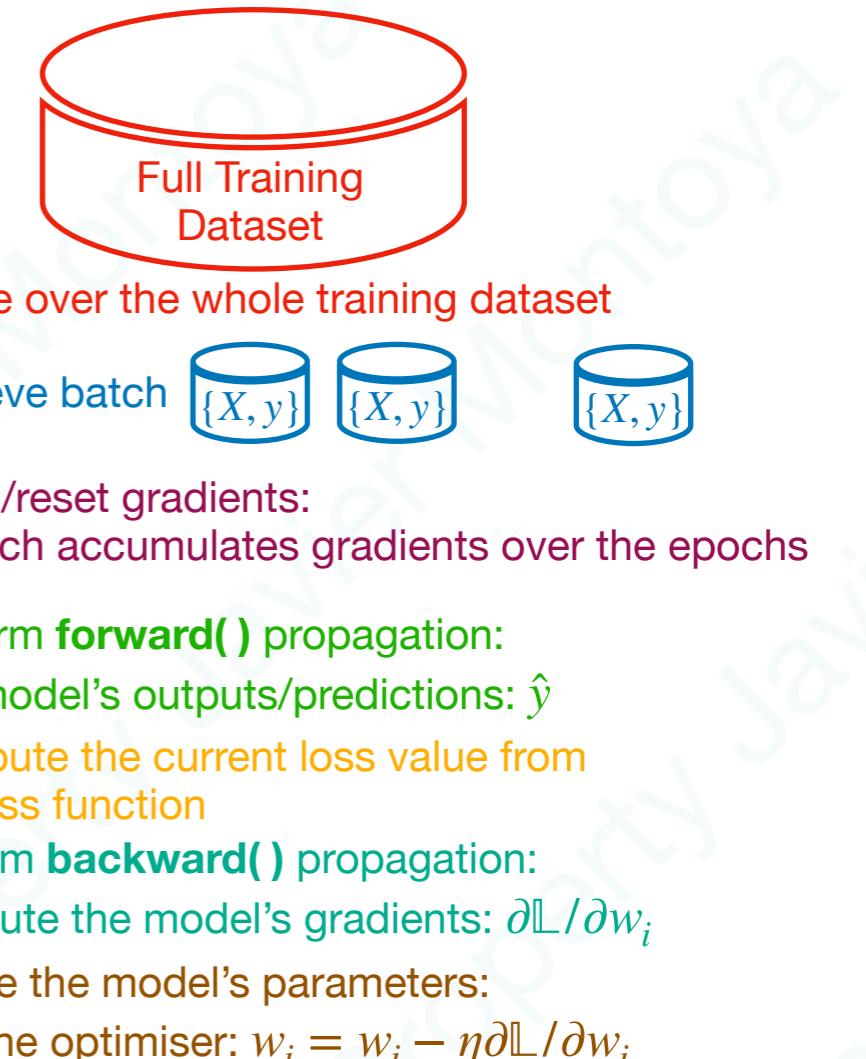
        # Make predictions for this batch
        outputs = model(inputs)

        # Compute the loss and its gradients
        loss = loss_fn(outputs, labels)
        loss.backward()

        # Adjust learning weights
        optimizer.step()

        # Gather data and report
        running_loss += loss.item()
        if i % 1000 == 999:
            last_loss = running_loss / 1000 # loss per batch
            print(' batch {} loss: {}'.format(i + 1, last_loss))
            tb_x = epoch_index * len(training_loader) + i + 1
            tb_writer.add_scalar('Loss/train', last_loss, tb_x)
            running_loss = 0.

    return last_loss
```



Deep Learning: From Theory to Practice

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