Introduction to Machine Learning

Foundations and Applications

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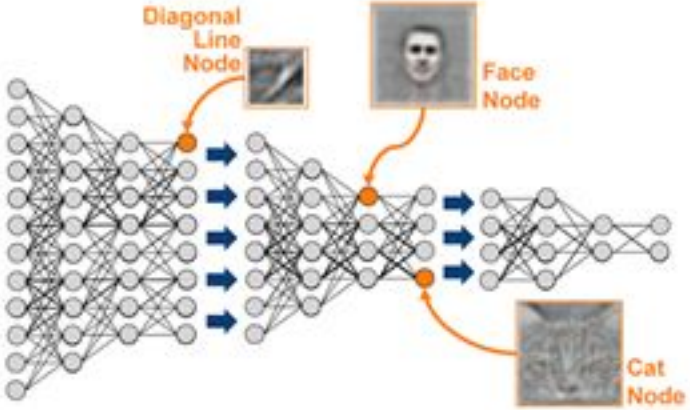
University of California
Santa Barbara

Deep Learning and Neural Networks

Deep Learning Overview

Machine Learning: Typical task is to try to learn a function $\mathrm{h}(\boldsymbol{x};\theta)$ from data $S = \{(x_i, y_i)\}$ that approximates y = f(x).



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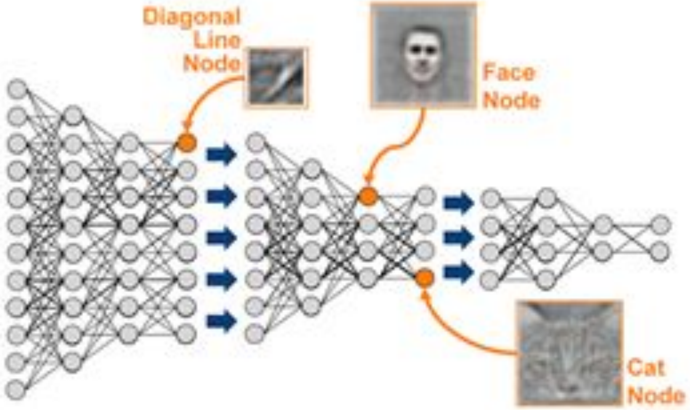

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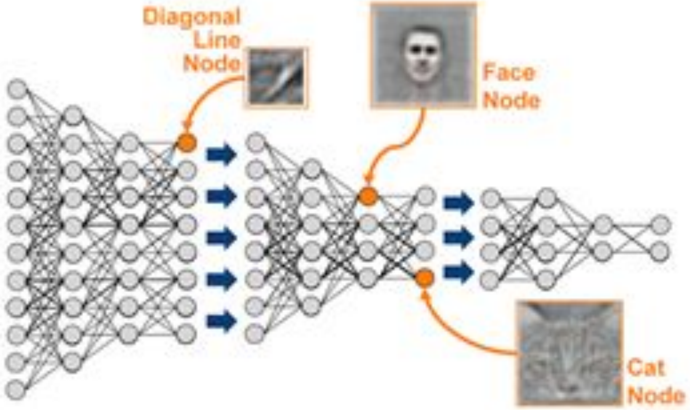

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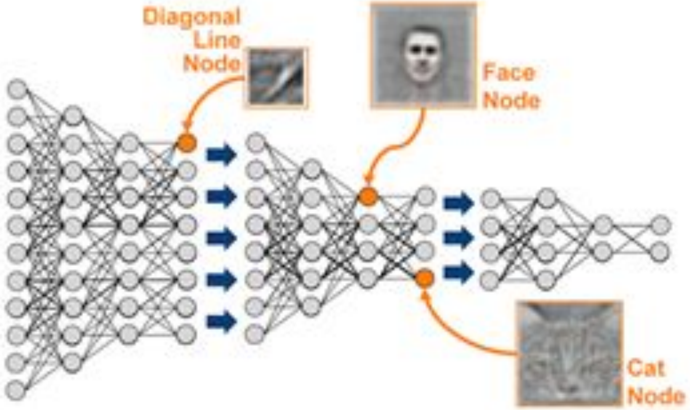

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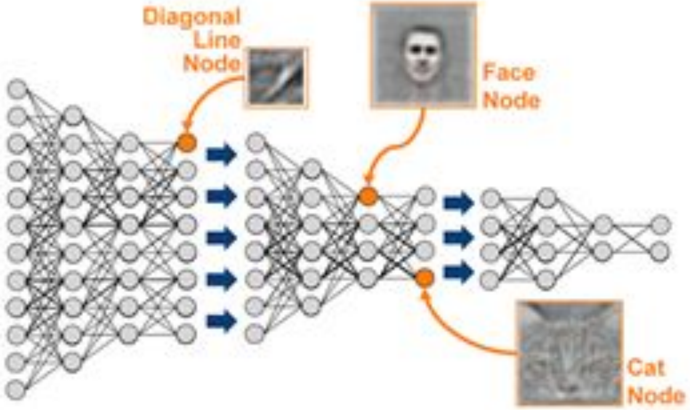

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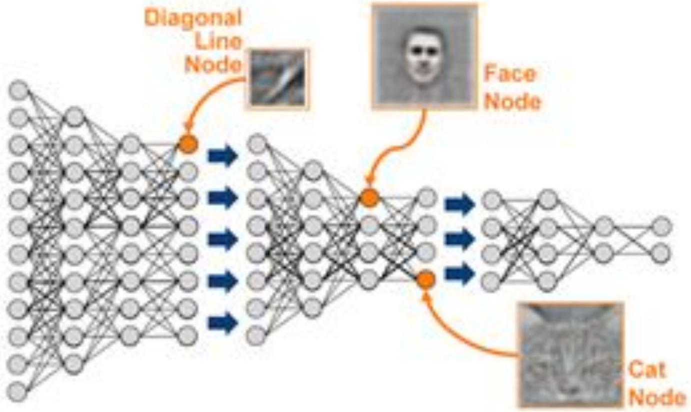

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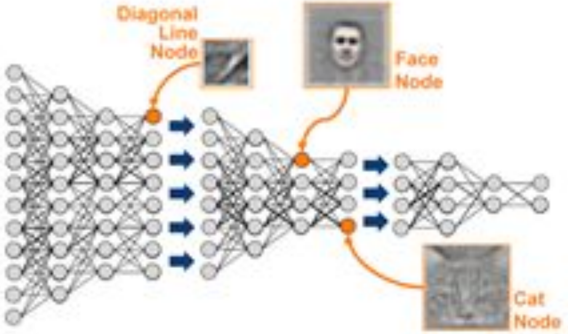

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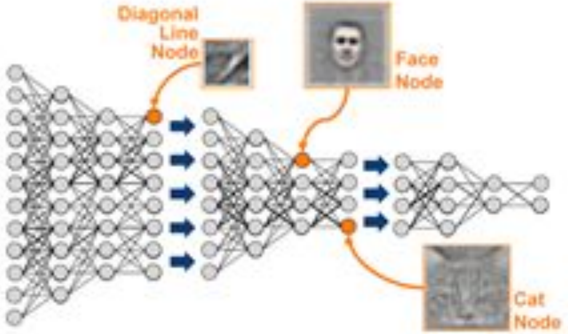

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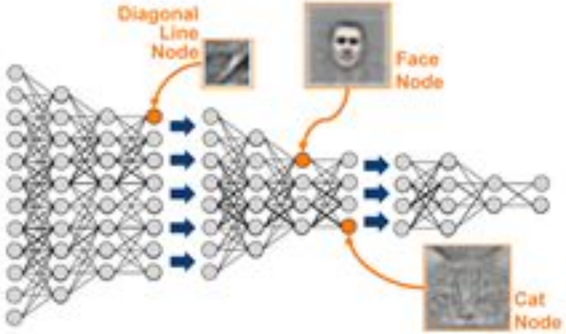

Ex: Regression $\mathrm{y} = |\cos(x_1 x_2) + 1|$ would have $f(x) = f^{(3)}\left(f^{(2)}\left(f^{(1)}(\boldsymbol{x})\right)\right)$ with $f^{(1)}(x_1, x_2) = x_1 x_2$ and $f^{(2)}\left(h^{(1)}\right) = \cos\left(h^{(1)}\right) + 1$ and $f^{(3)}\left(h^{(2)}\right) = \mathrm{abs}\left(h^{(2)}\right)$.

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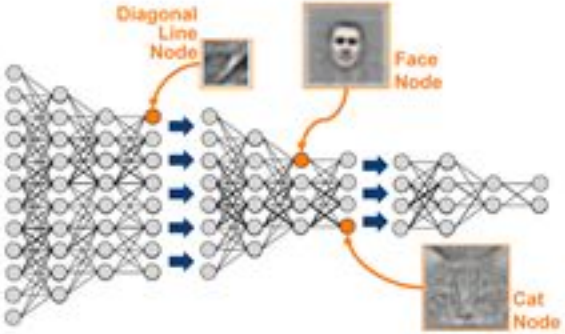

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Generally, we can think about $\mathrm{y} = \mathrm{f}(\boldsymbol{x}) = f^{(L)}\left(f^{(L-1)}\left(\ldots f^{(1)}(\boldsymbol{x})\ldots\right)\right)$ in terms of components as

$$\mathrm{y} = f(x_1, x_2, \ldots, x_N) = f^{(L)}\left(f_1^{(L-1)}\left(z_{i_1}, z_{i_2}, \ldots, z_{i_{N1}}\right), f_2^{(L-1)}\left(z_{j_1}, z_{j_2}, \ldots, z_{j_{N2}}\right), \ldots, f_{n2}^{(L-1)}\left(z_{k_1}, z_{k_2}, \ldots, z_{k_{Nn2}}\right)\right),\ z = f^{(L-2)}$$

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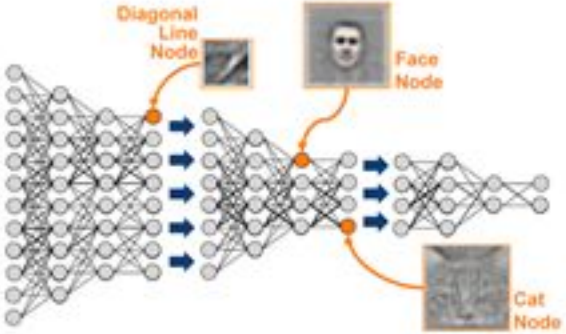

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Concepts represented by hierarchy of distributed features. For instance: position of robotic actuator from angles in arm, identity of person from parts of the face, meaning of a sentence from phrases/words.

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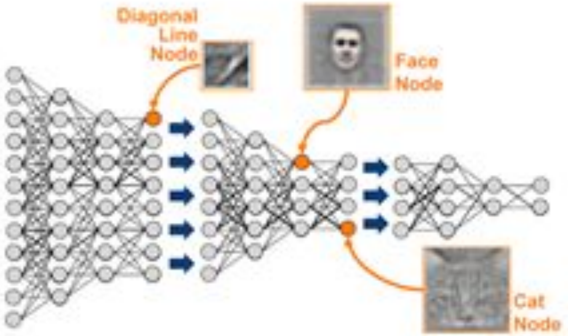

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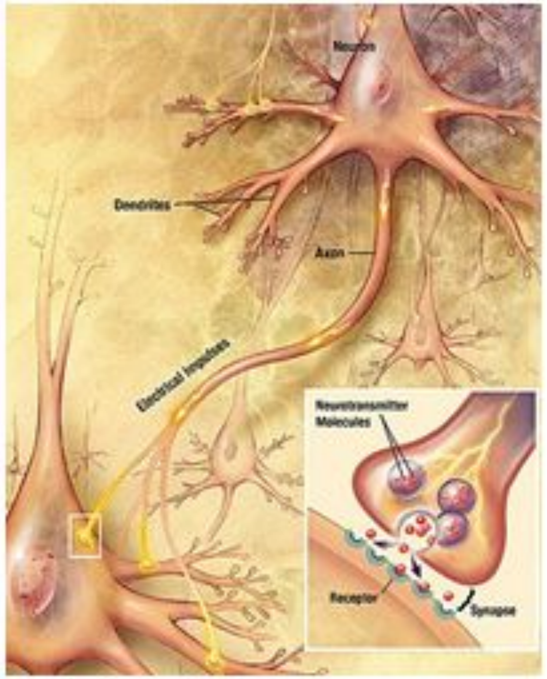
View as building up function from "hidden units" that detect particular features of input **z** as $h^{(k)} = f^{(k)}(\boldsymbol{z})$. Popular way to do this is to use Artificial Neural Networks (ANNs), $h^{(k)} = g(\boldsymbol{z}^T W + b)$.

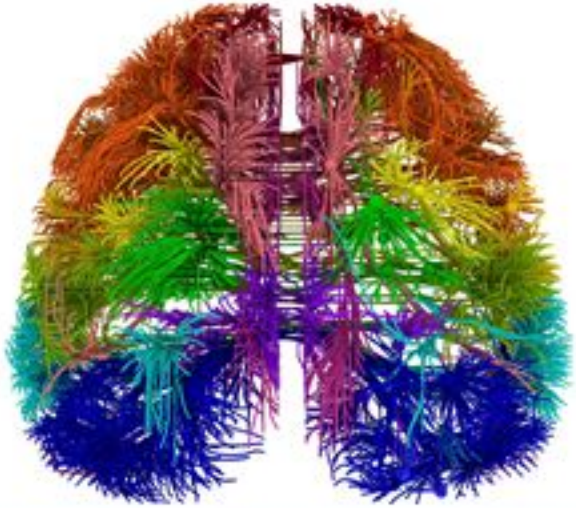
What are Artificial Neural Networks?

Biological neurons process information by firing to excite or inhibit neighbors:
action potentials → voltage-gated ion channels / neurotransmitters → collective neural activity.

Neuron: Axons and Dendrites



Human Connectome Project



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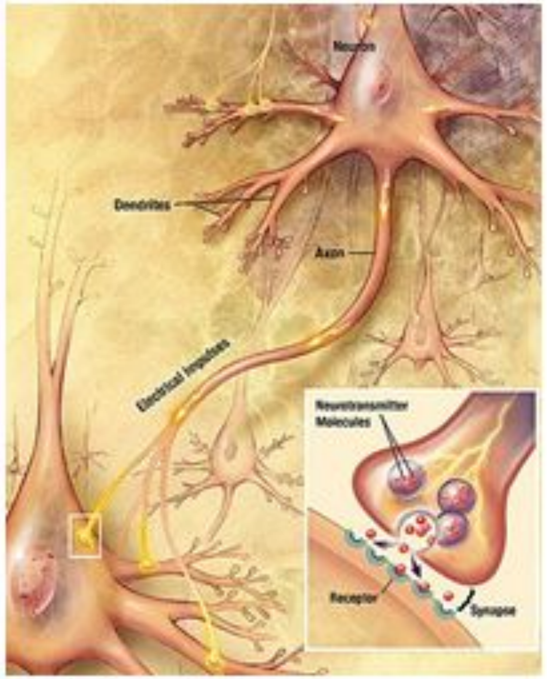

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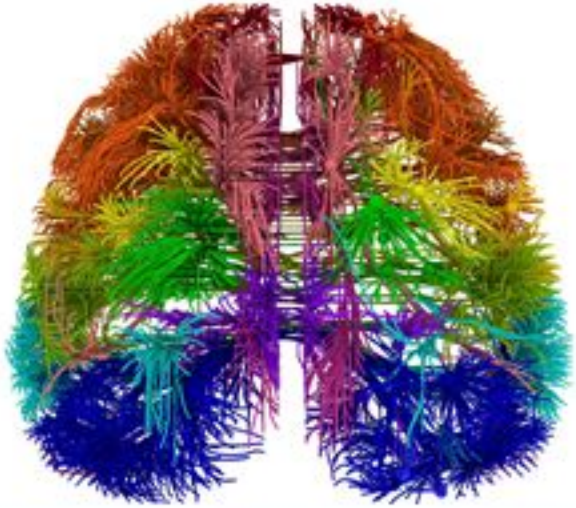

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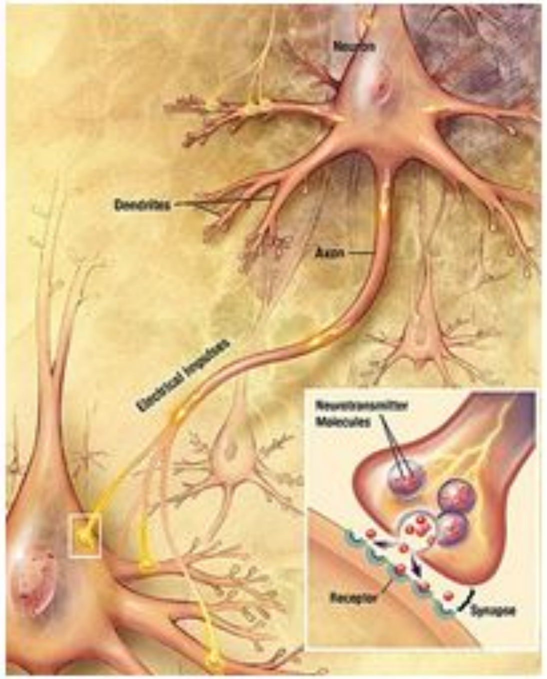

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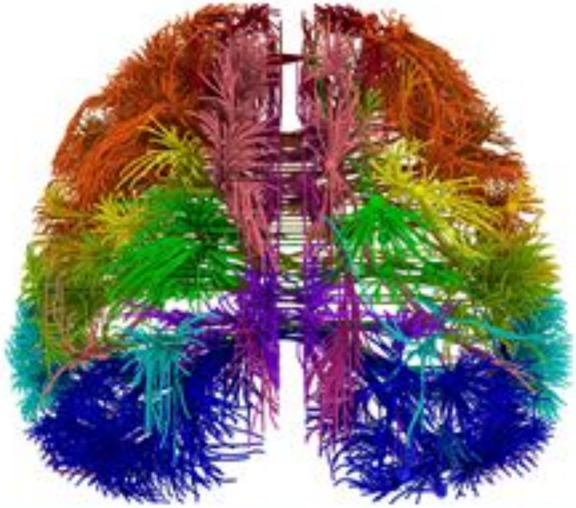

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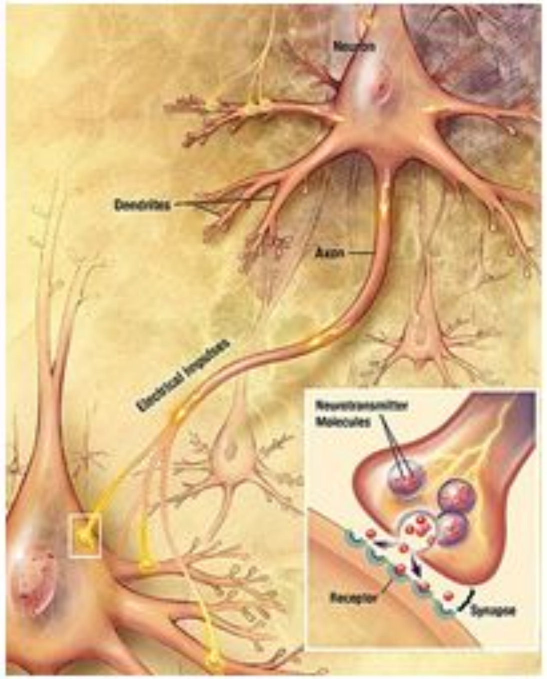

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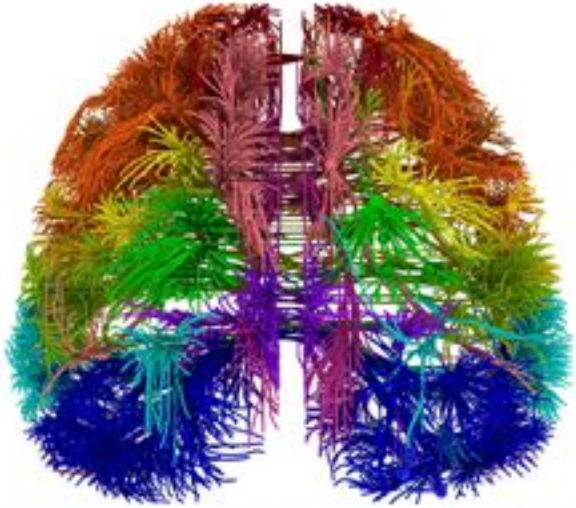

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inspiration →

Wright Brothers

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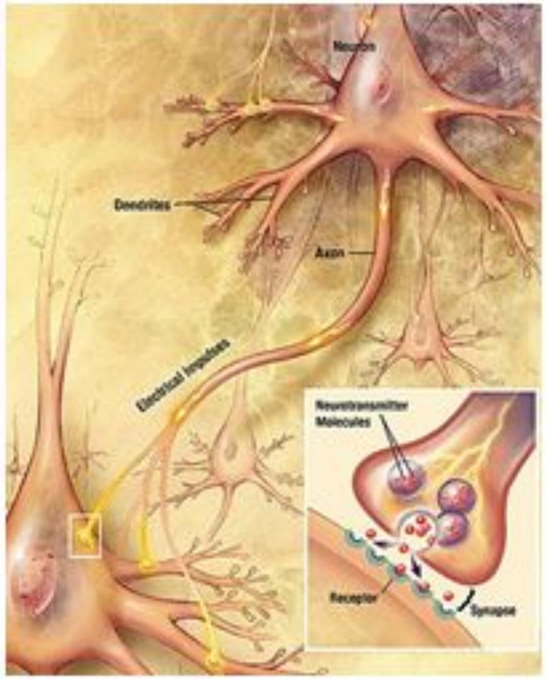

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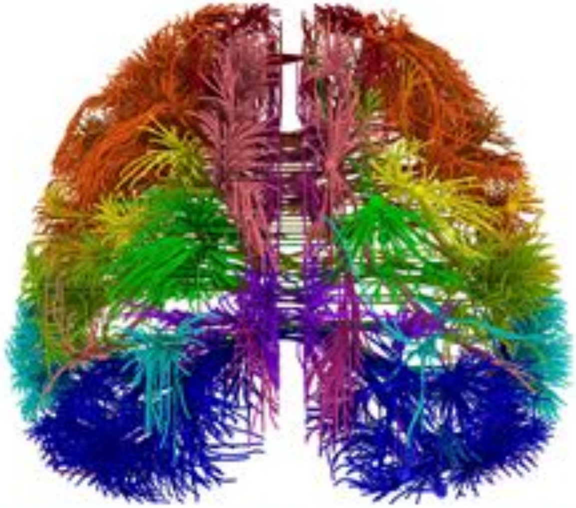

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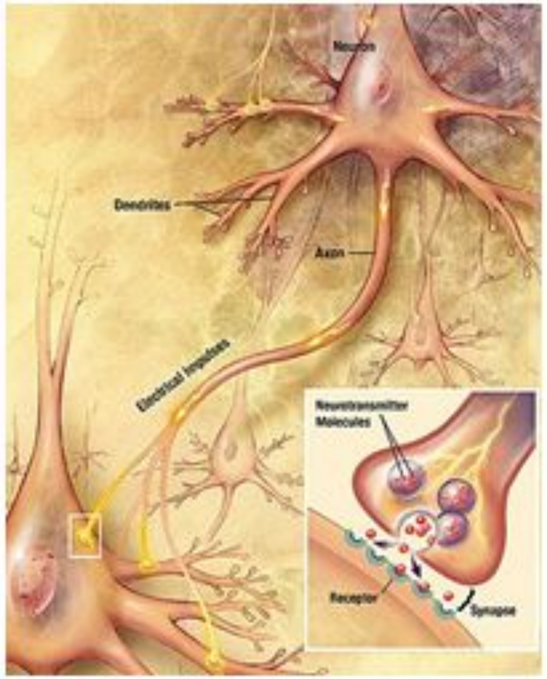

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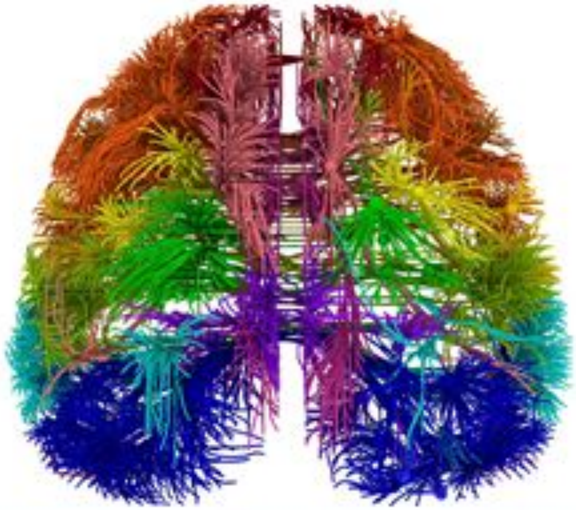

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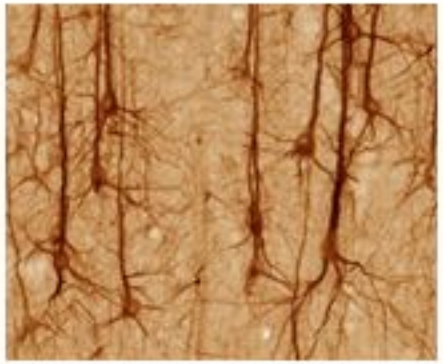

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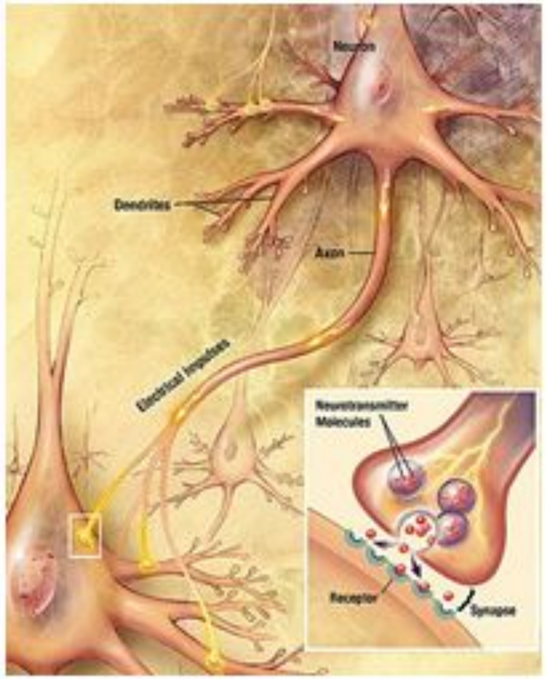

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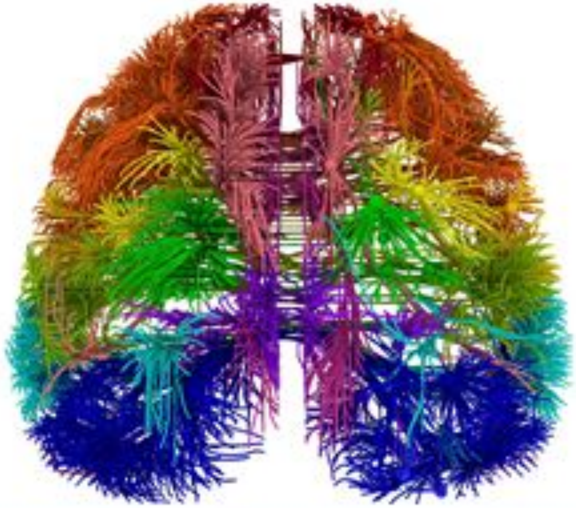

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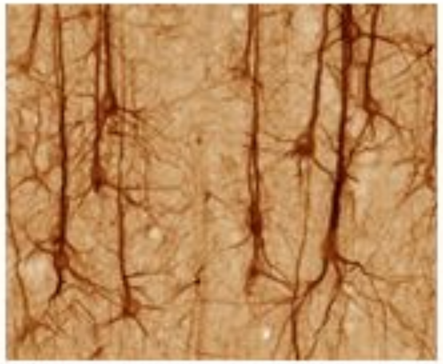
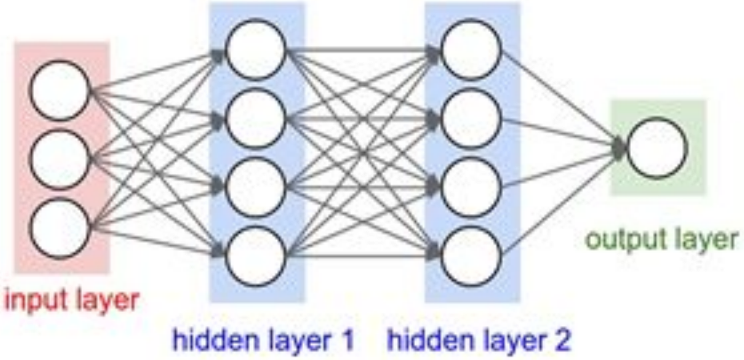


inspiration →

Artificial Neural Network (ANN)



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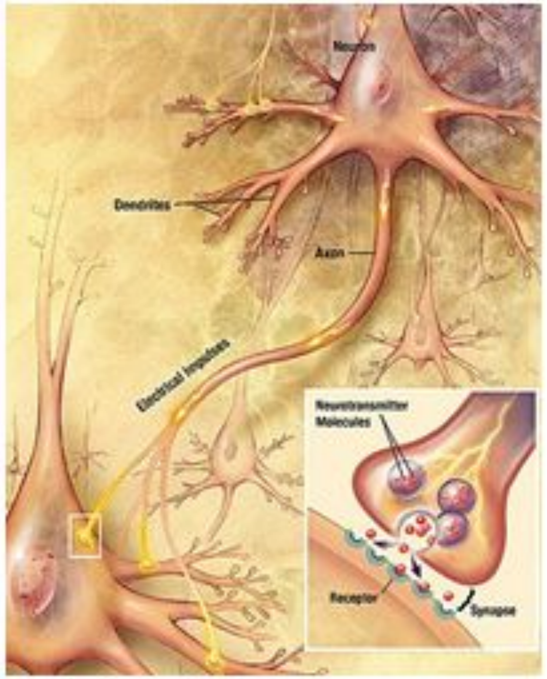

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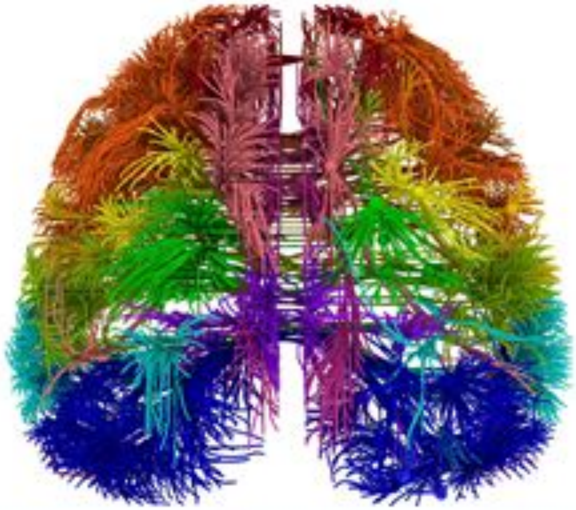

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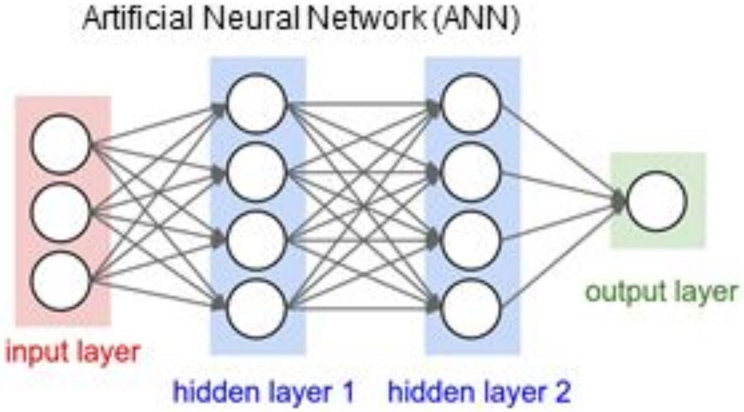

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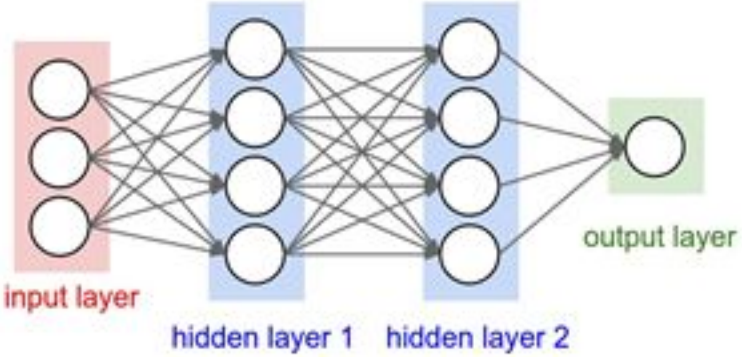

NN Transform: $y = f(\boldsymbol{x};\theta)$ where f is obtained by compositions $f^{(L)}\left(f^{(L-1)}(\ldots f^{(1)}(\boldsymbol{x})\ldots)\right)$ with $\boldsymbol{h}^k = f^{(k)}(\boldsymbol{h}^{k-1}) = g(\boldsymbol{h}^{k-1}\mathrm{W}^k + b^k)$.

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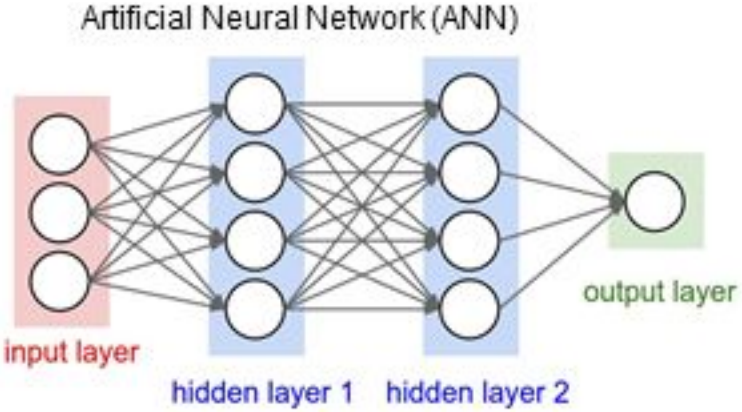

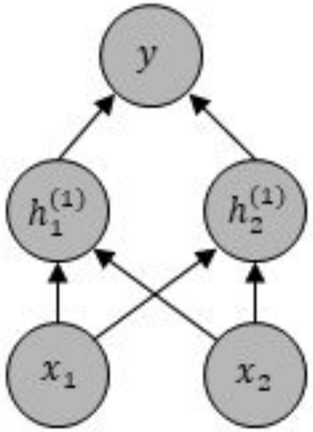

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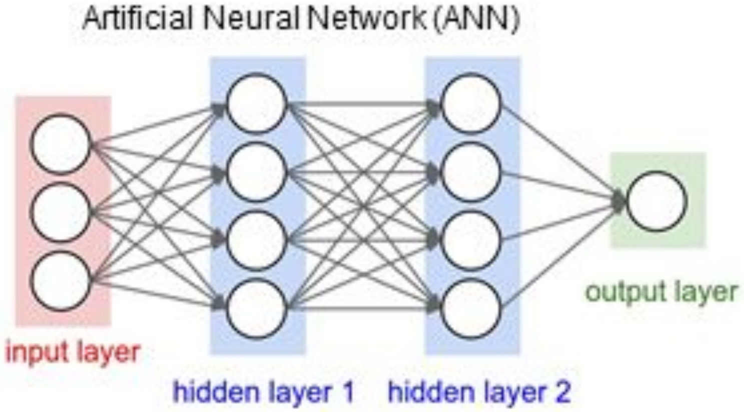

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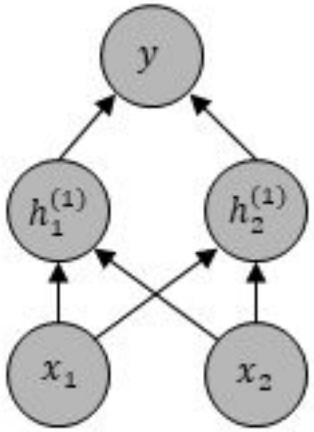

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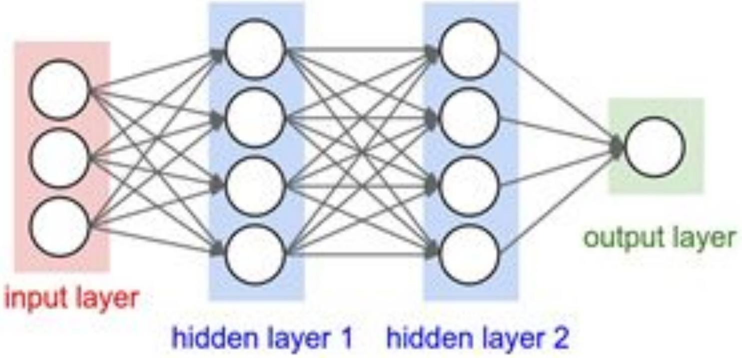
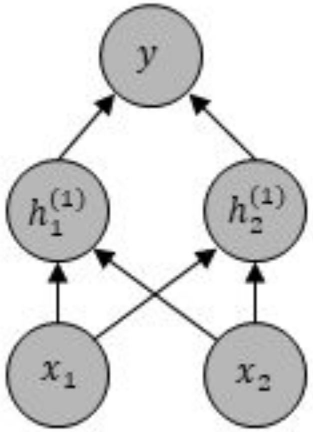
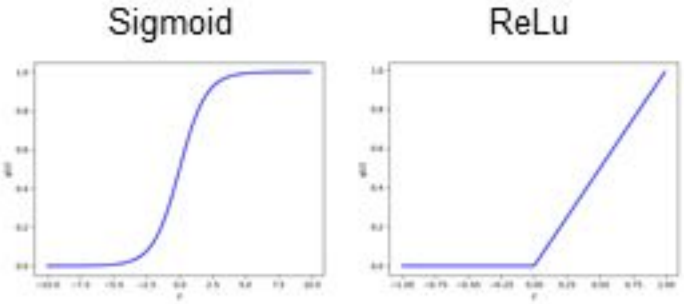
Artificial Neural Network (ANN)







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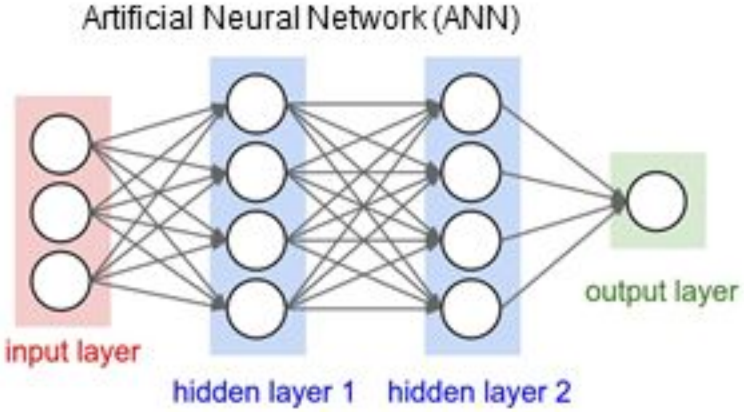

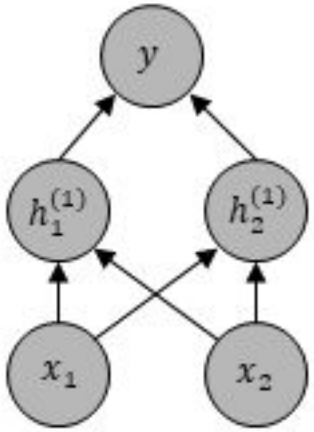

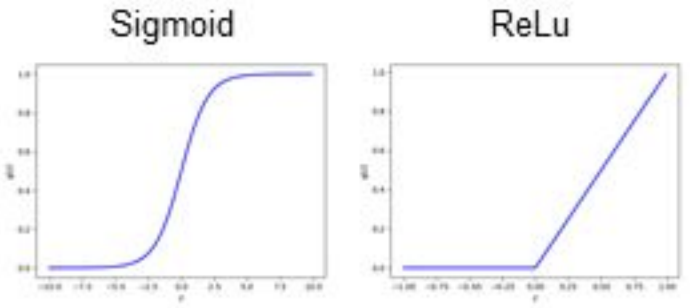

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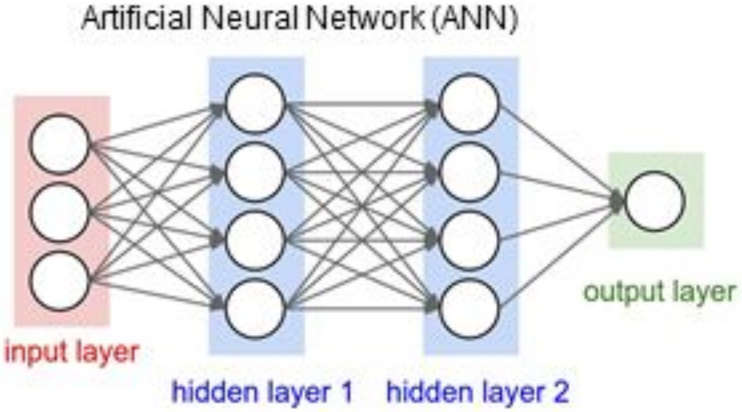

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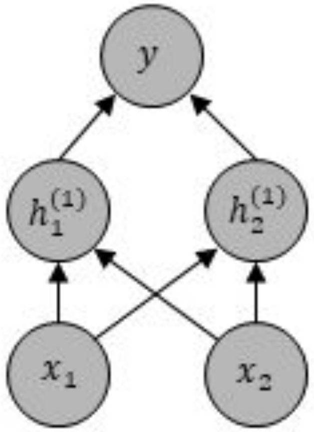

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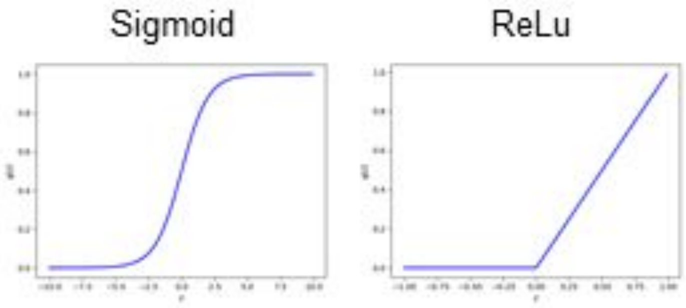

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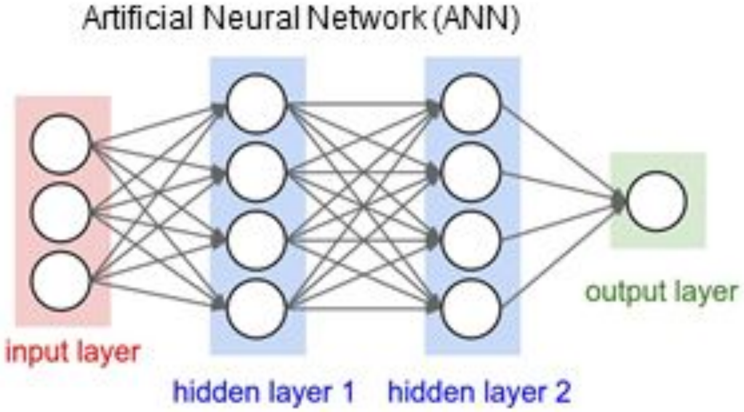

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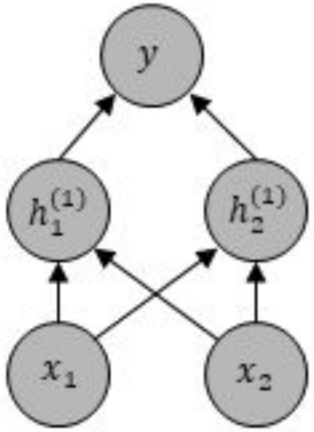

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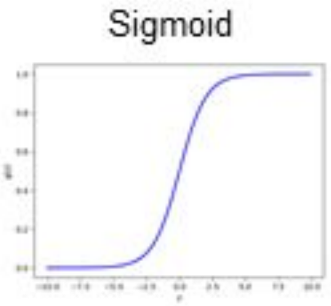

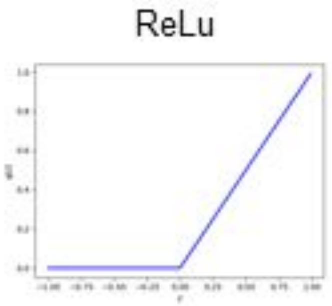

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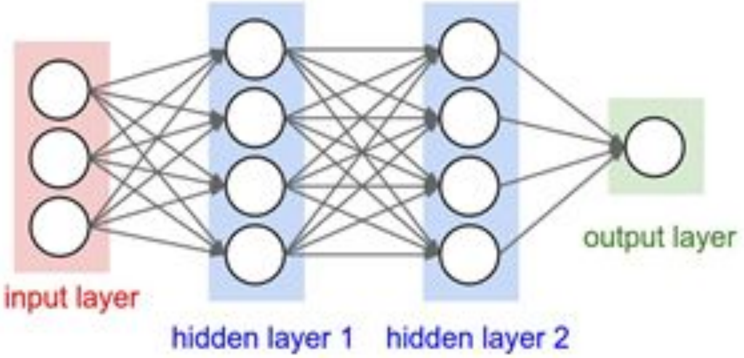

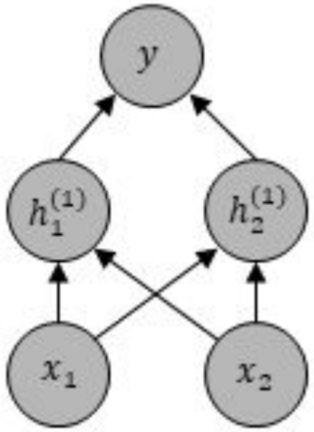

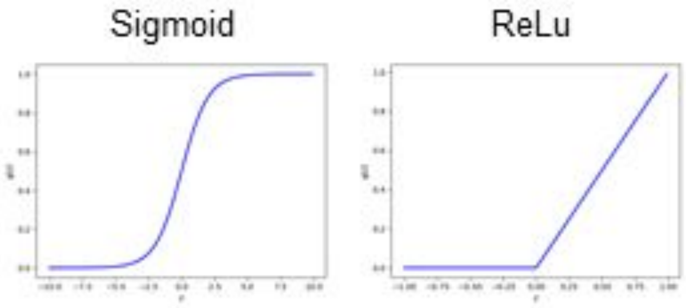

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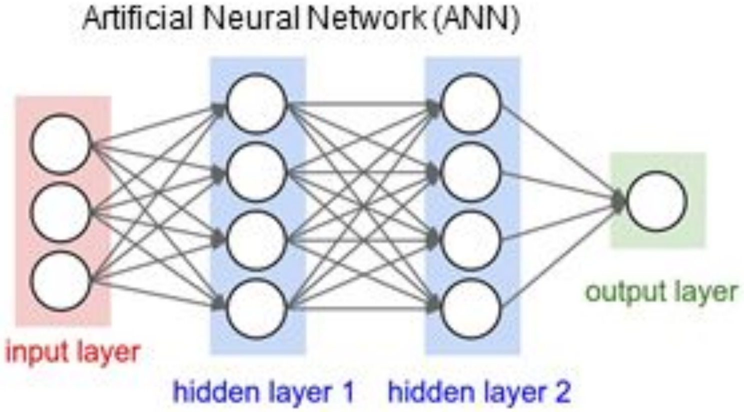

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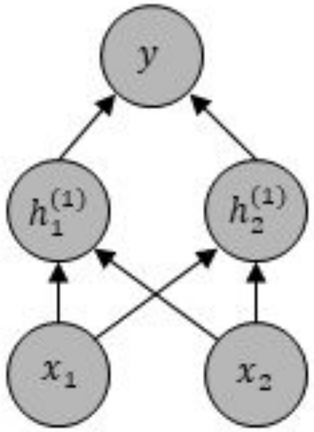

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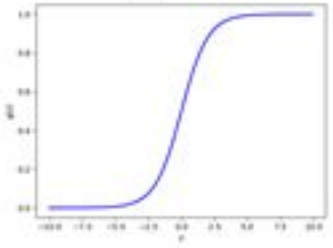
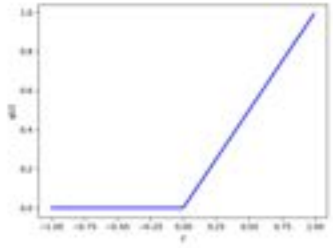


ReLu



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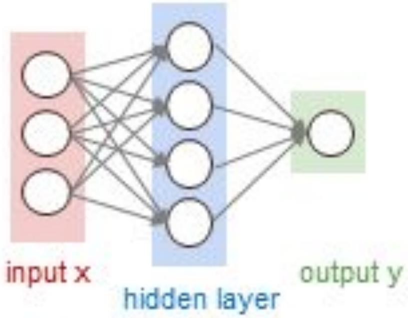
Many possible choices for network architectures, depth, activation functions.

Universal Approximation Theorem

For many activation functions g(z) just two layers is sufficient for universal approximation of any continuous function y = f(x) on a compact set.

Neural Network: 1-Hidden Layer



I_n is the unit cube in $\mathbb{R}^n$

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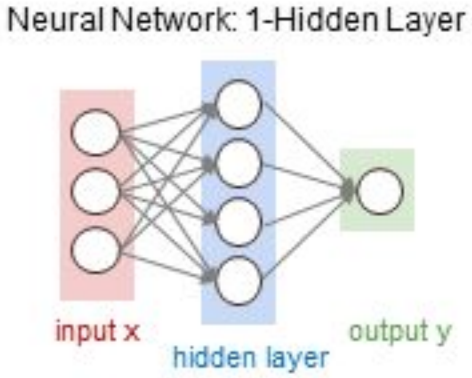
Definition: We say a function g(z) is **discriminatory** if for all $\boldsymbol{w}, b,$ we have $\int g(\boldsymbol{w}^T \boldsymbol{x} + b)\, d\mu(x) = 0$ then the measure must be zero $\mu \equiv 0$.



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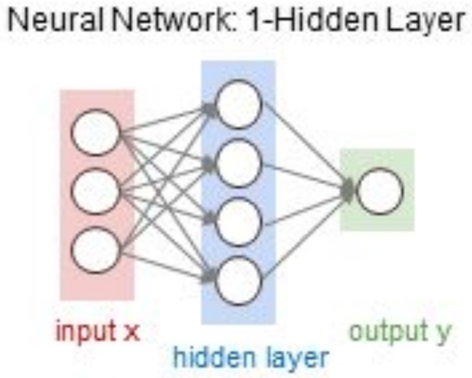

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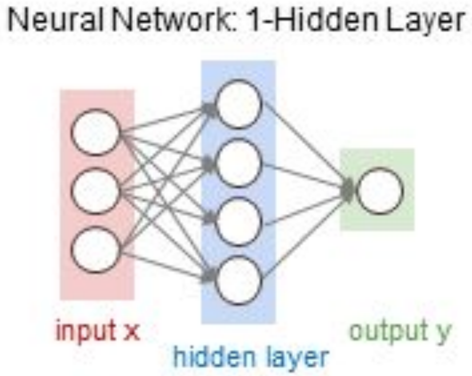

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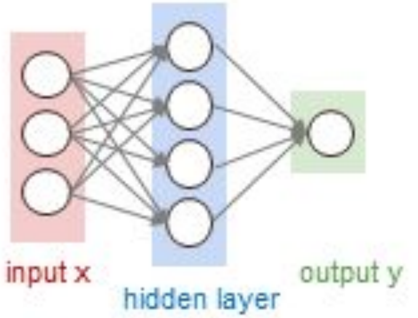

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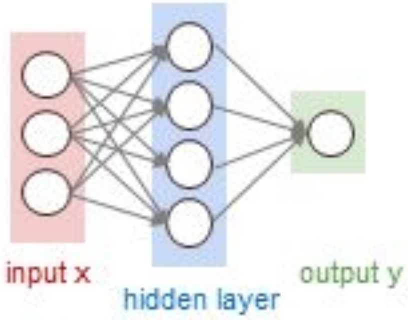

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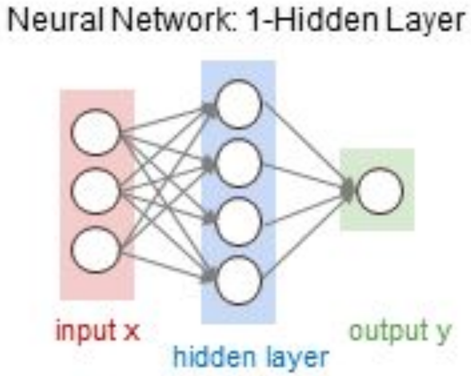

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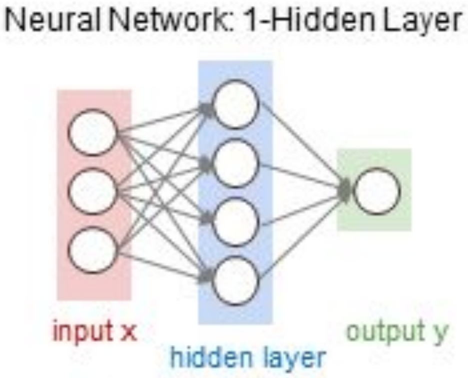
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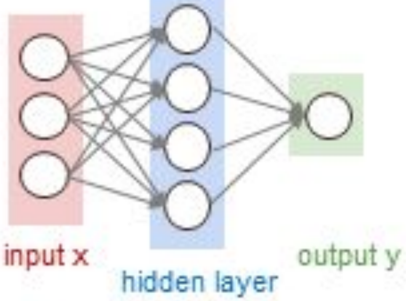

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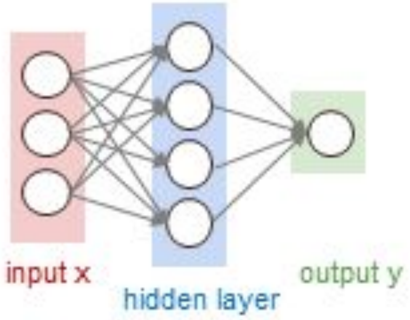
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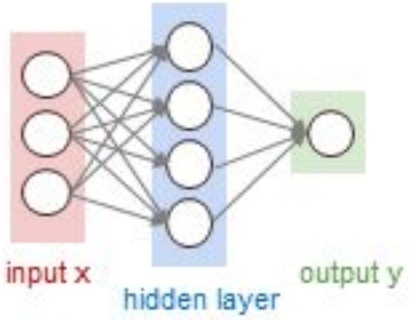
Neural Network: 1-Hidden Layer



Remark: For any function $\mathrm{f} \in C(\mathrm{I}_n)$ and $\varepsilon > 0$ there exists $\mathrm{q} \in V$ with N and weights $\alpha_j, \boldsymbol{w}_j^T, b_j$ such that $|f(x) - q(x)| < \epsilon$ for all $\mathrm{x} \in \mathrm{I}_n$.

Example: Linear/affine activation functions are ***not discrimantory***, $g(z) = c_1 z + c_2$.

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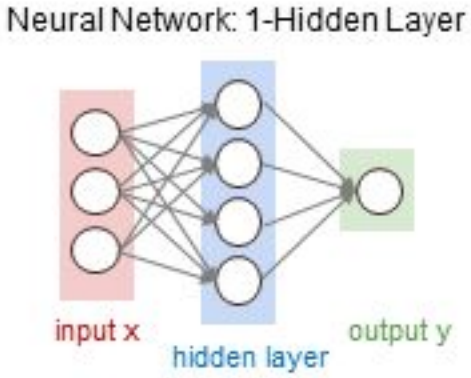

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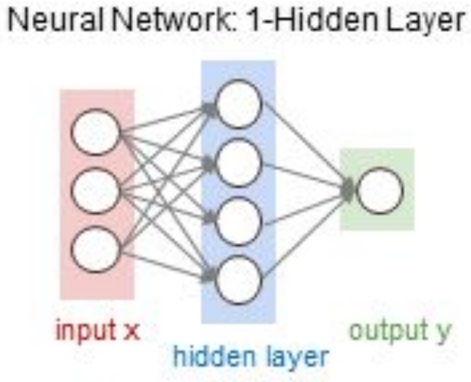

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ReLU-NN's include all pieces-wise linear approximations, realizable with enough hidden nodes, also provides another way to prove the universal approximation.

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Neural Networks: Example

NN Transform: $y = f(\boldsymbol{x};\theta)$ from compositions $\boldsymbol{h}^k = f^{(k)}\left(\boldsymbol{h}^{k-1}\right) = g(\boldsymbol{h}^{k-1}\mathrm{W}^k + \ b^k)$.

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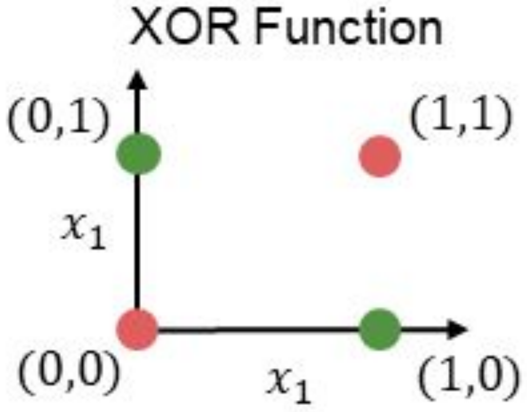

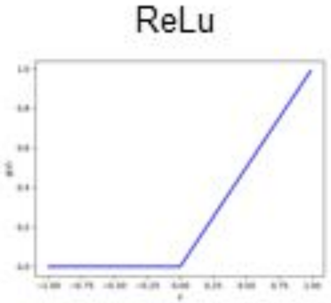

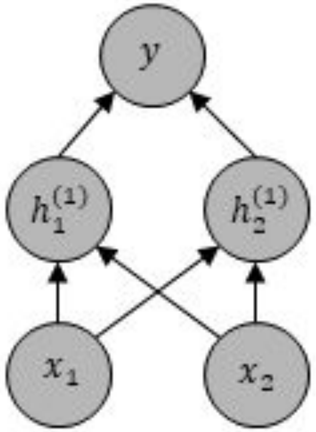

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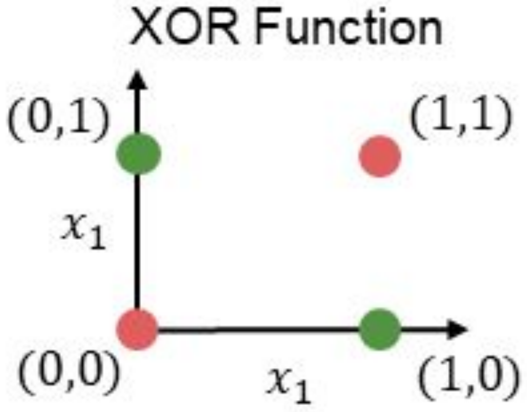

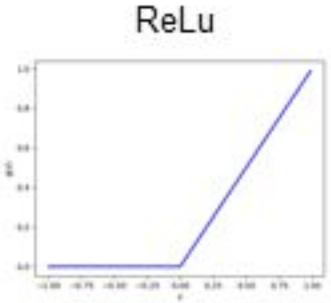

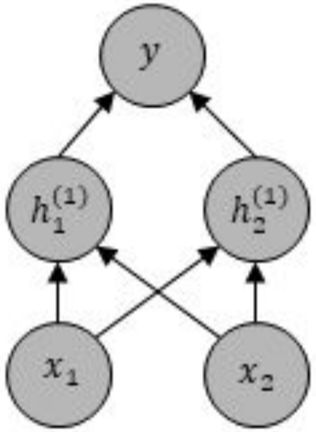

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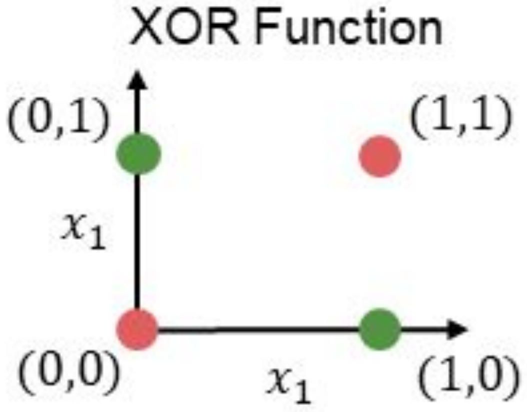

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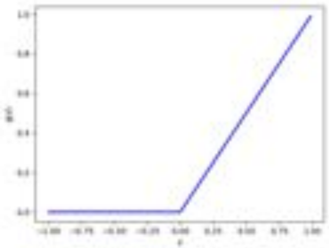
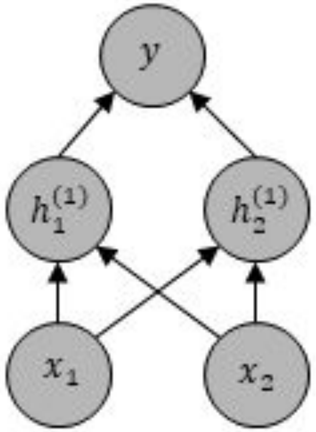
ReLu





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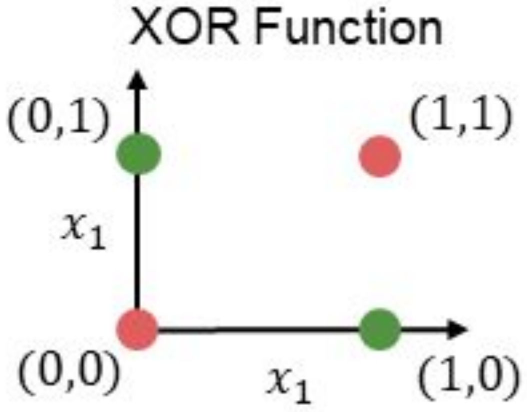

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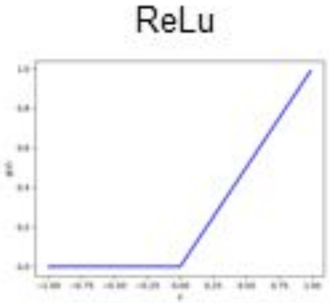

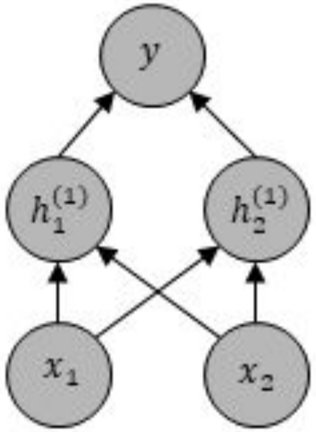

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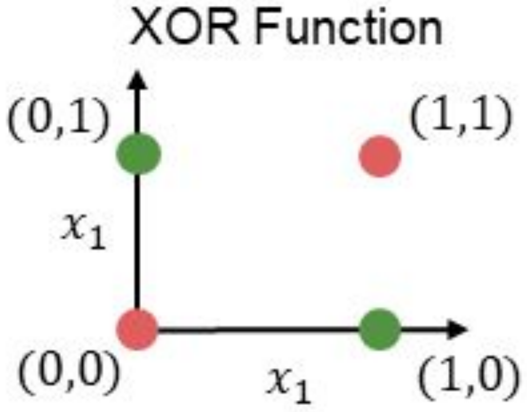

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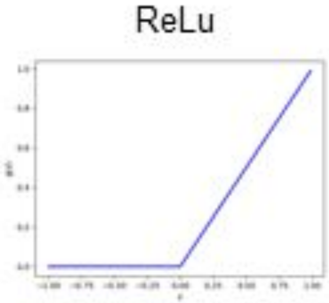

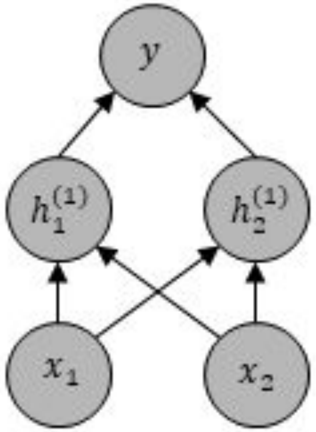

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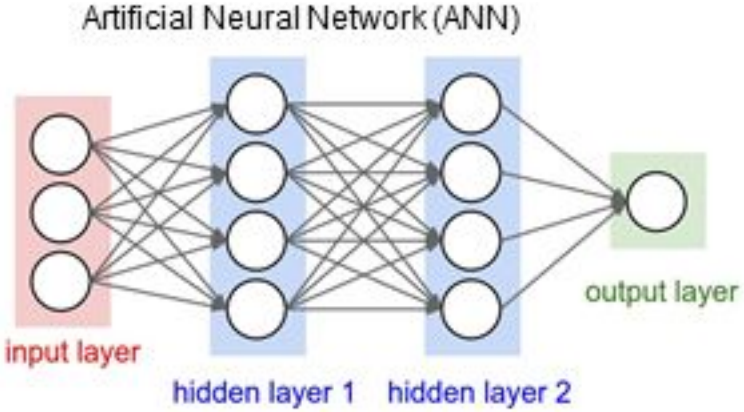
In general, we need methods to learn from data such weights to minimize a loss function.

Learning with Neural Networks

How do we find weights of Neural Networks?



Optimization Problem:

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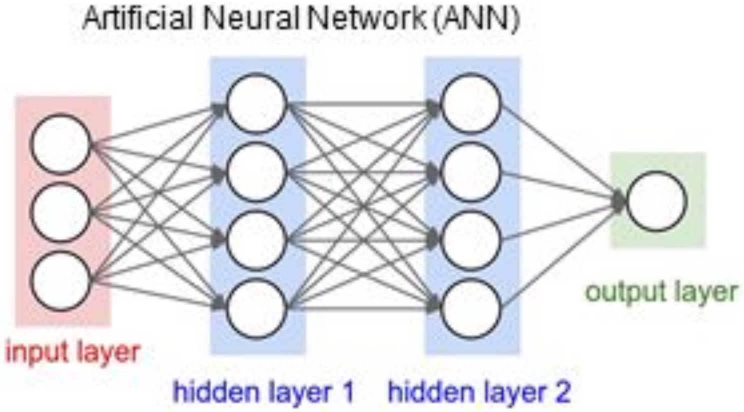

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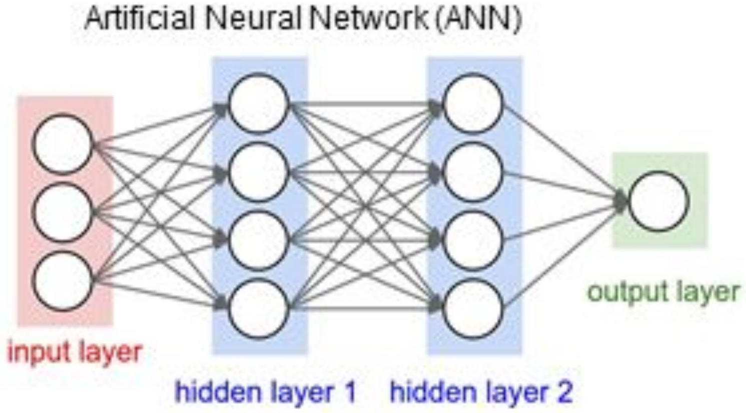

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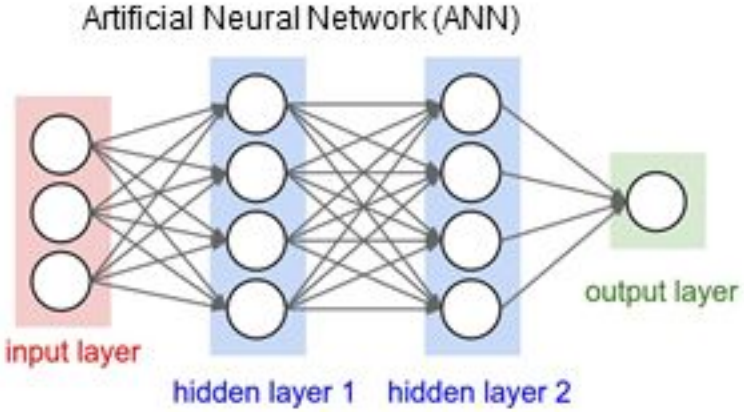

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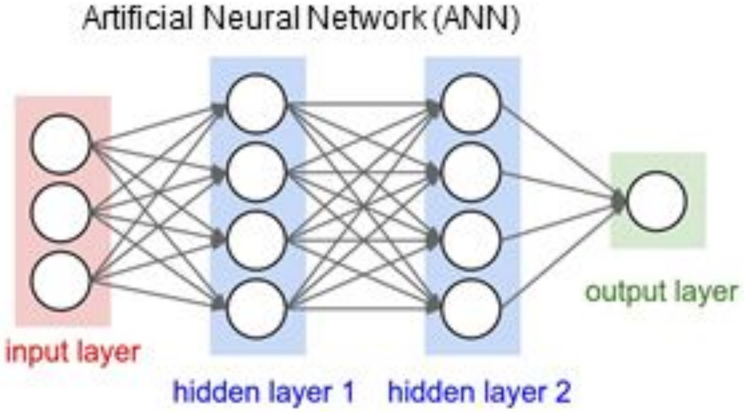

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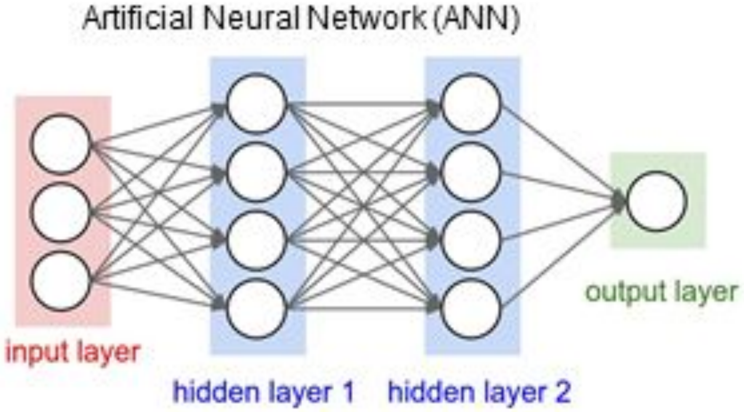

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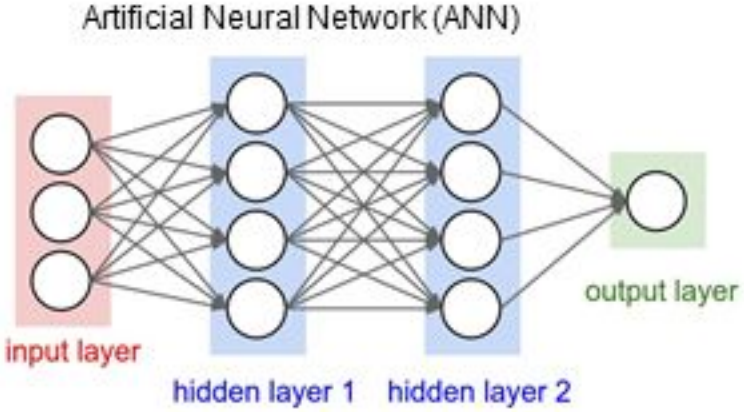

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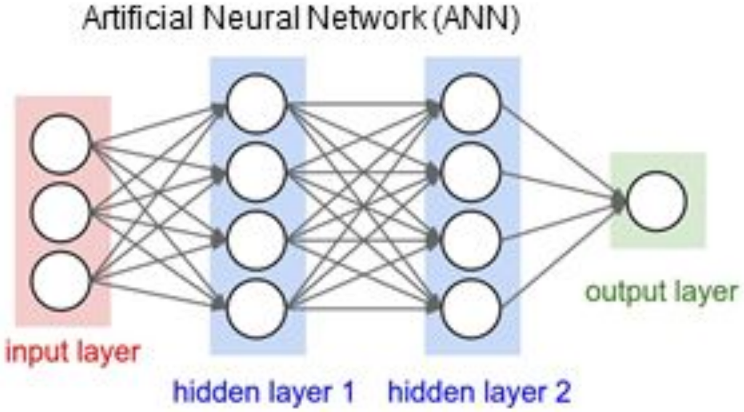

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Automatic differentiation used in practice called **back-propagation.**

Computational Graphs and Back-Propagation

Computational Graphs

Optimization methods often need gradients $\nabla_\theta f(\boldsymbol{X};\theta)$.

Symbolic representations of $f(\theta)$ useful for automatic differentiation to obtain $\nabla_\theta f$.

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Example: $\mathrm{y} = f(x) = \mathrm{x} + 5$.

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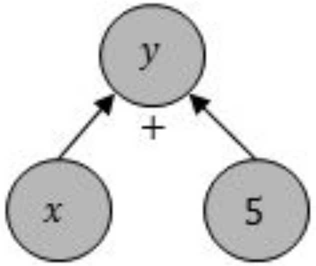

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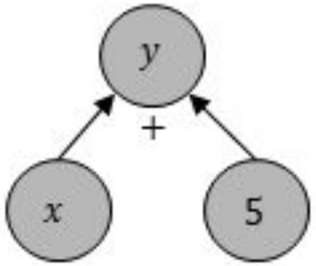

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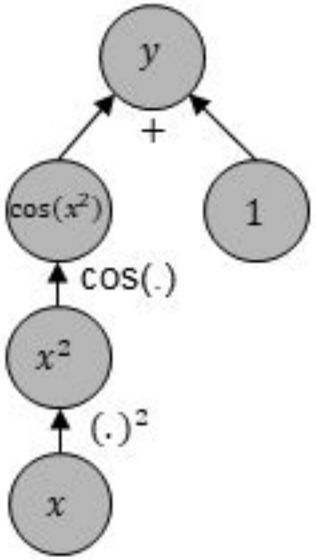

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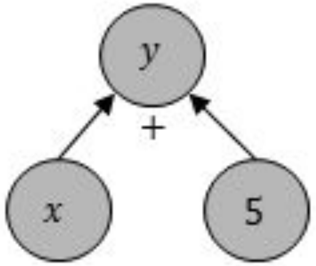
Computational Graphs



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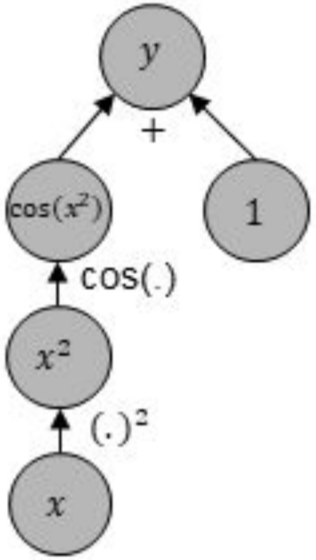
Computational graph represents function evaluation in terms of more basic operations.



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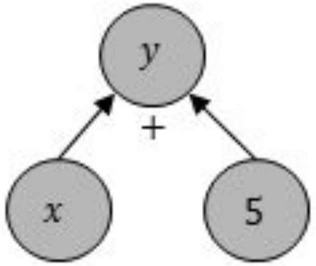

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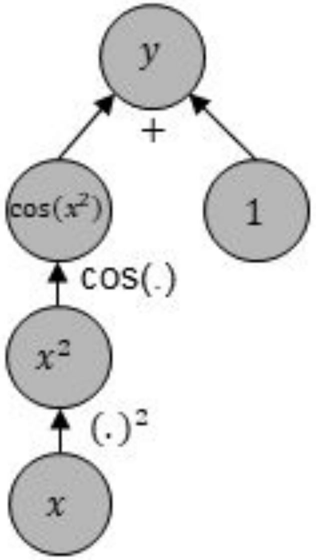

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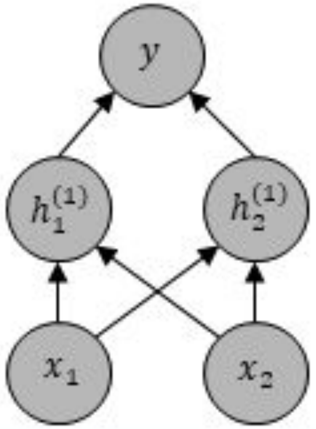

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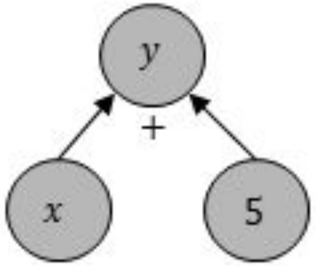

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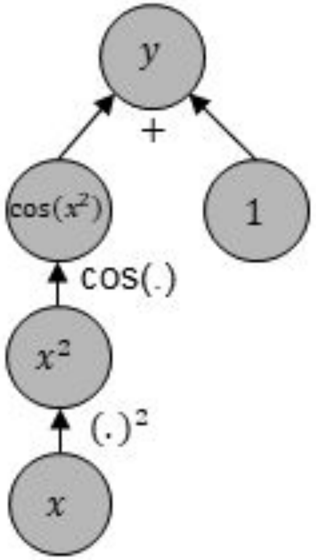

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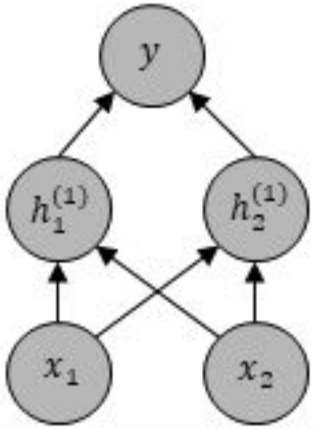

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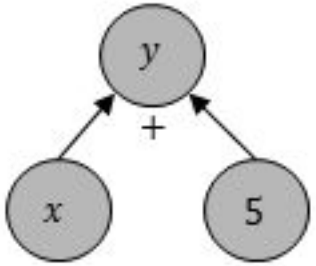

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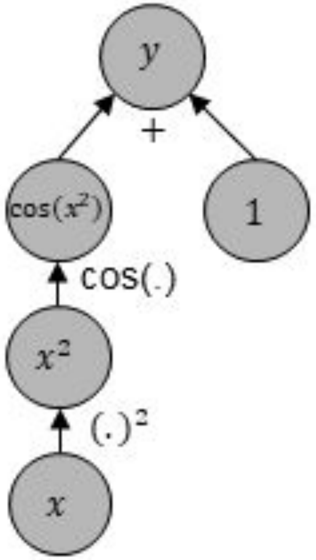

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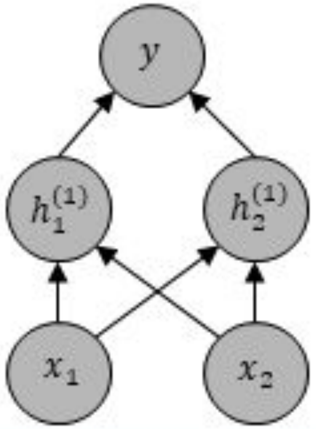

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Function derivatives can then be built up using the **chain-rule of calculus.**

Chain-Rule

Chain-Rule of Calculus:

$$\boldsymbol{u}^{(k)} = f\left(\boldsymbol{u}^{(k-1)}\right), \qquad \boldsymbol{u}^{(n)} = f\left(f\left(\dots f\left(\boldsymbol{u}^{(1)}\right)\dots\right)\right)$$

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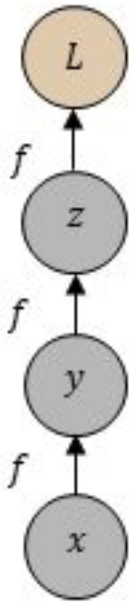

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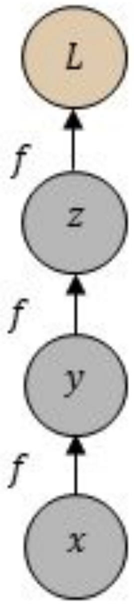

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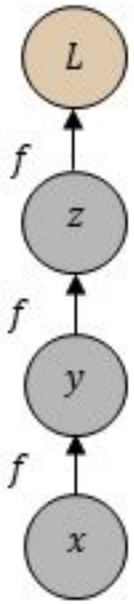

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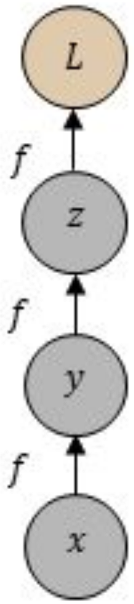

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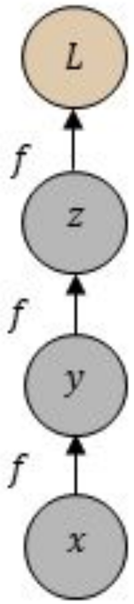

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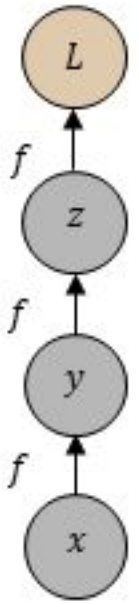

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Advantages of (i) when memory storage issues, otherwise (ii) is usually preferred.

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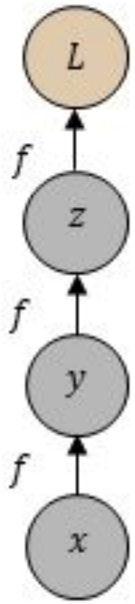

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Input: $x^{(1)}, x^{(2)}, \dots, x^{(n_I)}$
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  for $m = n_I + 1, \dots, n$
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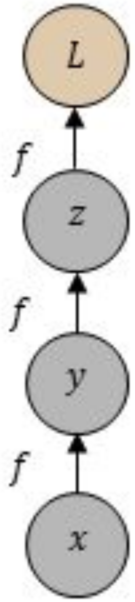

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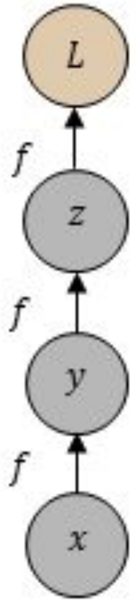

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Input: $u^{(m)}, m = 1,\dots n$.
grad_table[$u^{(n)}$] ← 1
For $j = n-1,\dots 1$
    grad_table[$u^{(j)}$] ← $\sum_{i:\, j\, \in \mathrm{Pa}(u^{(i)})}$ grad_table[$u^{(i)}$] $\frac{\partial \boldsymbol{u}^{(i)}}{\partial \boldsymbol{u}^{(j)}}$
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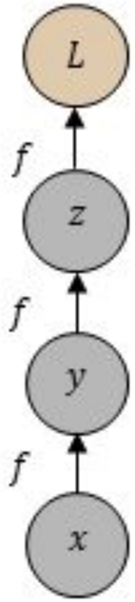

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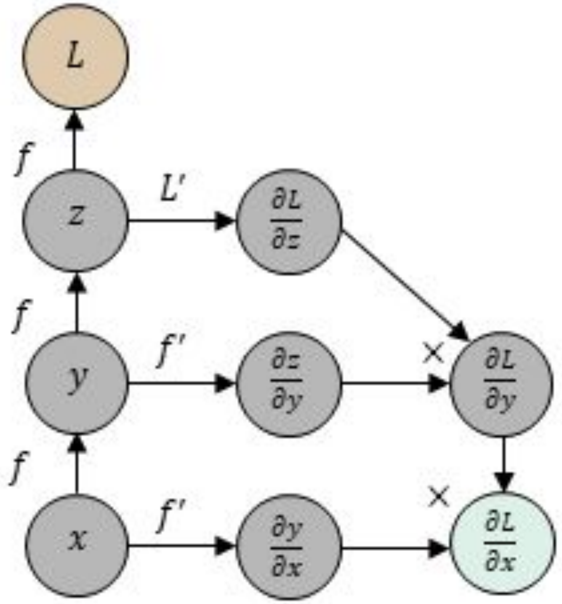

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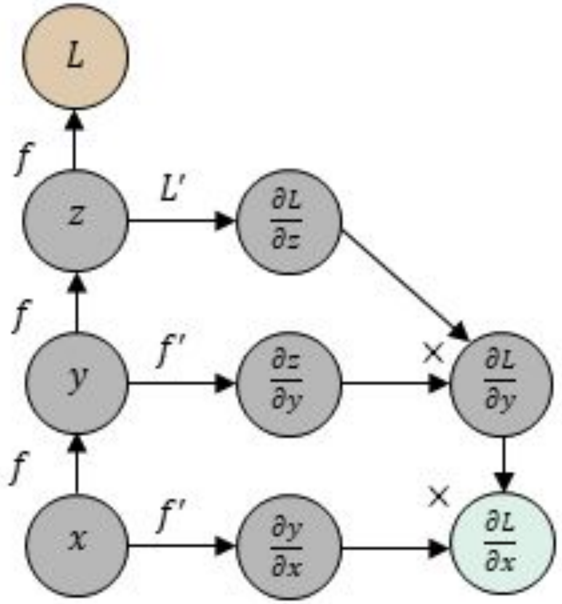

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Algorithm II maintains at each stage: grad_table$[u^{(j)}] = \frac{\partial \boldsymbol{u}^{(n)}}{\partial \boldsymbol{u}^{(j)}}$.

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Back-Propagation Method:

$$\boldsymbol{u}^{(k)} = f(\boldsymbol{u}^{(k-1)}),\ \boldsymbol{u}^{(n)} = f\left(f(\dots f(\boldsymbol{u}^{(1)})\dots)\right)$$

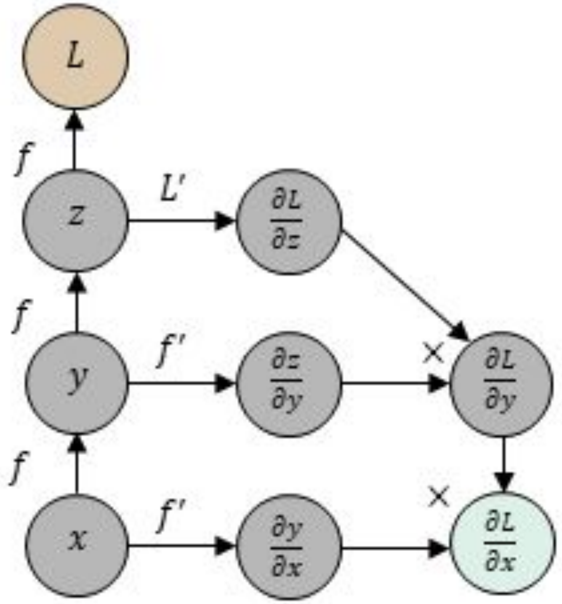
$$\frac{\partial \boldsymbol{u}^{(n)}}{\partial \boldsymbol{u}^{(j)}} = \sum_{i:\, j\, \in \mathrm{Pa}(u^{(i)})} \frac{\partial \boldsymbol{u}^{(n)}}{\partial \boldsymbol{u}^{(i)}} \frac{\partial \boldsymbol{u}^{(i)}}{\partial \boldsymbol{u}^{(j)}}$$

Algorithm I (Forward-Pass):

```
Input: $x^{(1)}, x^{(2)}, \dots, x^{(n_I)}$
  for $k = 1,2,\dots,n_I$
    $u^{(k)} \leftarrow x^{(k)}$
  for $m = n_I + 1, \dots, n$
    $\mathbb{U}^{(m)} \leftarrow \{u^{(j)} \mid j \in \mathrm{Pa}(u^{(m)})\}$
    $u^{(m)} \leftarrow f^{(m)}(\mathbb{U}^{(m)})$
Output: $u^{(n)}, \{u^{(i)}\}_{i=1}^{n}$.
```

Algorithm II (Backward-Pass):

```
Input: $u^{(m)}, m = 1, \dots n$.
grad_table$[u^{(n)}] \leftarrow 1$
For $j = n-1, \dots 1$
    grad_table$[u^{(j)}] \leftarrow \sum_{i:\, j\, \in \mathrm{Pa}(u^{(i)})}$grad_table$[u^{(i)}]\frac{\partial \boldsymbol{u}^{(i)}}{\partial \boldsymbol{u}^{(j)}}$
Output: $\frac{\partial \boldsymbol{u}^{(n)}}{\partial \boldsymbol{u}^{(k)}}$, $k = 1, \dots n_I$.
```



Algorithm I computes the functional evaluations $\{u^{(i)}\}_{i=1}^{n}$.

Algorithm II maintains at each stage: grad_table$[u^{(j)}] = \frac{\partial \boldsymbol{u}^{(n)}}{\partial \boldsymbol{u}^{(j)}}$.

Back-Propagation consists of the two steps (i) forward pass of algorithm I followed by (ii) backward pass of algorithm II.

Back-Propagation Method

Back-Propagation Method:

$$\boldsymbol{u}^{(k)} = f(\boldsymbol{u}^{(k-1)}),\ \boldsymbol{u}^{(n)} = f\left(f(\dots f(\boldsymbol{u}^{(1)})\dots)\right)$$

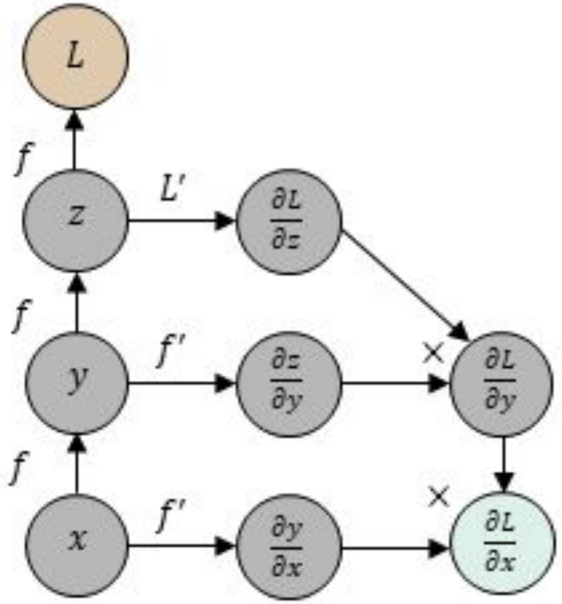
$$\frac{\partial \boldsymbol{u}^{(n)}}{\partial \boldsymbol{u}^{(j)}} = \sum_{i:\, j \in \mathrm{Pa}(u^{(i)})} \frac{\partial \boldsymbol{u}^{(n)}}{\partial \boldsymbol{u}^{(i)}} \frac{\partial \boldsymbol{u}^{(i)}}{\partial \boldsymbol{u}^{(j)}}$$

Algorithm I (Forward-Pass):

```
Input: $x^{(1)}, x^{(2)}, \dots, x^{(n_I)}$
  for $k = 1,2,\dots,n_I$
    $u^{(k)} \leftarrow x^{(k)}$
  for $m = n_I + 1,\dots,n$
    $\mathbb{U}^{(m)} \leftarrow \{u^{(j)} \mid j \in \mathrm{Pa}(u^{(m)})\}$
    $u^{(m)} \leftarrow f^{(m)}(\mathbb{U}^{(m)})$
Output: $u^{(n)}, \{u^{(i)}\}_{i=1}^{n}$.
```

Algorithm II (Backward-Pass):

```
Input: $u^{(m)}, m = 1,\dots n$.
grad_table$[u^{(n)}] \leftarrow 1$
For $j = n-1,\dots 1$
    grad_table$[u^{(j)}] \leftarrow \sum_{i:\, j \in \mathrm{Pa}(u^{(i)})}$grad_table$[u^{(i)}]\frac{\partial \boldsymbol{u}^{(i)}}{\partial \boldsymbol{u}^{(j)}}$
Output: $\frac{\partial \boldsymbol{u}^{(n)}}{\partial \boldsymbol{u}^{(k)}},\ k = 1,\dots n_I$.
```



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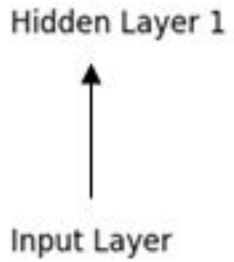
Back-Propagation consists of the two steps (i) forward pass of algorithm I followed by (ii) backward pass of algorithm II.

Parallelized versions and other variants also used for efficiency.

Feed-Forward Neural Networks (FFNNs)
Basic Examples of NN's

Feed-Forward Neural Networks

Neural network architecture with one processing layer feeding forward into the next processing layer.

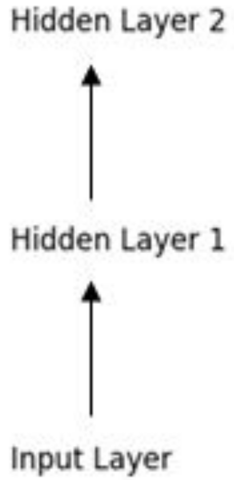


Hidden Layer 1

Input Layer

Feed-Forward Neural Networks

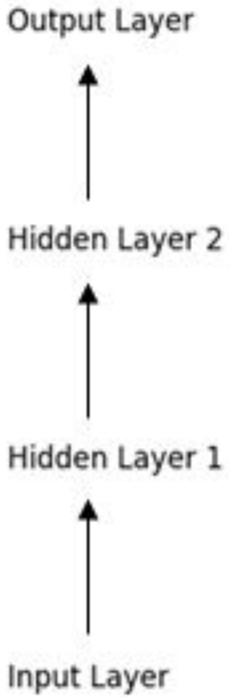
Neural network architecture with one processing layer feeding forward into the next processing layer.



Feed-Forward Neural Networks

Neural network architecture with one processing layer feeding forward into the next processing layer.

Neural Network Architecture



Output Layer

Hidden Layer 2

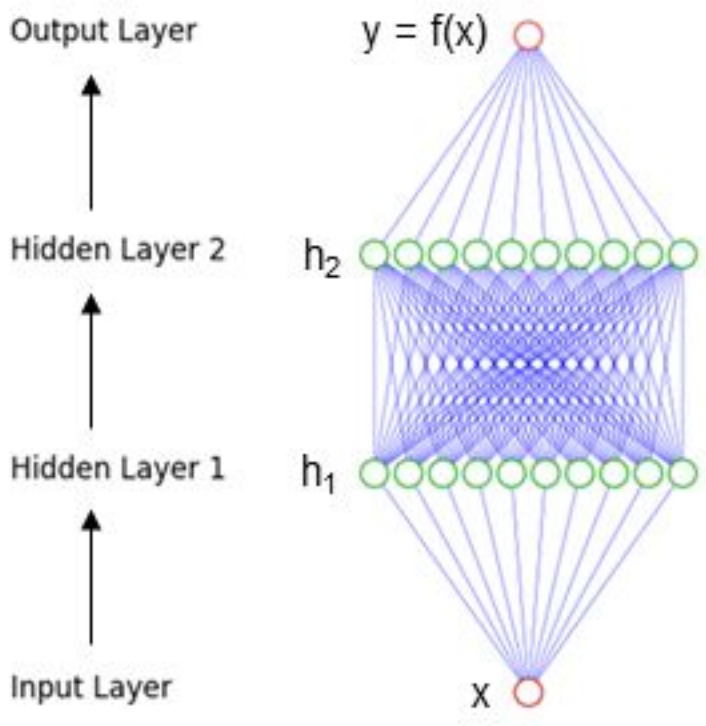
Hidden Layer 1

Input Layer

Feed-Forward Neural Networks

Neural network architecture with one processing layer feeding forward into the next processing layer.

Neural Network Architecture



Feed-Forward Neural Networks

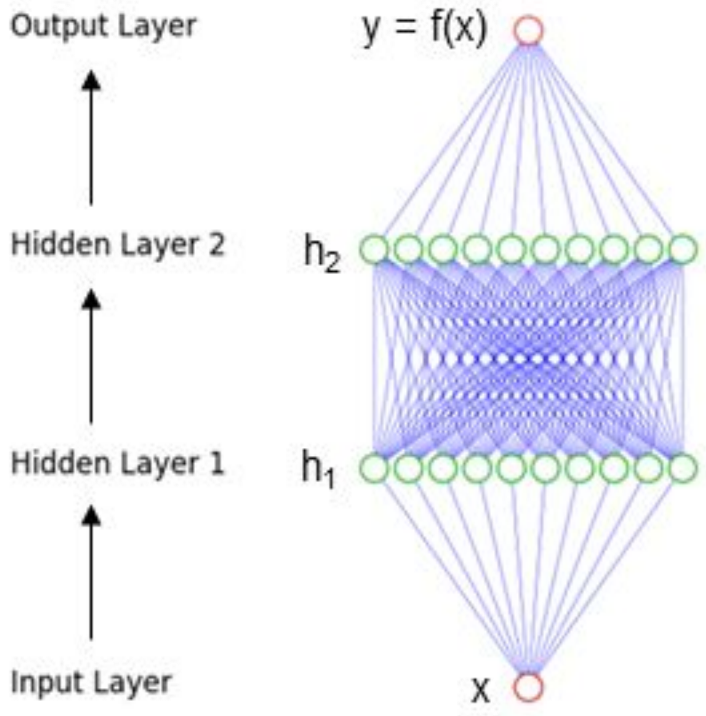
Neural network architecture with one processing layer feeding forward into the next processing layer.

Intermediate hidden processing layers of the form $g(XW + b)$.

Nonlinear transformation by some activation function $g(z)$.

Last processing layer typically is linear $XW + b$.

Neural Network Architecture



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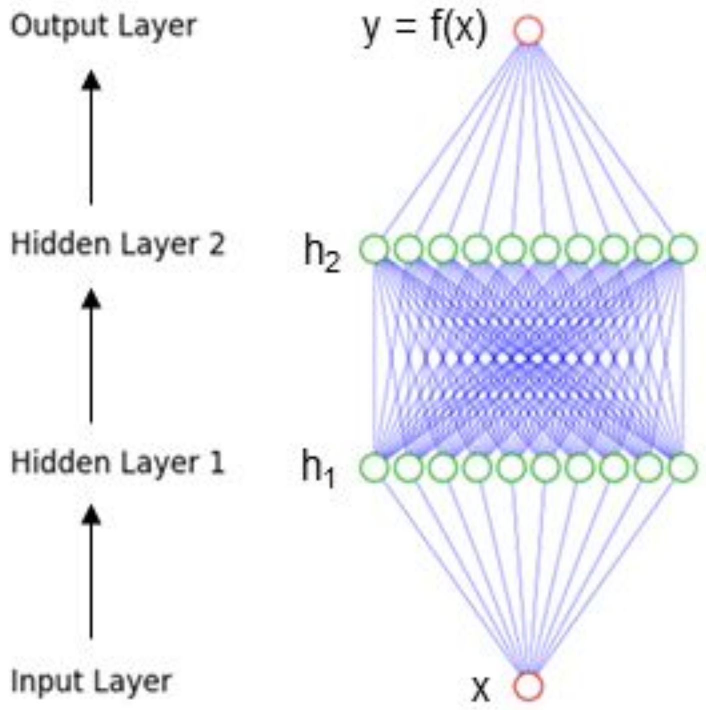
Feed-Forward Neural Network (FFNN) provide model for $y = f(x)$.

Neural Network Architecture



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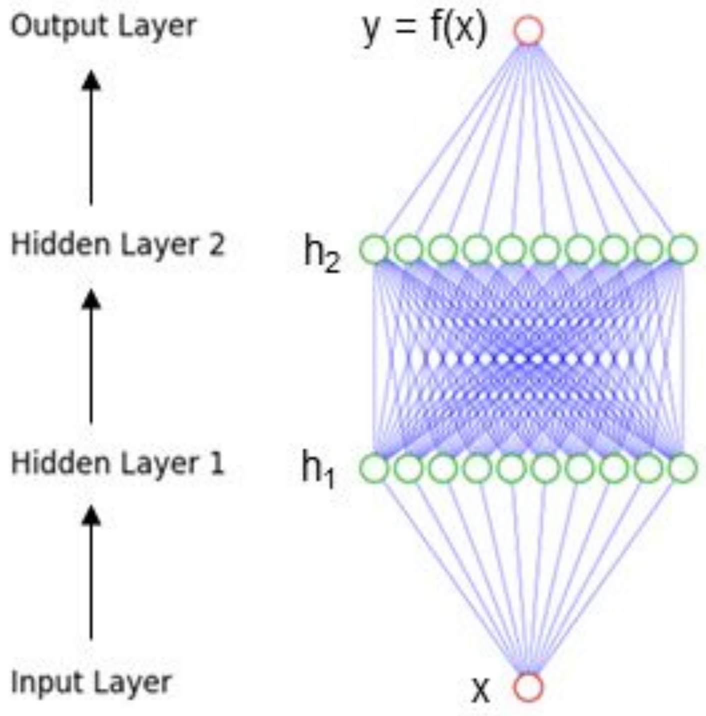
Learning involves adjusting weights W and bias b of layers.

Neural Network Architecture



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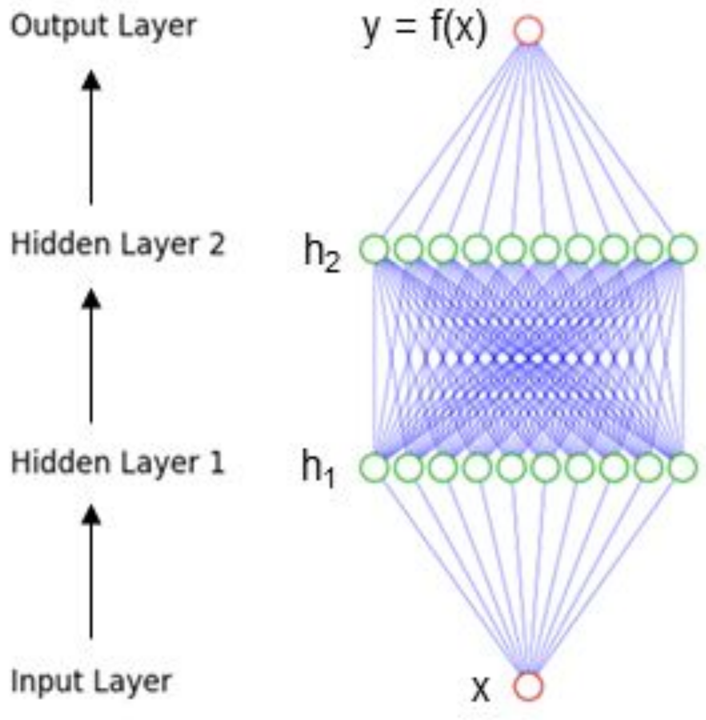
Learning involves adjusting weights W and bias b of layers.

Stochastic Gradient Descent (SGD) currently widely used for optimization of weights and bias.

Implicit regularization by choice of batch size and learning rates.

Neural Network Architecture



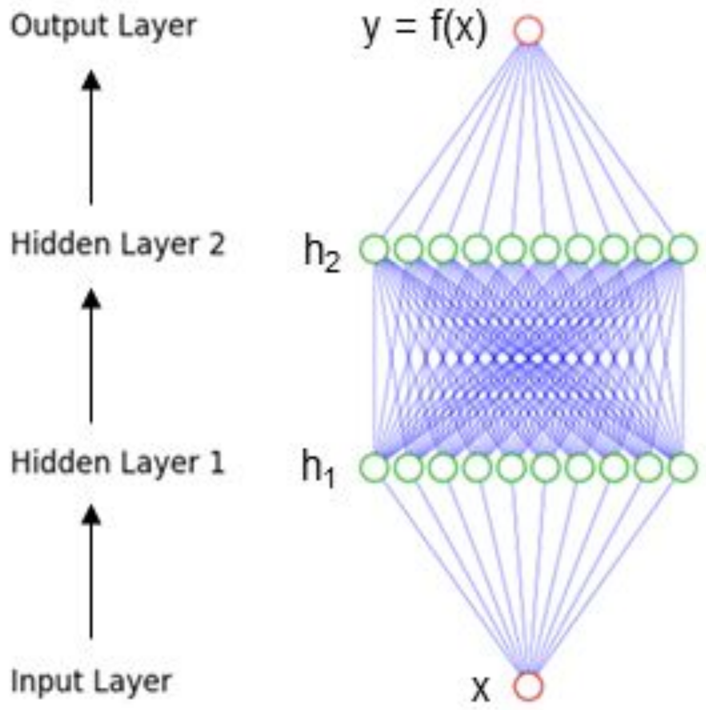
Feed-Forward Neural Networks: Example

Example: Approximate the function $y = \sin(x)$ using FFNN.

Architecture: 2-layers with 10-hidden ReLu nodes per layer.

This NN architecture spans piecewise linear functions (10 nodes).

Neural Network Architecture



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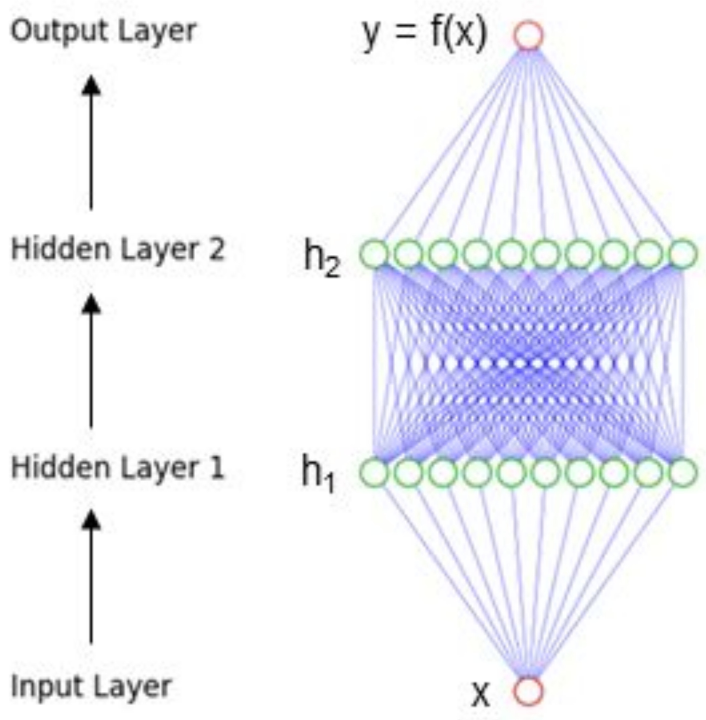
A notion of "loss" required to assess level of success in fit.

Neural Network Architecture



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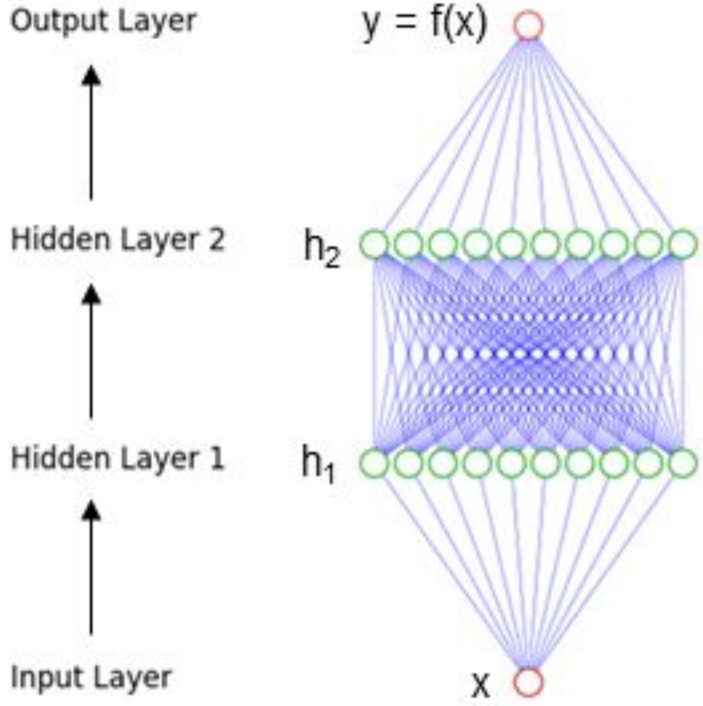
Neural Network Architecture



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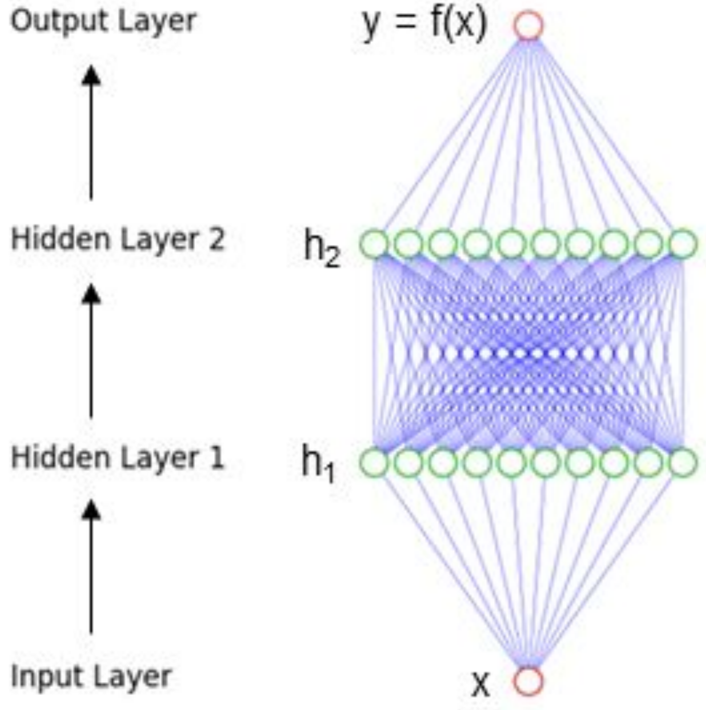
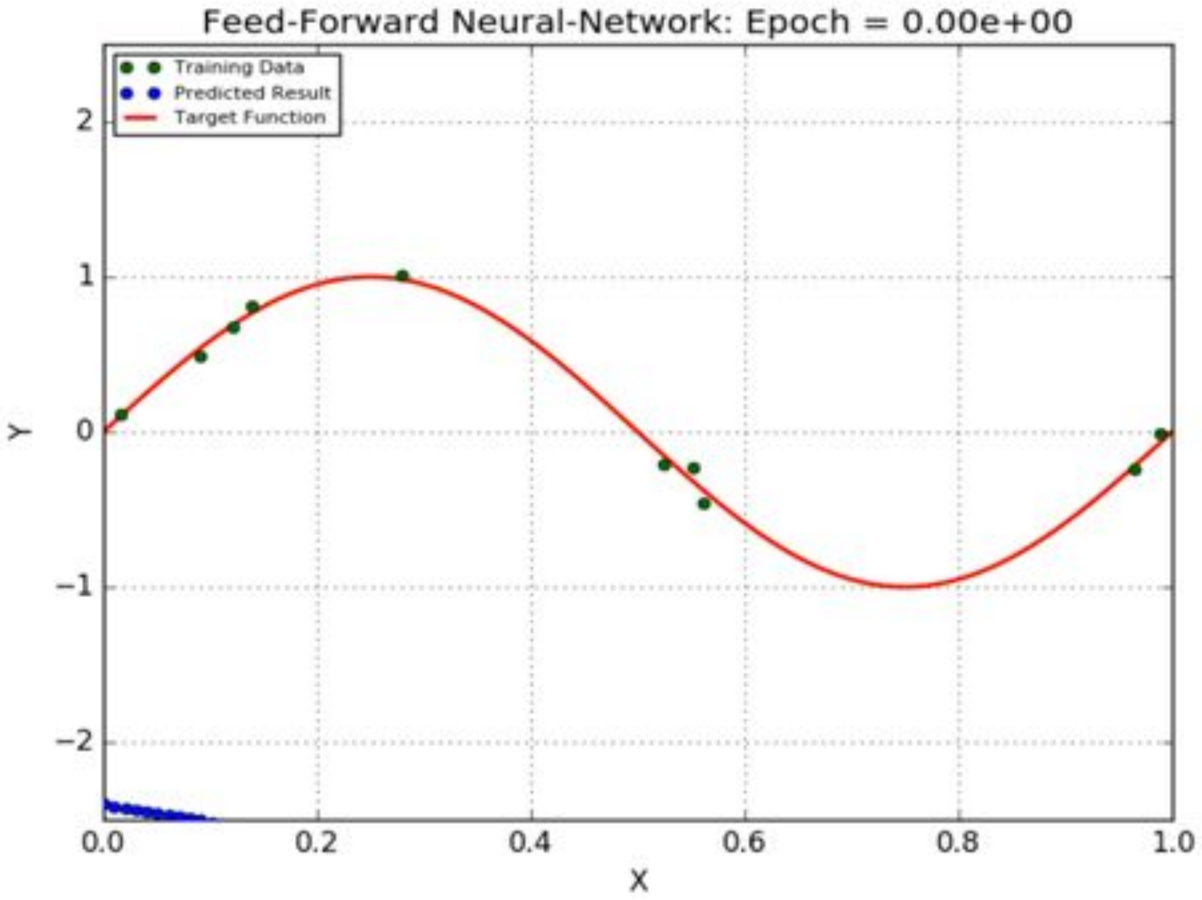
Neural Network Architecture



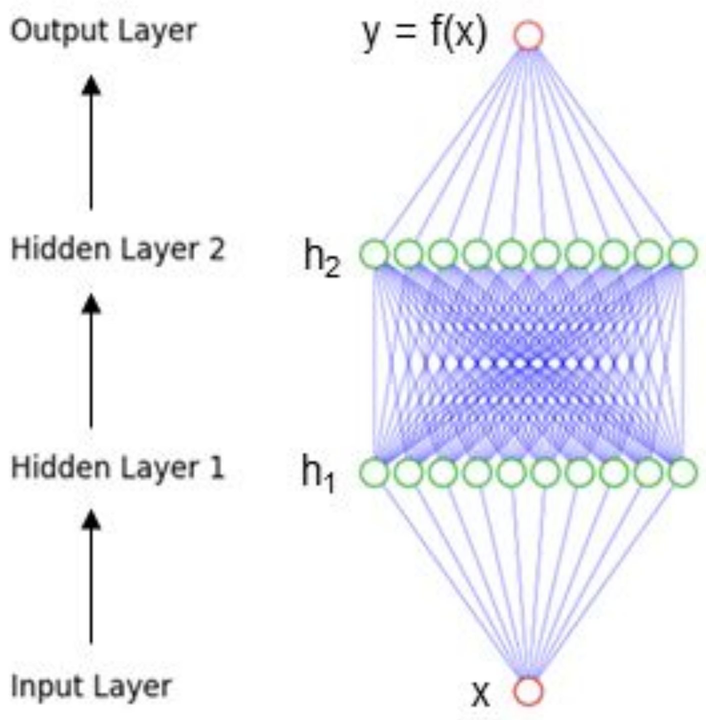
Feed-Forward Neural Networks: Example

Trained FFNN on set of 1000 samples $y_i = \sin(x_i) + \xi_i$.

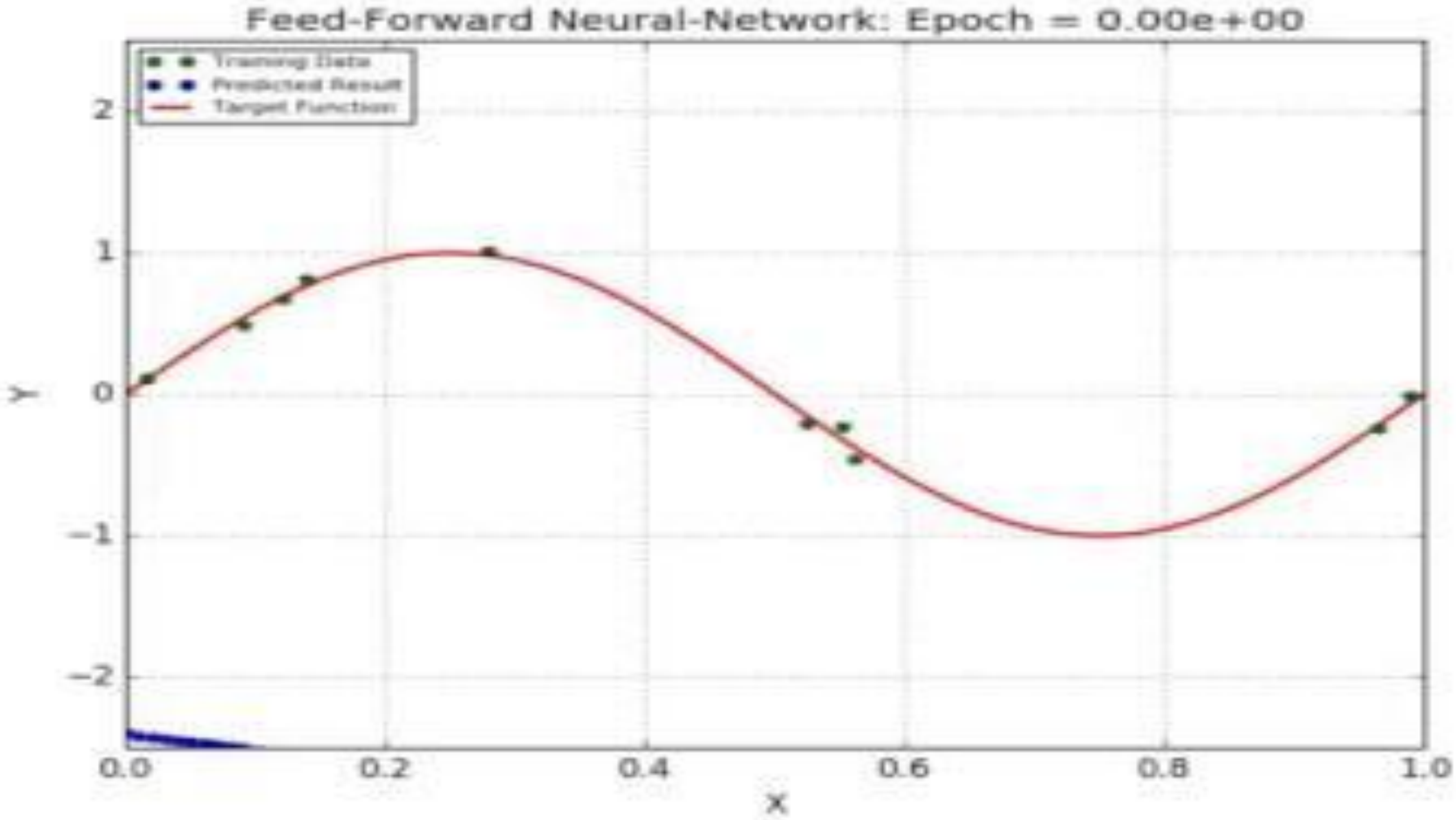
Stochastic Gradient Descent (SGD) used with batch size 10 and learning rate 10^{-4}.



Neural Network Architecture



Epoch = 1 step of SGD throughout these examples.


Feed-Forward Neural-Network: Epoch = 0.00e+00
Training Data
Predicted Result
Target Function
Y
2
1
0
−1
−2
X
0.0
0.2
0.4
0.6
0.8
1.0

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Trained FFNN on set of 1000 samples $y_i = \sin(x_i) + \xi_i$.

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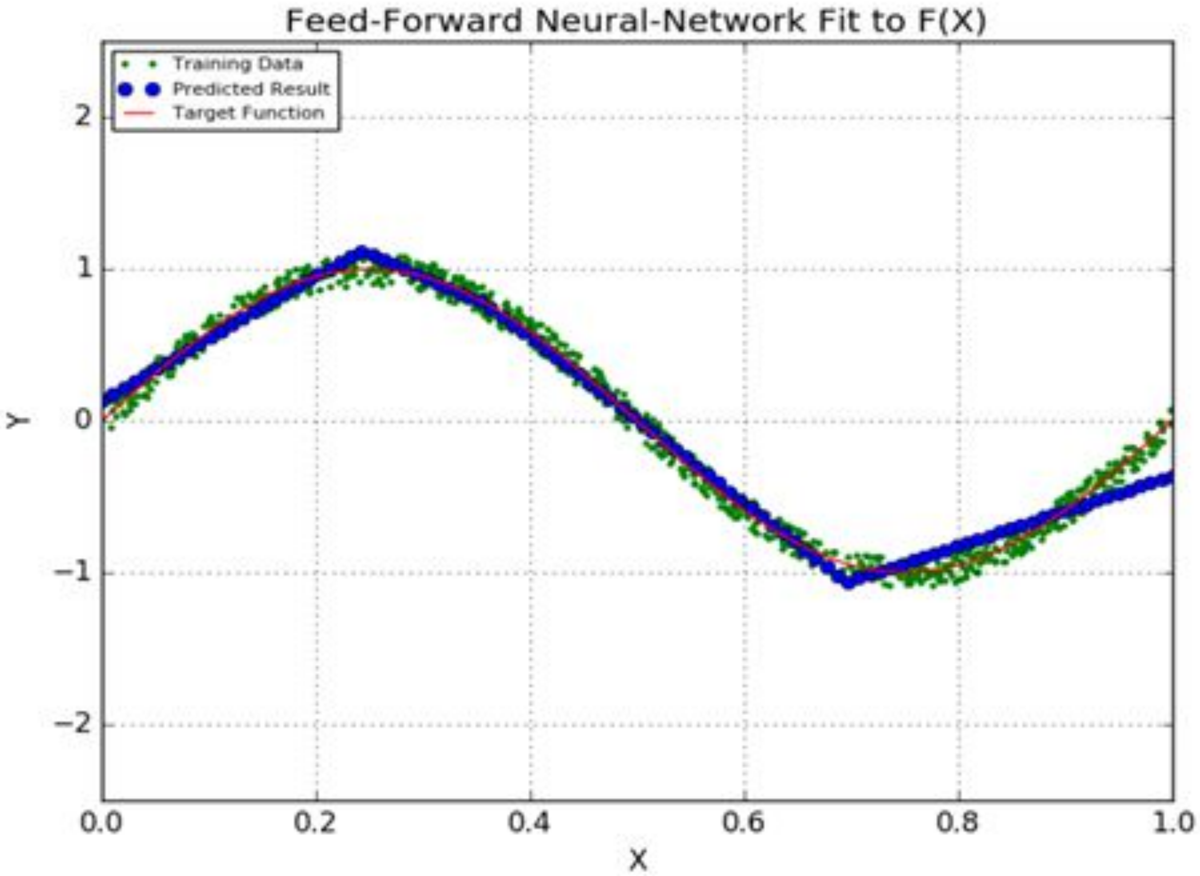
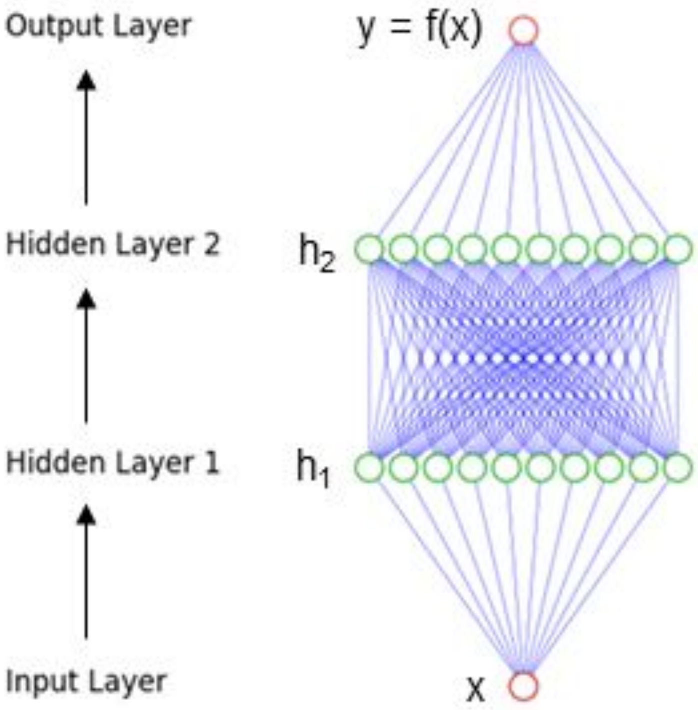


Neural Network Architecture



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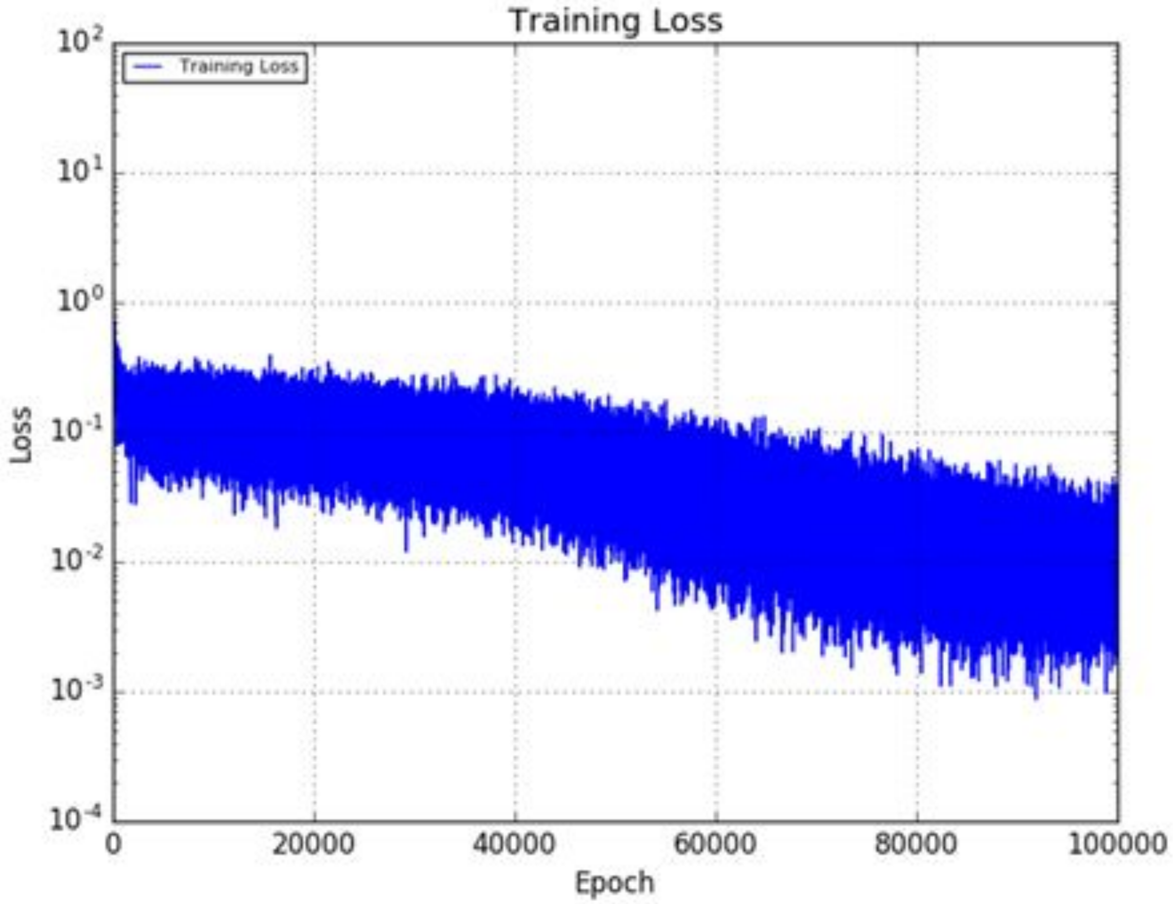
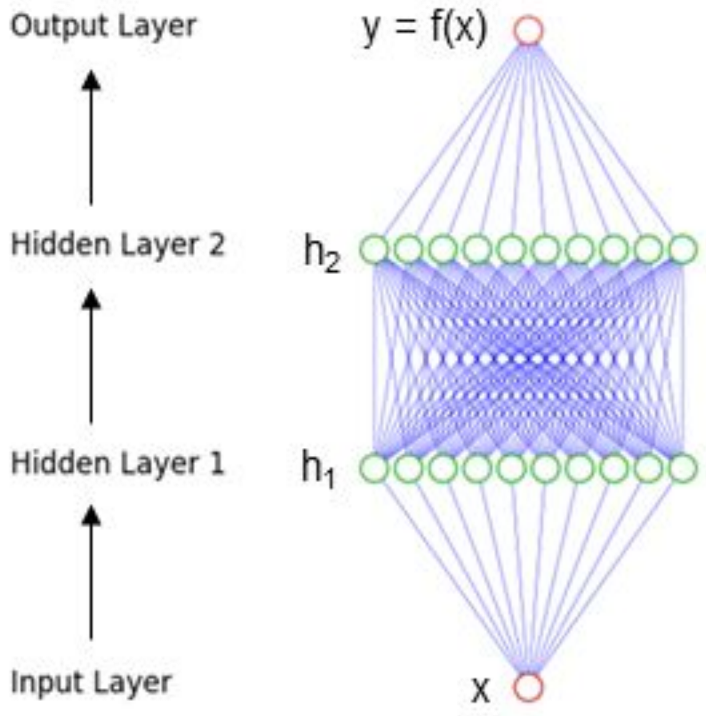
Stochastic Gradient Descent (SGD) used with batch size 10 and learning rate 10^{-4}.



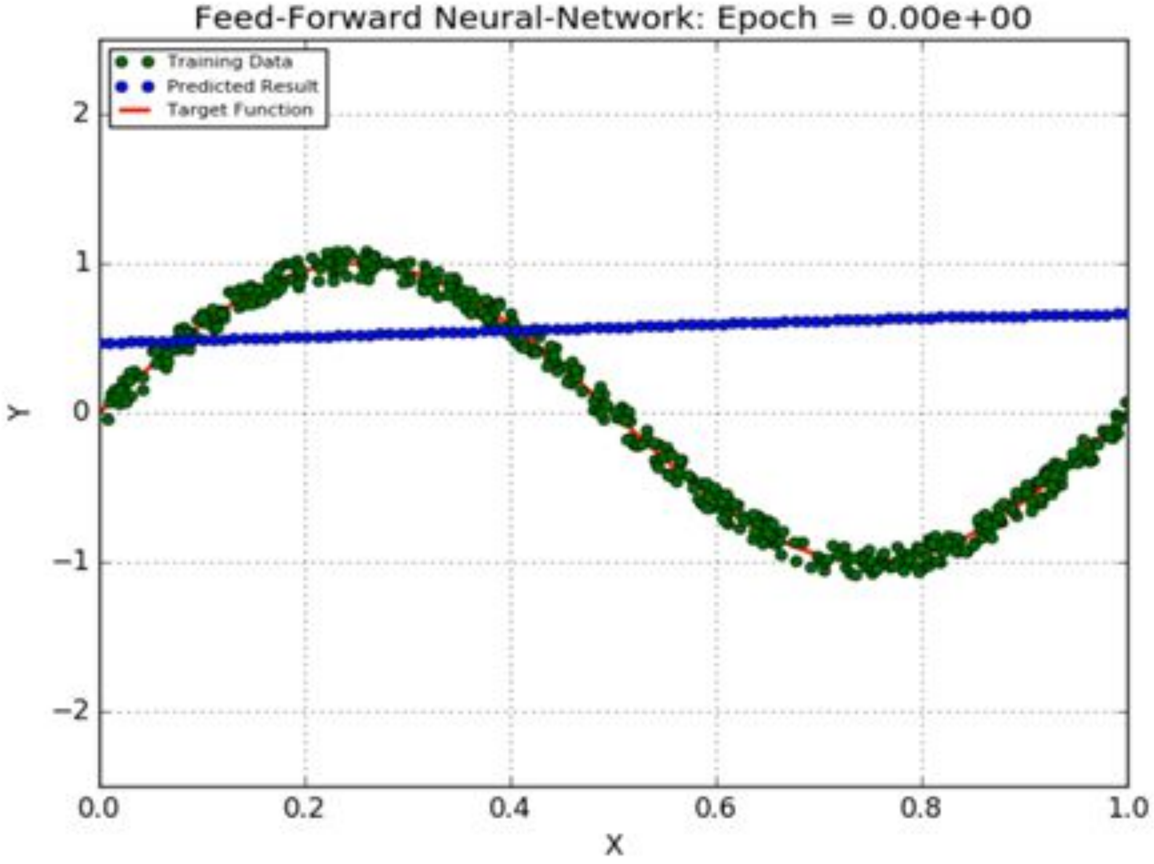
Neural Network Architecture



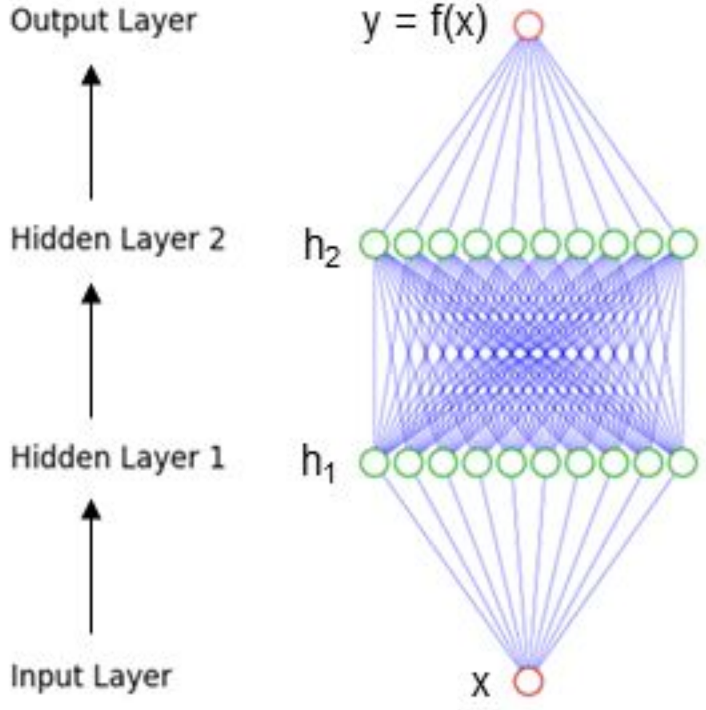
Feed-Forward Neural Networks: Example

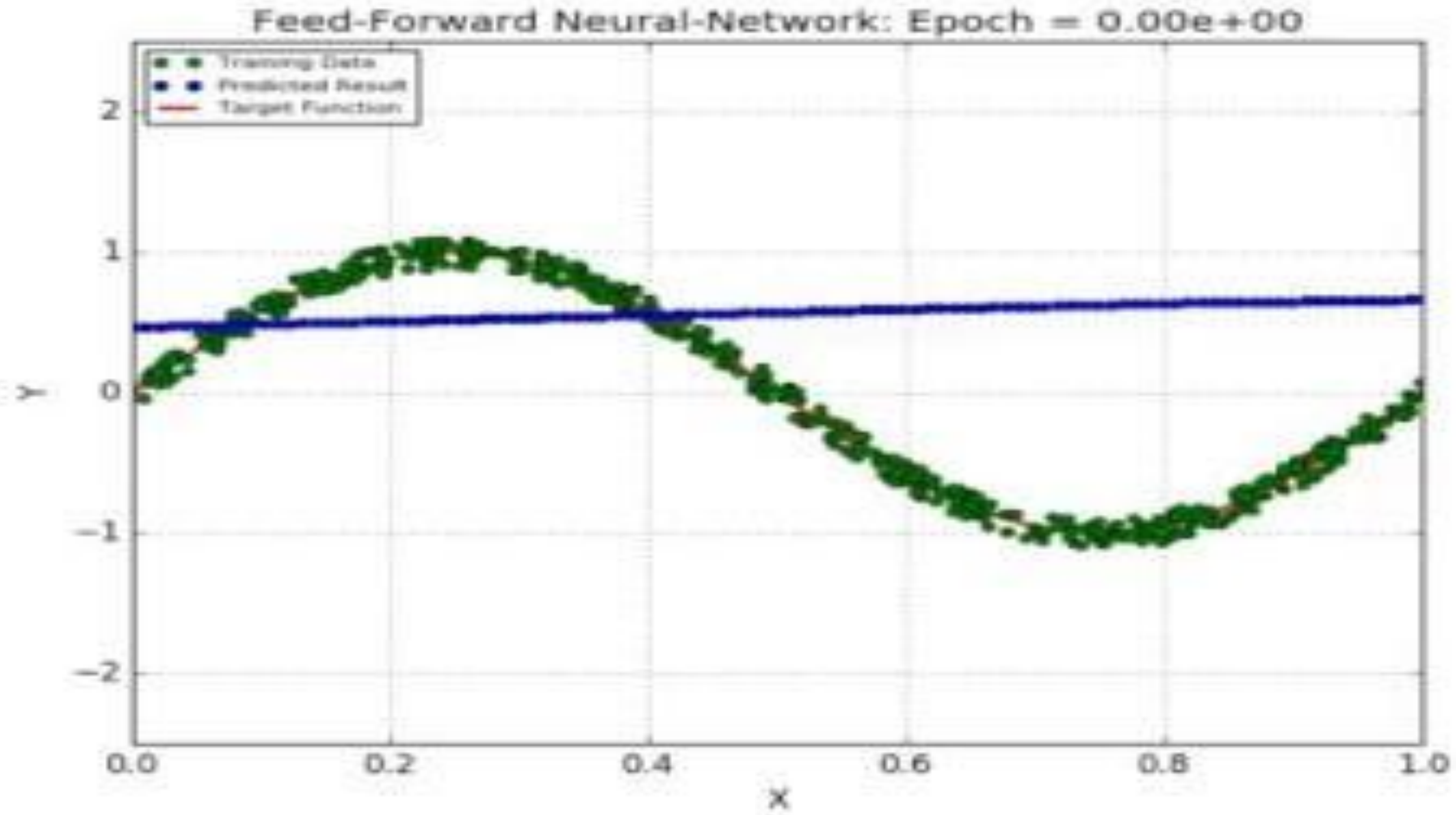
Trained FFNN on set of 1000 samples $y_i = \sin(x_i) + \xi_i$.

Stochastic Gradient Descent (SGD) used with batch size 500 and learning rate 10^{-4}.



Neural Network Architecture

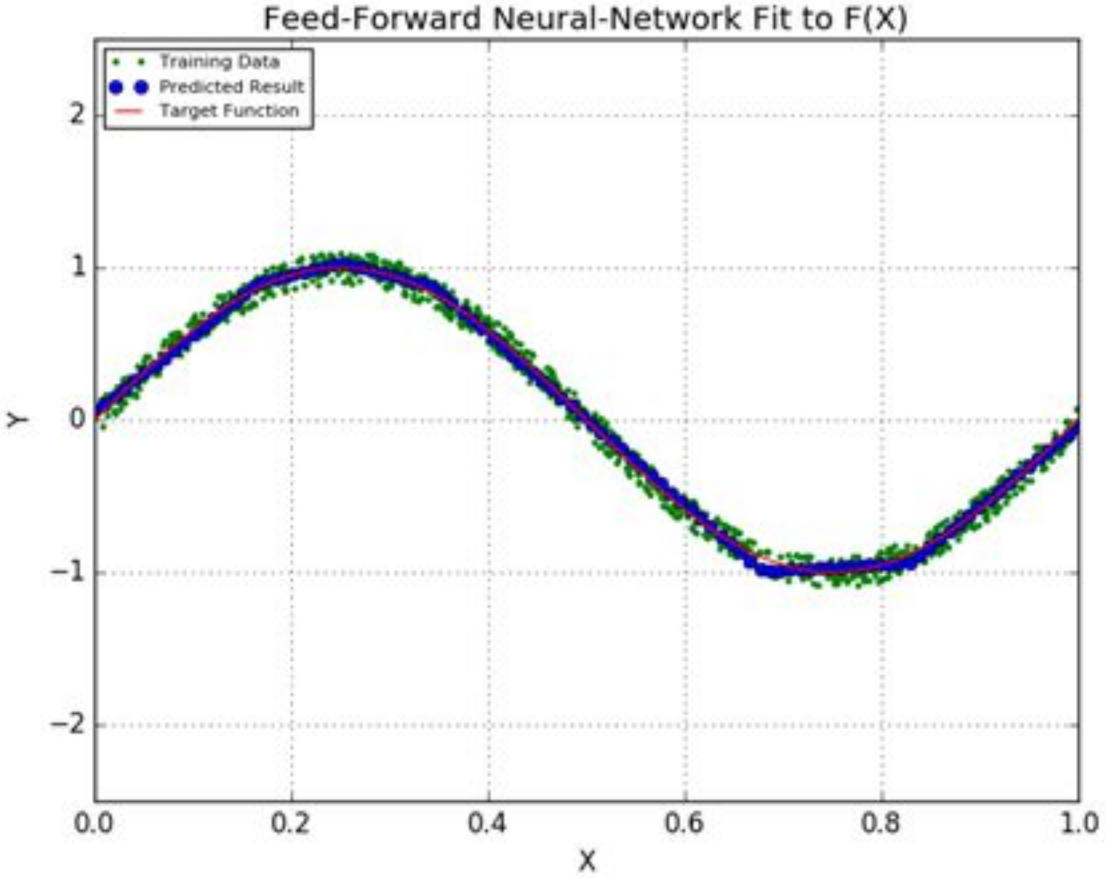



Feed-Forward Neural-Network: Epoch = 0.00e+00
Training Data
Predicted Result
Target Function
Y
2
1
0
−1
−2
X
0.0
0.2
0.4
0.6
0.8
1.0

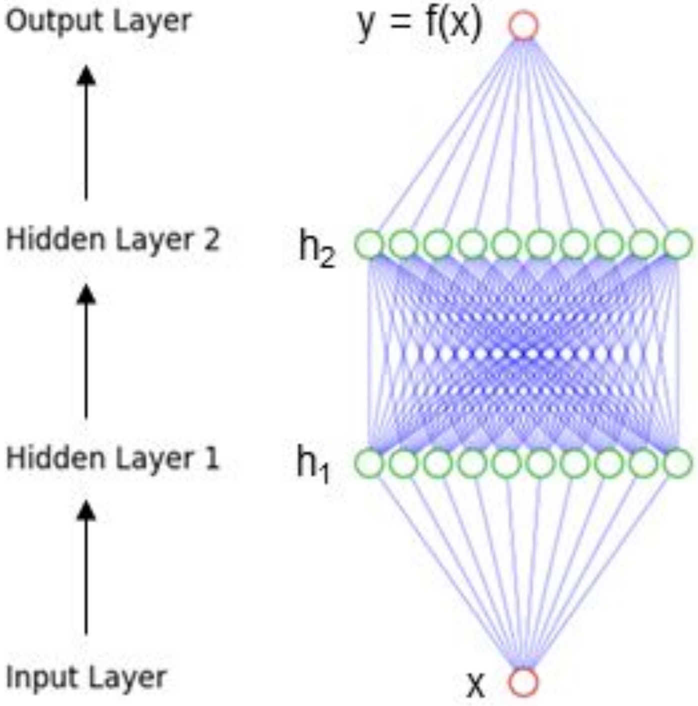
Feed-Forward Neural Networks: Example

Trained FFNN on set of 1000 samples $y_i = \sin(x_i) + \xi_i$.

Stochastic Gradient Descent (SGD) used with batch size 500 and learning rate 10^{-4}.



Neural Network Architecture



Feed-Forward Neural Networks: Example

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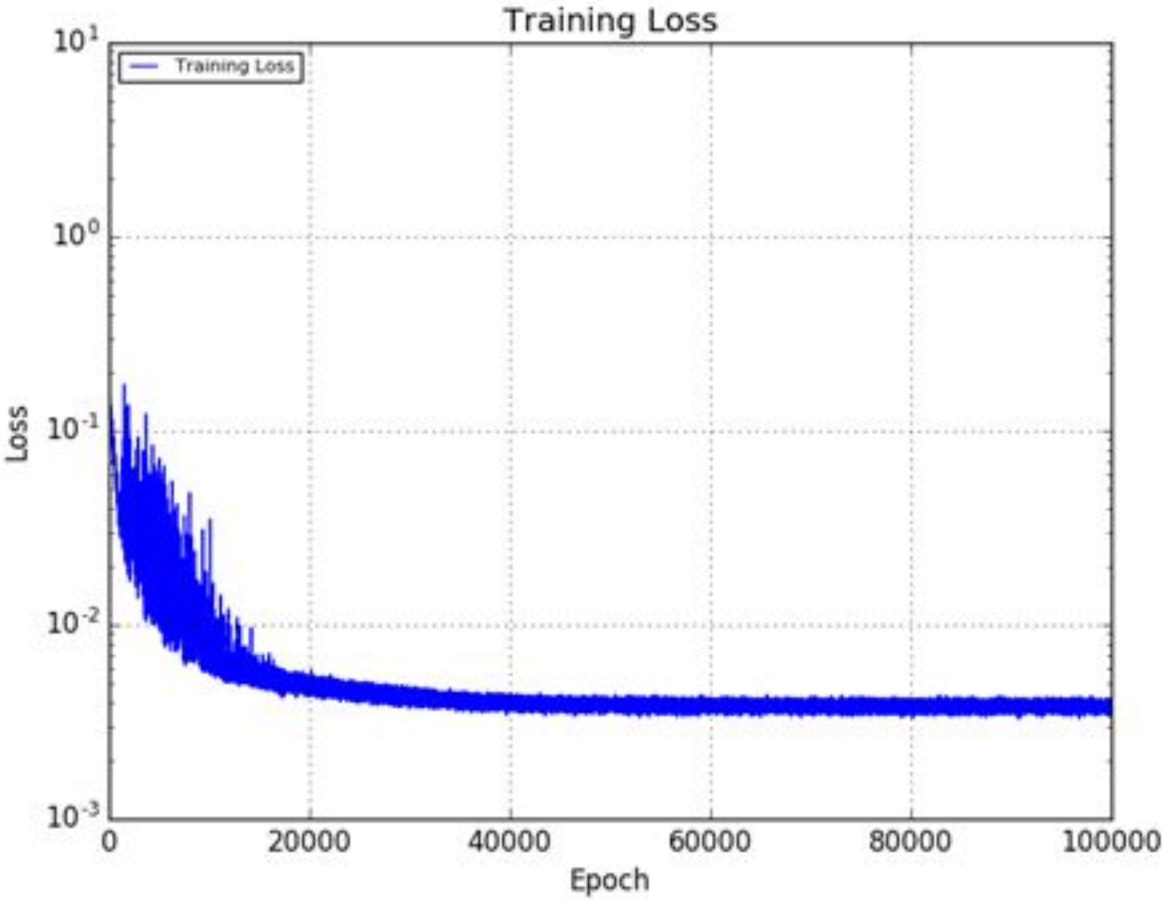
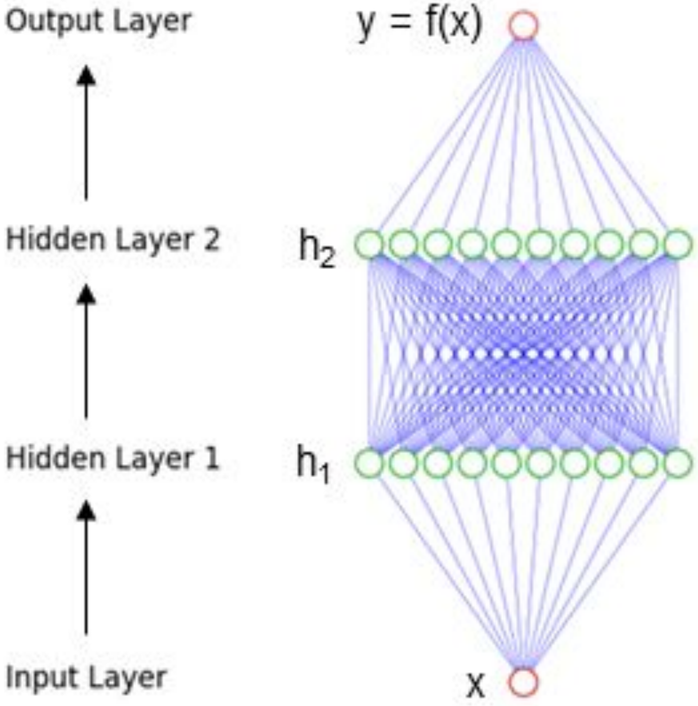
Stochastic Gradient Descent (SGD) used with batch size 500 and learning rate 10^{-4}.



Neural Network Architecture



Additional fine-tuning of hyper-parameters should be done to enhance efficiency of training.

Feed-Forward Neural Networks: Example

Example: Approximate the function $y = \sin(6\pi x) + 2x^2$ using FFNN.

Architecture: 2-layers with 100-hidden ReLu nodes per layer.

This NN architecture spans piecewise linear functions (100 nodes).

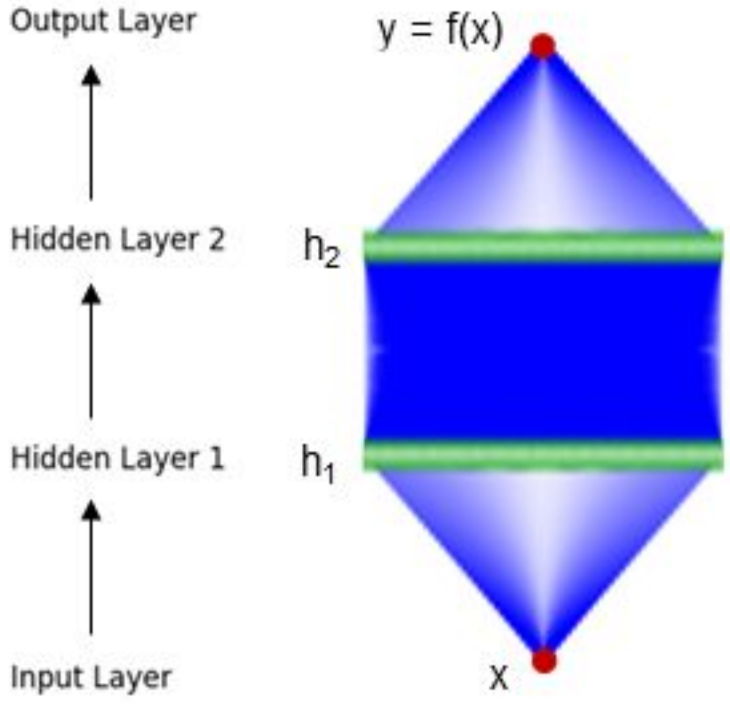
Explicitly: $f(X) = g(g(g(X \cdot W^{(1)} + b^{(1)}) \cdot W^{(2)} + b^{(2)}) \cdot W^{(3)} + b^{(3)}$
with $g(z) = \max(0, z)$.

A notion of "loss" required to assess level of success in fit.

Least-squares loss function $\ell(\{x_i, yi\}) = \sum_i (f(xi) - y_i)^2$.

Learning W,b proceeds by stochastic gradient descent.

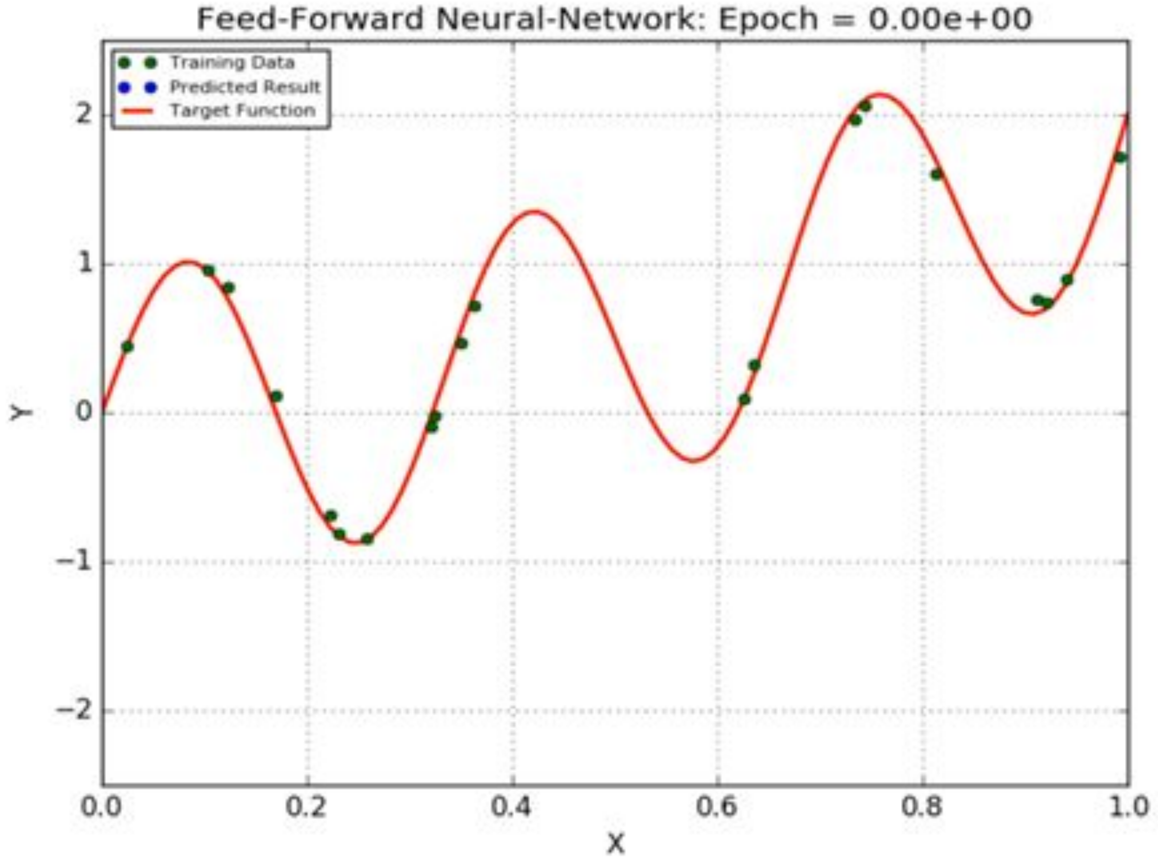
Neural Network Architecture



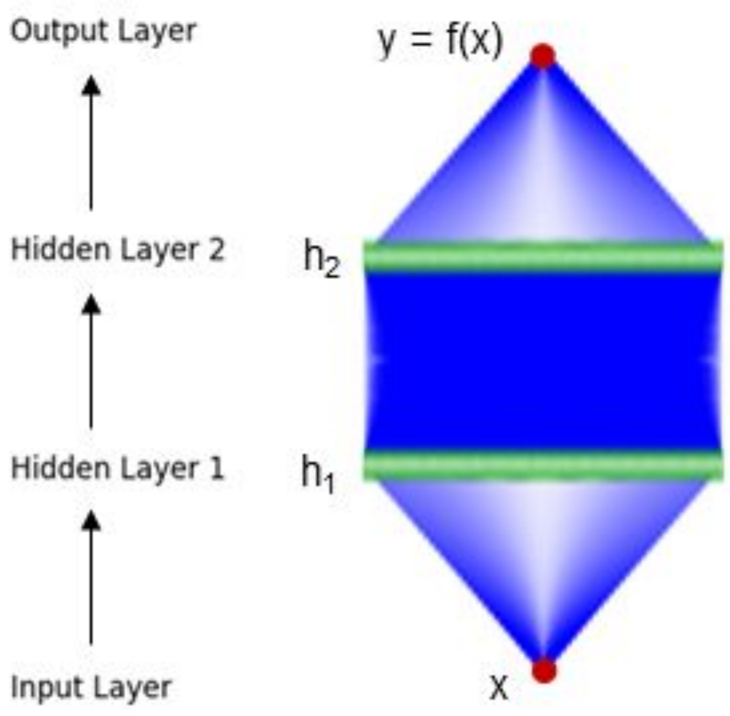
Feed-Forward Neural Networks: Example

Trained FFNN on set of 1000 samples $y_i = \sin(6\pi x_i) + 2x^2 + \xi_i$.

Stochastic Gradient Descent (SGD) used with batch size 20 and learning rate 10^{-4}.



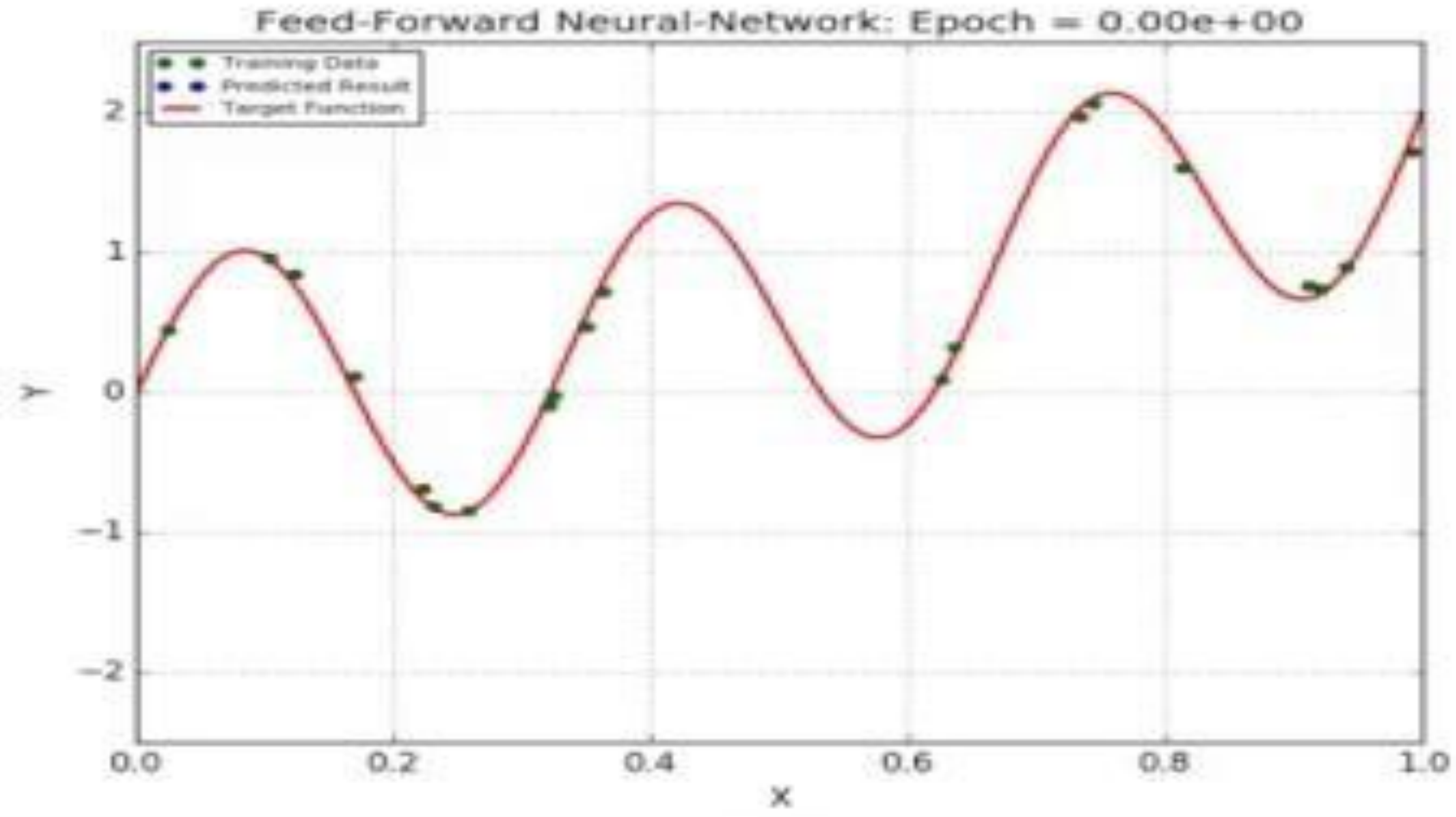
Neural Network Architecture


Output Layer

Hidden Layer 2

Hidden Layer 1

Input Layer


Feed-Forward Neural-Network: Epoch = 0.00e+00
Training Data
Predicted Result
Target Function
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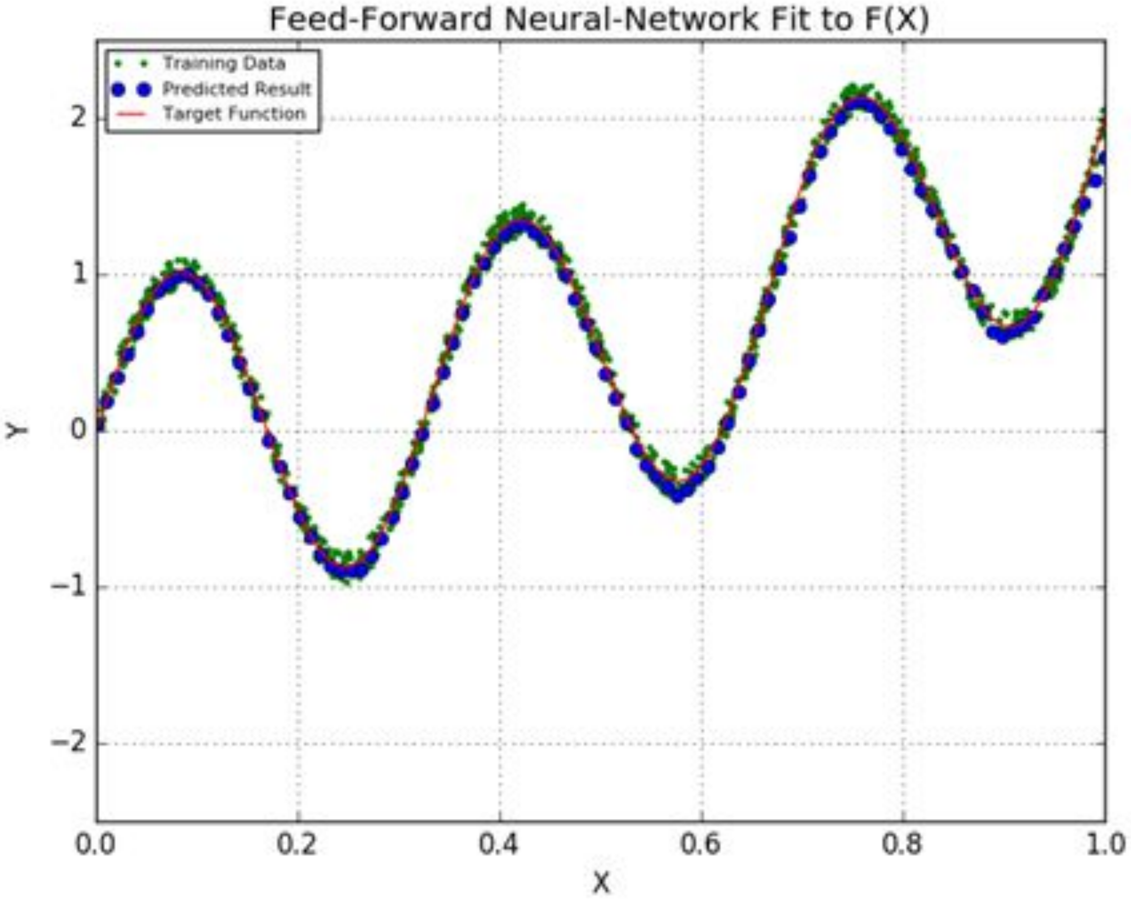
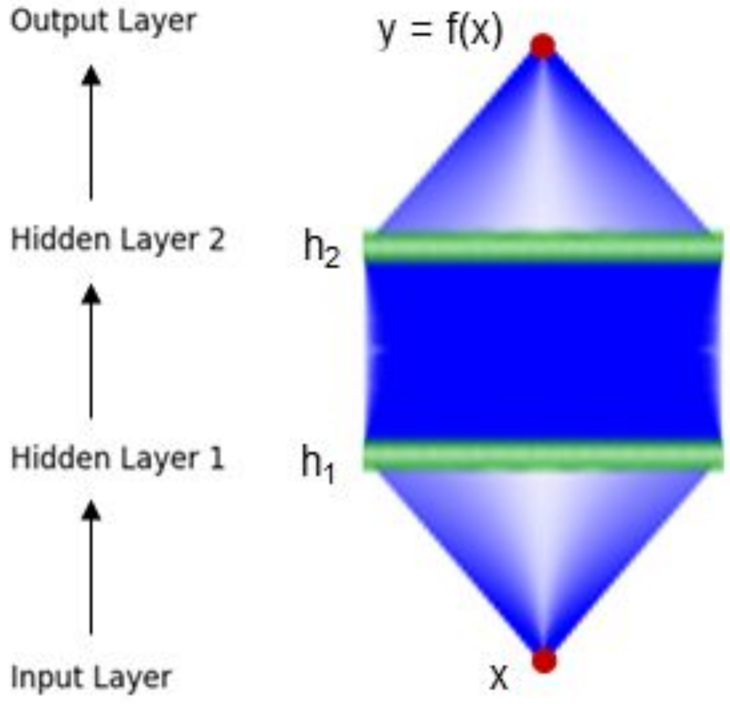


Neural Network Architecture



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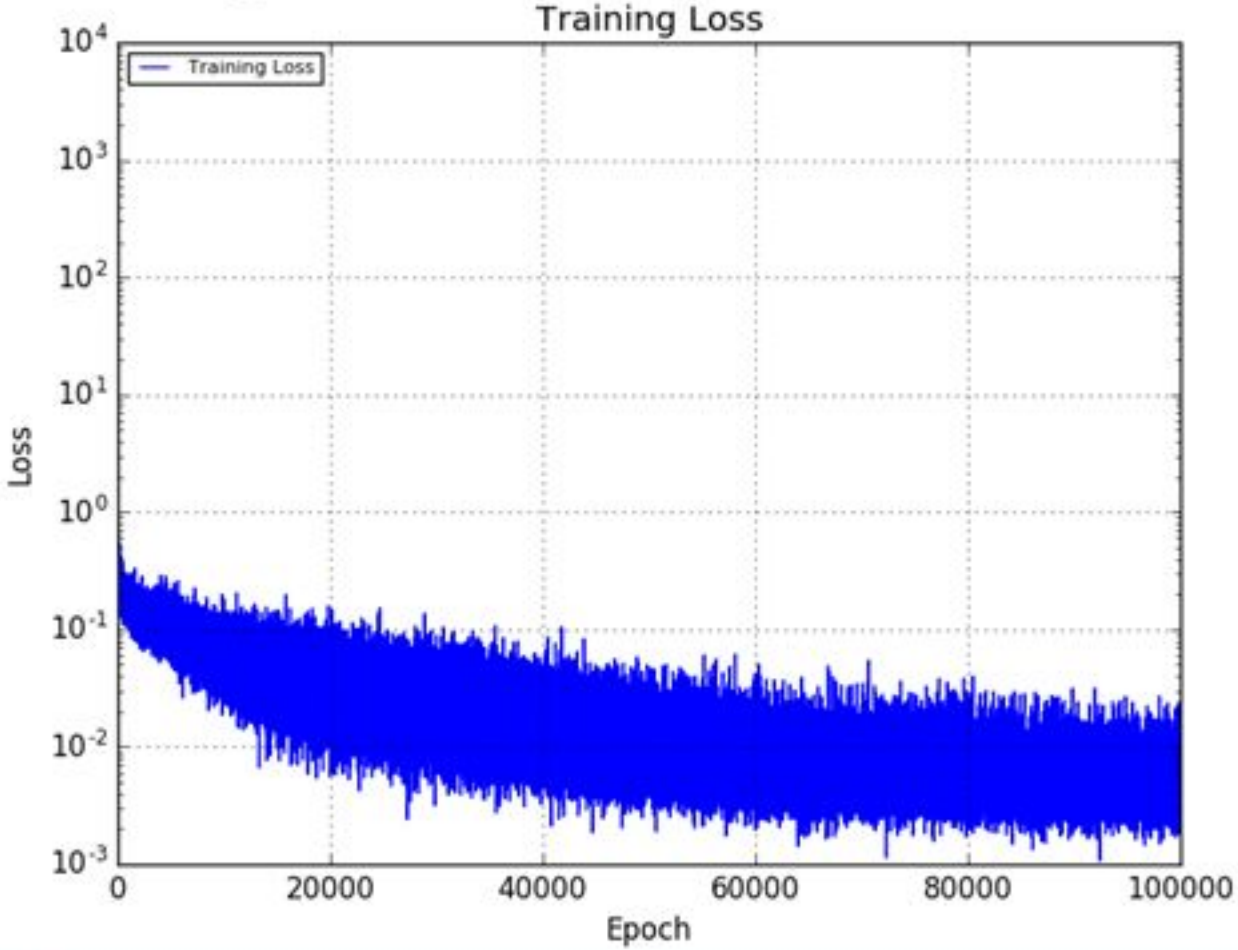
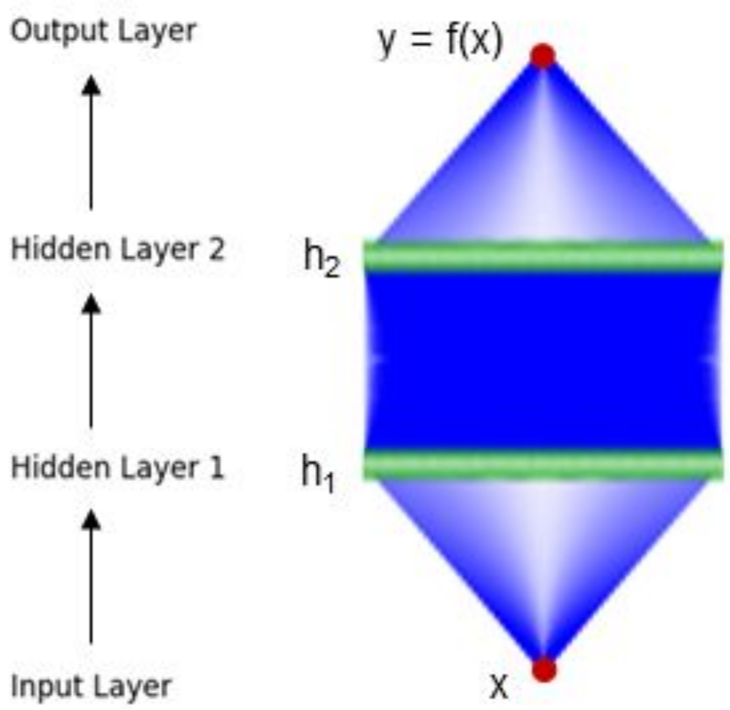
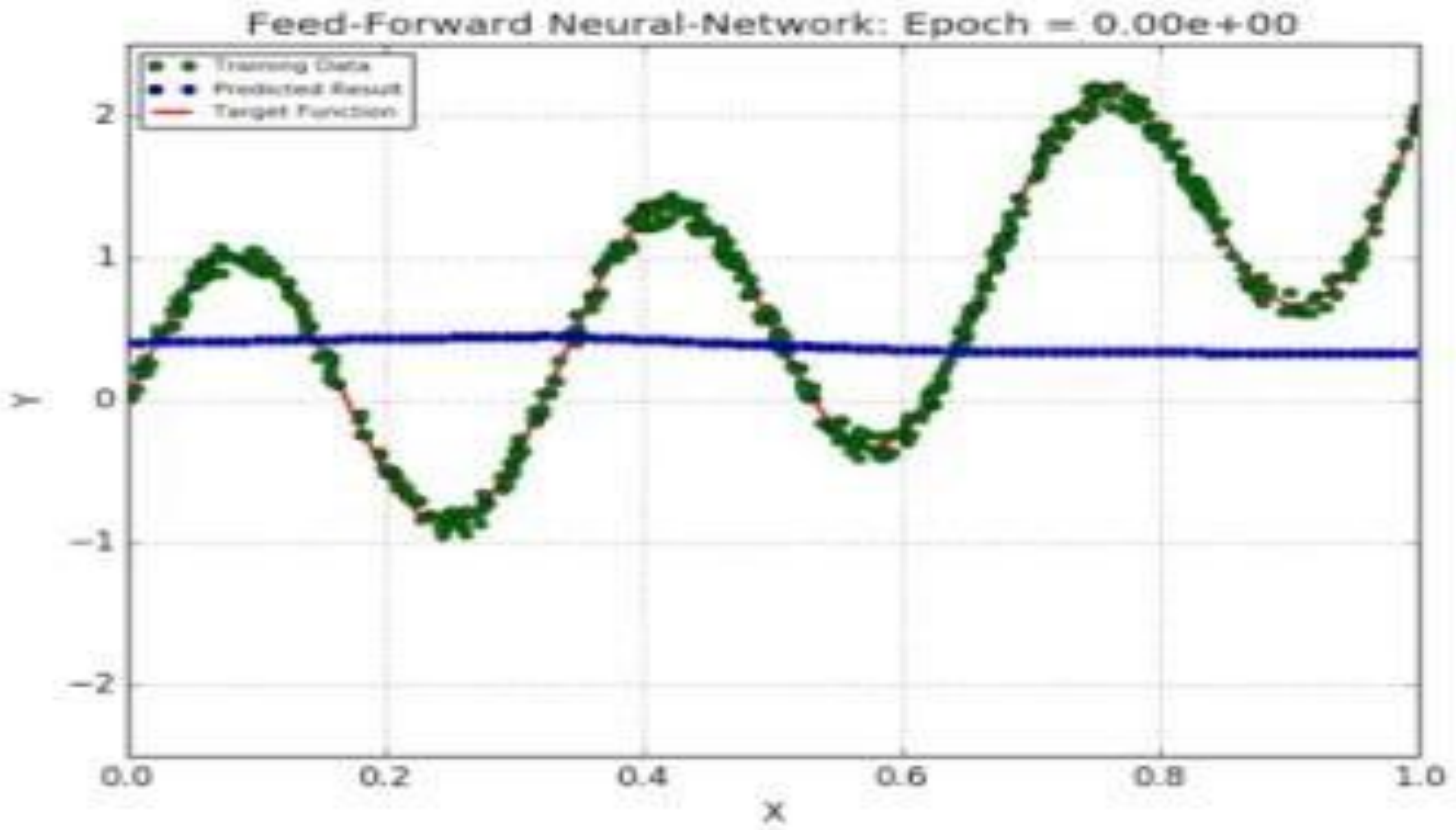


Neural Network Architecture



Additional fine-tuning of hyper-parameters should be done to enhance efficiency and robustness of training.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0.0
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X

Summary

Neural Networks: Summary

Deep Neural Network (DNN)

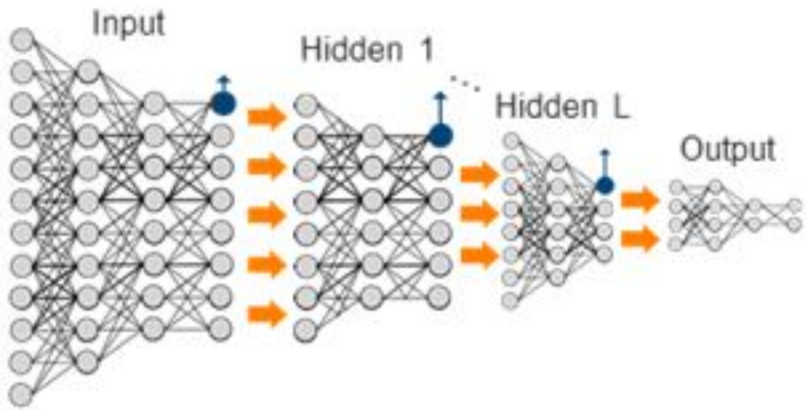
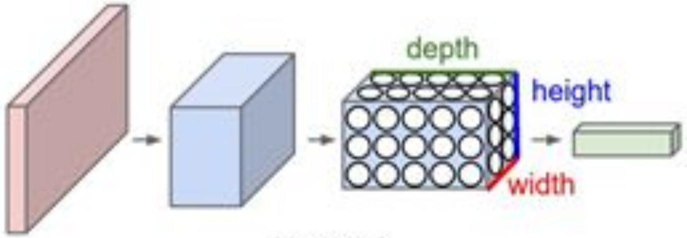
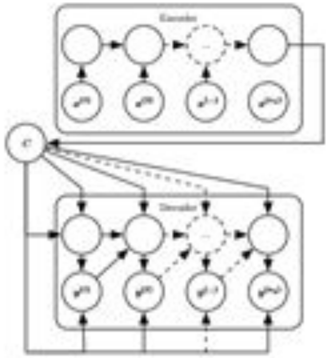


Image Classifier: Convolutional Neural Network (CNN)



LeCun 1989

Natural Language Processing
Recurrent Neural Network (RNN)



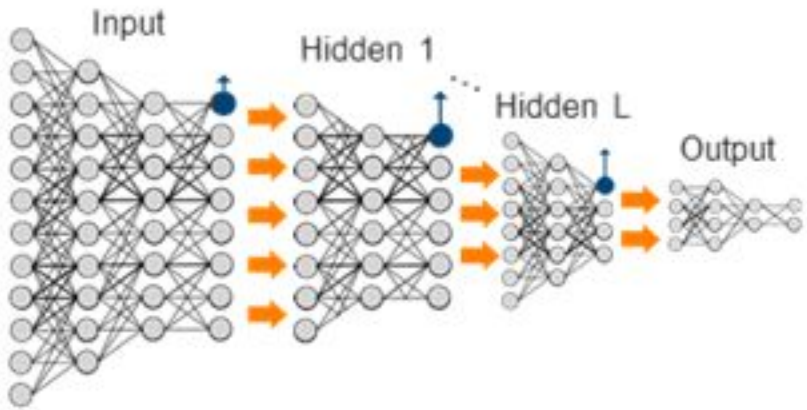
- **Neural Networks** are providing state-of-the-art results in many fields: (computer vision, natural language processing, reinforcement learning).

Alpha-Go

Google's Self-Driving Car

Neural Networks: Summary

Deep Neural Network (DNN)



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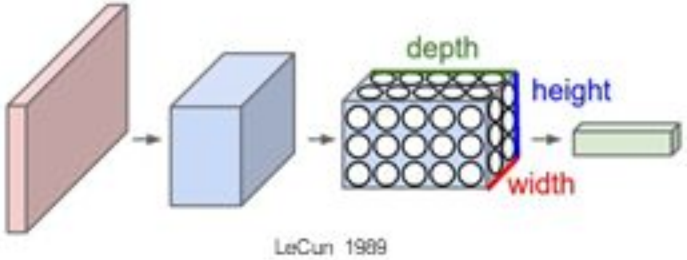
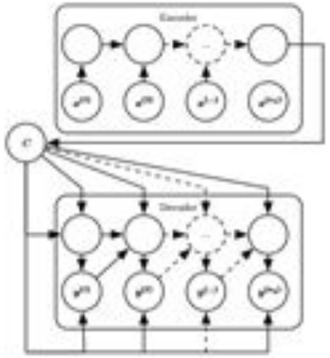


Natural Language Processing
Recurrent Neural Network (RNN)



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- **Powerful approximation properties:** target functions approximated by compositions, perform well in high dimensional spaces, many variants.

Alpha-Go

Google's Self-Driving Car

Neural Networks: Summary

Deep Neural Network (DNN)

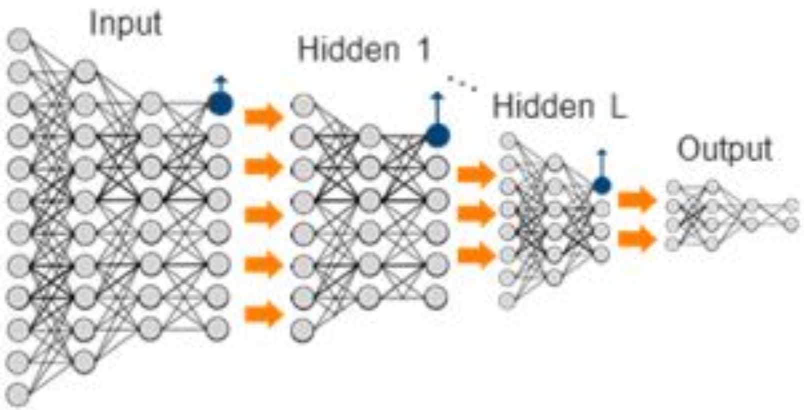
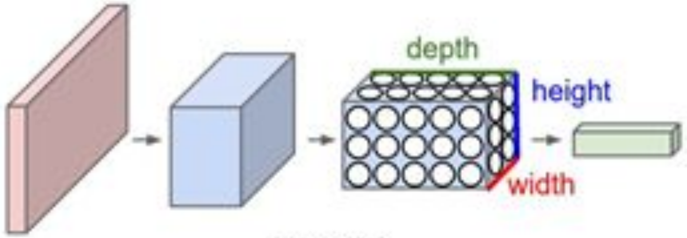
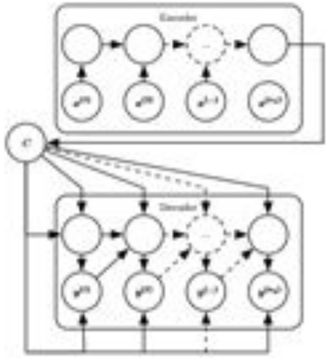


Image Classifier: Convolutional Neural Network (CNN)



LeCun 1989

Natural Language Processing
Recurrent Neural Network (RNN)



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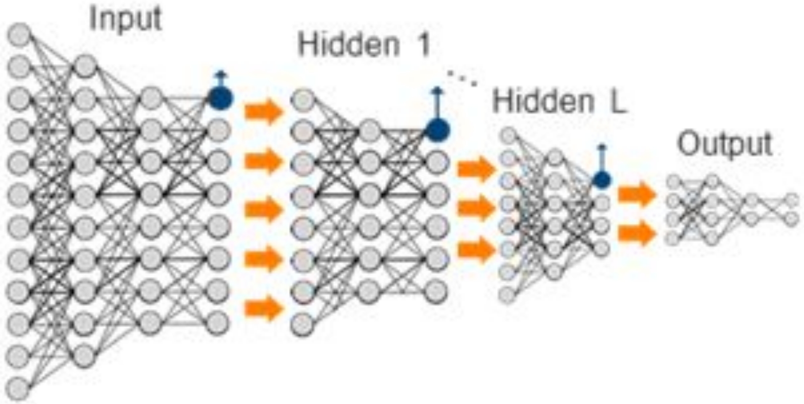

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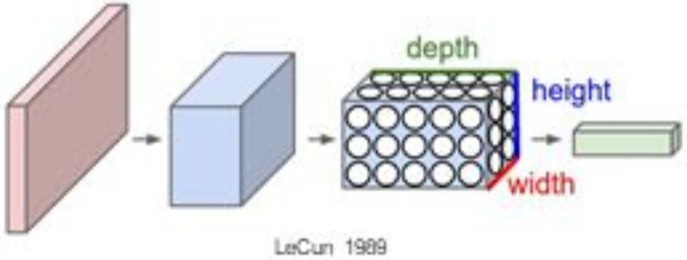
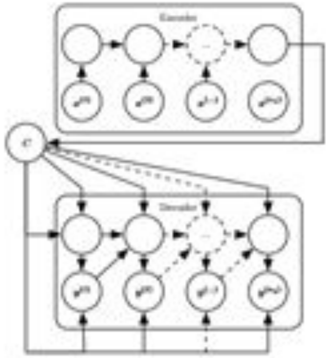


Natural Language Processing
Recurrent Neural Network (RNN)



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- **Current research to better understand NN's**: choice of architectures, training protocols, approximation properties, reliability, interpretability, …

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