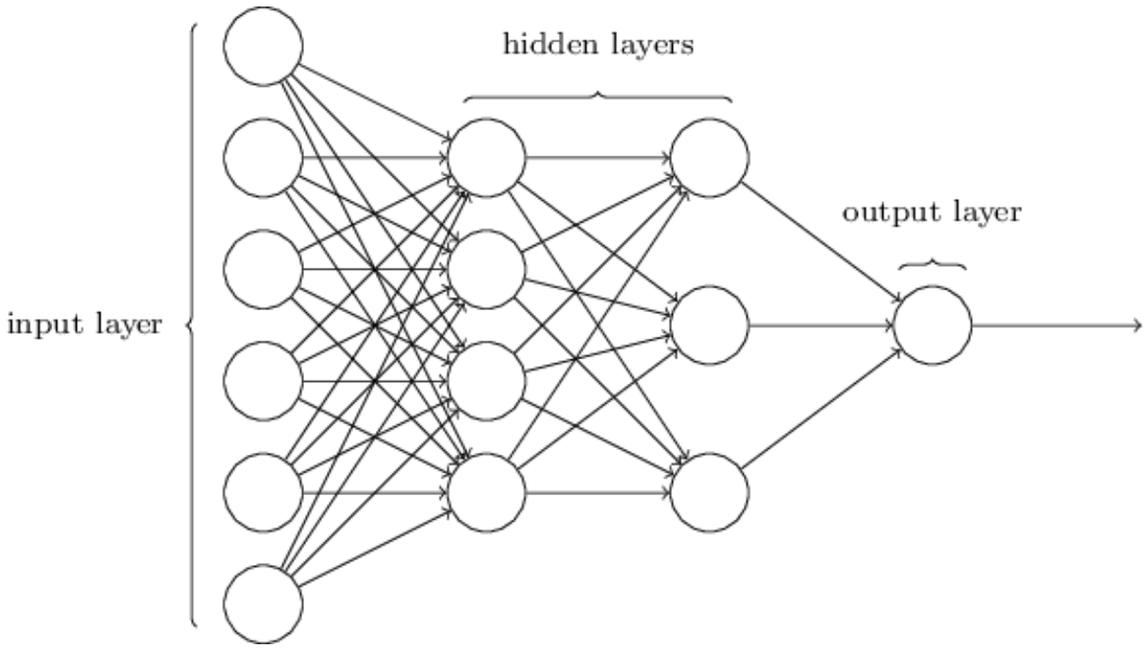
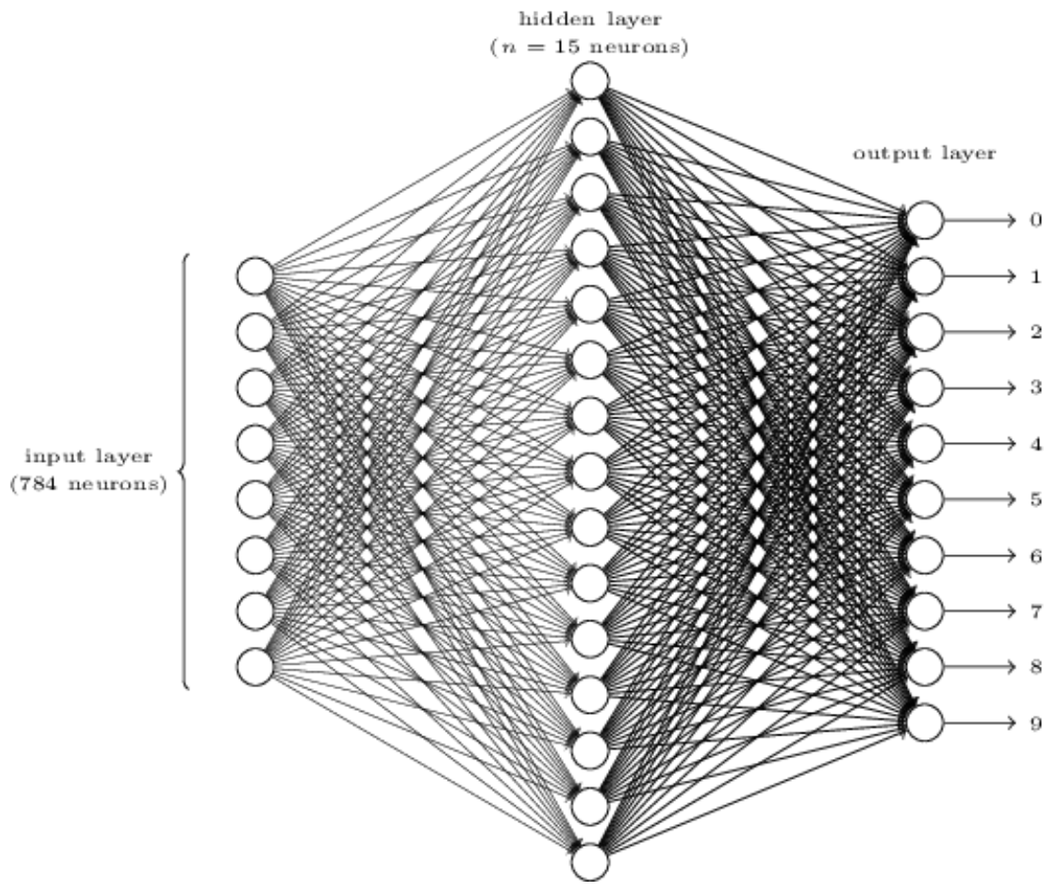
Content

Content

Four-layer network with two hidden layers

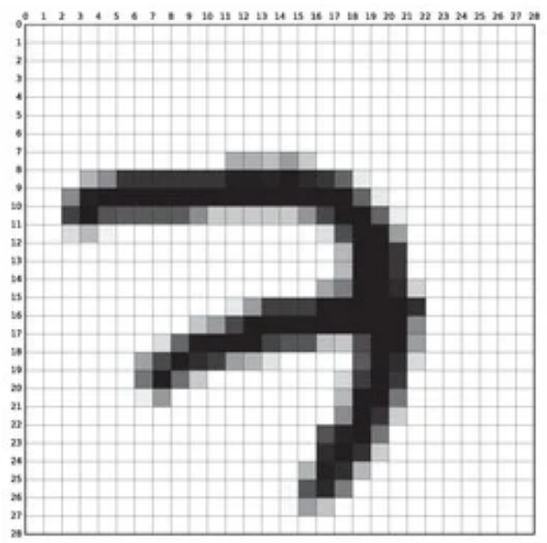




MNIST database of handwritten digits

Modified national institute of standards and technology database

60,000 training images and 10,000 testing images



(a) MNIST sample belonging to the digit '7'.

(b) 100 samples from the MNIST training set.

encode the intensities of the image pixels into the input neurons. If the image is a 28x28 greyscale image, then we'd have 28×28=784 input neurons, with the intensities scaled appropriately between 0 and 1.

Learning representations by back-propagating errors

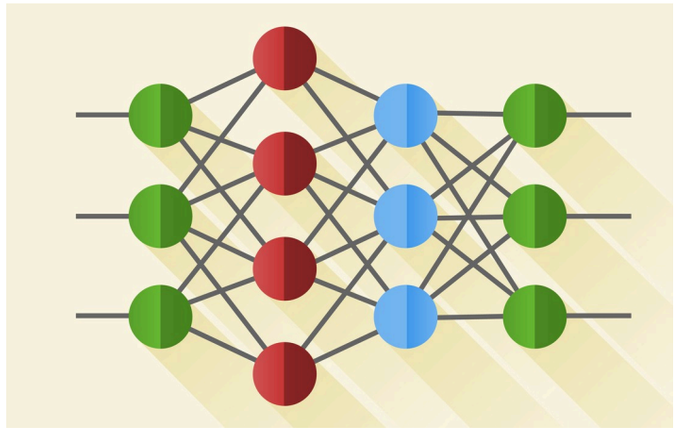
David E. Rumelhart, Geoffrey E. Hinton & Ronald J. Williams

Nature **323**, 533–536 (1986) | Cite this article

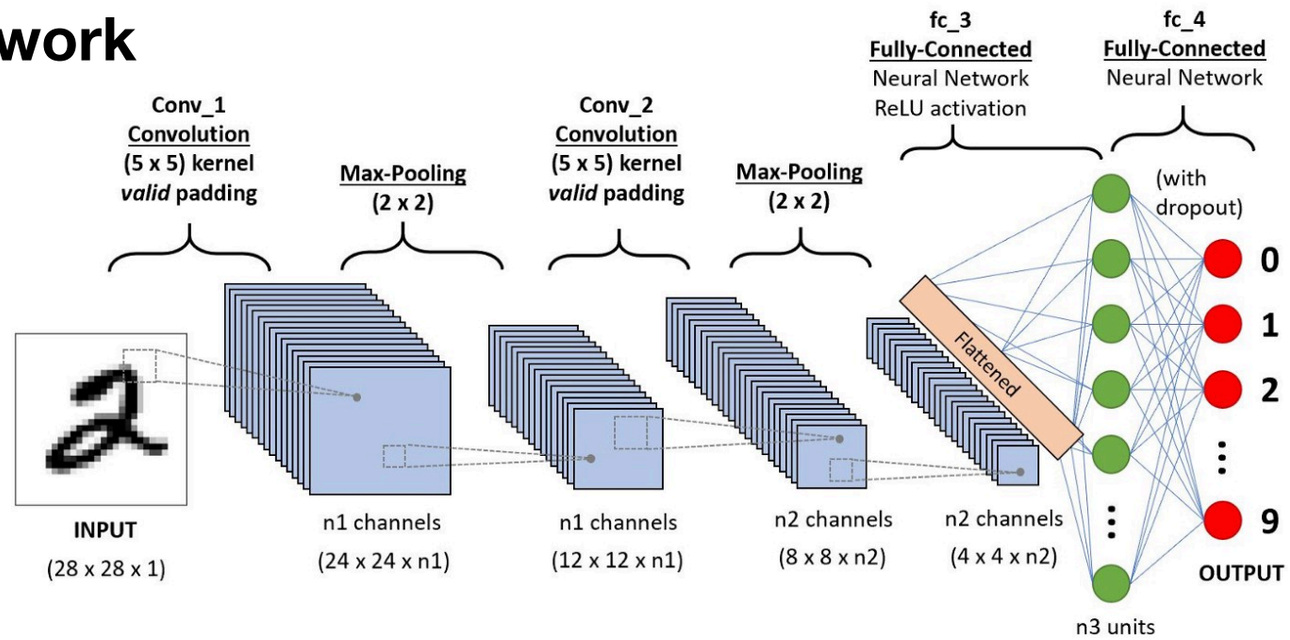
Connecting neurons to networks

Deep Learning: a network with 2 or more hidden layers with each layers containing large amount of neurons

Feed-forward network



Convolutional neural network

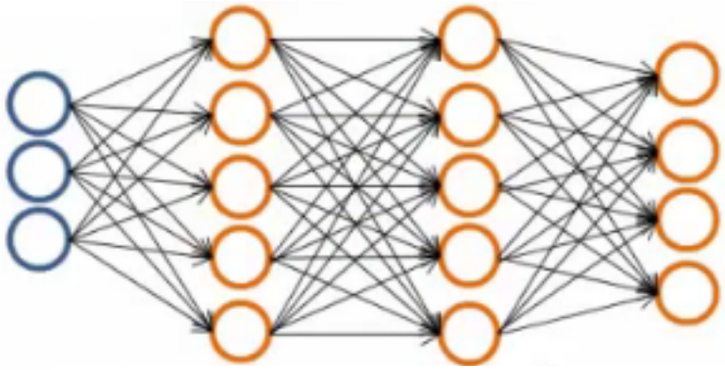


Generative neural network

Spiking neural network

https://towardsdatascience.com/introduction-to-math-behind-neural-networks-e8b60dbbdeba
https://towardsdatascience.com/nns-aynk-c34efe37f15a

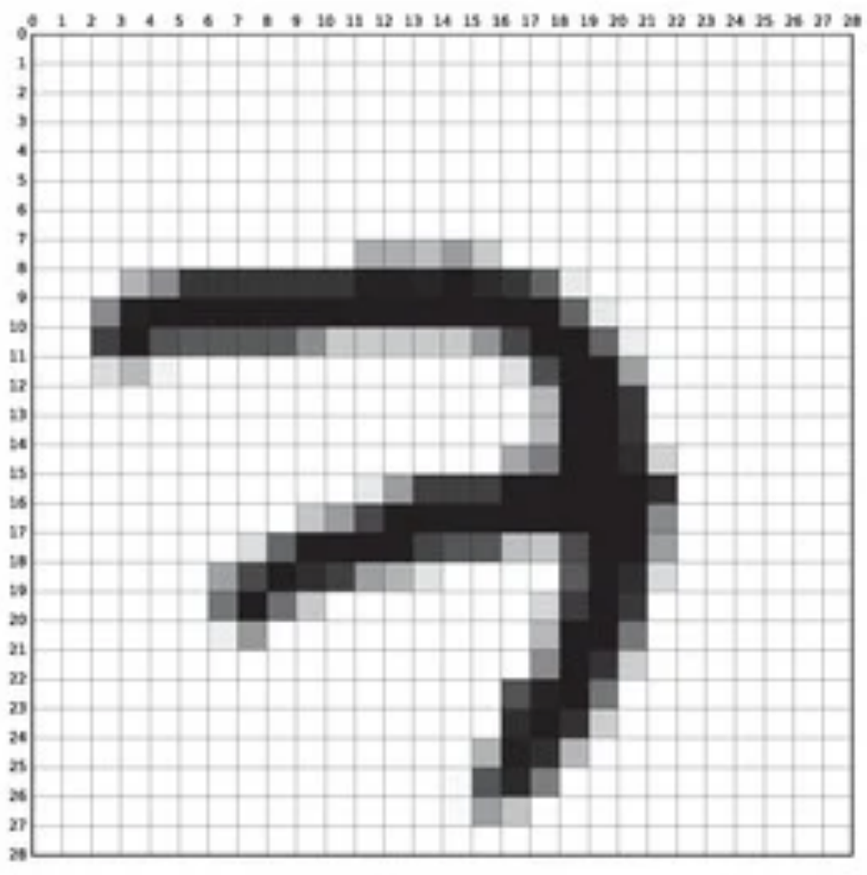
Neural network — Representation



$$h_\Theta(x) \in \mathbb{R}^4$$

Multiclass classification

Handwritten digital recognition problem - 10 possible categories (0-9)



(a) MNIST sample belonging to the digit '7'.

(b) 100 samples from the MNIST training set.

Mathematical representation for neutrons: Learning Algorithm

Backpropagation: backward propagation of errors

Computing the gradient of the cost function with respect to the weights

Cost function

$$J = \text{mean squared error} = \frac{1}{m}\sum_{i=1}^{m}(y_i - \hat{y}_i)^2$$

$$\frac{\partial J}{\partial w_i} = \frac{\partial J}{\partial \hat{y}} \times \frac{\partial \hat{y}}{\partial z} \times \frac{\partial z}{\partial w_i}$$

$$\frac{2}{m}\sum_{i=1}^{m}(y_i - \hat{y}_i) \qquad g(z)g(-z) \qquad x \qquad 1$$

$$\frac{\partial J}{\partial b} = \frac{\partial J}{\partial \hat{y}} \times \frac{\partial \hat{y}}{\partial z} \times \frac{\partial z}{\partial b}$$

$$z = w \cdot x + b = \theta^T x$$

$$y = \frac{1}{1 + \exp(-\theta^T x)}$$

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

1. $g(z) + g(-z) = 1$
2. $g'(z) = g(z)(1 - g(z)) = g(z)g(-z)$
3. $g'(-z) = g'(z)$

Optimization: select best weights and bias for the perceptron

$$w_i = w_i - \alpha\frac{\partial J}{\partial w_i} \qquad b = b - \alpha\frac{\partial J}{\partial b}$$

Andrew Ng, Stanford University

http://www.holehouse.org/mlclass/

https://github.com/mxc19912008/Andrew-Ng-Machine-Learning-Notes

Michael Nielsen, scientist at home, the best reading material

http://neuralnetworksanddeeplearning.com

http://neuralnetworksanddeeplearning.com/chap1.html

http://neuralnetworksanddeeplearning.com/chap2.html

https://machinelearningmastery.com/implement-backpropagation-algorithm-scratch-python/

Learning representations by back-propagating errors

David E. Rumelhart, Geoffrey E. Hinton & Ronald J. Williams

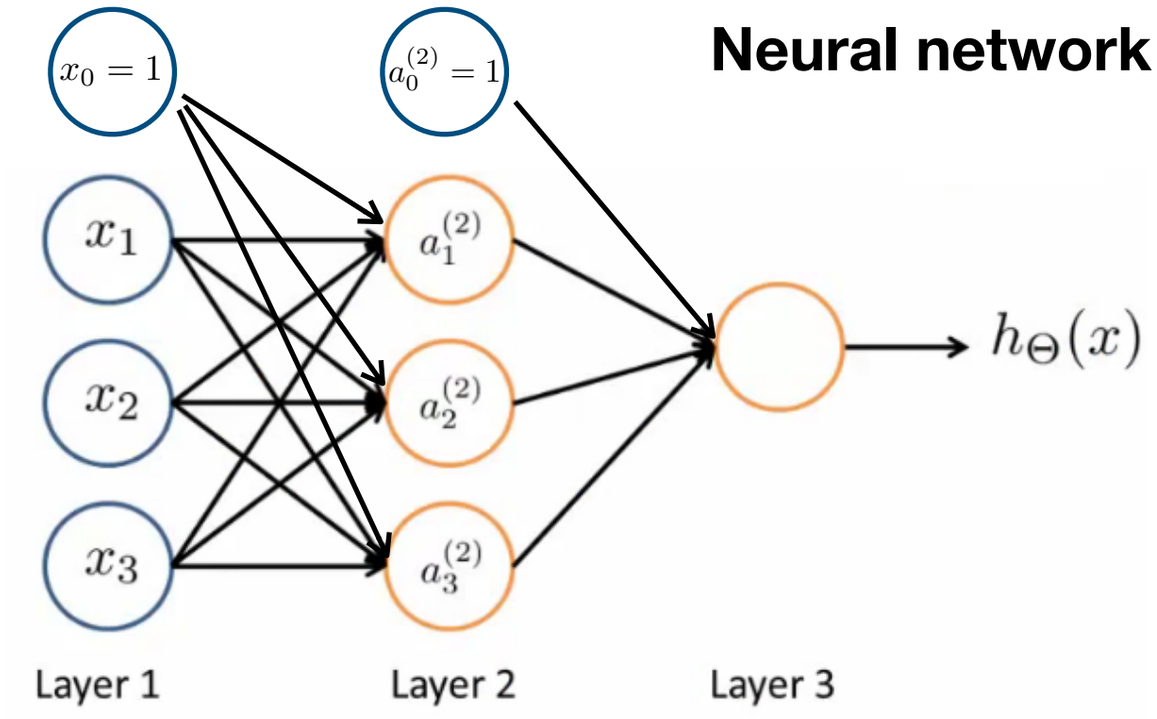
Nature **323**, 533–536 (1986) | Cite this article

84k Accesses | **12307** Citations | **239** Altmetric | Metrics

Early paper by
Li Wan, Matthew Zeiler, Sixin Zhang, Yann LeCun, Rob Fergus (2013)

http://yann.lecun.com/exdb/publis/pdf/wan-icml-13.pdf

Neural network — Representation



$a_i^{(l)}$ – activation of unit i in layer l

$\Theta^{(l)} : [s^{(l+1)} \times (s^{(l)} + 1)]$

the bias

Matrix of parameters mapping from layer (l) to layer (l+1)

Weights

$$x = \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \end{bmatrix} \quad \theta = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \theta_3 \end{bmatrix}$$

$$a_1^{(2)} = g(\Theta_{10}^{(1)} x_0 + \Theta_{11}^{(1)} x_1 + \Theta_{12}^{(1)} x_2 + \Theta_{13}^{(1)} x_3)$$
$$a_2^{(2)} = g(\Theta_{20}^{(1)} x_0 + \Theta_{21}^{(1)} x_1 + \Theta_{22}^{(1)} x_2 + \Theta_{23}^{(1)} x_3) \qquad \Theta^{(1)} : [3 \times 4]$$
$$a_3^{(2)} = g(\Theta_{30}^{(1)} x_0 + \Theta_{31}^{(1)} x_1 + \Theta_{32}^{(1)} x_2 + \Theta_{33}^{(1)} x_3)$$
$$h_\Theta(x) = a_1^{(3)} = g(\Theta_{10}^{(2)} a_0^{(2)} + \Theta_{11}^{(2)} a_1^{(2)} + \Theta_{12}^{(2)} a_2^{(2)} + \Theta_{13}^{(2)} a_3^{(2)}) \qquad \Theta^{(2)} : [1 \times 4]$$

$$(z_1^2 = \theta_{10}^{(1)} x_0 + \theta_{11}^{(1)} x_1 + \theta_{12}^{(1)} x_2 + \theta_{13}^{1} x_3 \ , z_2^2, z_3^2)$$

Vector representation

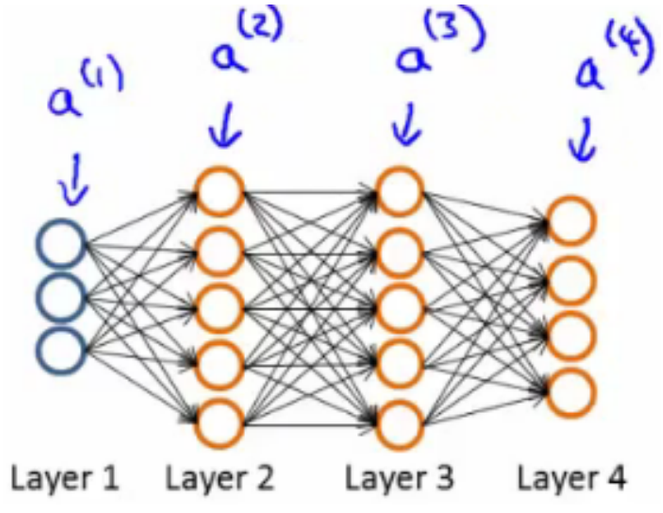
$$z^2 = \Theta^{(1)} x \qquad a^2 = g(z^2)$$

$$z^3 = \Theta^{(2)} a^2 \qquad h_\Theta(x) = a^3 = g(z^3)$$

Neural networks learns its own features

- Features in the hidden layer are calculated/learned - not original features
- Flexibility to learn whatever features it wants to feed into the final logistic regression calculation
- Hidden layers do the job, learn what gives the best final results to feed into final output layer
- Non-linear hypothesis

Neural network — Learning — back-propagation



Learning representations by back-propagating errors

David E. Rumelhart, Geoffrey E. Hinton & Ronald J. Williams

Nature **323**, 533–536 (1986) | Cite this article

$L = 4 \quad s^1 = 3 \quad s^2 = 5 \quad s^3 = 5 \quad s^4 = 4$

Training set (in vector form)

$$\{(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \cdots, (x^m, y^m)\}$$

Forward propagation

$$a^1 = x$$
$$z^2 = \Theta^1 a^1 \text{ (add } x_0)$$
$$a^2 = g(z^2)$$
$$z^3 = \Theta^2 a^2 \text{ (add } a_0^2)$$
$$a^3 = g(z^3)$$
$$z^4 = \Theta^3 a^3 \text{ (add } a_0^3)$$
$$a^4 = h_\Theta(x) = g(z^4)$$

Back propagation

δ_j^l – **the error of neuron j in layer l**

$$\delta^1 = (\Theta^1)^T \delta^2 - x$$
$$\delta^2 = (\Theta^2)^T \delta^3 .* g'(z^2)$$
$$\delta^3 = (\Theta^3)^T \delta^4 .* g'(z^3)$$
$$\delta^4 = (a^4 - y) .* g'(z^4)$$
$$\tilde{\delta}_j^4 = a_j^4 - y_j$$

from quadratic cost

$.*$ elementwise multiplication
Hadamard product

$$g'(z) = g(z) .* (1 - g(z))$$

$\Theta^3 : [4 \times 5]$ ($[4 \times 6]$ if include bias)

$(\Theta^3)^T : [5 \times 4]$

$\delta^4 : [4 \times 1]$

$g'(z^3) : [5 \times 1]$

Neural network — Learning — back-propagation

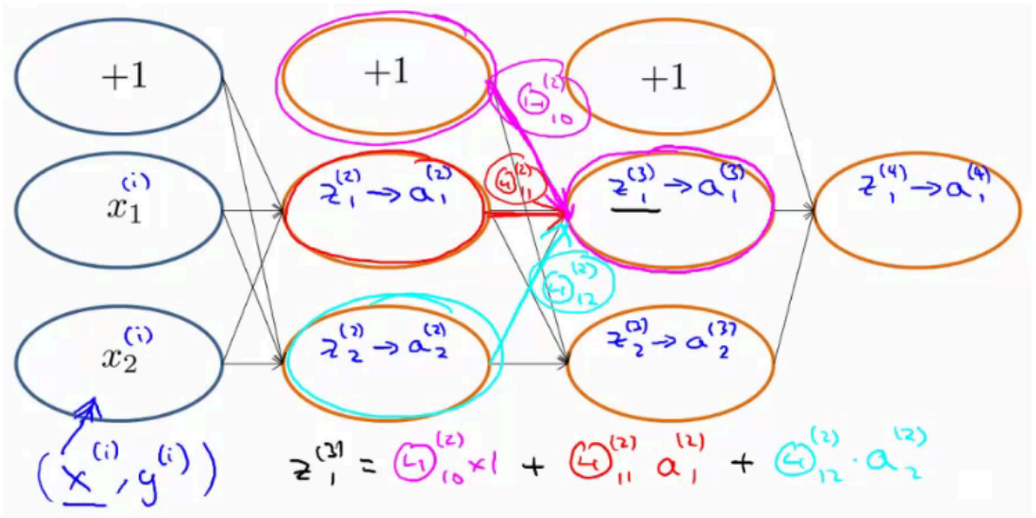
$$J(\Theta) = \frac{1}{2m}\sum_{x} ||y(x) - a^L(x)||^2 = \frac{1}{2m}\sum_{i} ||a_i^L - y_i||^2$$

Training set (in vector form) $\{(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \cdots, (x^m, y^m)\}$

$$\frac{\partial J(\Theta)}{\partial \Theta_{ij}^{(l)}} = a_j^{(l)} \delta_i^{(l+1)} = a_{\text{in}} \delta_{\text{out}}$$

Loop through the training set $i = 1$ to m

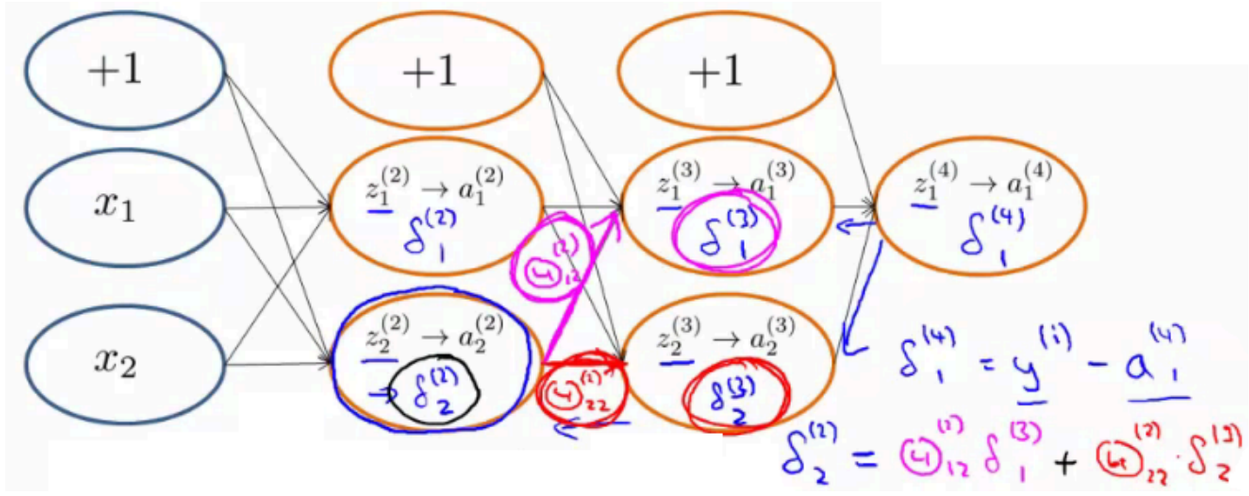
Forward propagation



Calculate activation values: weighted sum of the previous layer's activation values, weighted by the link parameters

Back propagation

How well is the network doing on example i ?



Calculate delta values: weighted sum of the next layer's delta values, weighted by the link parameters

After executing the loop

Update the cost function $\Theta_{ij}^{(l)} = \Theta_{ij}^{(l)} - \alpha \frac{\partial J(\Theta)}{\partial \Theta_{ij}^{(l)}}$

$$\frac{\partial J}{\partial \Theta_{10}^{(1)}} = \delta_1^{(2)} \qquad \frac{\partial J}{\partial \Theta_{10}^{(2)}} = \delta_1^{(3)}$$

$$\frac{\partial J}{\partial \Theta_{12}^{(1)}} = a_2^{(1)} \delta_1^{(2)} \qquad \frac{\partial J}{\partial \Theta_{12}^{(2)}} = a_2^{(2)} \delta_1^{(3)}$$

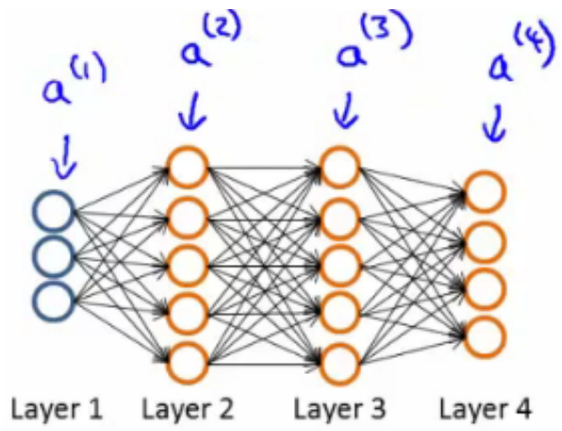
$$\frac{\partial J}{\partial \Theta_{22}^{(1)}} = a_2^{(1)} \delta_2^{(2)} \qquad \frac{\partial J}{\partial \Theta_{22}^{(2)}} = a_2^{(2)} \delta_2^{(3)}$$

Neural network — Learning put together

1) - pick a network architecture

Input units (x, a_1)
Output units (y)
Hidden units (Theta_1, a_2, Theta_2, a_3 …)

Normally more hidden units is better but more computationally expensive



2) - training a network

Randomly initiative the weights
Implement forward propagation to get a_L for any example x_i
Implement cost function J(Theta)
Implement back propagation to get partial derivatives

```
for i = 1:m {
     Forward propagation on (xⁱ, yⁱ) --> get activation (a) terms
     Back propagation on (xⁱ, yⁱ) --> get delta (δ) terms
     Compute Δ := Δˡ + δˡ⁺¹(aˡ)ᵀ
}

With this done compute the partial derivative terms
```

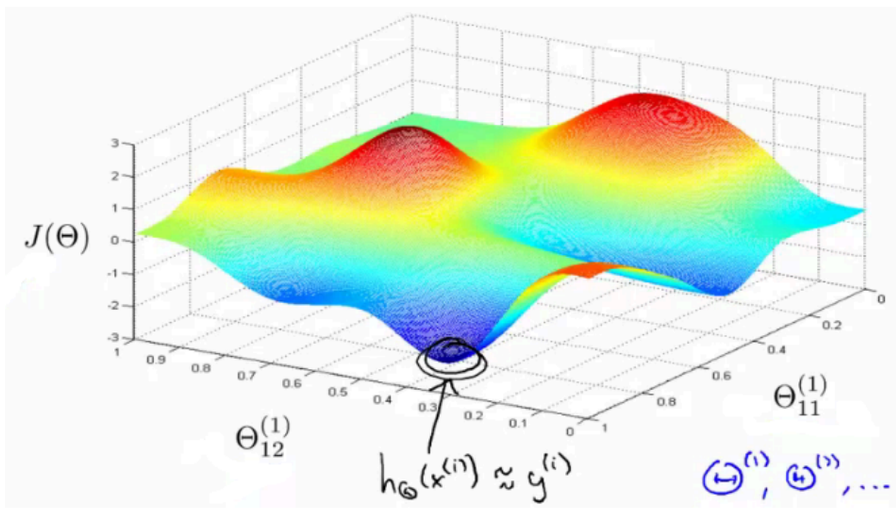
Use (gradient descent, CG or more advanced optimization) to minimise J(\Theta):
J(\Theta) is non-convex
Nonlinearity, local minimum, time, complexity …

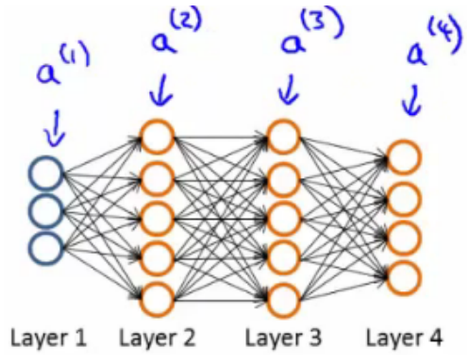
Learning representations by back-propagating errors

David E. Rumelhart, Geoffrey E. Hinton & Ronald J. Williams

Nature **323**, 533–536 (1986) | Cite this article

84k Accesses | **12307** Citations | **239** Altmetric | Metrics





$$\delta_j^l = \frac{\partial J}{\partial z_j^l} \text{ measures the error of neuron } j \text{ in layer } l$$

An equation for the rate of change of the cost with respect to any weight in the network

Partial derivatives $\frac{\partial}{\partial \Theta_{ij}^l} J(\Theta) = a_j^l \delta_i^{l+1}$

Learn slowly if either the input neuron is low-activation, or if the output neuron has saturated, i.e., is either high- or low-activation.

Summary: the equations of backpropagation

$\delta^L = \nabla_a C \odot \sigma'(z^L)$ (BP1)

$\delta^l = ((w^{l+1})^T \delta^{l+1}) \odot \sigma'(z^l)$ (BP2)

$\frac{\partial C}{\partial b_j^l} = \delta_j^l$ (BP3)

$\frac{\partial C}{\partial w_{j\,k}^l} = a_k^{l-1} \delta_j^l$ (BP4)

Prove this $\delta_j^2 = \frac{\partial J}{\partial z_j^2} = \sum_k \frac{\partial J}{\partial z_k^3} \frac{\partial z_k^3}{\partial z_j^2} = \sum_k \delta_k^3 \frac{\partial z_k^3}{\partial z_j^2}$

$z_k^3 = \sum_j \Theta_{kj}^2 a_j^2 = \sum_j \Theta_{kj}^2 g(z_j^2)$ $\frac{\partial z_k^3}{\partial z_j^2} = \Theta_{kj}^2 g'(z_j^2)$

$\delta_j^2 = \sum_k \Theta_{kj}^2 \, \delta_k^3 \, g'(z_j^2)$ $\delta^2 = (\Theta^2)^T \delta^3 .* g'(z^2)$

Notice the shift of l by 1, index jungle

Prove this $\frac{\partial J}{\partial \Theta^2} = \frac{\partial J}{\partial z^3} \frac{\partial z^3}{\partial \Theta^2} = \delta^3 a^2 = a^2 \delta^3$

$\delta^3 = \frac{\partial J}{\partial z^3}$ $z^3 = \Theta^2 a^2$

Michael Nielsen http://neuralnetworksanddeeplearning.com/chap2.html

In particular, given a mini-batch of m training examples, the following algorithm applies a gradient descent learning step based on that mini-batch

1. **Input a set of training examples**

2. **For each training example** x**:** Set the corresponding input activation $a^{x,1}$, and perform the following steps:

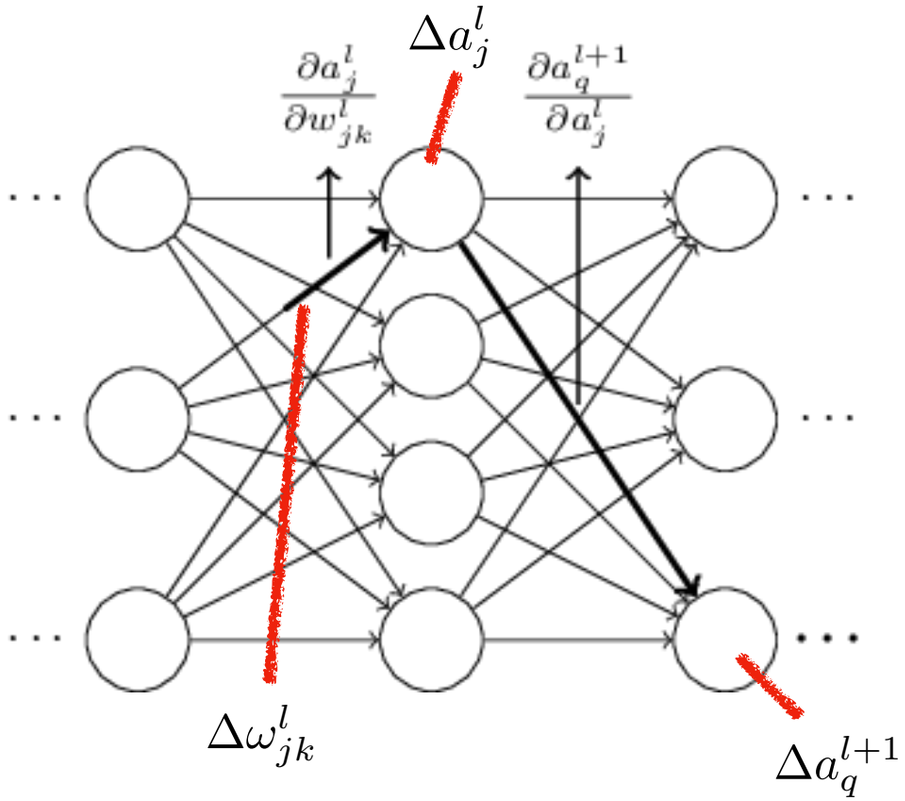
   - **Feedforward:** For each $l = 2, 3, \ldots, L$ compute $z^{x,l} = w^l a^{x,l-1} + b^l$ and $a^{x,l} = \sigma(z^{x,l})$.

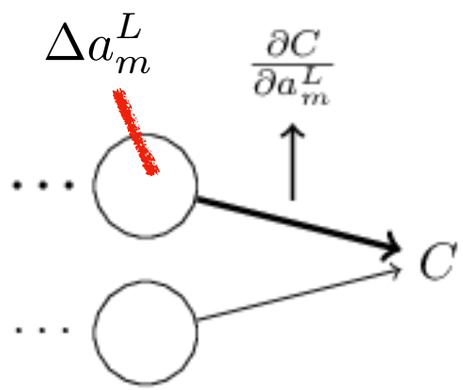
   - **Output error** $\delta^{x,L}$**:** Compute the vector $\delta^{x,L} = \nabla_a C_x \odot \sigma'(z^{x,L})$.

   - **Backpropagate the error:** For each $l = L-1, L-2, \ldots, 2$ compute $\delta^{x,l} = ((w^{l+1})^T \delta^{x,l+1}) \odot \sigma'(z^{x,l})$.

3. **Gradient descent:** For each $l = L, L-1, \ldots, 2$ update the weights according to the rule $w^l \to w^l - \frac{\eta}{m} \sum_x \delta^{x,l} (a^{x,l-1})^T$, and the biases according to the rule $b^l \to b^l - \frac{\eta}{m} \sum_x \delta^{x,l}$.

Michael Nielsen http://neuralnetworksanddeeplearning.com/chap2.html





Sigmoid is differentiable

$$\Delta C \approx \frac{\partial C}{\partial w_{jk}^l} \Delta w_{jk}^l.$$

$$\Delta a_j^l \approx \frac{\partial a_j^l}{\partial w_{jk}^l} \Delta w_{jk}^l \qquad \Delta a_q^{l+1} \approx \frac{\partial a_q^{l+1}}{\partial a_j^l} \frac{\partial a_j^l}{\partial w_{jk}^l} \Delta w_{jk}^l \qquad \cdots \qquad \Delta C \approx \frac{\partial C}{\partial a_m^L} \frac{\partial a_m^L}{\partial a_n^{L-1}} \frac{\partial a_n^{L-1}}{\partial a_p^{L-2}} \cdots \frac{\partial a_q^{l+1}}{\partial a_j^l} \frac{\partial a_j^l}{\partial w_{jk}^l} \Delta w_{jk}^l$$

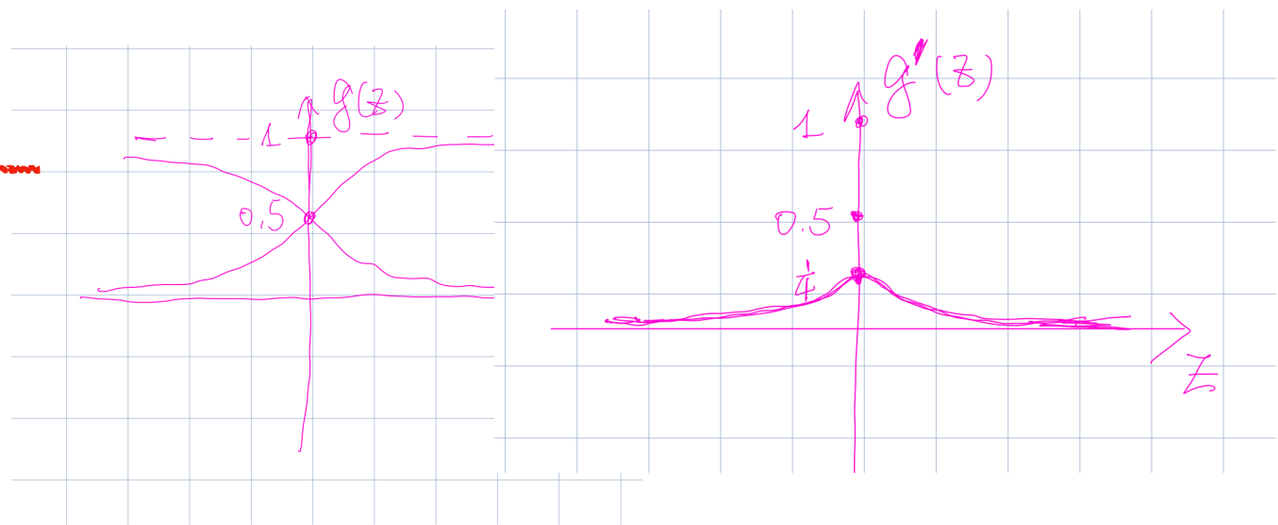
$$\Delta C \approx \sum_{mnp\ldots q} \frac{\partial C}{\partial a_m^L} \frac{\partial a_m^L}{\partial a_n^{L-1}} \frac{\partial a_n^{L-1}}{\partial a_p^{L-2}} \cdots \frac{\partial a_q^{l+1}}{\partial a_j^l} \frac{\partial a_j^l}{\partial w_{jk}^l} \Delta w_{jk}^l$$

$$\frac{\partial C}{\partial w_{jk}^l} = \sum_{mnp\ldots q} \frac{\partial C}{\partial a_m^L} \frac{\partial a_m^L}{\partial a_n^{L-1}} \frac{\partial a_n^{L-1}}{\partial a_p^{L-2}} \cdots \frac{\partial a_q^{l+1}}{\partial a_j^l} \frac{\partial a_j^l}{\partial w_{jk}^l}$$

http://neuralnetworksanddeeplearning.com/chap2.html

Improving the way neural networks learn

$$\frac{\partial}{\partial \Theta_{ij}^{l}} J(\Theta) = a_j^l \delta_i^{l+1} \qquad \delta^3 = (\Theta^3)^T \delta^4 .* g'(z^3)$$



Learning slowdown when output neuron saturates

Cross-entropy as cost function (cost function of logistic regression)

$$J(\Theta) = -\frac{1}{m} \sum_{i=1}^{m} [y_i \ln(a_i^L) + (1 - y_i) \ln(1 - a_i^L)]$$

$$\frac{\partial J}{\partial \theta_i} = \frac{1}{m} \sum_{i=1}^{m} x_i (g(z_i) - y_i)$$

Error in output control the learning

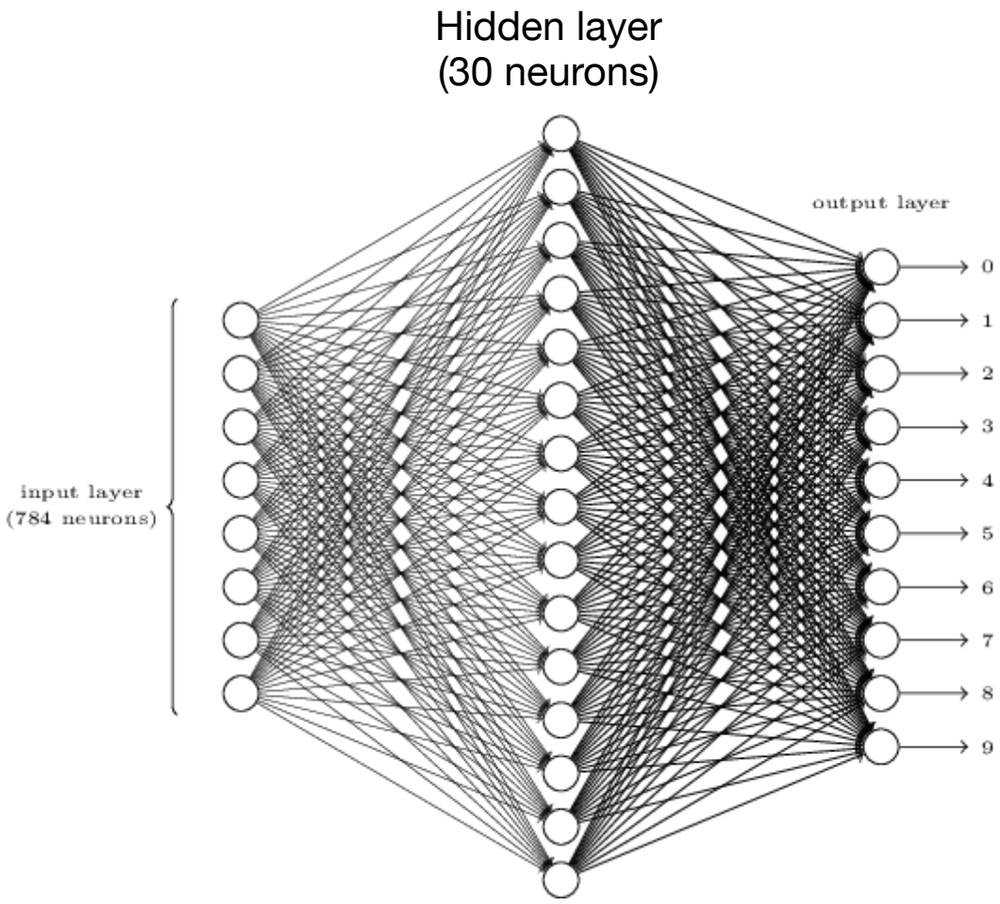
$$\frac{\partial J}{\partial b} = \frac{1}{m} \sum_{i=1}^{m} (g(z_i) - y_i)$$

Regularization $$J(\Theta) = -\frac{1}{m} \sum_{i=1}^{m} [y_i \ln(a_i^L) + (1 - y_i) \ln(1 - a_i^L)] + \frac{\lambda}{2m} \sum_{\Theta} \Theta^2$$

http://neuralnetworksanddeeplearning.com/chap3.html

Hyperparameters: learning rate, mini-batch size

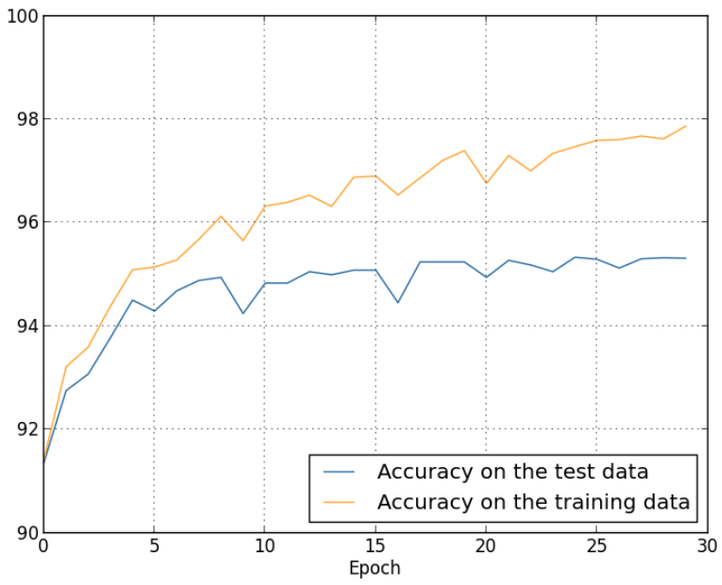
Requires thorough optimisation process



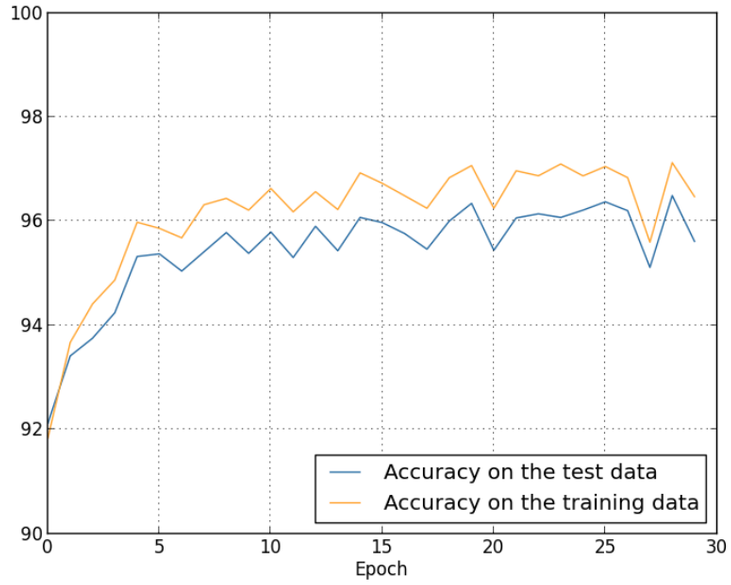
785x30 + 10x31 = 23,860

Fermi: "I remember my friend Johnny von Neumann used to say, with four parameters I can fit an elephant, and with five I can make him wiggle his trunk.".

Training_data	validation_data	test_data
$\{\Theta_{ij}^{(l)}\}$	Hyperparameters	
50,000 images 30 epochs, mini-batch size 10	10,000 images	10,000 images



Without regularisation

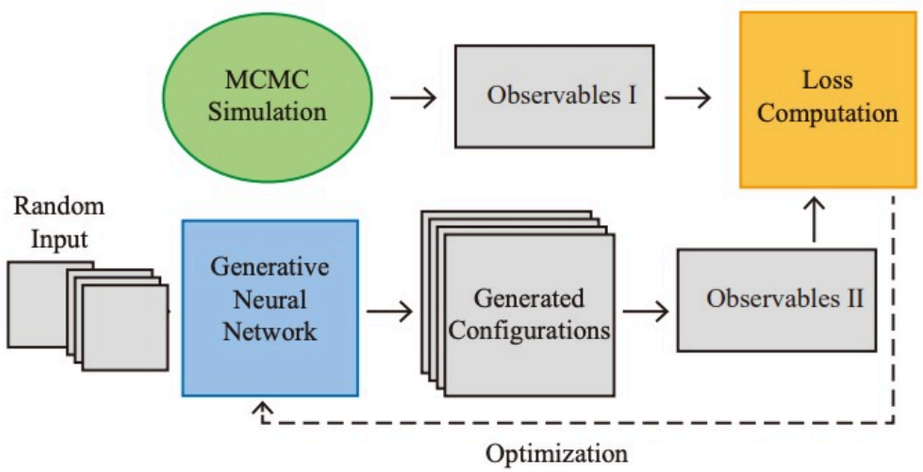


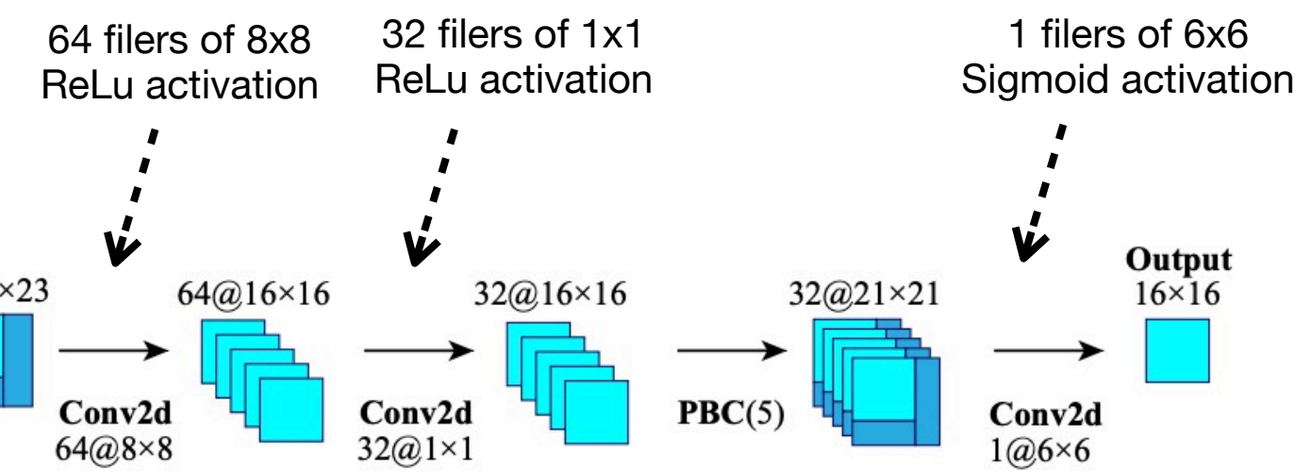
With regularisation

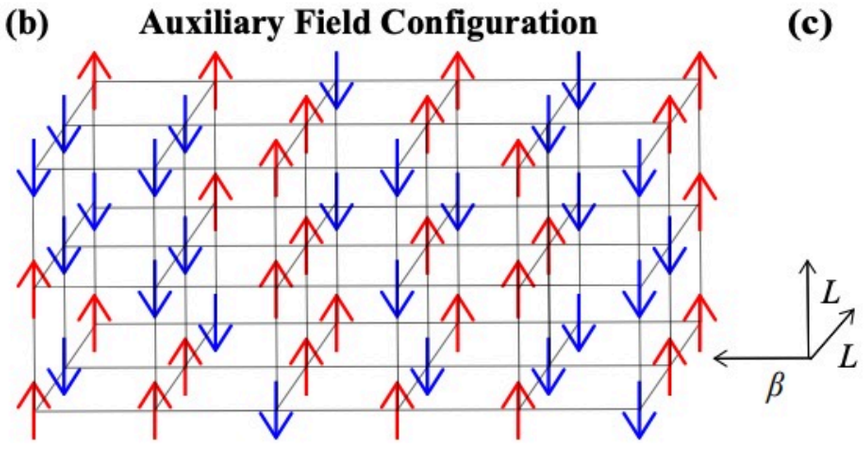
Chin. Phys. Lett. **39**, 050701 (2022)

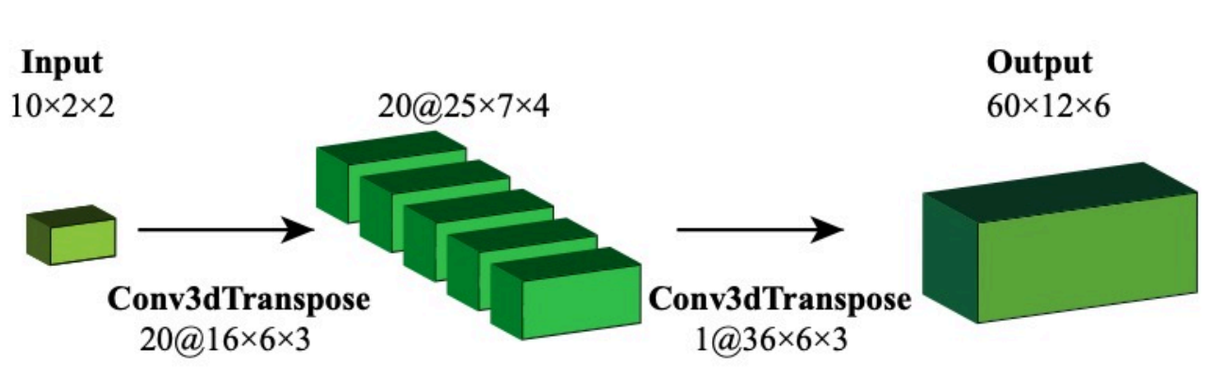
Network-Initialized Monte Carlo Based on Generative Neural Networks

Hongyu Lu, Chuhao Li, Bin-Bin Chen, …, ZYM





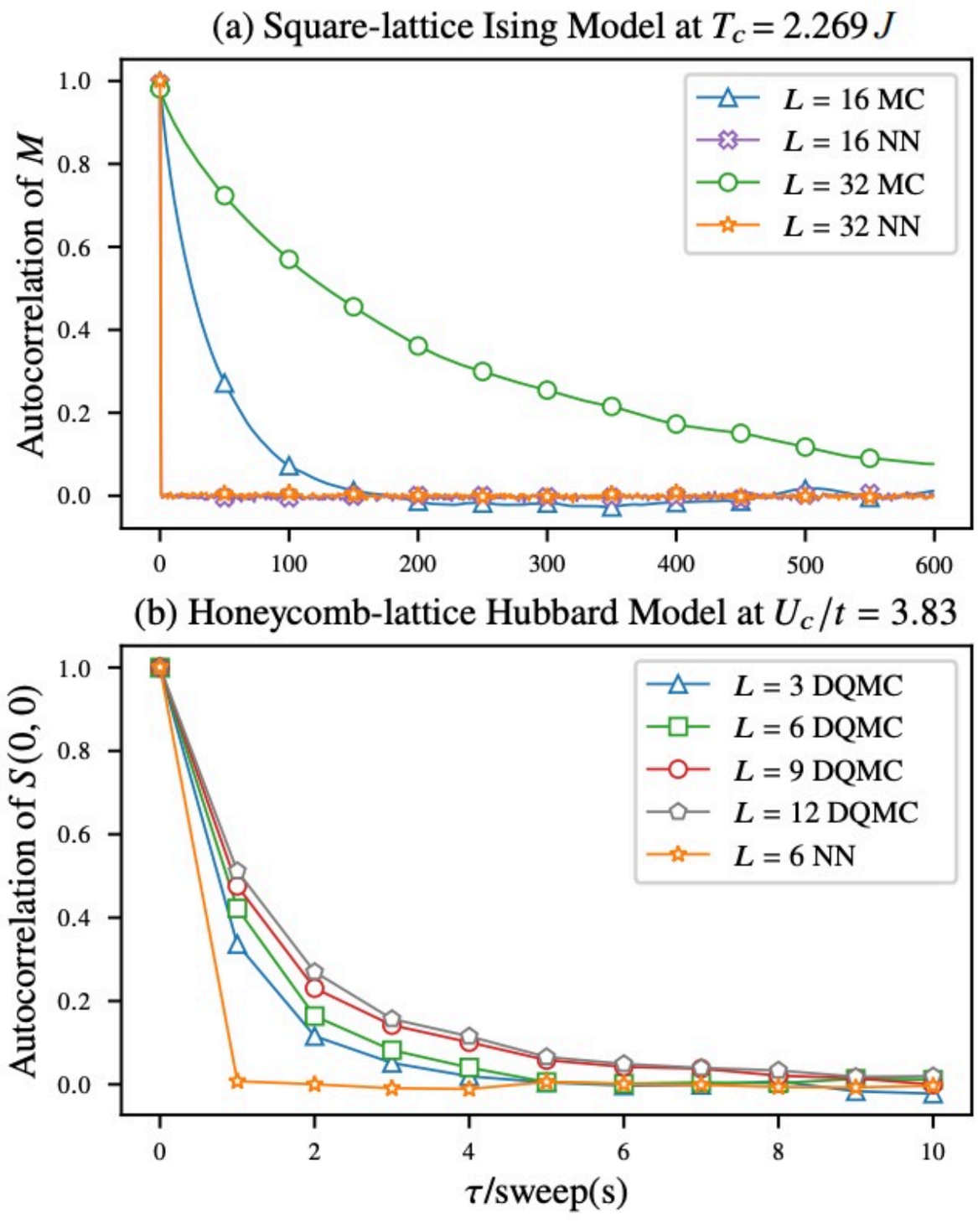


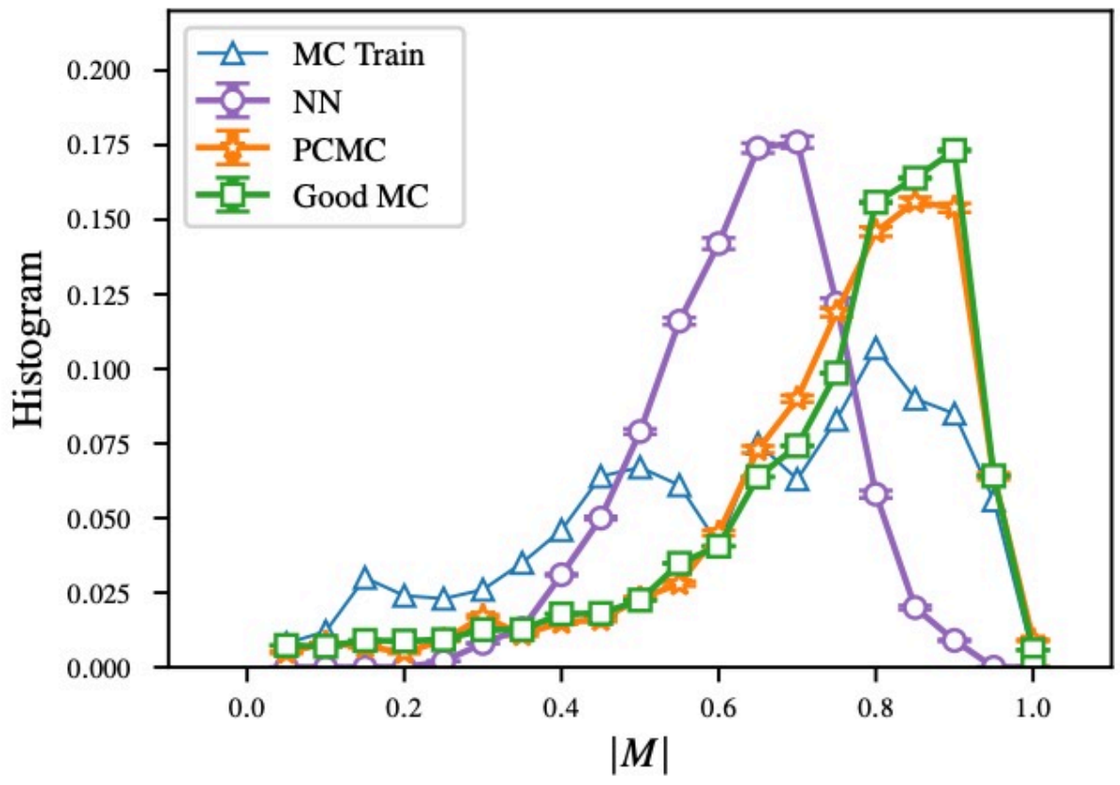


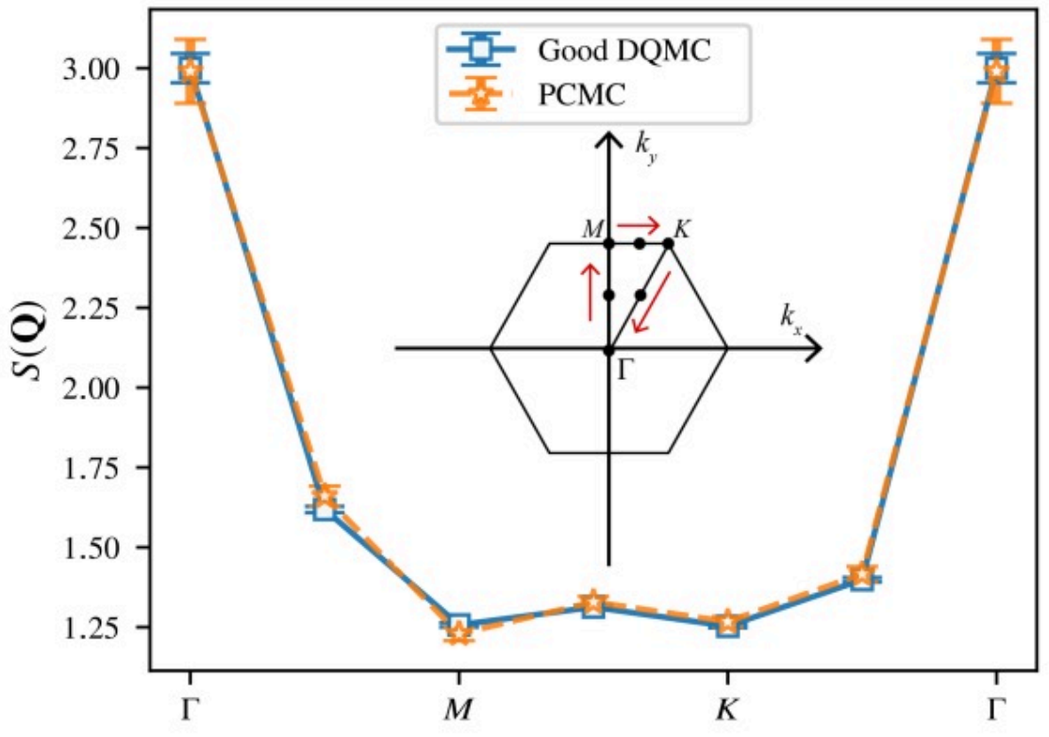
In order to optimize such neural networks, for both classical and quantum models, we prepare 1000 sets of observables measured from MC simulations and take 1000 input random configurations which will be processed into generated configurations. The comparison in loss function is randomly distributed without any grouping. For the choice of observables in the defined loss functions, we simply pick some from the ones we usually focus on. In the Ising case, we take the batch size to be 5 and epoch number to be up to 150 as the computation is quite easy. While in the Hubbard case, we run at most 15 epochs with a batch size of 3. We optimize the network parameters using Adam[63] with conventional learning rate 10^{-3}, $\beta_1 = 0.9$, and $\beta_2 = 0.999$.

$$Loss(\boldsymbol{G}_l; M_l, E_l) = w_1 \sum_l [|M(\boldsymbol{G}_l)| - |M_l|]^2 + w_2 \sum_l [M^2(\boldsymbol{G}_l) - M_l^2]^2 + w_3 \sum_l [E(\boldsymbol{G}_l) - E_l]^2 \quad (2)$$

where $\boldsymbol{G}_l$ is the l-th generated configuration, M_l and E_l refer to the magnetization $\frac{1}{N}|\sum_j \sigma_j|$ and the energy density $\frac{1}{N}\langle H \rangle$

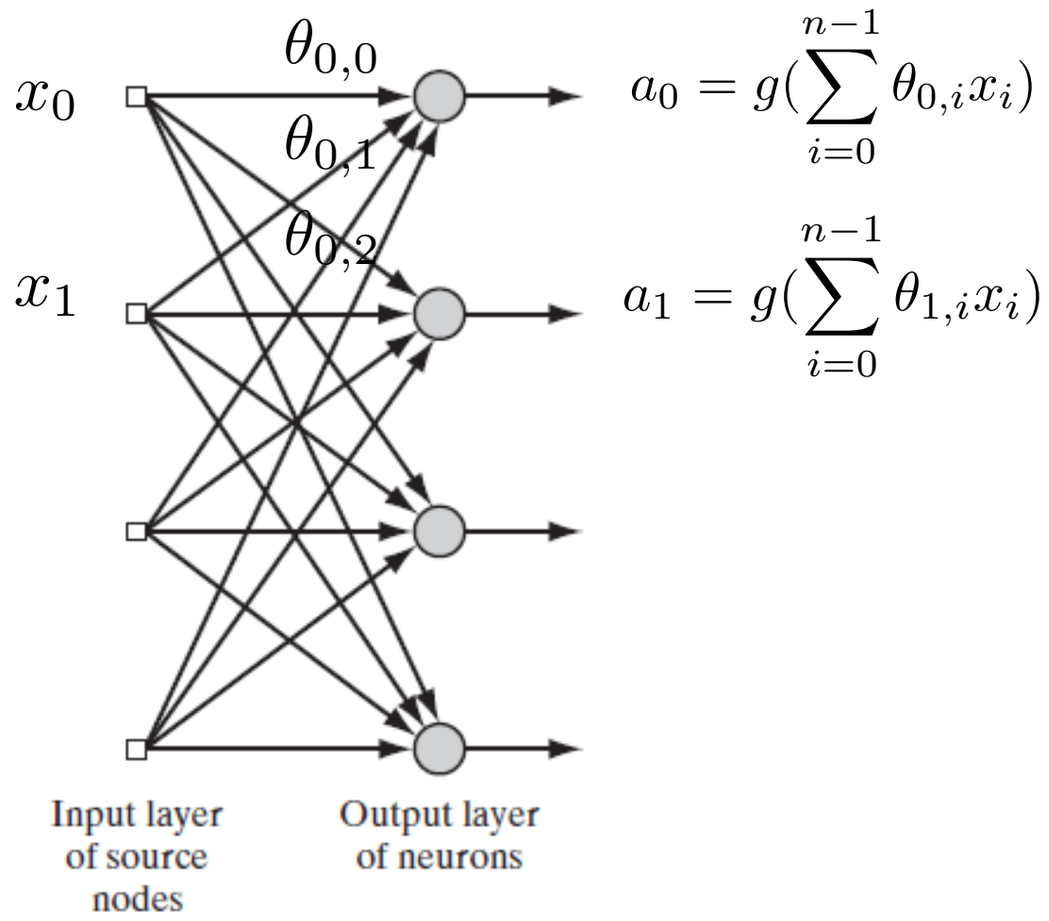



MC Train
NN
PCMC
Good MC
Histogram
|M|
0.000
0.025
0.050
0.075
0.100
0.125
0.150
0.175
0.200
0.0
0.2
0.4
0.6
0.8
1.0


Good DQMC
PCMC
S(Q)
Γ
M
K
Γ
1.25
1.50
1.75
2.00
2.25
2.50
2.75
3.00
k_y
k_x
M
K
Γ

Feed-forward neural networks

Single layer

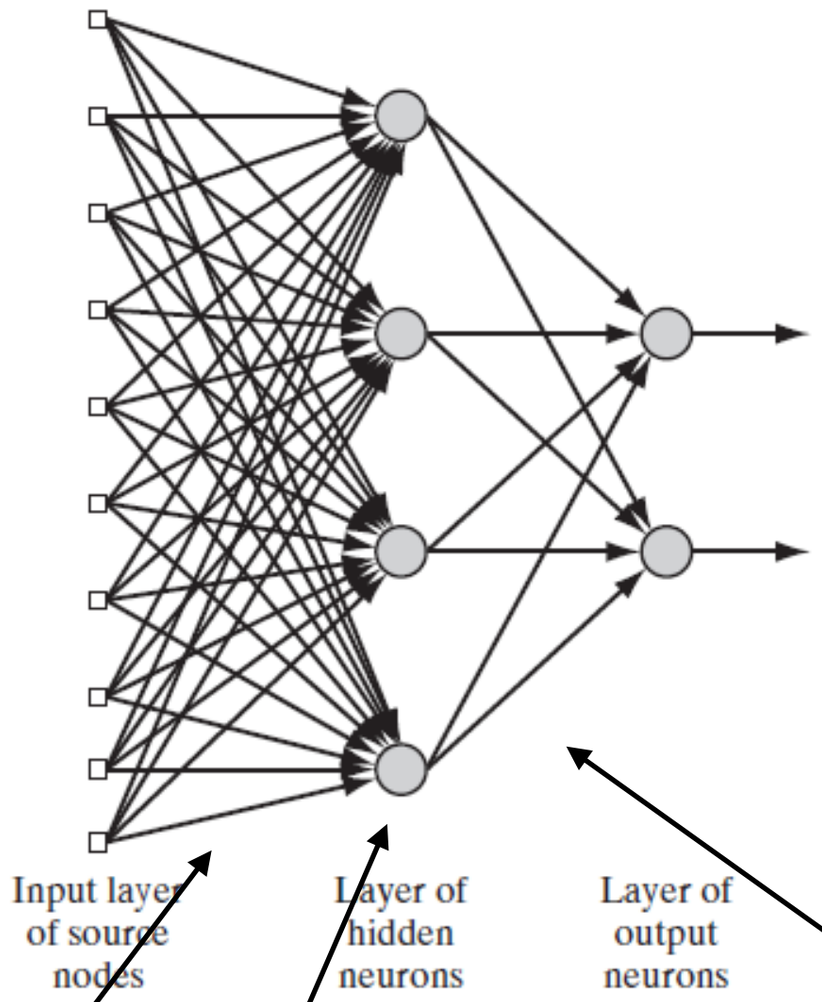


$\{x_0, x_1, \cdots, x_{n-1}\}$ $\quad \{\Theta_{i,j}\} \quad$ $\{a_0 = g(\sum_{i=0}^{n-1} \theta_{0,i} x_i), a_1 = g(\sum_{i=0}^{n-1} \theta_{1,i} x_i), \cdots, a_{n-1} = g(\sum_{i=0}^{n-1} \theta_{n-1,i} x_i)\}$

activation function g Sigmoid

Feed-forward neural networks

Multi-layer



$\{x_0, x_1, \cdots, x_{n-1}\}$ $\{\Theta_{i,j}^{(l)}\}$ $\{a_0^{(l+1)} = g(\sum_{i=0}^{n} \theta_{0,i}^{(l)} x_i), a_1^{(l+1)} = g(\sum_{i=0}^{n} \theta_{1,i}^{(l)}), \cdots\}$ $\{\Theta_{i,j}^{(l+1)}\}$ $\cdots$