機械学習特論

~理論とアルゴリズム~

第9回

(Neural Networks)

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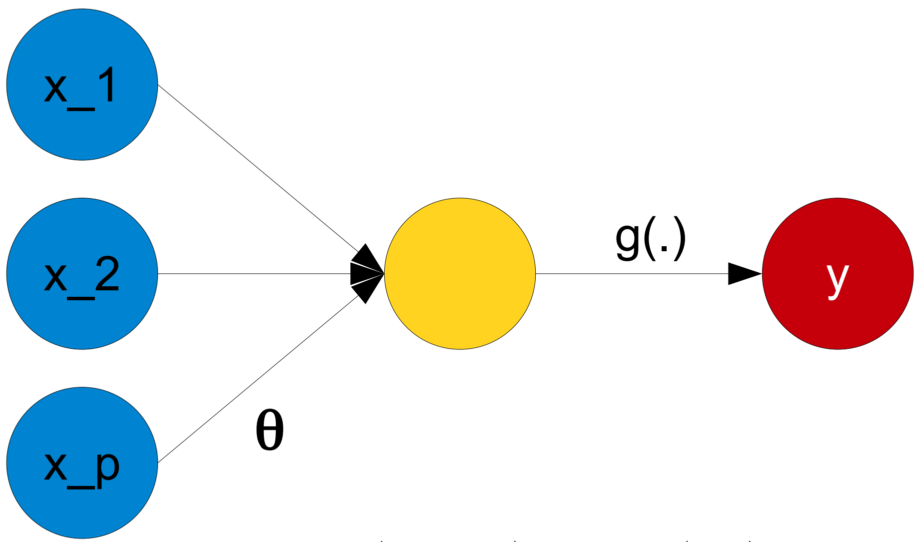
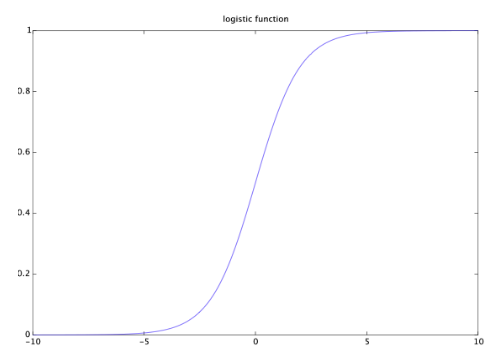
Neural Network; what is it ?

- Originally developed in 1950's by mimicking the network of neurons in human brain.

Single layer network
(a.k.a. linear / logistic regression)



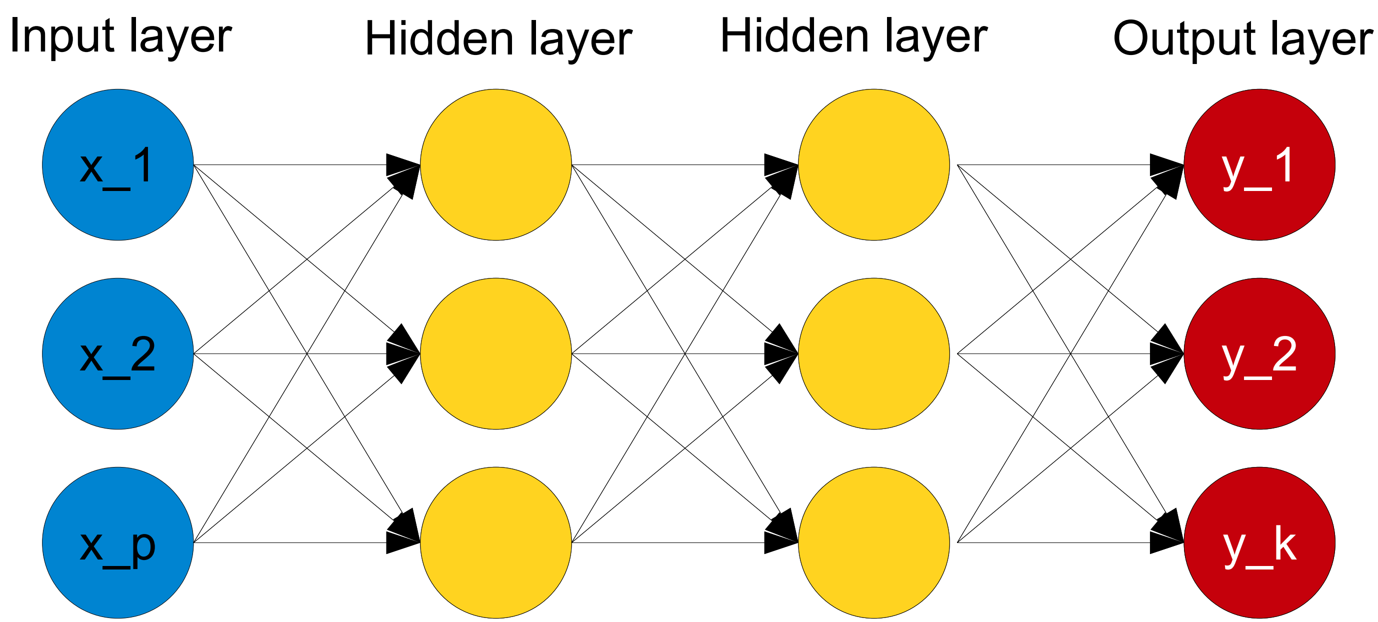
$$y = g(\boldsymbol{x}'\boldsymbol{\theta}) = h_{\Theta}(\boldsymbol{x})$$



g(.) is a logistic sigmoid function

$$g(\boldsymbol{x}) = \frac{\exp(-\boldsymbol{x})}{1 + \exp(-\boldsymbol{x})}$$

Multi-layer network for multi-class classification

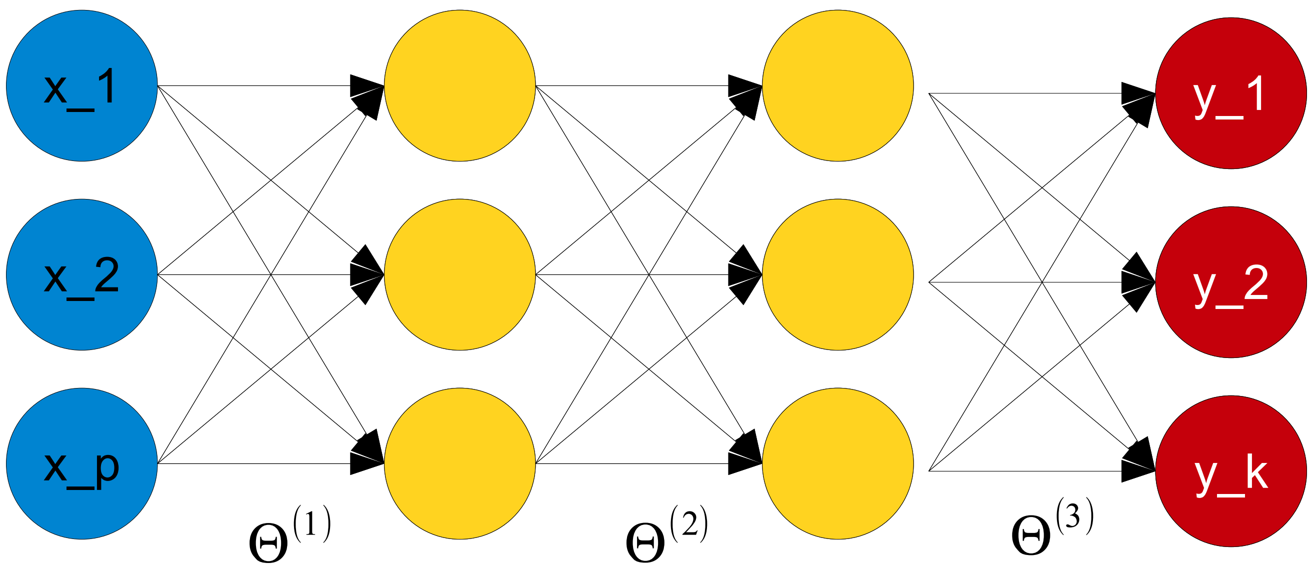


$$\boldsymbol{x}_1 = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_p \end{pmatrix}$$

$$\boldsymbol{y}_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \boldsymbol{y}_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \boldsymbol{y}_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

Multi-layer network model parameters

- a^(l): input to the l-th layer
- z^(l): output of the l-th layer



$\boldsymbol{a}^{(1)} = \boldsymbol{x}$

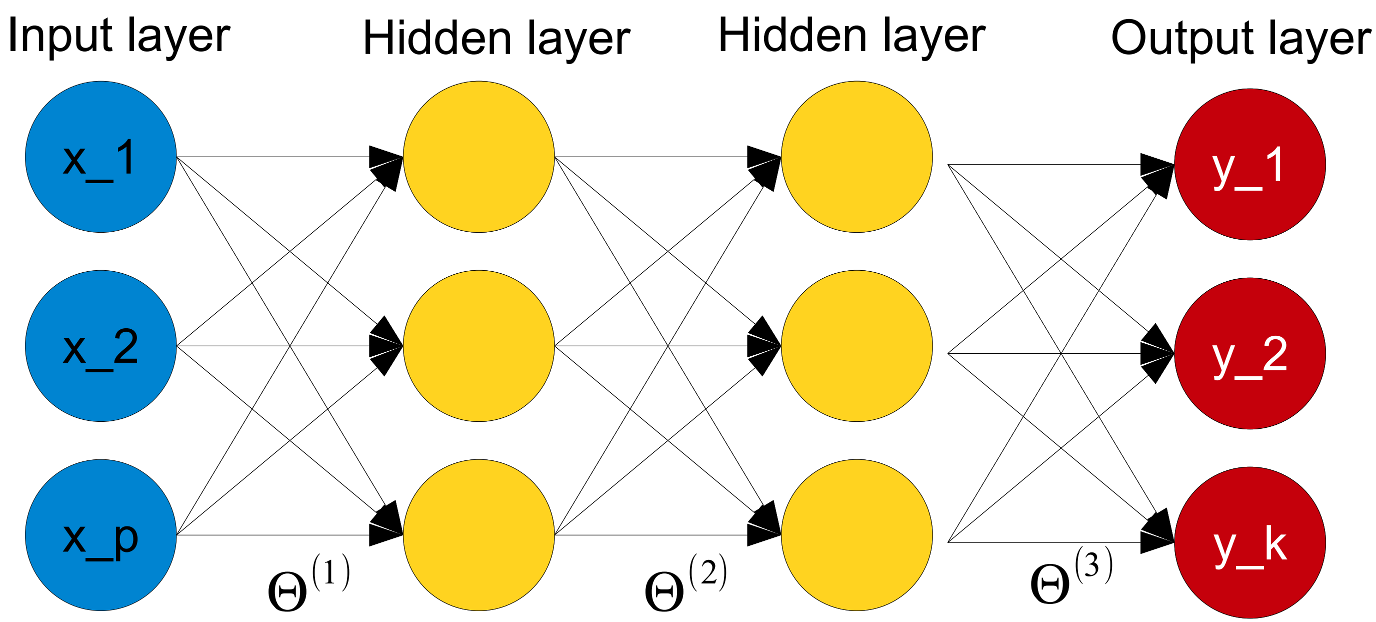
$\boldsymbol{z}^{(2)} = \Theta^{(1)} \boldsymbol{a}^{(1)}$
$\boldsymbol{a}^{(2)} = g\left(\boldsymbol{z}^{(2)}\right)$

$\boldsymbol{z}^{(3)} = \Theta^{(2)} \boldsymbol{a}^{(2)}$
$\boldsymbol{a}^{(3)} = g\left(\boldsymbol{z}^{(3)}\right)$

$\boldsymbol{z}^{(4)} = \Theta^{(3)} \boldsymbol{a}^{(3)}$
$\boldsymbol{a}^{(4)} = g\left(\boldsymbol{z}^{(4)}\right)$

$h_{\Theta}\left(\boldsymbol{x}\right) = \boldsymbol{a}^{(4)}$

Difficulty in training multi-layer network



- Number of parameters in this example:

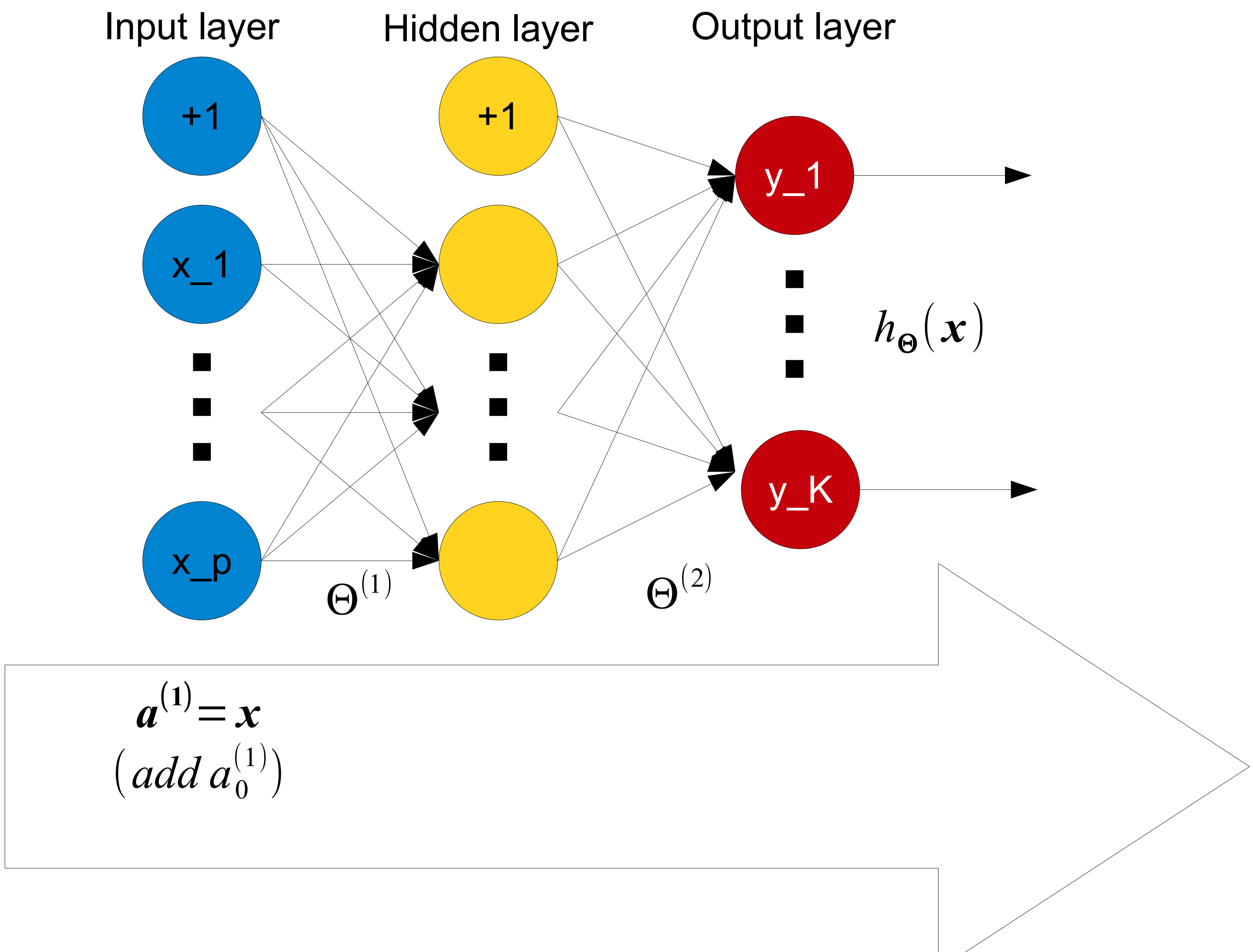
$$|\Theta^{(1)}| + |\Theta^{(2)}| + |\Theta^{(3)}| = 3\times3 + 3\times3 + 3\times3 = 27$$

- More formerly: $p\times h_1 + h_1\times h_2 + h_2\times k$
  - Easily above millions !

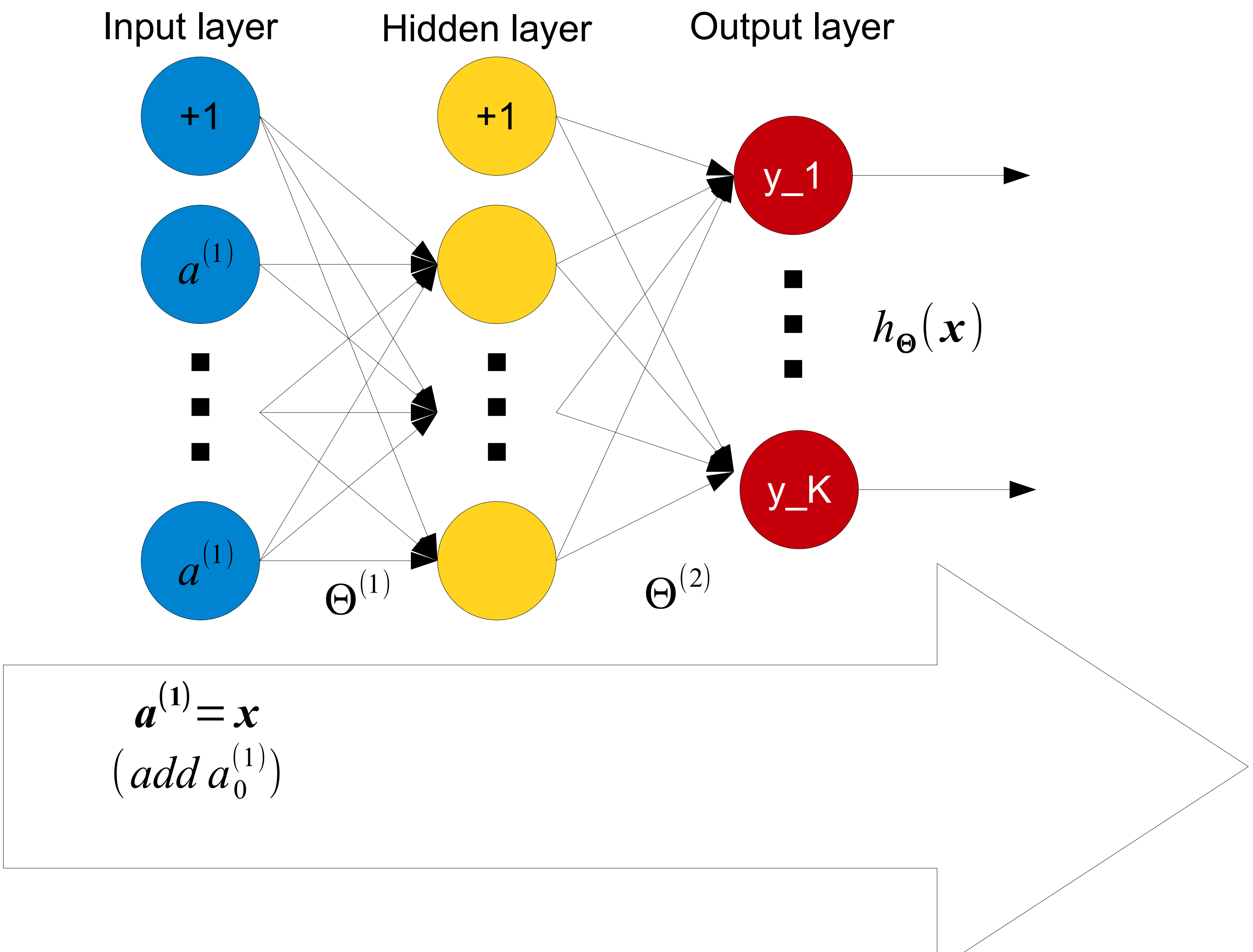
Efficiently updating parameters via forward/backward propagation

- For handling large number of parameters, an efficient updating technique is necessary.
- Forward propagation algorithm computes variables **a** and **z** from left (input) to right (output).
- Backward propagation algorithm computes δ from right (output) to left (input).

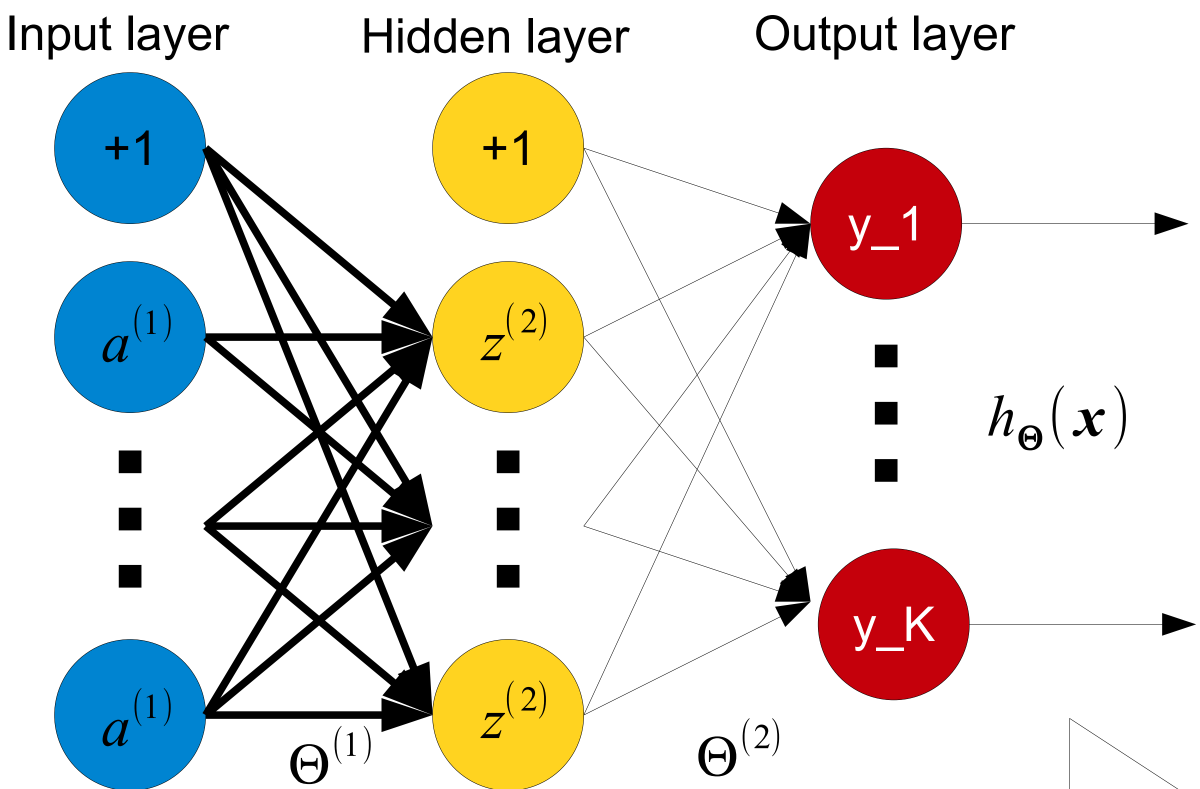
Feedforward Propagation



Feedforward Propagation



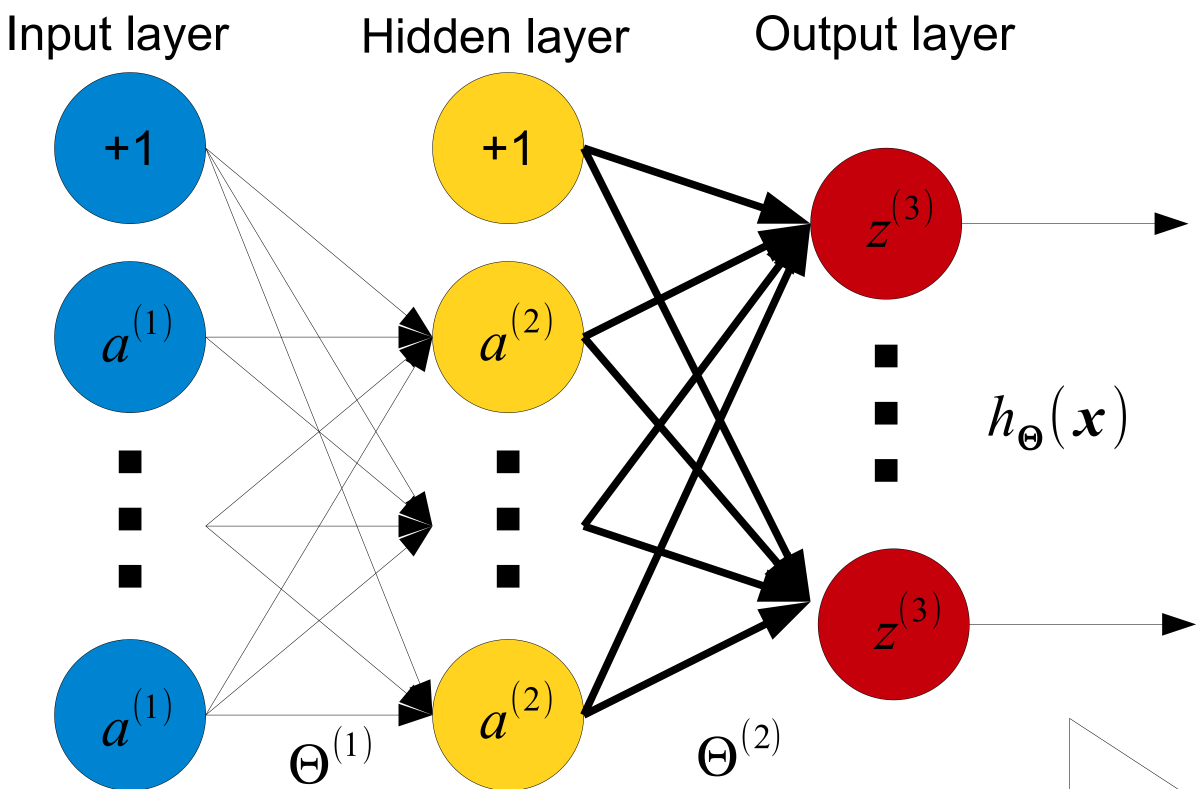
Feedforward Propagation



$$\boldsymbol{a}^{(1)} = \boldsymbol{x}$$
$$\left(add\; a_0^{(1)} \right)$$

$$\boldsymbol{z}^{(2)} = \Theta^{(1)} \boldsymbol{a}^{(1)}$$

Feedforward Propagation

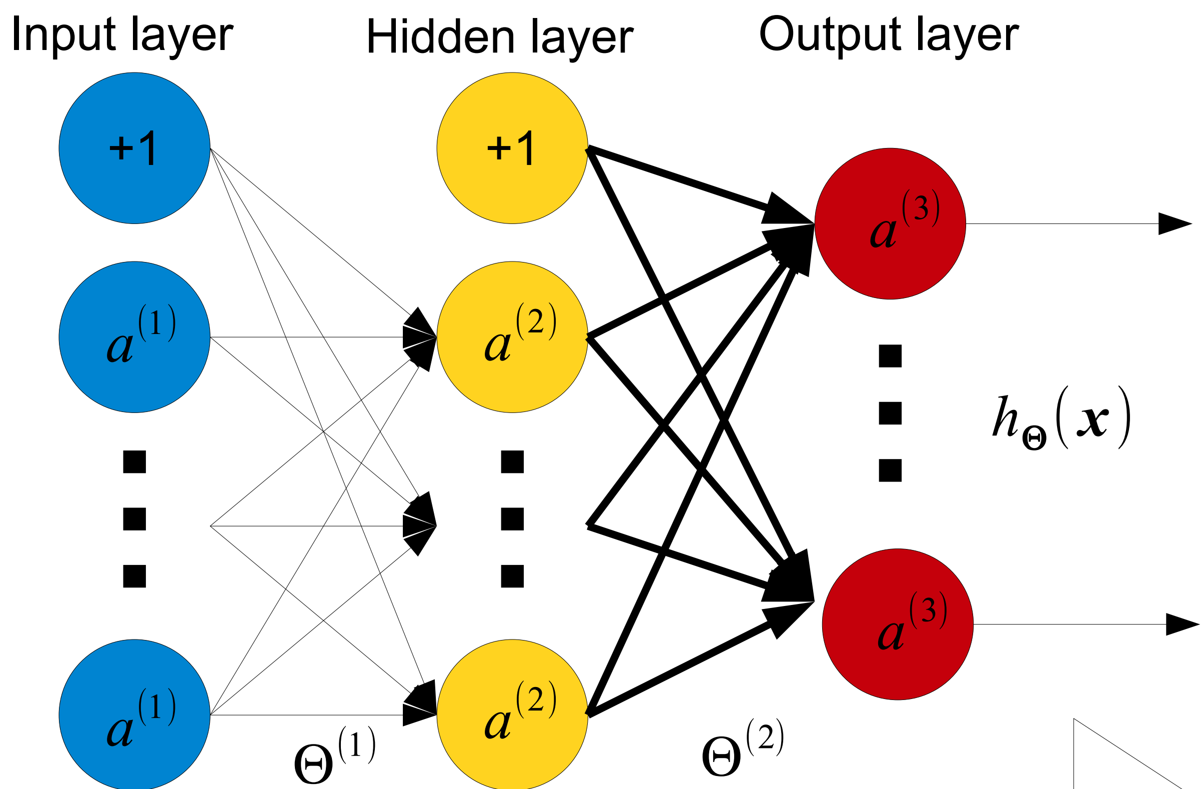


$\boldsymbol{a}^{(1)} = \boldsymbol{x}$
$\left(add\ a_0^{(1)}\right)$

$\boldsymbol{z}^{(2)} = \Theta^{(1)} \boldsymbol{a}^{(1)}$
$\boldsymbol{a}^{(2)} = g\left(\boldsymbol{z}^{(2)}\right)$
$\left(add\ a_0^{(2)}\right)$

$\boldsymbol{z}^{(3)} = \Theta^{(2)} \boldsymbol{a}^{(2)}$

Feedforward Propagation



$$\boldsymbol{a}^{(1)} = \boldsymbol{x}$$
$$\left(add\ a_0^{(1)}\right)$$

$$\boldsymbol{z}^{(2)} = \Theta^{(1)} \boldsymbol{a}^{(1)}$$
$$\boldsymbol{a}^{(2)} = g\left(\boldsymbol{z}^{(2)}\right)$$
$$\left(add\ a_0^{(2)}\right)$$

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

Algorithm: Feedforward Propagation

- Input $\{(x_1),\ldots,(x_m)\},\Theta_{ij}^{(l)}$
- Output $\{h_\Theta(x_1),\ldots,h_\Theta(x_m)\}$
- Procedure
  - Set $\boldsymbol{a}^{(\mathbf{1})}=\boldsymbol{x}$
  - For i=2:L

$$\boldsymbol{z}^{(\boldsymbol{l})}=\Theta^{(l-1)}\boldsymbol{a}^{(\boldsymbol{l}-\mathbf{1})}$$
$$\boldsymbol{a}^{(\boldsymbol{l})}=g\left(\boldsymbol{z}^{(\boldsymbol{l})}\right)$$

  - $h_\Theta(\boldsymbol{x})=\boldsymbol{a}^{(\boldsymbol{L})}$

Ex 1: Feedforward propagation (Prediction)

- Load data and variables by
  - load('MNIST.mat')
  - load('Weights.mat');
- Complete the following function
  - Function pred = feedforward(Theta1, Theta2, X)
    - where pred is 5000 x 10 matrix of prediction results
- If implemented correctly,
  - [M I] = max(pred, [], 2)
    - returns 0...,0, 1...,1, 2...,2, 3...,3 …

Dataset

- MNIST dataset
  - X: 5000 x 256 (digits 0-9 from 500 people. Each image consists of 16 x 16 pixels)
    - Visualization: `> imagesc(reshape(X(1,:),[16 16]))`
  - Xy: 5000 x 1 true digits
  - Theta1: 25 x 257 learnt parameters for the first layer.
  - Theta2: 10 x 26 learnt parameters for the second layer.
  - Tips: you need to augment matrices with a column of ones from left; X = [ones(5000,1) X]
  - Tips; you need “sigmoid” function, or h.m from the previous exercise.

Objective function

- L2-Logistic regression

$$y_i = \{0, 1\},\ h(.) \in R$$

$$J(\boldsymbol{\theta}) = -\sum_{i=1}^{n} \{y_i \log g(\boldsymbol{\theta}' \boldsymbol{x_i}) + (1 - y_i) \log(1 - g(\boldsymbol{\theta}' \boldsymbol{x_i}))\} + \frac{\lambda}{2} \sum_{j=1}^{p} \theta_j^2$$

- Multi-output neural nets for classification

$$y_i^{(k)} = \{0\ ,1\}^k,\ h_k \in R^k$$

$$J(\boldsymbol{\Theta}) = -\sum_{i=1}^{n} \sum_{k=1}^{K} \{y_i^{(k)} \log h_{\boldsymbol{\Theta}}(\boldsymbol{x_i})^k + (1 - y_i^{(k)}) \log(1 - h_{\boldsymbol{\Theta}}(\boldsymbol{x_i})^k)\}$$
$$+ \frac{\lambda}{2} \sum_{l=1}^{L-1} \sum_{i=1}^{n} \sum_{j=1}^{p} (\Theta_{ij}^{(l)})^2$$

Gradient of the objective

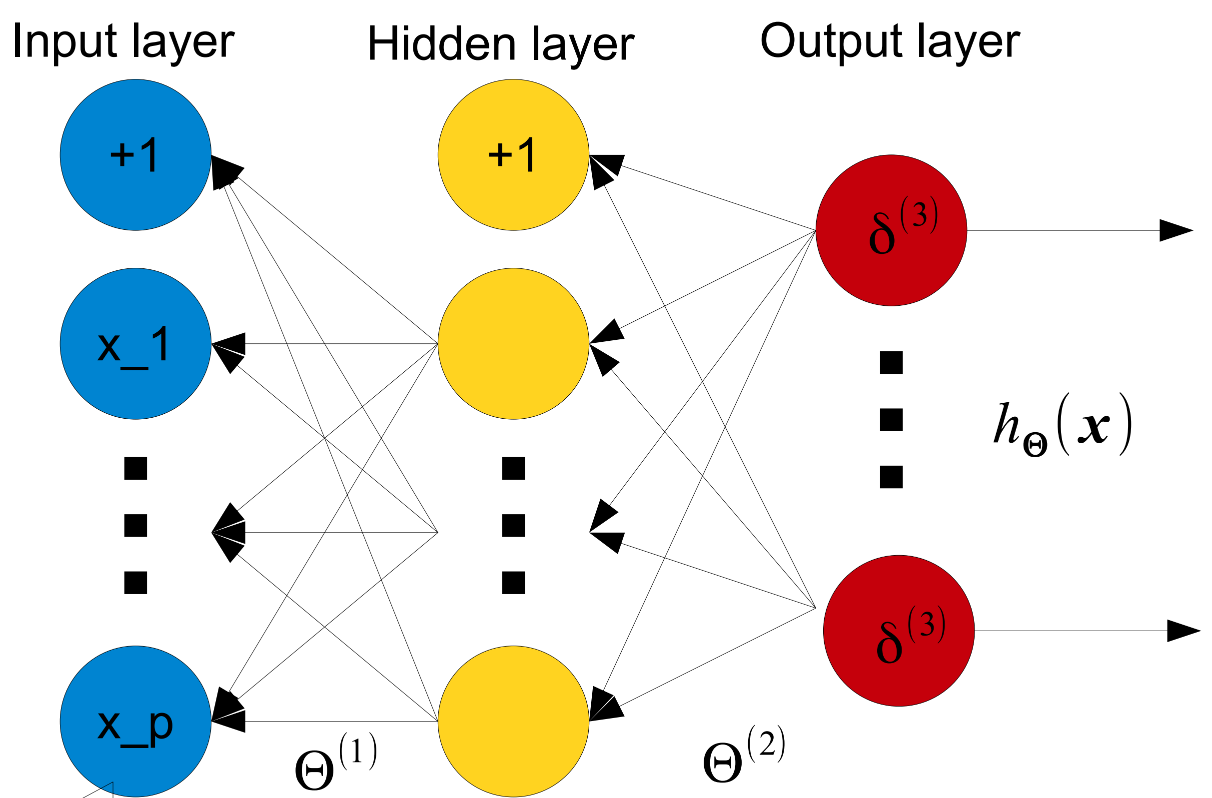
- Gradient of the objective w.r.t. parameters $\frac{\partial J(\Theta)}{\partial \Theta_{ji}^{(l)}}$
  - using a chain rule $\frac{\partial J(\Theta)}{\partial \Theta_{ji}^{(l)}} = \frac{\partial J(\Theta)}{\partial z_i^{(l)}} \frac{\partial z_i^{(l)}}{\partial \Theta_{ji}^{(l)}}$
  - Let $\delta_i^{(l+1)} = \frac{\partial J(\Theta)}{\partial z_i^{(l)}}$ be an "error" (at node j in the l-th layer) propagated from the (l+1)-th layer
  - Since $z_i^{(l)} = \sum_i \Theta_{ji}^{(l)} a_j^{(l)}$, $\frac{\partial z_i^{(l)}}{\partial \Theta_{ji}^{(l)}} = \frac{\partial}{\partial \Theta_{ji}^{(l)}} \left(\sum_i \Theta_{ji}^{(l)} a_j^{(l)} \right) = a_j^{(l)}$
  - Plugging in the above relations obtains

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

Gradient Computation

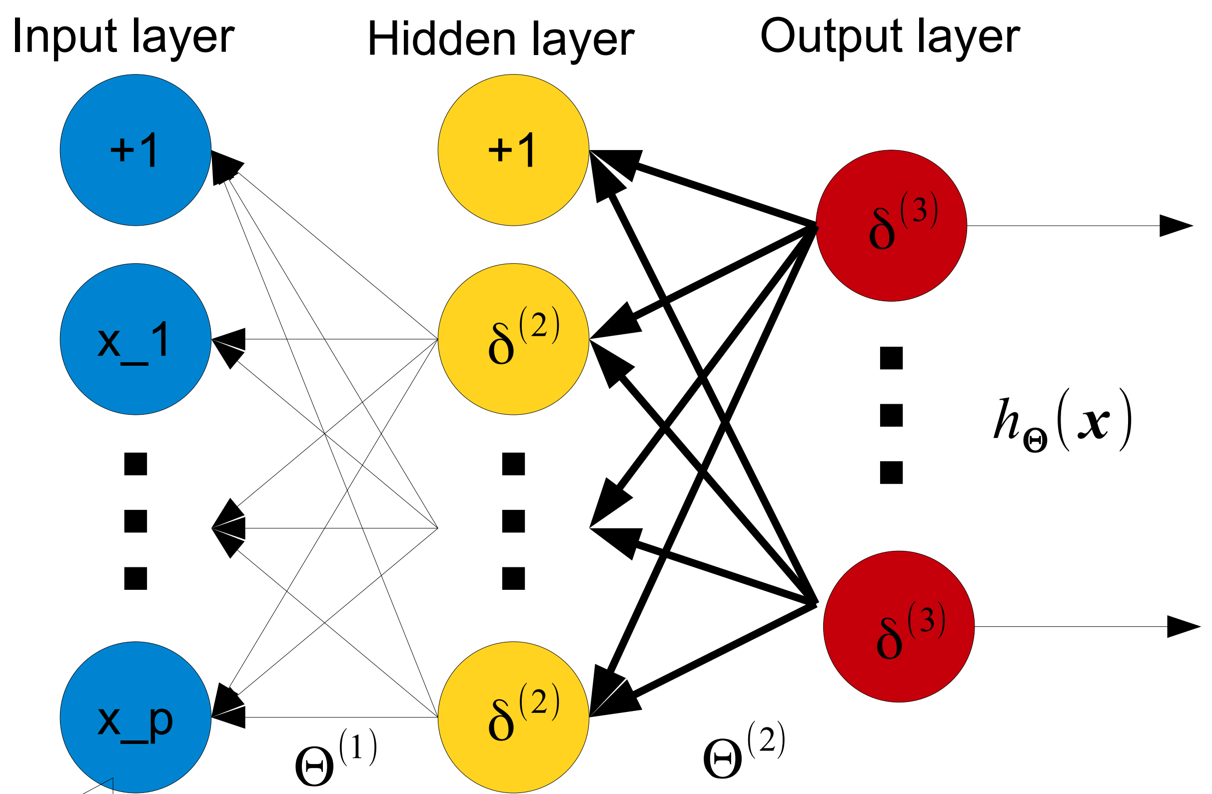
- Input: $\{(x_{1,}y_1),\ldots,(x_m,y_m)\},\Theta_{ij}^{(l)}$
- Output: $\Delta_{ij}^{(l)}=\frac{\partial J(\Theta)}{\partial\Theta_{ij}^{(l)}}=a_j^{(l)}\delta_i^{(l+1)}$
- Procedure
  - For i=1:m (each example) Feedforward propagation
    - Set $a^{(1)}=x^{(i)}$
    - For l=1:L Feedforward propagation to compute $a^{(l)}$
    - Compute $\delta^{(L)}=a^{(L)}-y$
    - For l=L:2 Compute $\delta^{(l)}=(\Theta^{(l)})^T\delta^{(l+1)}.*g'(z^{(l)})$
    - Update $\Delta_{ij}^{(l)}=\Delta_{ij}^{(l)}+a_j^{(l)}\delta_i^{(l+1)}$ Backward propagation

Backward Propagation (L=3)



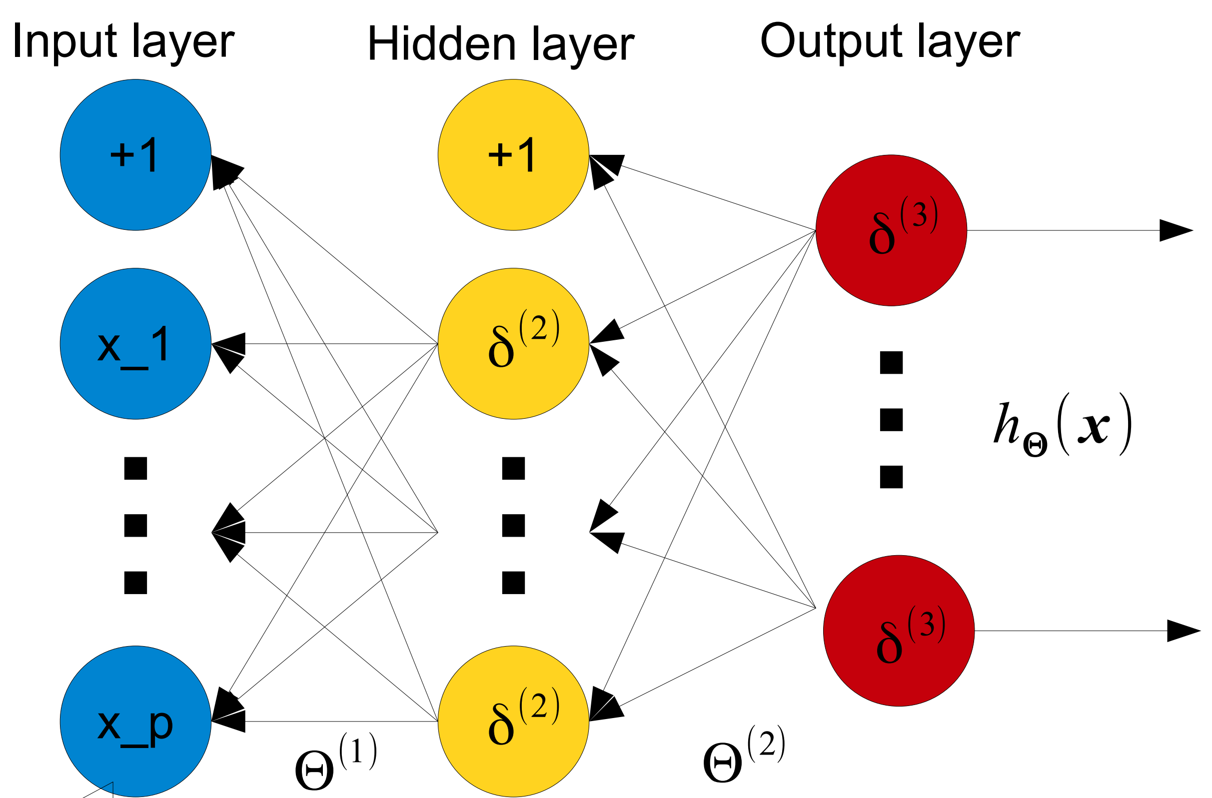
Difference between current prediction and label $\delta^{(3)} = a^{(3)} - y$

Backward Propagation (L=3)



$$\delta^{(2)} = (\Theta^{(2)})^T \delta^{(3)} .* g'(z^{(2)}) \qquad \delta^{(3)} = a^{(3)} - y$$

Backward Propagation (L=3)



Until the end (beginning).. $\delta^{(2)} = (\Theta^{(2)})^T \delta^{(3)} .* g'(z^{(2)})$ $\delta^{(3)} = a^{(3)} - y$

Understanding the update rule

$$\delta^{(l)} = (\Theta^{(l)})^T \delta^{(l+1)} .* g'(z^{(l)})$$

$$\delta_i^{(l+1)} = \frac{\partial J(\Theta)}{\partial z_i^{(l)}}$$

- We focus on one delta (j), and apply chain rule.

$$\delta_j^{(l)} = \frac{\partial J(\Theta)}{\partial z_j^{(l)}} = \sum_k \frac{\partial J(\Theta)}{\partial z_k^{(l)}} \frac{\partial z_k^{(l)}}{\partial z_j^{(l)}} = \sum_k \delta_k^{(l+1)} \frac{\partial z_k^{(l)}}{\partial z_j^{(l)}}$$

- Since $z_k^{(l)} = \sum_j \Theta_{kj}^{(l)} a_j^{(l)}$ and $a_j^{(l)} = g(z_j^{(l)})$,

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

- Plugging in the above relationships obtains

$$\delta_j^{(l)} = \sum_k \delta_k^{(l+1)} \frac{\partial z_k^{(l)}}{\partial z_j^{(l)}} = g'(z_j^{(l)}) \sum_k \delta_k^{(l+1)} \Theta_{kj}^{(l)} = (\Theta^{(l)})^T \delta^{(l+1)} .* g'(z_j^{(l)})$$

Gradient Computation

- Input: $\{(x_{1,}y_1),\ldots,(x_m,y_m)\},\Theta_{ij}^{(l)}$
- Output: $\Delta_{ij}^{(l)}=\dfrac{\partial J(\Theta)}{\partial\Theta_{ij}^{(l)}}=a_j^{(l)}\delta_i^{(l+1)}$
- Procedure
  - $\boxed{\text{For i=1:m}}$ (each example) Feedforward propagation
    - Set $a^{(1)}=x^{(i)}$
    - For l=1:L Feedforward propagation to compute $a^{(l)}$
    - Compute $\delta^{(L)}=a^{(L)}-y$
    - For l=L:2 Compute $\delta^{(l)}=(\Theta^{(l)})^T\delta^{(l+1)}.*g'(z^{(l)})$
    - Update $\Delta_{ij}^{(l)}=\Delta_{ij}^{(l)}+a_j^{(l)}\delta_i^{(l+1)}$

Backward propagation

Optimization by gradient descent

$$\Theta_{ij}^{(l)} = \Theta_{ij}^{(l)} + \epsilon \Delta_{ij}^{(l)}$$

- Once gradient is computed, then variants of gradient descent methods are available
  - SGD, Momentum, AdaGrad, Adam

- Newton’s method is too expensive.

- Only local convergence is guaranteed.

Ex 2: neural net training

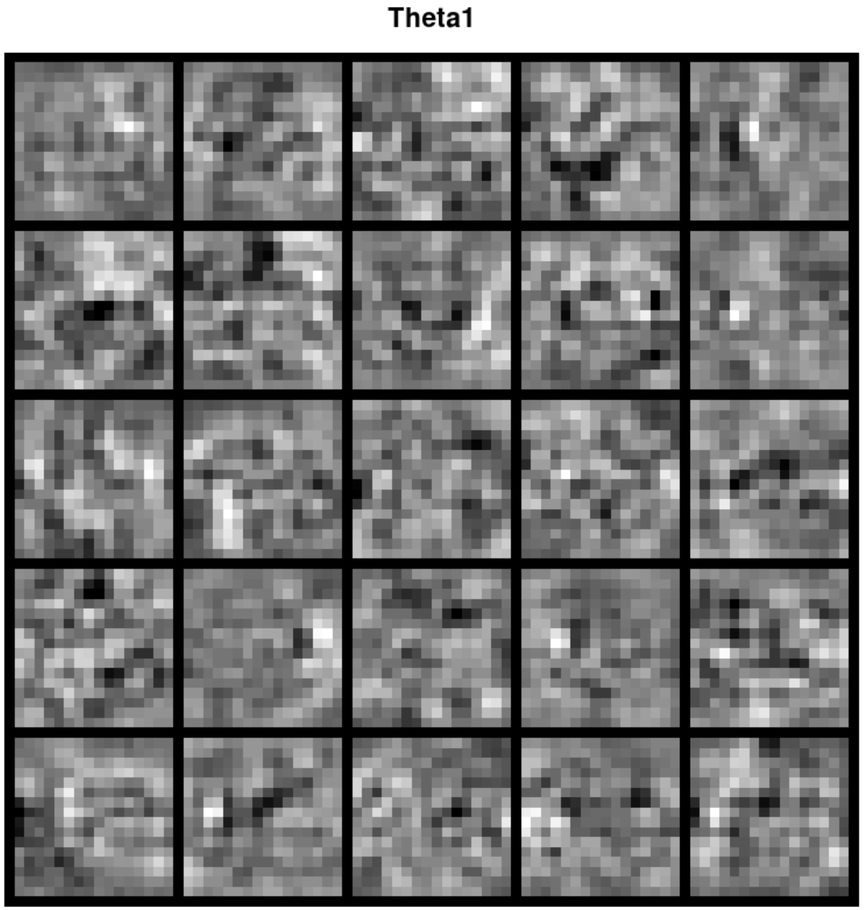
- Try “nn_demo.m”

```
> nn_demo
```

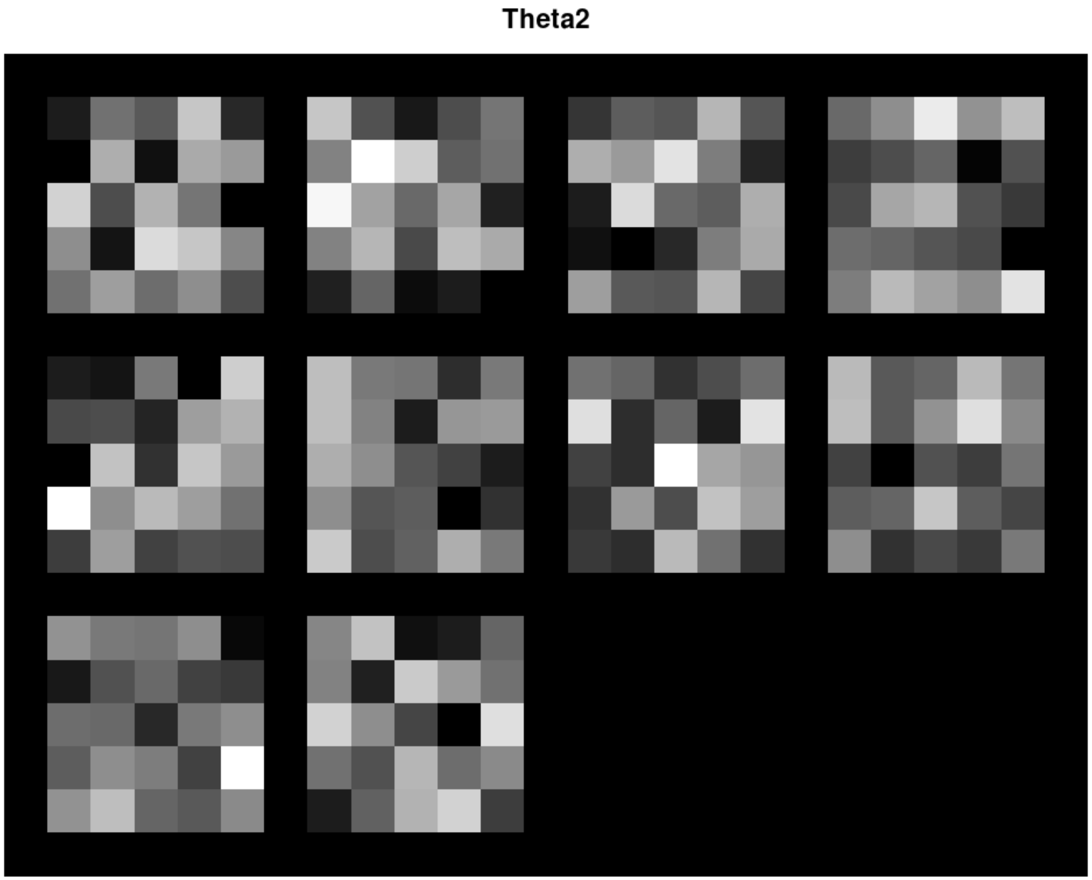
- “nnCostFunction.m” performs gradient computation. Read and compare the code with lecture slides.

- Try different # of iterations, lambda by editing nn_demo.m
  - Can you achieve 100% accuracy ?

Theta1: 256 x 25



Theta2: 25 x 10



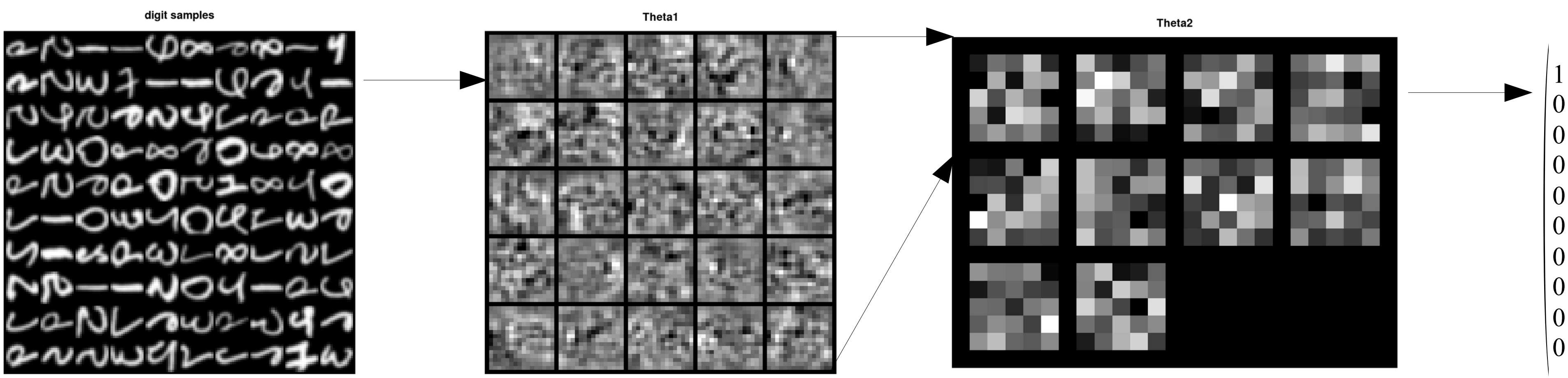
Overall structure

Input layer
n x 16 x 16

Hidden layer 1
16 x 16 x 5 x 5

Hidden layer 2
5 x 5 x 10

Output layer
n x 10



Objective computation in nnCostfunction.m

```
p_vec = zeros(size(X, 1), 1); % prediction vector
for i=1:m

  h1 = sigmoid([1 X(i,:)] * Theta1');
  h2 = sigmoid([1 h1] * Theta2');
  p_vec = h2';

  y_vec = (1:num_labels == y(i))'; % one hot encoding for y, such as y(2) -> [ 0 1 0 0 0 ]

  J += -( y_vec'*log(p_vec) + (1-y_vec)'*log(1-p_vec) ); % objective function
end

J = J/m + lambda/(2*m)*( norm(Theta1(:,2:end)(:)).^2 + norm(Theta2(:,2:end)(:)).^2 ); % +regularization
```

Forward/Backward computation in nnCostfunction.m

```
for t=1:m

% Feedforward
  a_1 = [1; X(t,:)'];
  z_2 = Theta1 * a_1;
  a_2 = [1; sigmoid(z_2)];
  z_3 = Theta2 * a_2;
  a_3 = sigmoid(z_3);

% Backward propagation
  y_vec = (1:num_labels == y(t))'; % label vector in one-hot encoding

  delta_3 = a_3 - y_vec;
  delta_2 = Theta2(:,2:end)' * delta_3 .* sigmoidGradient(z_2);

% Gradient update
  Theta2_grad += delta_3 * a_2';
  Theta1_grad += delta_2 * a_1';

end
```

Appendix

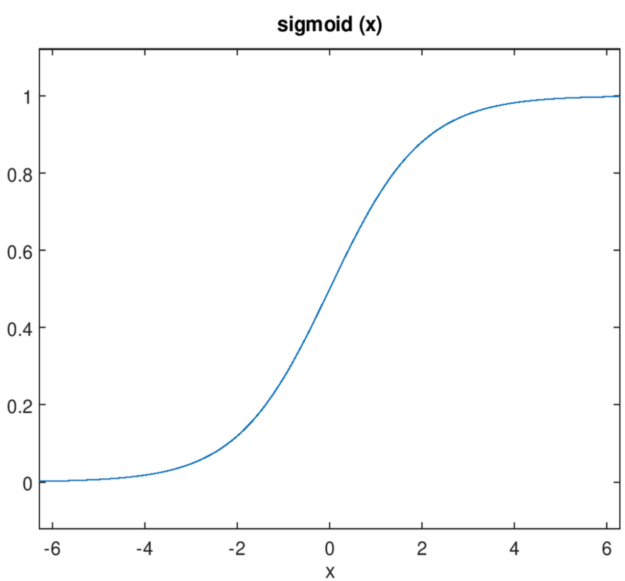
- Index
  - Random initialization
  - Model zoo
  - Activation functions
  - Network design
  - Gradient Checking
  - Software

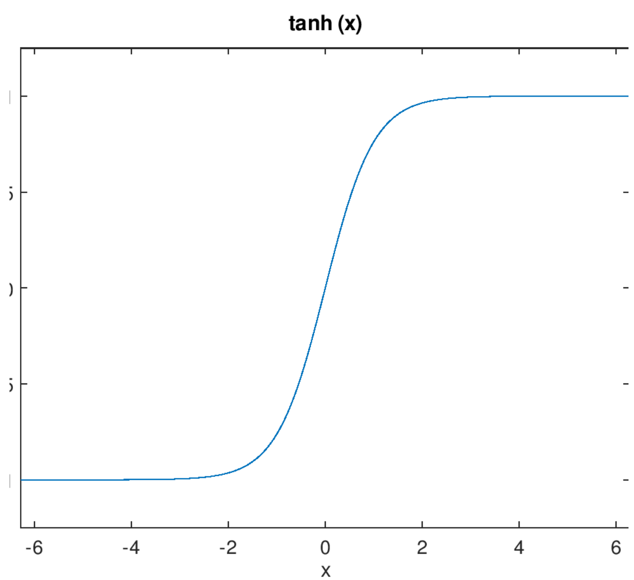
Random Initialization

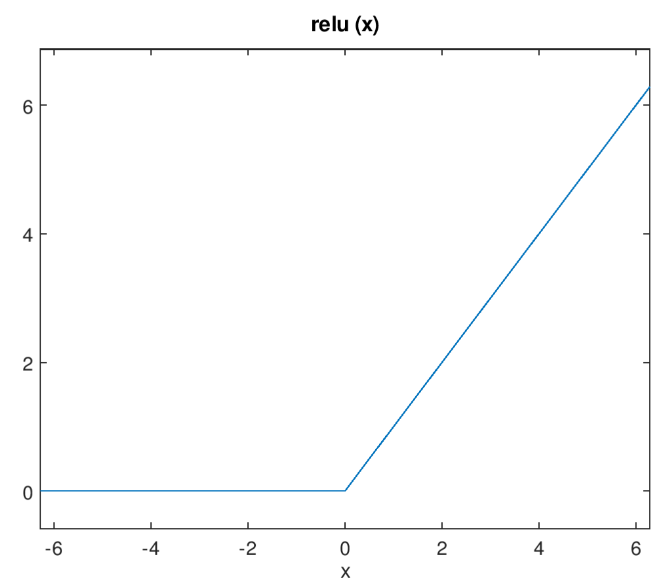
- Suppose that weights are initialized by zeros. Then all a and z become zeros as well, and we cannot compute gradients by backprop.
- Thereby weights must be initialized by random values.
- Implemented in “randInitializeWeights.m”

Activation functions

- Logistic sigmoid $g(\boldsymbol{x}) = \dfrac{\exp(-\boldsymbol{x})}{1 + \exp(-\boldsymbol{x})}$
- Tanh $g(\boldsymbol{x}) = \tanh(x)$
- Relu $g(\boldsymbol{x}) = x > 0\, ?\, x : 0$



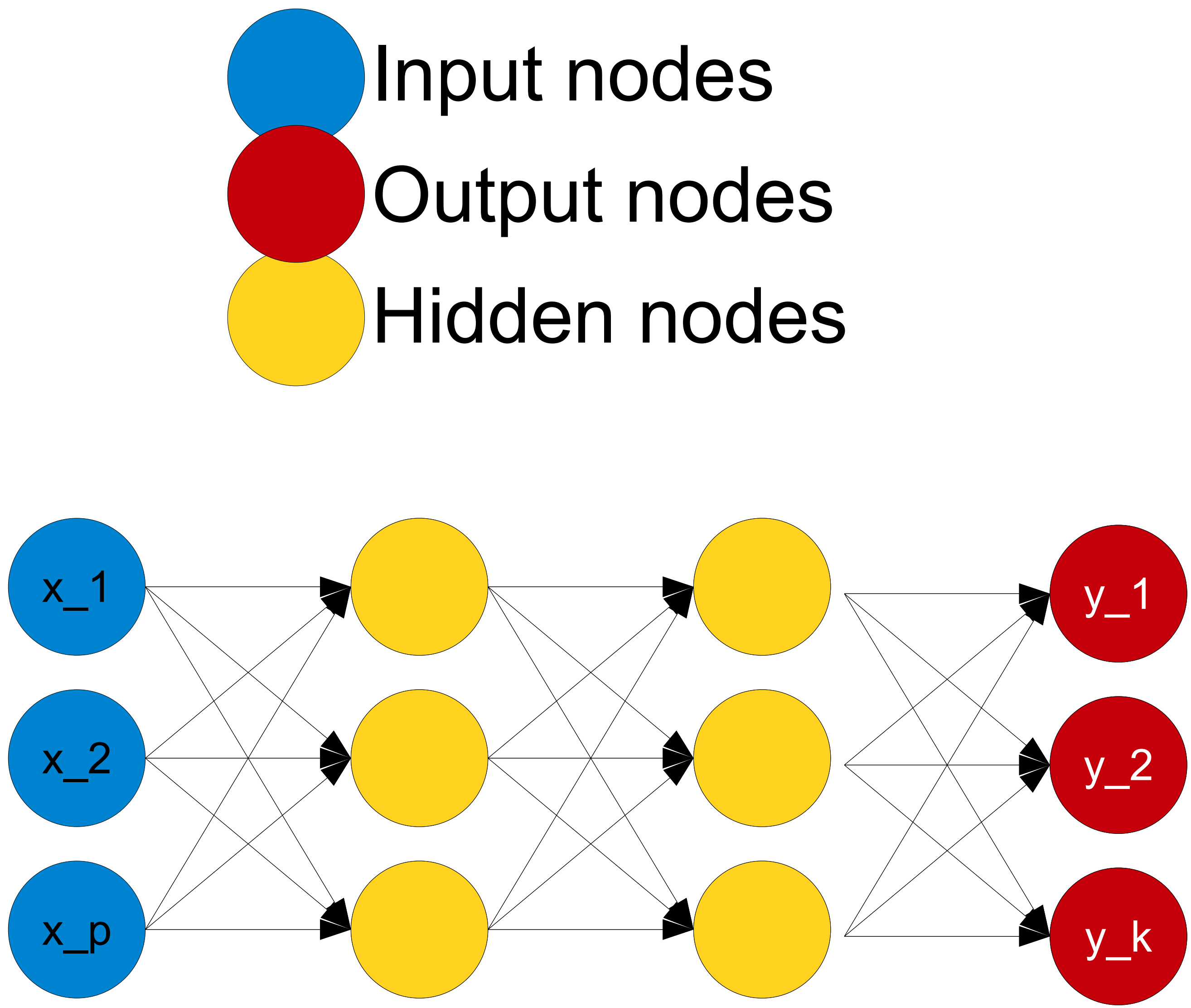




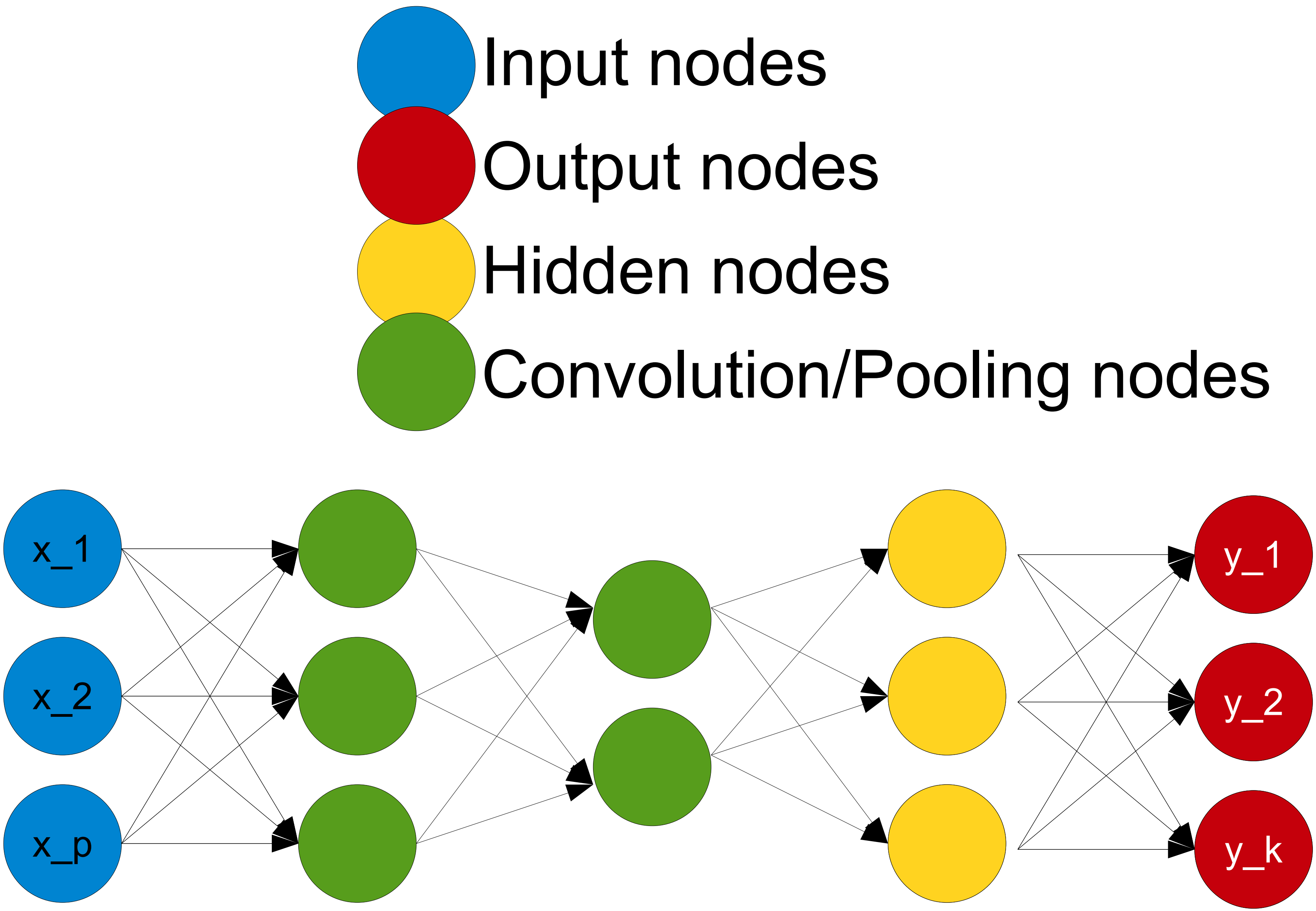
Network design tips

- Number of input units is the same as the number of features.
- Number of output units is the same as the number of classes.
- Number of hidden units is approximately the number of features.
- More number of layers can represent more complex decision boundary.

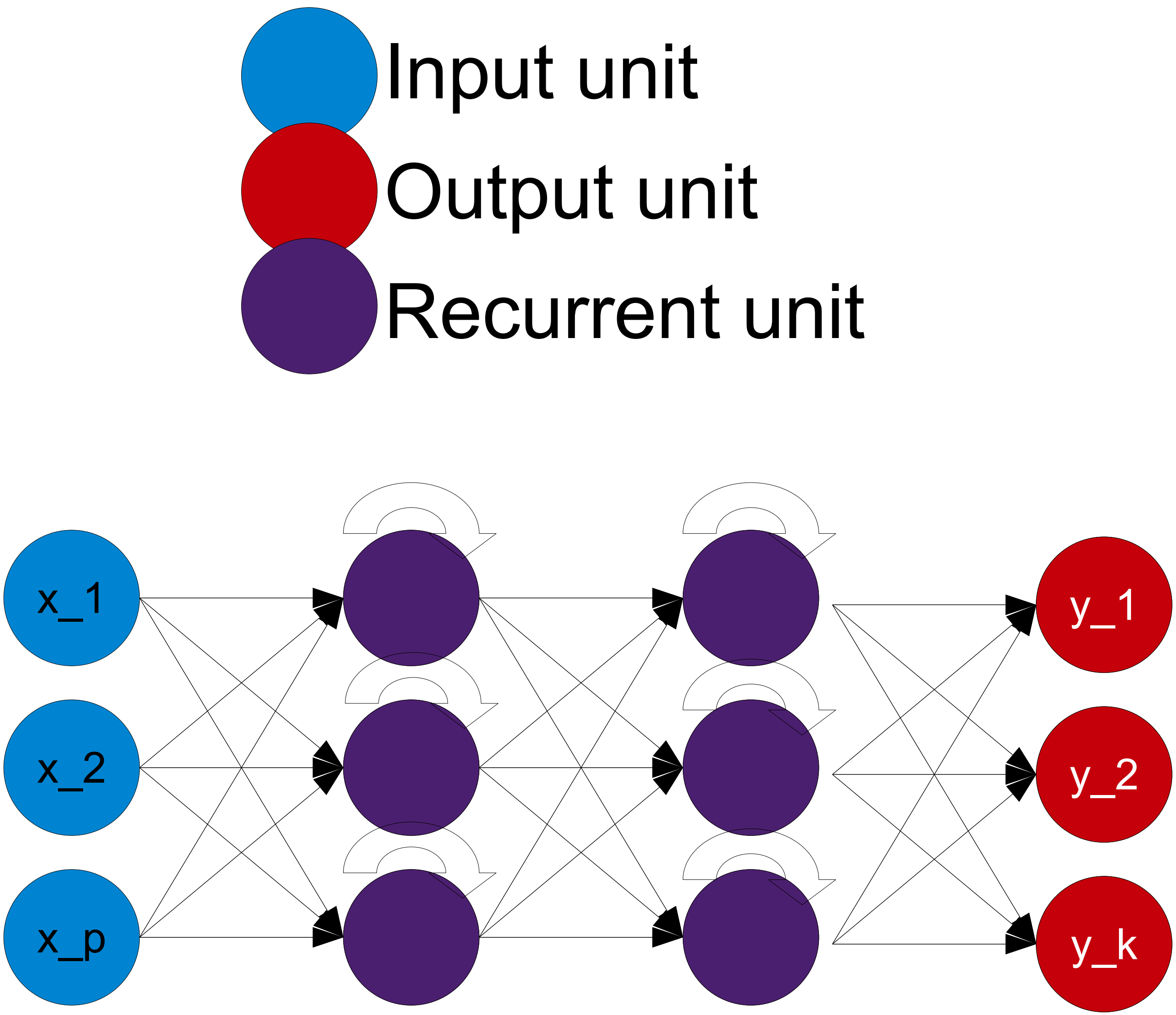
Multi-layer perceptron (MLP)



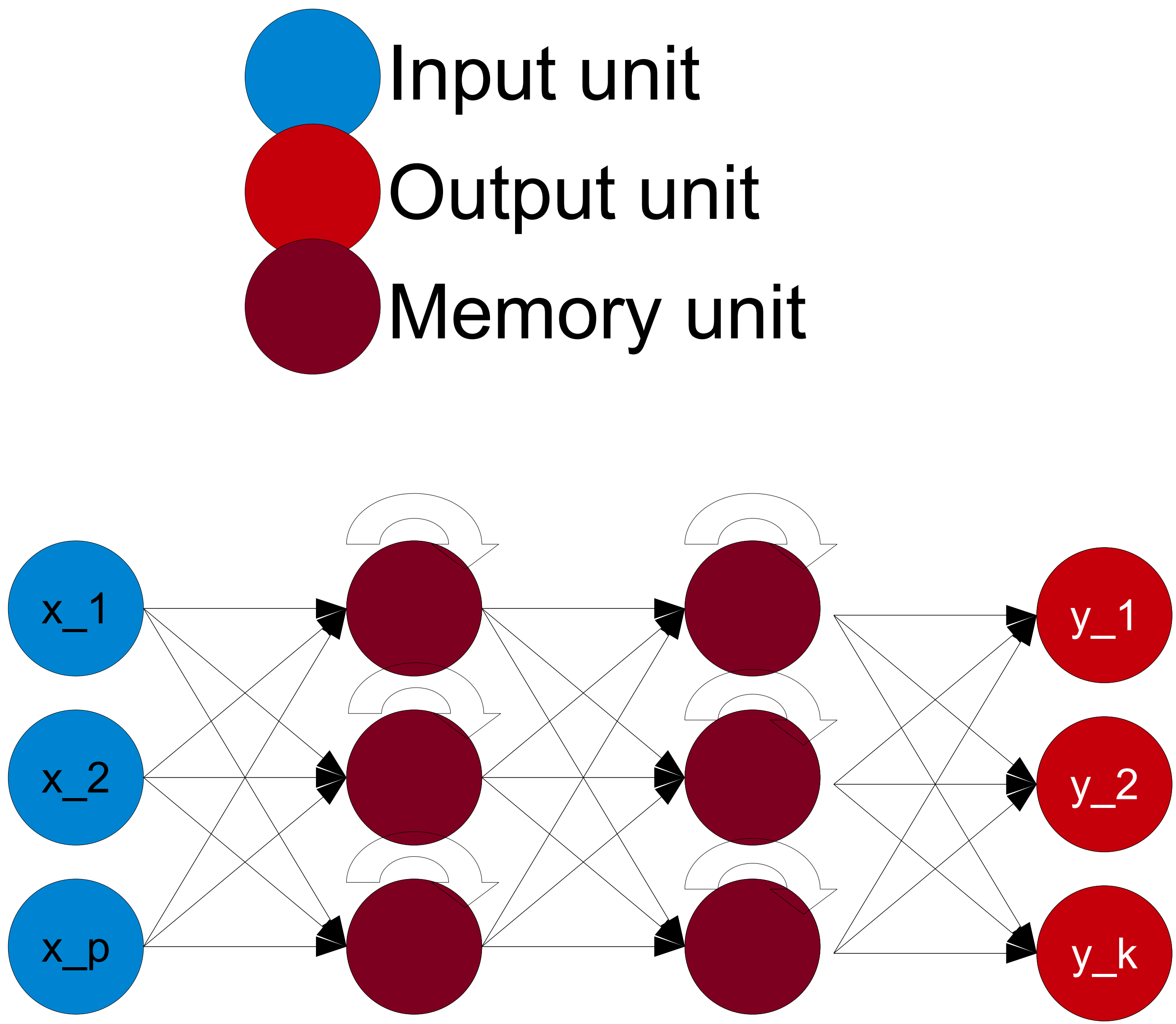
Convolution Neural Network (CNN)



Rucurrent Neural Network (RNN)



Long/Short Term Memory (LSTM)



Types of nodes

- Input nodes
- Output nodes
- Hidden nodes
- Convolution nodes
- Pooling nodes
- Memory nodes
- Recurrent nodes

Software

- For handling large dataset, use of optimization packages with GPU support is highly recommended.
- Popular packages
  - TensorFlow + Keras (C++/Python)
    - Google
  - Pytorch (C++/Python)
    - Facebook