Understanding Deep Neural Networks

Chapter Four

BP: An Illustrating Example

Zhang Yi, *IEEE Fellow* Autumn 2019

Outline

- ■Brief Review of Backpropagation Algorithm
- ■An Illustrating Example
- Experiments
- Assignment

Brief History of BP

CHAPTER 8

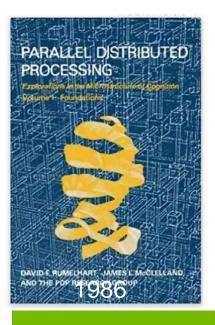
Learning Internal Representations by Error Propagation

D. E. RUMELHART, G. E. HINTON, and R. J. WILLIAMS

THE PROBLEM

We now have a rather good understanding of simple two-layer associative networks in which a set of input patterns arriving at an input layer are mapped directly to a set of output patterns at an output layer. Such networks have no hidden units. They involve only input and output units. In these cases there is no internal representation. The coding provided by the external world must suffice. These networks have proved useful in a wide variety of applications (cf. Chapters 2, 17, and 18). Perhaps the essential character of such networks is that they map similar input patterns to similar output patterns. This is what allows these networks to make reasonable generalizations and perform reasonably on patterns that have never before been presented. The similarity of patterns in a PDP system is determined by their overlap. The overlap in such networks is determined outside the learning system itself—by whatever produces the patterns.

The constraint that similar input patterns lead to similar outputs can lead to an inability of the system to learn certain mappings from input to output. Whenever the representation provided by the outside world is such that the similarity structure of the input and output patterns are very different, a network without internal representations (i.e., a







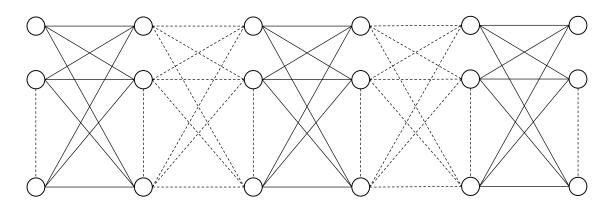


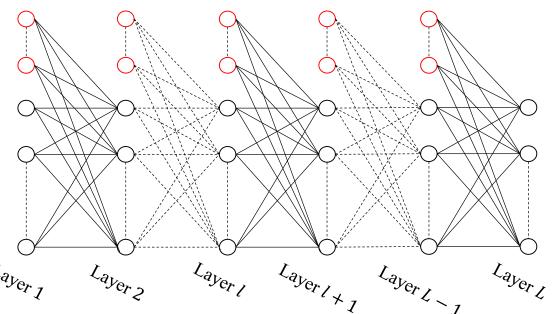
Professor P. Werbos

Computational Model of Neural Networks

Two important characters:

- No any connection in any layer
- No any connection across any layer



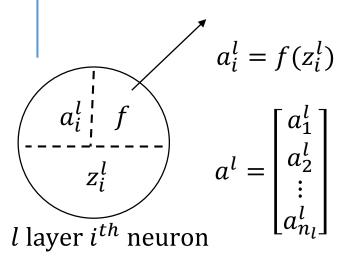


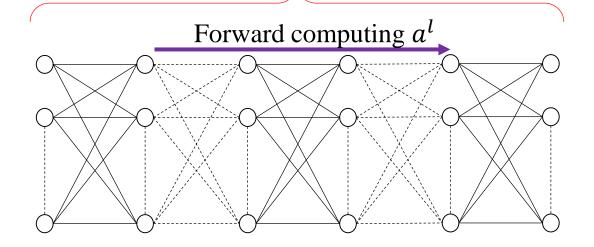
External inputs

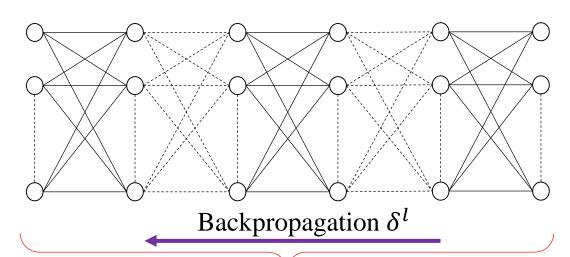


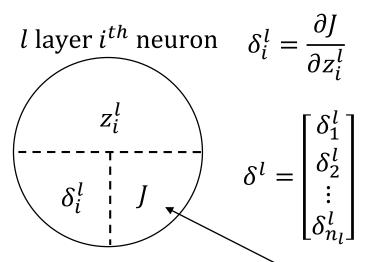
Local function defined on neuron

Local activation function f

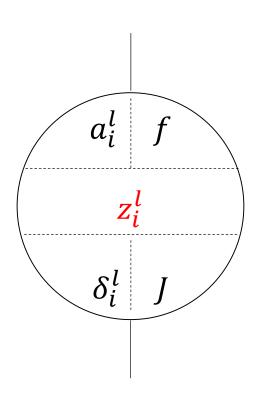




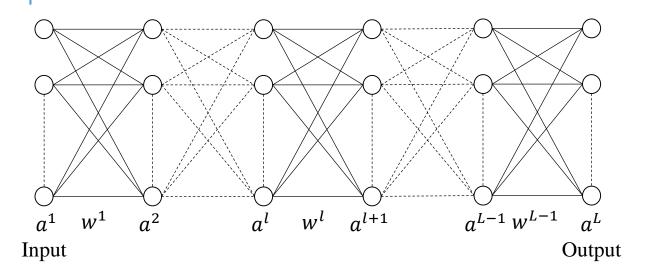




Global function defined on network



Network Performance: Cost Function



A cost function *J* describes the performance of the network. If the J is small, it implies that the network prediction a^L close to the target y^L , the network is called in good performance. Since *J* is a function with variables (w^1, \dots, w^L) , good performance means to find suitable (w^1, \dots, w^L) such that J is small. The process of looking for suitable (w^1, \dots, w^L) is called network learning.

Target

Network prediction

$$y^{L} = \begin{bmatrix} y_{1}^{L} \\ \vdots \\ y_{n_{L}}^{L} \end{bmatrix} \qquad \qquad a^{L} = \begin{bmatrix} a_{1}^{L} \\ \vdots \\ a_{n_{L}}^{L} \end{bmatrix}$$

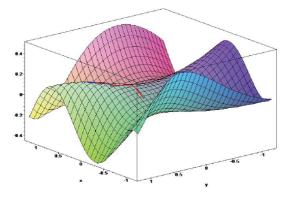
$$a^L = \begin{bmatrix} a_1^L \\ \vdots \\ a_{n_L}^L \end{bmatrix}$$

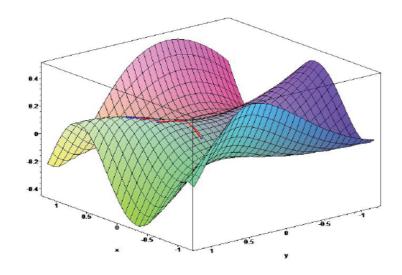
There are many ways to construct cost functions. A frequently used cost is as follows:

$$e_{j} = a_{j}^{L} - y_{j}^{L}$$

$$J = \frac{1}{2} \sum_{j=1}^{n_{L}} e_{j}^{2} = J(w^{1}, \dots, w^{L})$$

Clearly, I is a function of w^1, \dots, w^L .

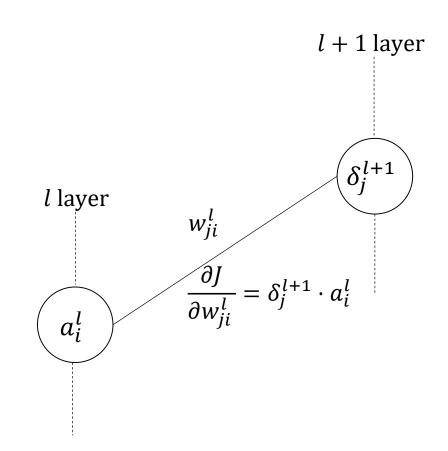




$$J=J(\cdots,w_{ij}^l,\cdots)$$

Steepest Descent Method

$$w_{ji}^l \leftarrow w_{ji}^l - \alpha \cdot \frac{\partial J}{\partial w_{ji}^l}$$



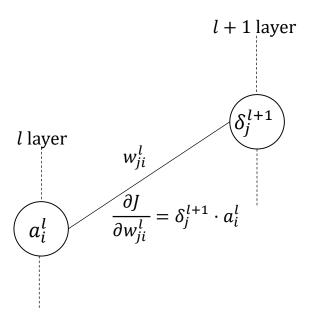
One Page to Understand BP

Cost function: $J(w^1, \dots, w^L)$

Relationship: $\frac{\partial J}{\partial w_{ji}^l} = \delta_j^{l+1} \cdot a_i^l$

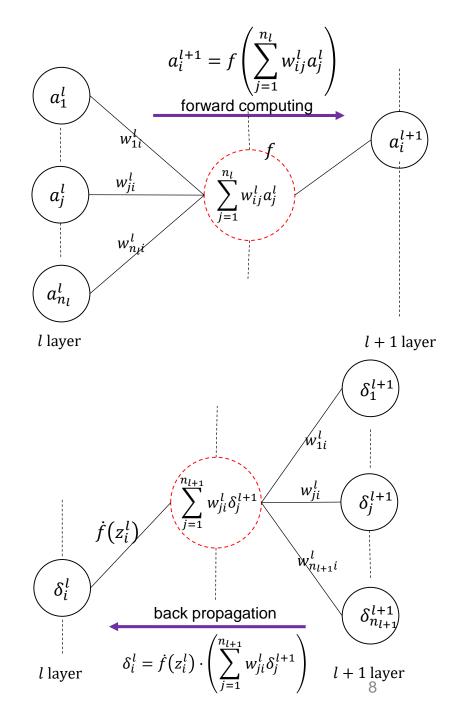
Updating rule: $w_{ji}^l \leftarrow w_{ji}^l - \alpha \cdot \frac{\partial J}{\partial w_{ji}^l}$

forward computing a^l $a^l \quad w^l \quad a^{l+1}$ backpropagation δ^l



$$\delta_i^l = f(z_i^l)$$

$$\delta_i^l = \frac{\partial J}{\partial z_i^l}$$



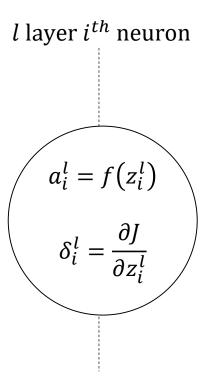
BP Functions

Cost function: $J(w^1, \dots, w^L)$

Updating rule: $w_{ji}^l \leftarrow w_{ji}^l - \alpha \cdot \frac{\partial J}{\partial w_{ii}^l}$

Relationship: $\frac{\partial J}{\partial w_{ii}^l} = \delta_j^{l+1} \cdot a_i^l$

forward computing a^l v^l l layer l+1 layer $backpropagation <math>\delta^l$



% forward computing function
$$fc(w^l, a^l)$$
 for $i = 1: n_{l+1}$
$$z_i^{l+1} = \sum_{j=1}^{n_l} w_{ij}^l a_j^l$$

$$a_i^{l+1} = f(z_i^{l+1})$$
 end

%backpropagation function
$$bc(w^l, \delta^{l+1})$$
 for $i=1:n_l$
$$\delta_i^l = \dot{f}(z_i^l) \cdot \left(\sum_{j=1}^{n_{l+1}} w_{ji}^l \delta_j^{l+1}\right)$$
 end

Step 1. Input the training data set $D = \{(x, y)\}$

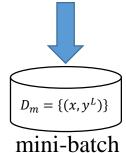
Step 2. Initialize each w_{ij}^l , and choose a learning rate α .

Step 3. for each mini-batch sample $D_m \subseteq D$

for each
$$x \in D_m$$
;
 $a^1 \leftarrow x \in D_m$;
for $l = 1: L-1$
 $a^{l+1} \leftarrow fc(w^l, a^l)$;
end
 $\delta^L = \frac{\partial J(x)}{\partial z^L}$;
for $l = L - 1: 2$
 $\delta^l \leftarrow bc(w^l, \delta^{l+1})$;
end
 $\frac{\partial J}{\partial w^l_{ji}} \leftarrow \frac{\partial J}{\partial w^l_{ji}} + \delta^{l+1}_j \cdot a^l_i$;
end
 $w^l_{ji} \leftarrow w^l_{ji} - \alpha \cdot \frac{\partial J}{\partial w^l_{ji}}$;
end

training data

$$D = \{(x, y^L)\}$$



The BP Algorithm

function $fc(w^l, a^l)$ $for i = 1: n_{l+1}$ $z_i^{l+1} = \sum_{j=1}^{n_l} w_{ij}^l a_j^l$ $a_i^{l+1} = f(z_i^{l+1})$ end

Relationship:

$$\frac{\partial J}{\partial w_{ji}^l} = \delta_j^{l+1} \cdot a_i^l$$

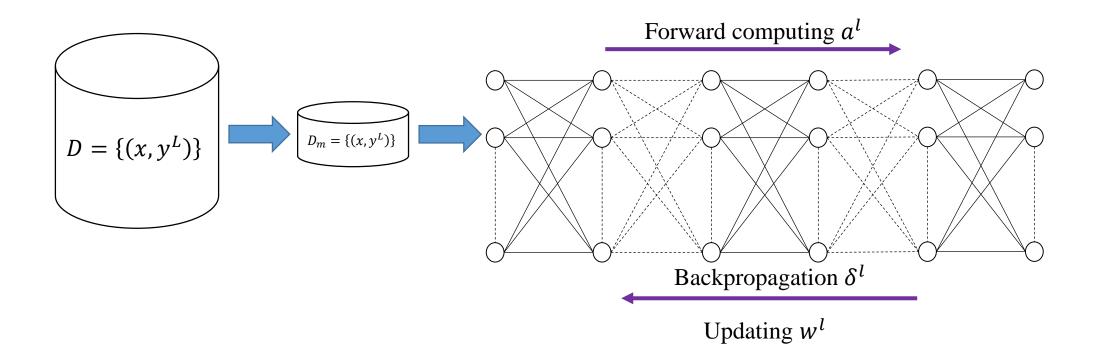
function $bc(w^l, \delta^{l+1})$ $for i = 1: n_l$

end

$$\delta_i^l = \dot{f}(z_i^l) \cdot \left(\sum_{j=1}^{n_{l+1}} w_{ji}^l \delta_j^{l+1}\right)$$

Step 4. Return to Step 3 until each w^l converge.

Network Training



Network Training Steps

Step 1: Data Preparation Step 2: Design
Network Architecture

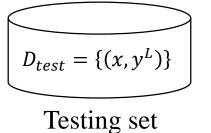
Step 3: Initialize Parameters

Step 4: Define Cost Function

Step 5: Define
Evaluation Index

 $D_{train} = \{(x, y^L)\}$

Training set



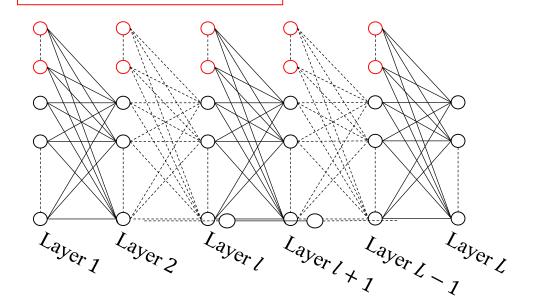
■ Number of layers

- Number of neurons in each layer
- Activation function

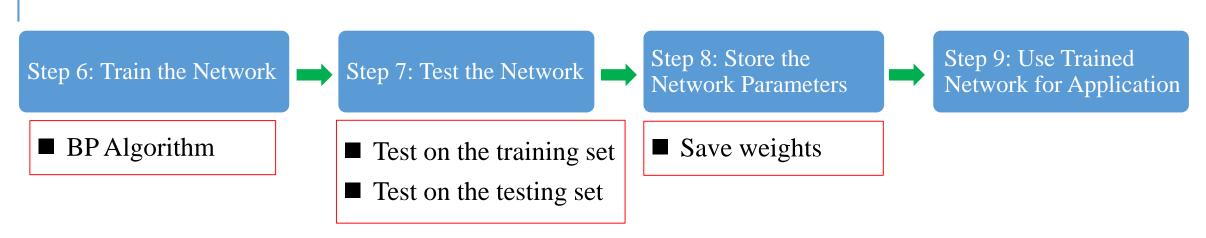
- Weights
- Learning rate

$$J = \frac{1}{2} \sum_{j=1}^{n_L} e_j^2$$
$$= J(w^1, \dots, w^L)$$

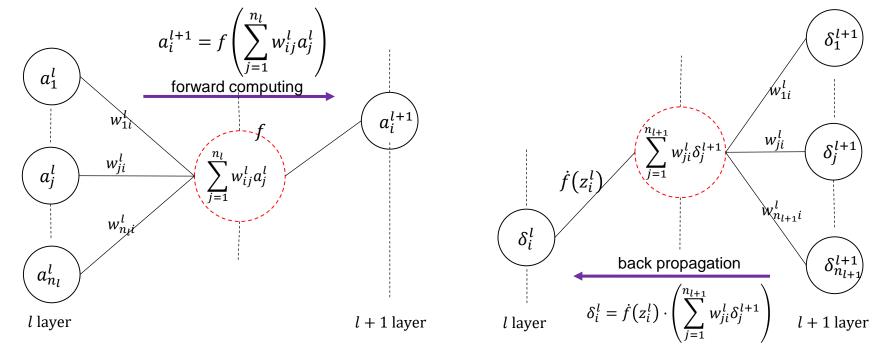
Accuracy



Network Training Steps



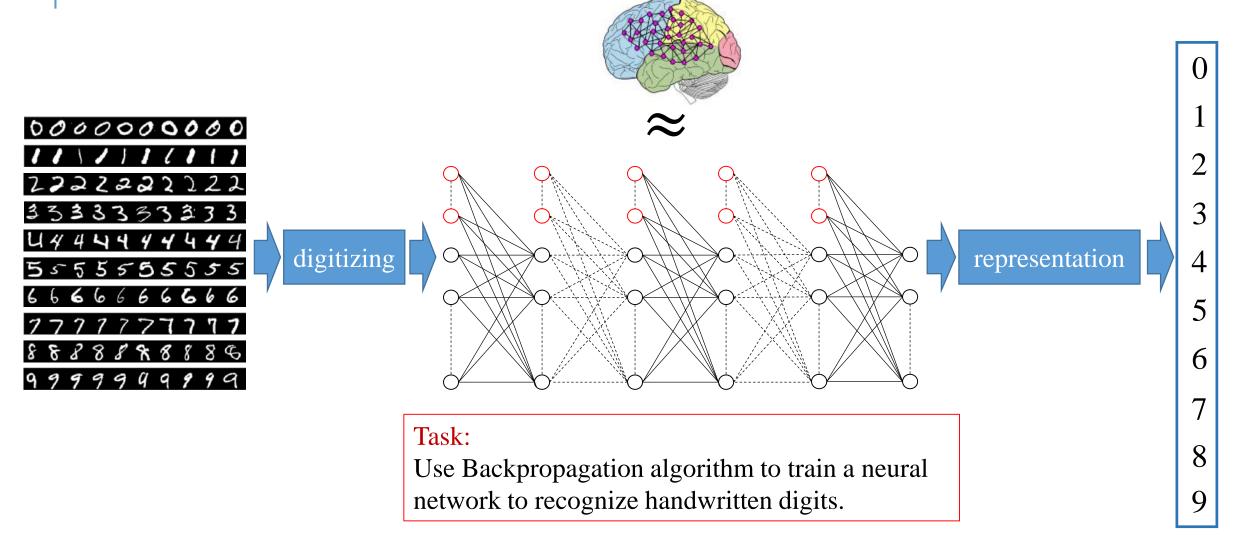
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Outline

- ■Brief Review of Backpropagation Algorithm
- ■An Illustrating Example
- **Experiments**
- Assignment

Handwritten digits recognition problem



Dataset: MNIST_small

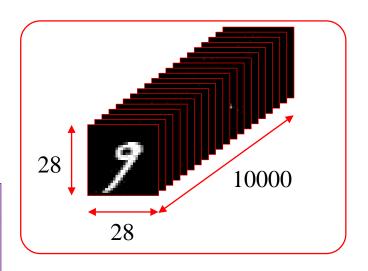
MNIST is a database of handwritten digits created by "re-mixing" the samples from MNIST's original datasets. It contains digits written by high school students and employees of the United States Census Bureau. The digits have been size-normalized and centered in 28 × 28 images.

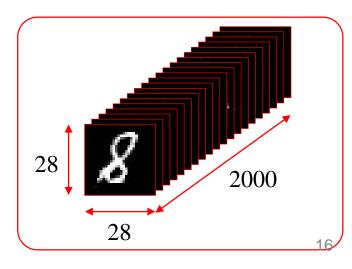
MNIST_small dataset is a subset of MNIST containing 10000 training samples and 2000 testing samples.





Data

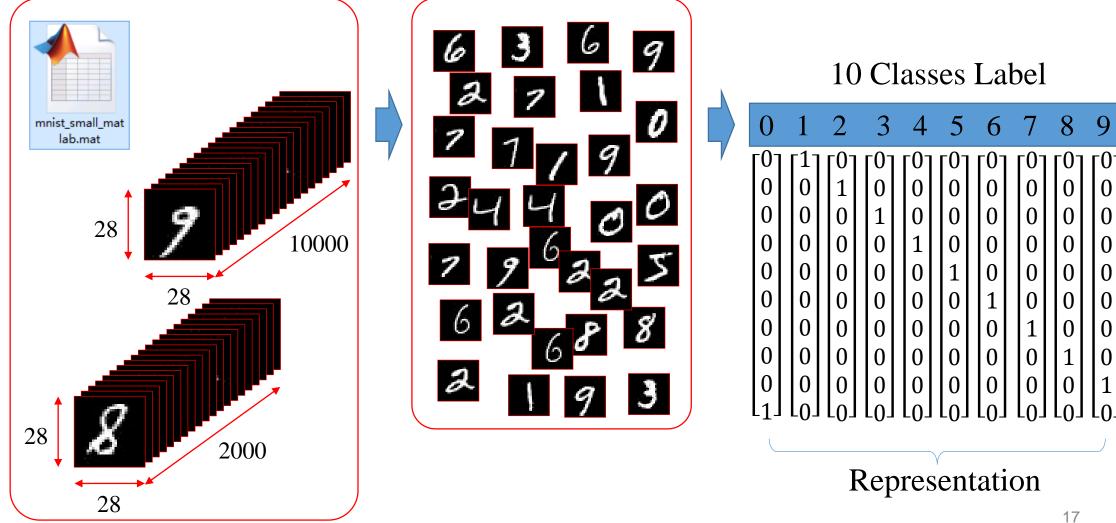




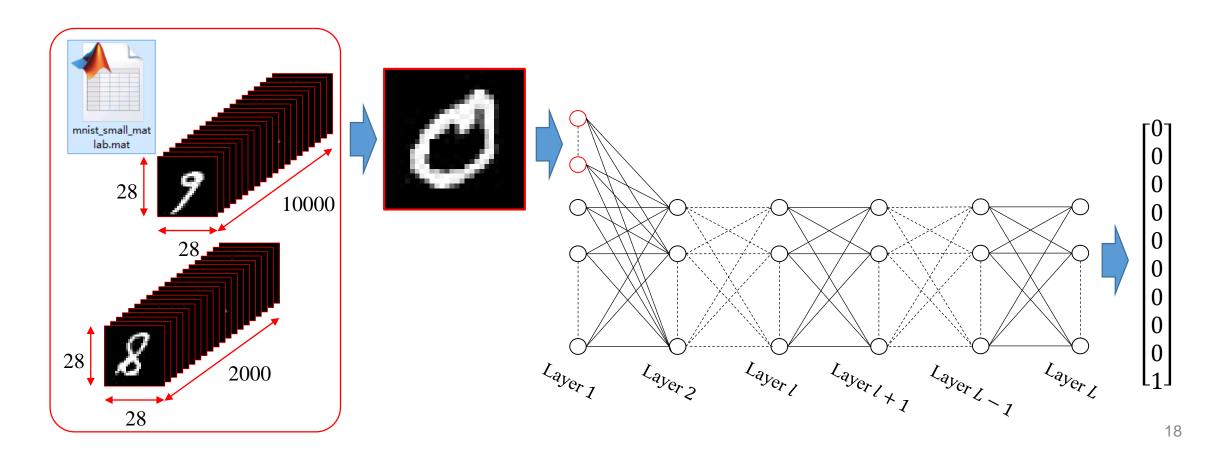
Download link:

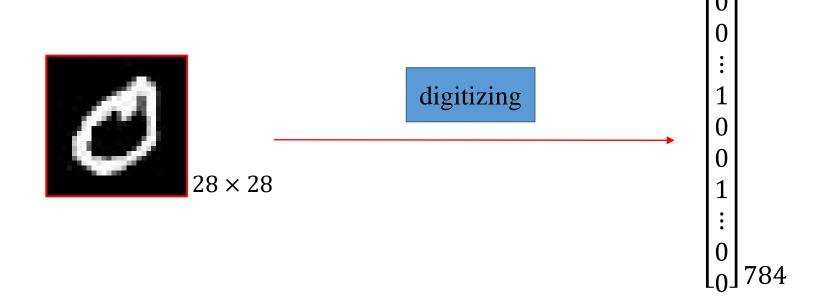
MNIST http://yann.lecun.com/exdb/mnist/

MNIST_small: https://github.com/kswersky/nnet/blob/master/mnist_small.mat



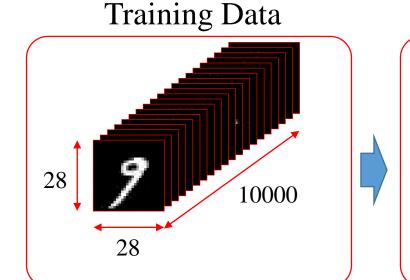
The input image is a $28 \times 28 = 784$ dimensional vector.



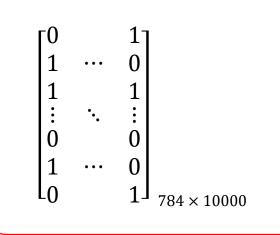


Training set

- ☐ Used for training network
- ☐ 10000 samples



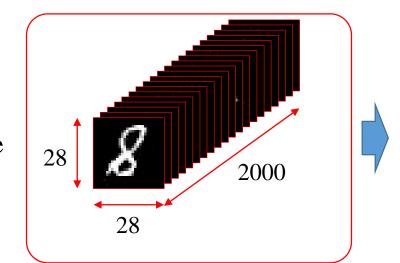
Training Data

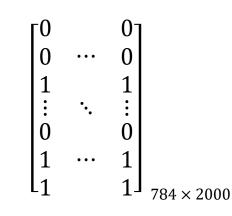




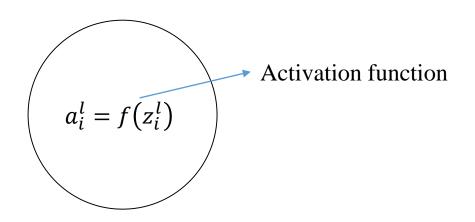
Testing set

- ☐ Used for evaluating network performance
- □ 2000 samples



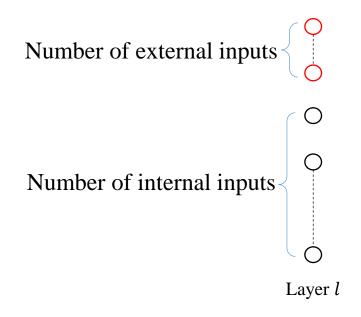


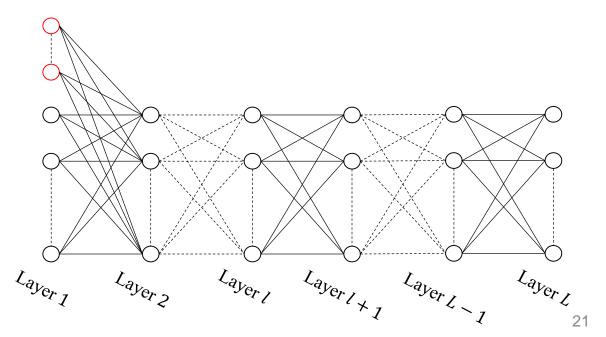
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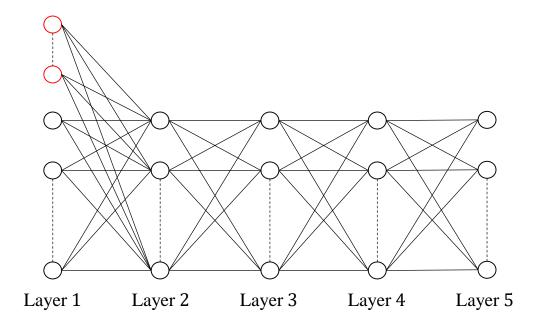
Network architecture design:

- 1. Number of layers
- 2. Number of neurons in each layer (external neurons and internal neurons)
- 3. Activation function

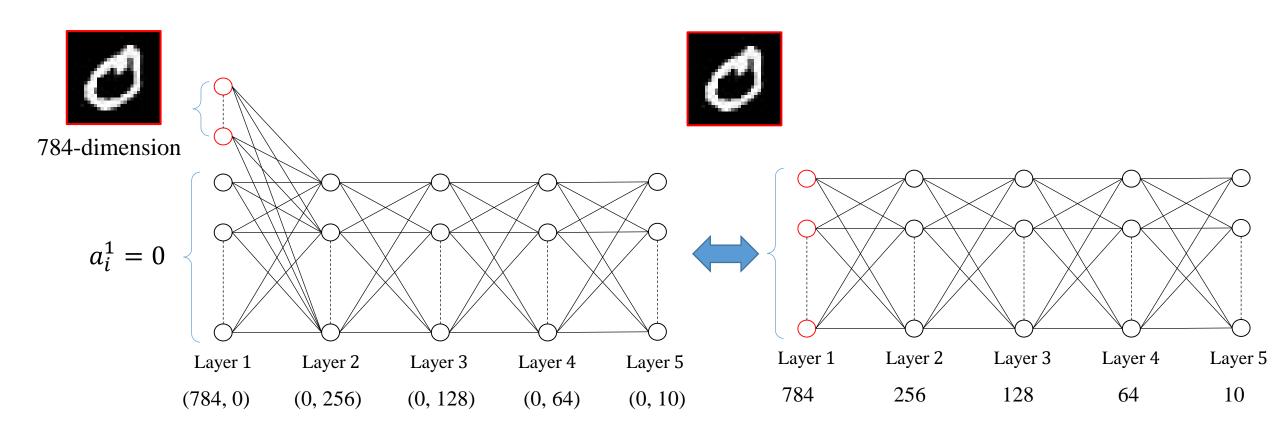




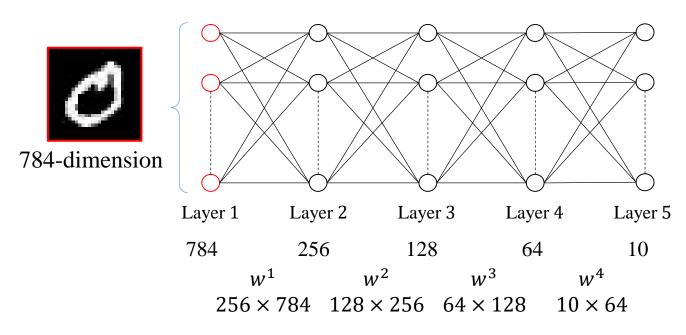
Define Number of Layers

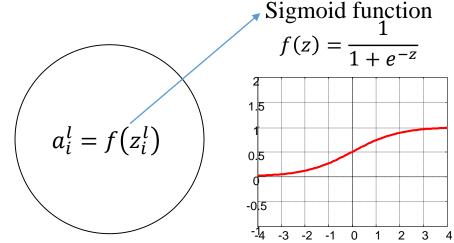


Define Number of Neurons in Each Layer



Define Activation Function



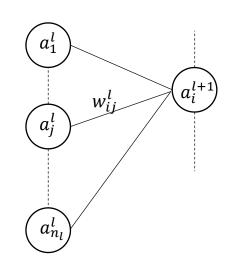


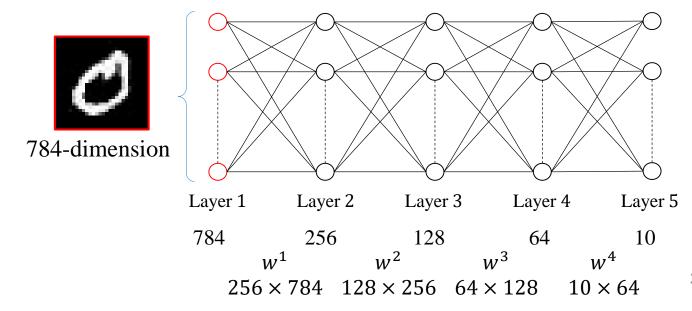
Step 3: Initialize Parameters

Initialize connection weights

Random initialization:

Gaussian distribution: $w_{ij}^l \sim N(0,1)$



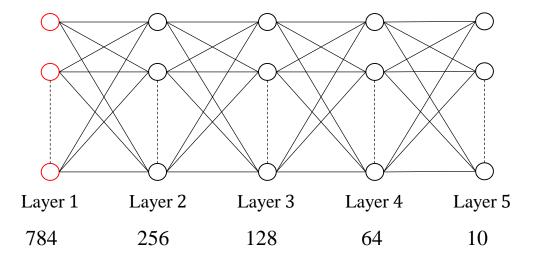


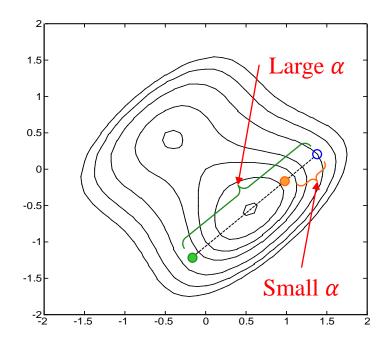
Step 3: Initialize Parameters

Learning rate:

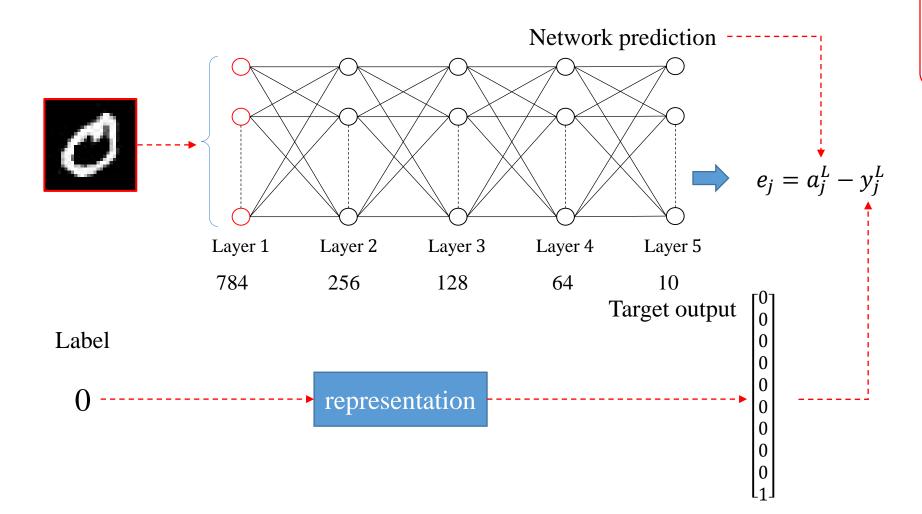
- Small: slow learning, long learning time.
- Large: fast learning, possibly not converge to minima.

$$w_{ji}^l \leftarrow w_{ji}^l - \alpha \cdot \frac{\partial J}{\partial w_{ji}^l} \qquad \alpha = \cdots, 0.005, 0.01, 0.02, 0.04, \cdots$$





Step 4: Define Cost Function

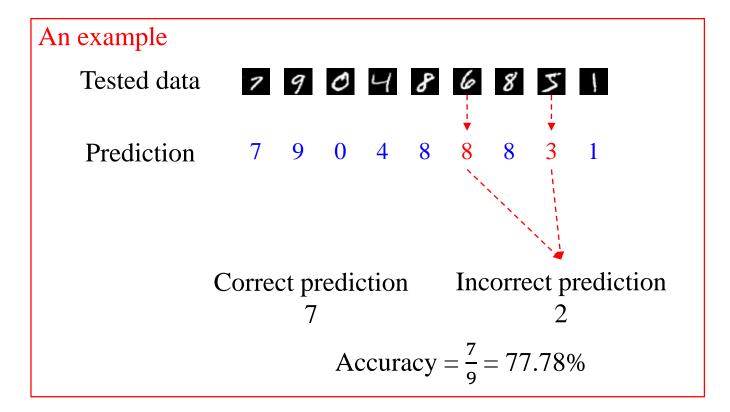


Cost function

$$J = \frac{1}{2} \sum_{j=1}^{n_L} e_j^2$$

Step 5: Define Evaluation Index

$$Acc = \frac{number\ of\ correct\ prediction}{number\ of\ samples}$$



Test on training set:

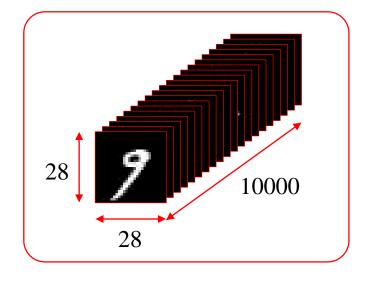
• Evaluate the ability of the model to fit given data.

Test on testing set:

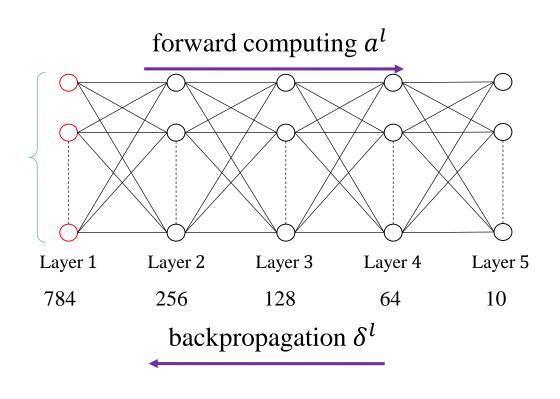
• Evaluate the ability of the model to generalize the knowledge.

Step 6: Train the Network

Training Data

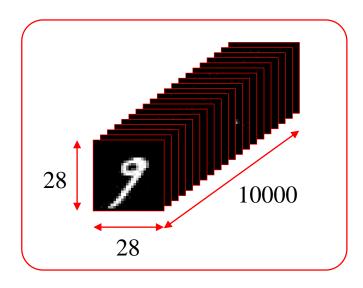


Updating weights
$$w_{ji}^{l} \leftarrow w_{ji}^{l} - \alpha \cdot \frac{\partial J}{\partial w_{ji}^{l}}$$



Step 7: Test the Network

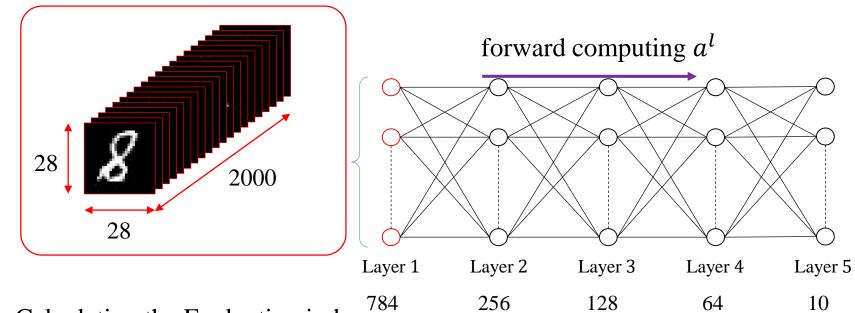
Training Data



Calculating the Evaluation index on training set

$$Acc = \frac{number\ of\ correct\ prediction}{10000}$$

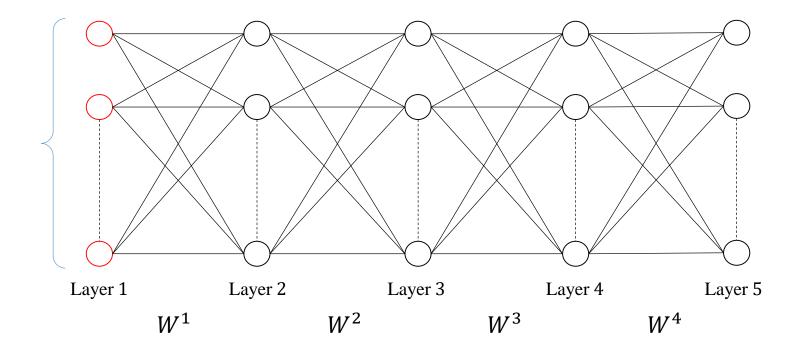
Testing Data



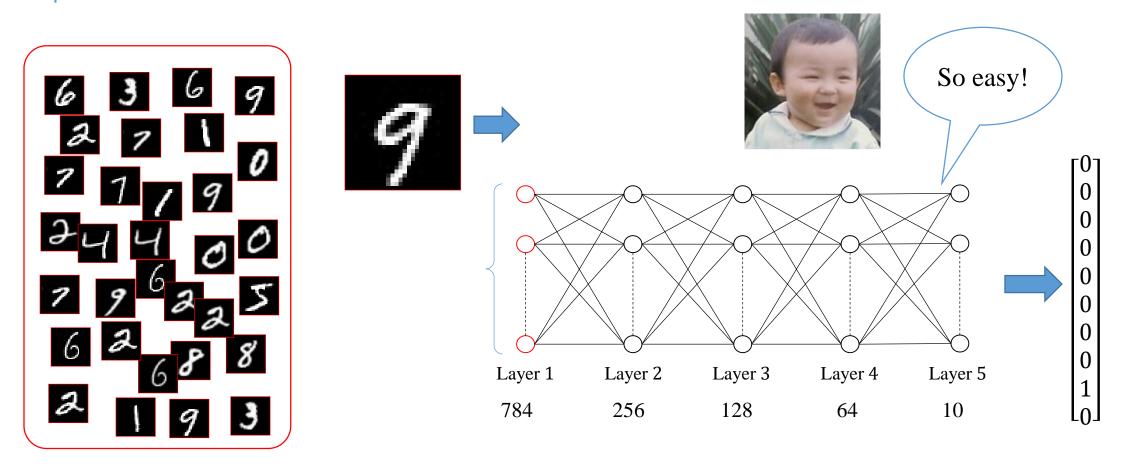
Calculating the Evaluation index on testing set

$$Acc = \frac{number\ of\ correct\ prediction}{2000}$$

Step 8: Store the Network Parameters

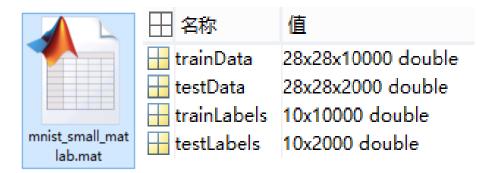


Step 9: Use Trained Network for Application



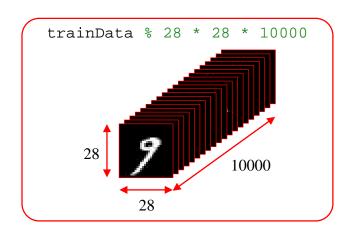
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- **■**Experiments
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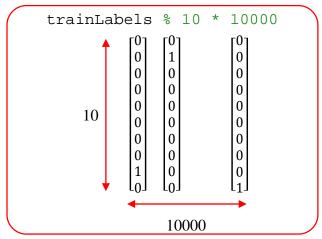


```
%% Step 1: Data Preparation
% loading dataset
load mnist_small_matlab.mat
% trainData: a matrix with size of 28x28x10000
% trainLabels: a matrix with size of 10x10000
% testData: a matrix with size of 28x28x2000
% testLabels: a matrix with size of 10x2000
```

Training Data



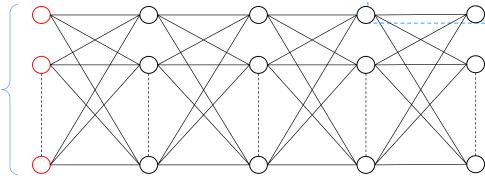
Label



```
% prepare the external input for training set
train_size = 10000; % number of training samples
% input in the 1st layer
X_train = reshape(trainData, 784, train_size);
```

TTPs

- X_train and X_test are cells in Matlab
- reshape and zeros are built-in functions in Matlab



Layer 1	Layer 2	Layer 3	Layer 4	Layer 5
784	256	128	64	10

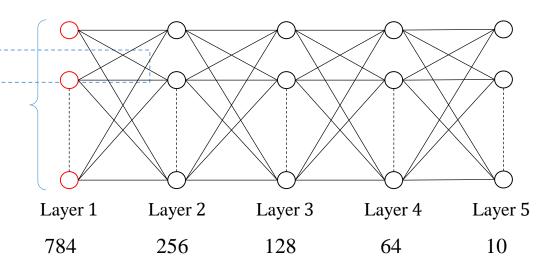
Step 3: Initialize Parameters

Gaussian distribution: $w_{ij}^l \sim N(0,1)$

```
% initialize weights
for l = 1:L-1
    w{l} = 0.1*randn(layer_size(l+1,1), sum(layer_size(l,:)));
end
```

Initialize learning rate

alpha = 0.005; % initialize learning rate



Step 4, 5: Define Cost Function and Evaluation Index

```
%% Step 4: Define Cost Function
function [J] = cost(a, y)
    J = 1/2 * sum((a - y).^2);
end
%% Step 5: Define Evaluation Index
function [ acc ] = accuracy(a, y)
    mini batch = size(a, 2);
    [\sim,idx a] = max(a);
    [\sim,idx_y] = max(y);
    acc = sum(idx a==idx y) / mini batch;
end
                                                          Layer 1
                                                                    Layer 2
                                                                               Layer 3
                                                                                         Layer 4
                                                                                                    Layer 5
                                                          784
                                                                     256
                                                                                128
                                                                                           64
                                                                                                     10
```

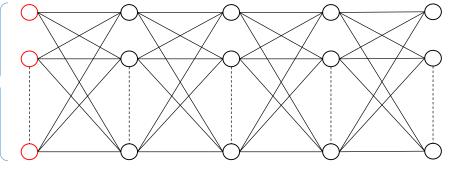
Cost function

$$J = \frac{1}{2} \sum_{j=1}^{n_L} e_j^2$$

$$Acc = \frac{number\ of\ correct\ prediction}{number\ of\ samples}$$

```
%% Step 6: Train the Network
J = []; % array to store cost of each mini batch
Acc = []; % array to store accuracy of each mini batch
max_epoch = 200; % number of training epochs
mini_batch = 100; % number of sample in each mini batch
```

Mini-batch BP implement



Layer 1

Layer 2

Layer 3

Layer 4

Layer 5

BP Algorithm:

Step 1. Input the training data set $D = \{(x, y)\}$

Step 2. Initialize each w_{ij}^l , and choose a learning rate α .

Step 3. for each mini-batch sample $D_m \subseteq D$

for each
$$x \in D_m$$

 $a^1 \leftarrow x \in D_m$;
for $l = 1: L-1$
 $a^{l+1} \leftarrow fc(w^l, a^l)$;
end
 $\delta^L = \frac{\partial J}{\partial z^L}$;
for $l = L - 1: 2$
 $\delta^l \leftarrow bc(w^l, \delta^{l+1})$;
end
 $\frac{\partial J}{\partial w^l_{ji}} \leftarrow \frac{\partial J}{\partial w^l_{ji}} + \delta^{l+1}_j \cdot a^l_i$;
end
 $w^l_{ji} \leftarrow w^l_{ji} - \alpha \cdot \frac{\partial J}{\partial w^l_{ji}}$;

Step 4. Return to Step 3 until each w^l converge.

end

```
% randomly permutate the indexes of samples in training set
idxs = randperm(train size);
% for each mini-batch
for k = 1:ceil(train size/mini batch)
   % prepare internal inputs in 1st layer denoted by a{1}
   end idx = min(k*mini batch, train size); % end index of kth mini-batch
   a{1} = X_train(:,idxs(start_idx:end_idx));
   % prepare labels
   y = trainLabels(:, idxs(start_idx:end_idx));
   % forward computation
   % cost function
   9
   % backward computation
   %
   % update weight
   90
end
```

TIPs

 randperm is a built-in function in Matlab

% forward computation for l=1:L-1 $[a\{1+1\}, z\{1+1\}] = fc(w\{1\}, a\{1\});$ end % Compute delta of last layer $delta\{L\} = (a\{L\} - y).* a\{L\} .*(1-a\{L\});$ % backward computation for l=L-1:-1:2 $delta{1} = bc(w{1}, z{1}, delta{1+1});$ end % update weight for l=1:L-1 % compute the gradient grad_w = delta{l+1} * a{l}'; $w\{1\} = w\{1\} - alpha*grad_w;$ end end

BP Algorithm:

Step 1. Input the training data set $D = \{(x, y)\}$ Step 2. Initialize each $w_{i,i}^l$, and choose a learning rate α .

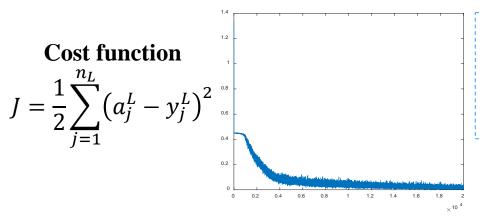
Step 3. for each mini-batch sample $D_m \subseteq D$

for each
$$x \in D_m$$
;
$$a^1 \leftarrow x \in D_m;$$
for $l = 1: L-1$

$$a^{l+1} \leftarrow fc(w^l, a^l);$$
end
$$\delta^L = \frac{\partial J}{\partial z^L};$$
for $l = L-1: 2$

$$\delta^l \leftarrow bc(w^l, \delta^{l+1});$$
end
$$\frac{\partial J}{\partial w^l_{ji}} \leftarrow \frac{\partial J}{\partial w^l_{ji}} + \delta^{l+1}_j \cdot a^l_i;$$
end
$$w^l_{ji} \leftarrow w^l_{ji} - \alpha \cdot \frac{\partial J}{\partial w^l_{ji}};$$
end

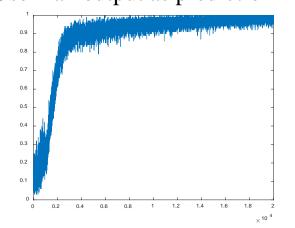
Step 4. Return to Step 3 until each w^l converge.



```
% training cost on training batch
J = [J 1/mini_batch*cost(a{L}, y)];
figure
plot(J);
```

Accuracy

 $Acc = \frac{number\ of\ correct\ prediction}{number\ of\ samples}$ Use max output as prediction



```
% accuary on training batch
Acc =[Acc accuracy(a{L}, y)];
figure
plot(Acc);
```

Step 7: Test the Network

```
%test on training set
a{1} = X_train;
for l = 1:L-1
  a{l+1} = fc(w{l}, a{l});
end
train_acc = accuracy(a{L}, trainLabels);
fprintf('Accuracy on training dataset is %f%%\n', train_acc*100);
```

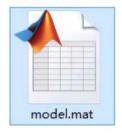
Accuracy on training dataset is 98.160000%

```
%test on testing set
a{1} = X_test;
for l = 1:L-1
    a{l+1} = fc(w{l}, a{l});
end
test_acc = accuracy(a{L}, testLabels);
fprintf('Accuracy on testing dataset is %f%%\n', test_acc*100);
```

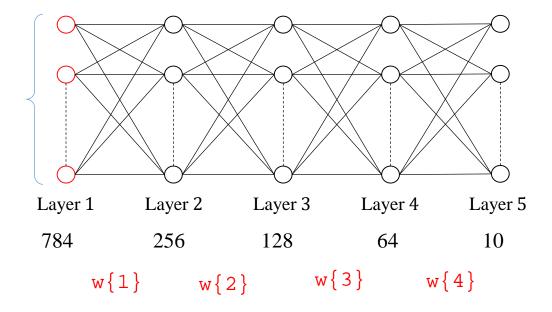
Accuracy on testing dataset is 95.550000%

Experiments: Store the Network Parameters

```
% save model
save model.mat w layer_size
```



This is very important!



Experiments: Code Structure











The main running script

Forward computing function

Backward computing function

Cost function

Evaluation Index

```
% Step 1: Data Preparation
% loading dataset
load mnist_small_matlab.mat
% trainData: a matrix with size of 28x28x10000
% trainLabels: a matrix with size of 10x10000
% testData: a matrix with size of 28x28x2000
% testLabels: a matrix with size of 10x2000
```

```
train_size = 10000; % number of training samples
% input in the 1st layer
X_train = reshape(trainData, 784, train_size);
```

```
test_size = 2000; % number of testing samples
% external input in the 1st layer
X_test = reshape(testData, 784, test_size);
```

```
%% Step 3: Initial Parameters
% initialize weights in each layer with Gaussian distribution
for 1 = 1:L-1
    w\{l\} = 0.1 * randn(layer_size(l+1,1), sum(layer_size(l,:)));
end
alpha = 0.005; % initialize learning rate
%% Step 4: Define Cost Function
% cost function is defined in cost.m
%% Step 5: Define Evaluation Index
% accuracy defined in accuracy.m
```

```
%% Step 6: Train the Network
J = []; % array to store cost of each mini batch
Acc = []; % array to store accuracy of each mini batch
max epoch = 200; % number of training epoch
mini batch = 100; % number of sample of each mini batch
figure % plot the cost
for iter=1:max_epoch
    % randomly permute the indexes of samples in training set
idxs = randperm(train size);
% for each mini-batch
for k = 1:ceil(train size/mini batch)
    % prepare internal inputs in 1st layer denoted by a{1}
    start idx = (k-1)*mini batch+1; % start index of kth mini-batch
    end_idx = min(k*mini_batch, train_size); % end index of kth mini-batch
    a{1} = X_train(:,idxs(start_idx:end_idx));
    % prepare labels
    y = trainLabels(:, idxs(start_idx:end_idx));
```

```
% forward computation
for l=1:I_{i-1}
    [a\{1+1\}, z\{1+1\}] = fc(w\{1\}, a\{1\});
end
% Compute delta of last layer
delta\{L\} = (a\{L\} - y).* a\{L\} .*(1-a\{L\}); %delta\{L\} = {partial J}/{partial z^L}
% backward computation
for 1=I_1-1:-1:2
    delta{1} = bc(w{1}, z{1}, delta{1+1});
end
% update weight
for l=1:I_{i-1}
    % compute the gradient
    grad_w = delta{l+1} * a{l}';
    w\{1\} = w\{1\} - alpha*grad_w;
end
```

```
% training cost on training batch
    J = [J 1/mini_batch*sum(cost(a{L}, y))];
    Acc = [Acc accuracy(a{L}, y)];
    % plot training error
    plot(J);
    pause(0.000001);
    end
end
% end training
% plot accuracy
figure
plot(Acc);
```

```
%% Step 7: Test the Network
%test on training set
a\{1\} = X_{train};
for 1 = 1:L-1
  a\{1+1\} = fc(w\{1\}, a\{1\});
end
train_acc = accuracy(a{L}, trainLabels);
fprintf('Accuracy on training dataset is %f%%\n', train_acc*100);
%test on testing set
a\{1\} = X \text{ test};
for 1 = 1:L-1
   a\{l+1\} = fc(w\{l\}, a\{l\});
end
test_acc = accuracy(a{L}, testLabels);
fprintf('Accuracy on testing dataset is %f%%\n', test acc*100);
%% Step 8: Store the Network Parameters
save model.mat w layer size
```

Experiments: Code—fc.m and bc.m

```
% fc.m
% This is forward computation function

function [a_next, z_next] = fc(w, a)
    % define the activation function
    f = @(s) 1 ./ (1 + exp(-s));

    % forward computing
    z_next = w * a;
    a_next = f(z_next);
end
```

```
% bc.m
% This is backward computation function
function delta = bc(w, z, delta next)
   % activation function
    f = @(s) 1 ./ (1 + exp(-s));
    % derivative of activation function
    df = @(s) f(s) .* (1 - f(s));
    % backward computing
    delta = (w' * delta next) .* df(z);
end
```

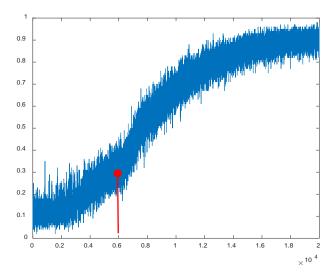
Experiments: Code—cost.m and accuracy.m

```
%% Step 4: Define Cost Function
function [J] = cost(a, y)
    J = 1/2 * sum((a - y).^2);
end
```

```
%% Step5: Define Evaluation Index
function [ acc ] = accuracy( a, y )
    mini_batch = size(a, 2);
    [~,idx_a] = max(a);
    [~,idx_y] = max(y);
    acc = sum(idx_a==idx_y) / mini_batch;
end
```

Results: Learning Rate

% learning rate
alpha = 0.001;

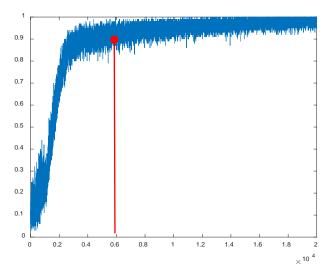


Accuracy

- Training=90.24%
- Testing=89.10%

Too Slow

% learning rate
alpha = 0.005;

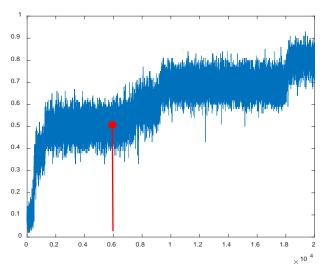


Accuracy

- Training=98.15%
- Testing=95.25%

Good

% learning rate
alpha = 0.08;



Accuracy

- Training=79.66%
- Testing=76.65%

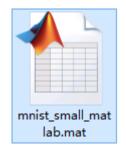
Too Fast

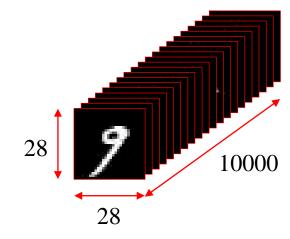
Outline

- ■Brief Review of Backpropagation Algorithm
- ■An Illustrating Example
- Experiments
- Assignment

Assignment

- 1. Copy and run the handwritten digits recognition code by MATLAB using only one layer of external input.
- 2. Try different network layers with different neurons and plot the results (such as L = 2, 3, 8).





Thanks