Deep Learning Book

Chapter 6
Deep Feedforward Networks

Botian Shi botianshi@bit.edu.cn March 7, 2017



- · A type of neural network
 - · Deep feedforward network
 - · Feedforward neural network
 - · Multilayer perceptron (MLP)
- For a classifier, $y = f^*(x)$ maps an input x to category y
- · Defines a mapping

$$y = f(x; \theta)$$

- · Learns the best approximation of f^* with parameter $oldsymbol{ heta}$
- · Feedforward only, no feedback connections
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Feedforward networks are ...

- 1. Extreme important.
- 2. Stepping stone on the path to many neural network models.

Example: convolutional neural network

Figure 1: A type of convolutional neural network: LeNet-5 (LeCun et al. [1998])

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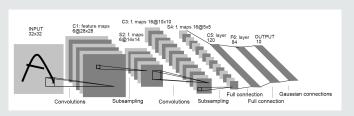


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Why called networks?

- Composing together many different functions
- Model is associated with a DAG describing the composition:

$$f(x) = f^{(3)} (f^{(2)} (f^{(1)} (x)))$$

- $\cdot f^{(1)}$ called first layer of the network
- $f^{(2)}$ called second layer, and so on
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• During training, we drive f(x) to match $f^*(x)$

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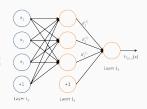


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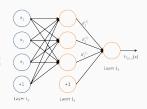


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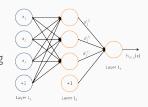


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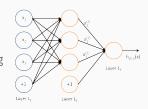


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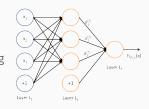


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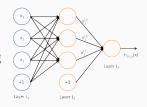


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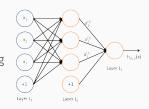


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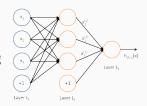


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- · Each element of the vector may be interpreted as a neuron.
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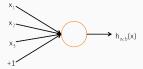


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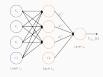


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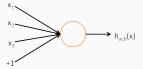


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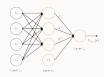


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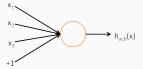


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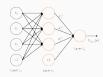


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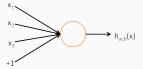


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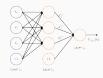


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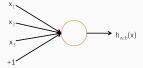


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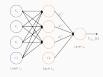


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$$\theta = \underset{\theta}{\operatorname{arg\,min}} \mathbf{J}(\theta; \mathbf{X}) = \underset{\theta}{\operatorname{arg\,min}} \frac{1}{2} \sum_{i=1}^{m} (h_{\theta}(\mathbf{x}^{(i)}) - \mathbf{y}^{(i)})^2$$

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 - • High dimension \Leftrightarrow enough capacity to fit the training set.

 - · 😀 No-free-lunch: Runge phenomenon; Gibbs phenomenon.
 - 2. Manually engineer ϕ
 - Require human effort for each separate task.
 - Need practitioners specializing in different domains.
 - 3. Deep learning
 - Strategy: learn a ϕ automatically.
 - $y = f(x; \theta, w) = \phi(x; \theta)^T w$
 - We have parameters θ to learn ϕ from a broad class of functions.
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 - We have parameters w to map from $\phi(x)$ to the desired output.
 - · Here in example, ϕ defining a hidden layer.
 - Deep learning is not simply a "deep" neural network. The ϕ is crucial!

· Why deep learning?

- 1. Parametrize the representation as $\phi(\mathbf{x};oldsymbol{ heta})$
- 2. We can use optimization algorithm to find the θ that corresponds to a good representation.
- Capture the benefit of first and second approach.
 - Being highly generic: using a very broad family $\phi(x; \theta)$
 - Human practitioners can encode their knowledge by designing families $\phi(\mathbf{x}; \boldsymbol{\theta})$.
 - Human designer only needs to find the right general function family rather than finding precisely the right function.
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- Target: $y = f^*(x)$
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 to make f as similar as possible to f*
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Table 1: XOR

X_2	У
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0	1
1	0
	0 1 0

$$J(\boldsymbol{\theta}) = \frac{1}{4} \sum_{\mathbf{x} \in \mathbb{X}} (f^*(\mathbf{x}) - f(\mathbf{x}; \boldsymbol{\theta}))^2$$

Figure 5: XOR problem

Suppose our model is:

$$f(\mathbf{x}; \mathbf{w}, \mathbf{b}) = \mathbf{x}^{\mathsf{T}} \mathbf{w} + \mathbf{b}$$

- After solving the equations, we obtain w=0 and $b=\frac{1}{2}$; $f(x)=\frac{1}{2}$; $J(\theta)=\frac{1}{4}$
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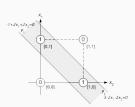
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Figures from colah's blog

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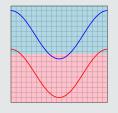
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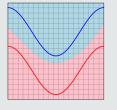
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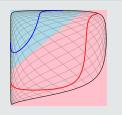
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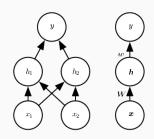




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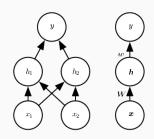
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- The values of these hidden units are then used as the input for a second layer.
- The output layer is still just a linear regression model, but now it is applied to h rather than to x.
- The network now contains two functions chained together:
 h = f⁽¹⁾(x; W, c) and y = f⁽²⁾(h; w, b)
- the complete model is: $f(x; W, c, w, b) = f^{(2)}(f^{(1)}(x))$

Figure 6: A feedforward network with one hidden layer and two hidden units



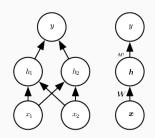
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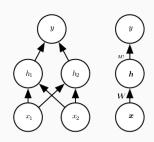
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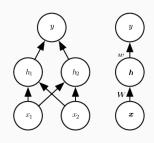
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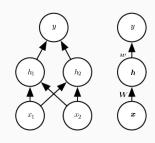
- $h = f^{(1)}(x; W, c)$ and $y = f^{(2)}(h; w, b)$
- What function should $f^{(1)}$ compute? We may be tempting to make $f^{(1)}$ be linear as well?
- Unfortunately, if f⁽¹⁾ were linear, then the feedforward network as a whole would remain a linear function of its input.
- suppose f⁽¹⁾(x) = W^Tx and f⁽²⁾(h) = h^Tw. Then f(x) = w^TW^Tx. We could represent this function as f(x) = x^Tw' where w' = Ww
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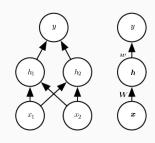
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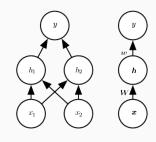
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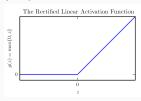


- Most neural networks describe the features using an affine transformation controlled by learned parameters, followed by a fixed, nonlinear function called an activation function.
- We define: $h = g(W^Tx + c)$, where W provides the weights of a linear transformation and c the biases.
- The activation function g is typically chosen to be a function that is applied element-wise, with $h_i = g(\mathbf{x}^T \mathbf{W}^{:,i} + c_i)$.
- In modern neural networks, the default recommendation is to use the rectified linear unit or ReLU (Jarrett et al. [2009], Nair and Hinton [2010], Glorot et al. [2011]) defined by the activation function g(z) = max{0, z}

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We can now specify our complete network as

$$f(\mathbf{x}; \mathbf{W}, \mathbf{c}, \mathbf{w}, b) = \mathbf{w}^{\mathsf{T}} \max\{0, \mathbf{W}^{\mathsf{T}} \mathbf{x} + \mathbf{x}\} + b$$

We can now specify a solution to the XOR problem. Let

$$W = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}, c = \begin{bmatrix} 0 \\ -1 \end{bmatrix}, w = \begin{bmatrix} 1 \\ -2 \end{bmatrix}, b = 0$$

Let X be the design matrix containing all four points in the binary input space:

$$\mathbf{x} = \begin{bmatrix} 0 & 0 \\ 0 & 1 \\ 1 & 0 \\ 1 & 1 \end{bmatrix}$$

We can now specify our complete network as

$$f(\mathbf{x}; \mathbf{W}, \mathbf{c}, \mathbf{w}, b) = \mathbf{w}^{\mathsf{T}} \max\{0, \mathbf{W}^{\mathsf{T}} \mathbf{x} + \mathbf{x}\} + b$$

We can now specify a solution to the XOR problem. Let

$$W = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}, c = \begin{bmatrix} 0 \\ -1 \end{bmatrix}, w = \begin{bmatrix} 1 \\ -2 \end{bmatrix}, b = 0$$

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To finish computing the value of h for each example, we apply the rectified linear transformation and then, we can use a linear model to solve the problem. We finish by multiplying by the weight vector \mathbf{w}

$$\operatorname{ReLU}(XW+c) = \begin{bmatrix} 0 & 0 \\ 1 & 0 \\ 2 & 0 \\ 2 & 1 \end{bmatrix}; \qquad \operatorname{ReLU}(XW+c) \times W = \begin{bmatrix} 0 \\ 1 \\ 1 \\ 0 \end{bmatrix};$$

The neural network has obtained the correct answer for every example in the batch.

In this example, we simply specified the solution, then showed that it obtained zero error. In a real situation, there might be billions of model parameters and billions of training examples, so one cannot simply guess the solution as we did here.

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- The cost functions for neural networks are more or less the same as those for other parametric models, such as linear models.
- Parametric model defines a distribution $p(y|x;\theta)$ and we simply use the principle of maximum likelihood.
- The total cost function = primary cost functions + regularization term.
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$$J(W,b) = \left[\frac{1}{m} \sum_{i=1}^{m} (\frac{1}{2} \|h_{W,b}(x^{(i)}) - y^{(i)}\|^2)\right] + \frac{\lambda}{2} \sum_{l=1}^{n_l-1} \sum_{i=1}^{s_l} \sum_{j=1}^{s_l+1} \left(W_{ji}^{(l)}\right)^2$$

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Cross-entropy cost function in logistic regression with 1 unit

 We can use MSE to be the cost function:

$$C = \frac{1}{2}(y-a)^2$$
 where $a = \sigma(z)$ and $z = WX+b$

· The gradient of the cost function *C*:

$$\frac{\partial C}{\partial w} = (a - y)\sigma'(z)x = a\sigma'(z)$$

• Then update parameters:

$$w \leftarrow w - \eta \frac{\partial C}{\partial w} = w - \eta \times a \times \sigma'(z)$$

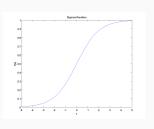


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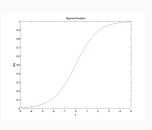


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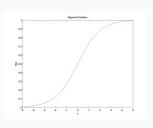


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- Here, we focus on the use of these units as outputs of the model, but in principle they can be used internally as well.
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- One kind of output unit is based on an affine transformation with no nonlinearity. (Linear Units)
- Given features h, a layer of linear output units produces a vector $\hat{y} = W^T h + b$
- Linear output layers are often used to produce the mean of a conditional Gaussian distribution:

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The sigmoid function is:

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

- We can think of the sigmoid output unit as having two components.
 - 1. A linear layer to compute $z = \mathbf{w}^{\mathsf{T}} \mathbf{h} + b$
 - Convert z into a probability by the sigmoid activation function.

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$$\hat{y} = \sigma(\mathbf{w}^\mathsf{T} \mathbf{h} + b)$$

The sigmoid function is:

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

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- Softmax functions are most often used as the output of a classifier, to represent the probability distribution over n different classes.
- To generalize to the case of a discrete variable with n values, we now need to produce a vector \hat{y} , with $\hat{y_i} = P(y = i | x)$.
- We require not only that each element of $\hat{y_i}$ between 0 and 1, but also that the entire vector sums to 1.

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From a neuroscientific point of view, it is interesting to think of the softmax as a way to create a form of competition between the units that participate in it: the softmax outputs always sum to 1 so an increase in the value of one unit necessarily corresponds to a decreases in the value of others.

This is analogous to the lateral inhibition that is believed to exist between nearby neurons in the cortex. At the extreme it becomes a form of winner - take - all (one of the outputs is nearly 1 and the others are nearly 0).

$$g(z) = \max\{0,z\}$$

- A variety of generalizations of ReLU guarantee that they receive gradient everywhere.
- Three generalizations of rectified linear units are based on using a non-zero slope \(\alpha_i\) when \(z_i < 0\):

$$h_i = g(\mathbf{z}, \boldsymbol{\alpha})_i = \max(0, z_i) + \alpha_i \min(0, z_i)$$

- 1. Absolute value rectification (Jarrett et al. [2009]) fixes $\alpha_i = -1$ to obtain g(z) = |z|
- 2. A leaky ReLU (Maas et al. [2013]) fixes α_i to a small value like 0.01
- 3. A parametric ReLU or PReLU (He et al. [2015]) treats α_i as a learnable parameter.
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Hidden Units Retified Linear Units and Their Generalizations

· Easy to optimize: similar to linear units

$$g(z) = \max\{0, z\}$$

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Hidden Units Logistic Sigmoid and Hyperbolic Tangent

 Prior to the introduction of rectified linear units, most neural networks used the logistic sigmoid activation function

$$g(z) = \sigma(z)$$

Or the hyperbolic tangent activation function

$$g(z) = \tanh(z)$$

• These activation functions are closely related because $\tanh(z) = 2\sigma(2z) - 1$

Hidden Units Other Hidden Units

· Radial basis function or RBF unit

$$h_i = \exp\left(-\frac{1}{\sigma_i^2} \|\mathbf{W}_{:,i} - \mathbf{x}\|^2\right)$$

· Softplus (Dugas et al. [2001])

$$g(a) = \xi(a) = \log(1 + e^a)$$

Hard tanh (Collobert [2004])

$$g(a) = \max(-1, \min(1, a))$$

- Another key design consideration for neural networks is determining the architecture.
- The word architecture refers to the overall structure of the network:
 - 1. How many units it should have
 - 2. How these units should be connected to each other.
- · Most networks are organized into groups of units called layers.
- Most network architecture arrange these layers in a chain structure.
- In this structure, the layers are given by

$$h^{(1)} = g^{(1)}(W^{(1)T}x + b^{(1)})$$

$$h^{(2)} = g^{(2)}(W^{(1)T}h^{(1)} + b^{(2)})$$

and so on.

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Universal Approximation Properties and Depth

- The reason why linear models are easy to train is their loss functions are convex.
- · Unfortunately, we often want to learn nonlinear functions.
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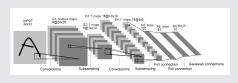
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Other Architectural Considerations

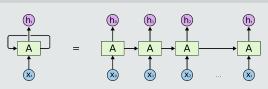
· Convolutional Networks for computer vision

Convolutional Network (LeNet-5 LeCun et al. [1998])



· Recurrent Neural Networks for sequence modeling

Recurrent Neural Network



- · input x provide information \rightarrow hidden layers \rightarrow an output \hat{y}
- This process called forward propagation
- During training, forward propagation can continue onward until it produces a scalar cost $J(\theta)$
- Computing an analytical expression for gradient: computationally expensive.
- The back-propagation algorithm (Rumelhard and Williams [1986]) allows the information from the cost to then flow backward through the network, in order to compute the gradient.
- The gradient we require is the gradient of the cost function with respect to the parameters

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- To compute the derivatives of composite function
- Back-propagation is an algorithm that computes the chain rule, with a specific order of operations that is highly efficient.

$$y = g(x)$$
 and $z = f(y) = f(g(x))$

· The chain rule states that

$$\frac{dz}{dx} = \frac{dz}{dy}\frac{dy}{dx}$$

• Generalize beyond the scalar case. Suppose that $x \in \mathbb{R}^m$, $y \in \mathbb{R}^n$, g maps from $\mathbb{R}^m to \mathbb{R}^n$, and f maps from \mathbb{R}^n to \mathbb{R} . If y = g(x) and z = f(y) then

$$\frac{\partial z}{\partial x_i} = \sum_{j} \frac{\partial z}{\partial y_j} \frac{\partial y_j}{\partial x_j}$$

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$$\frac{\partial z}{\partial x_i} = \sum_{j} \frac{\partial z}{\partial y_j} \frac{\partial y_j}{\partial x_i}$$

- Using the chain rule is straightforward.
- However, actually evaluating that expression in a computer introduces some extra considerations
- · Repeat computation of subexpressions
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Algorithm 1 Forward Propagation

Algorithm 2 Forward Propagation

```
Require: Network depth, l
```

Algorithm 3 Forward Propagation

```
Require: Network depth, l
Require: W^{(i)}, i \in \{1, ..., l\}, the weight matrix of the model
```

Algorithm 4 Forward Propagation

```
Require: Network depth, l
Require: W^{(i)}, i \in \{1, ..., l\}, the weight matrix of the model
Require: b^{(i)}, i \in \{1, ..., l\}, the bias parameters of the model
```

Algorithm 5 Forward Propagation

```
Require: Network depth, l
Require: W^{(i)}, i \in \{1, ..., l\}, the weight matrix of the model
Require: b^{(i)}, i \in \{1, ..., l\}, the bias parameters of the model
Require: x, the input to process
```

Algorithm 6 Forward Propagation

Require: Network depth, lRequire: $W^{(i)}$, $i \in \{1, ..., l\}$, the weight matrix of the model

Require: $b^{(i)}, i \in \{1, ..., l\}$, the bias parameters of the model

Require: *x*, the input to process **Require:** *y*, the target output

```
h^{(0)} = x

for k = 1, ..., l do

a^{(k)} = b^{(k)} + W^{(k)} h^{(k-1)}

h^{(l)} = f(a^{(k)})

end for

\hat{y} = h^{(l)}

l = l(\hat{v}, v) + \lambda \Omega(\theta)
```

Algorithm 7 Forward Propagation

```
Require: Network depth, l
Require: W^{(i)}, i \in \{1, ..., l\}, the weight matrix of the model
Require: b^{(i)}, i \in \{1, ..., l\}, the bias parameters of the model
Require: x, the input to process
Require: y, the target output
  h^{(0)} = x
```

Forward Propagation

Algorithm 8 Forward Propagation

```
Require: Network depth, l
Require: W^{(i)}, i \in \{1, ..., l\}, the weight matrix of the model
Require: b^{(i)}, i \in \{1, ..., l\}, the bias parameters of the model
Require: x, the input to process
Require: y, the target output
  h^{(0)} = x
  for k = 1, ..., l do
    a^{(k)} = b^{(k)} + W^{(k)}h^{(k-1)}
    h^{(l)} = f(a^{(k)})
  end for
```

Forward Propagation

Algorithm 9 Forward Propagation

```
Require: Network depth, l
Require: W^{(i)}, i \in \{1, ..., l\}, the weight matrix of the model
Require: b^{(i)}, i \in \{1, ..., l\}, the bias parameters of the model
Require: x, the input to process
Require: y, the target output
  h^{(0)} = x
  for k = 1, ..., l do
     a^{(k)} = b^{(k)} + W^{(k)}h^{(k-1)}
     h^{(l)} = f(a^{(k)})
  end for
  \hat{\mathbf{v}} = \mathbf{h}^{(l)}
```

Forward Propagation

Algorithm 10 Forward Propagation

```
Require: Network depth, l
Require: W^{(i)}, i \in \{1, ..., l\}, the weight matrix of the model
Require: b^{(i)}, i \in \{1, ..., l\}, the bias parameters of the model
Require: x, the input to process
Require: y, the target output
   h^{(0)} = x
  for k = 1, ..., l do
     a^{(k)} = b^{(k)} + W^{(k)}h^{(k-1)}
     h^{(l)} = f(a^{(k)})
   end for
  \hat{\mathbf{v}} = \mathbf{h}^{(l)}
  J = L(\hat{\mathbf{y}}, \mathbf{y}) + \lambda \Omega(\theta)
```

Algorithm 11 Backward computation

After the forward computation, compute the gradient on the output layer:

$$g \leftarrow \nabla_{\hat{y}} J = \nabla_{\hat{y}}(\hat{y}, y)$$
for $k = 1, l = 1$

Convert the gradient on the layer's output into a gradient into the pre-nonlinearity activation:

$$g \leftarrow \nabla_{\hat{a}^{(k)}} J = g \otimes f'(a^{(k)})$$

Compute gradients on weights and biases (including the regularization term):

$$abla_{b^{(k)}}J = g + \lambda
abla_{b^{(k)}}\Omega(\theta)
abla_{W^{(k)}}J = gh^{(k-1)T} + \lambda
abla_{W^{(k)}}\Omega(\theta)
abla_{w^{(k)}}D(\theta)
abla_{$$

Propagate the gradients w.r.t. the next lower level hidden layer's activations:

$$g \leftarrow \nabla_{\hat{h}^{(k-1)}} J = W^{(k)T} g$$

Algorithm 12 Backward computation

After the forward computation, compute the gradient on the output layer:

$$g \leftarrow \nabla_{\hat{y}} J = \nabla_{\hat{y}}(\hat{y}, y)$$

for
$$k = l, l - 1, ..., 1$$
 do

Convert the gradient on the layer's output into a gradient into the pre-nonlinearity activation:

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Compute gradients on weights and biases (including the regularization term):

$$\nabla_{b^{(k)}}J = g + \lambda \nabla_{b^{(k)}}\Omega(\theta)$$

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Algorithm 13 Backward computation

After the forward computation, compute the gradient on the output layer:

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Compute gradients on weights and biases (including the regularization term):

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 $\nabla_{W^{(k)}}J = gh^{(k-1)T} + \lambda \nabla_{W^{(k)}}\Omega(\theta)$

Propagate the gradients w.r.t. the next lower level hidden layer's activations:

$$g \leftarrow \nabla_{\hat{\mathbf{h}}_{(k-1)}} J = \mathbf{W}^{(k)\mathsf{T}} \mathbf{g}$$

end for

Algorithm 14 Backward computation

After the forward computation, compute the gradient on the output layer:

$$g \leftarrow \nabla_{\hat{y}} J = \nabla_{\hat{y}}(\hat{y}, y)$$

for $k = l, l - 1, ..., 1$ do

Convert the gradient on the layer's output into a gradient into the pre-nonlinearity activation:

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Compute gradients on weights and biases (including the regularization term):

$$\nabla_{b^{(k)}} J = g + \lambda \nabla_{b^{(k)}} \Omega(\theta)$$
$$\nabla_{w^{(k)}} J = gh^{(k-1)T} + \lambda \nabla_{w^{(k)}} \Omega(\theta)$$

Propagate the gradients w.r.t. the next lower level hidden layer's activations:

$$g \leftarrow \nabla_{\hat{h}(k-1)} J = W^{(k)T} g$$

end for

Algorithm 15 Backward computation

After the forward computation, compute the gradient on the output layer:

$$g \leftarrow \nabla_{\hat{y}} J = \nabla_{\hat{y}}(\hat{y}, y)$$

for $k = l, l - 1, ..., 1$ do

Convert the gradient on the layer's output into a gradient into the pre-nonlinearity activation:

$$g \leftarrow \nabla_{\hat{a}^{(k)}} J = g \otimes f'(a^{(k)})$$

Compute gradients on weights and biases (including the regularization term):

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abla_{oldsymbol{b}^{(k)}} J &= g + \lambda
abla_{oldsymbol{b}^{(k)}} \Omega(heta) \
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- · <u>UFLDL</u> (Unsupervised Feature Learning and Deep Learning)
- Backpropagation Algorithm

- Suppose we have a fixed training set
 {(x⁽¹⁾, y⁽¹⁾),...,(x^(m), y^(m))} of m training examples.
- For a single training example (x, y), cost function:

$$J(W, b; x, y) = \frac{1}{2} ||h_{W, b}(x) - y||^2$$

· Given a training set of *m* examples, the overall cost function:

$$J(W,b) = \left[\frac{1}{m}\sum_{i=1}^{m}J(W,b;x^{(i)},y^{(i)})\right] + \frac{\lambda}{2}\sum_{l=1}^{n_{l}-1}\sum_{i=1}^{s_{l}}\sum_{j=1}^{s_{l}+1}\left(W_{ji}^{(l)}\right)^{2}$$

$$= \left[\frac{1}{m}\sum_{i=1}^{m}\left(\frac{1}{2}\|h_{W,b}(x^{(i)})-y^{(i)}\|^{2}\right)\right] + \frac{\lambda}{2}\sum_{l=1}^{n_{l}-1}\sum_{i=1}^{s_{l}}\sum_{j=1}^{s_{l}+1}\left(W_{ji}^{(l)}\right)^{2}$$

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 One iteration of gradient descent updates the parameters W, b as follows:

$$W_{ij}^{(l)} = W_{ij}^{(l)} - \alpha \frac{\partial}{\partial W_{ij}^{(l)}} J(W, b)$$

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- The intuition behind the backpropagation algorithm is as follows.
 - Given a training example (x, y): run a "forward pass" to compute all the activations.
 - 2. Then, for each node *i* in layer *l*: compute an "error term" $\delta_i^{(i)}$.
 - 3. For an output node, we can measure the difference between the network's activation and the true target value, and use that to define $\delta_i^{(n_l)}$ (where layer n_l is the output layer).
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In detail, here is the backpropagation algorithm:

- 1. Perform a feedforward pass, computing the activations for layers L_2 , L_3 , and so on up to the output layer L_{n_l} .
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Q&A

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