A Capsule-unified Framework of Deep Neural Networks for Graphical Programming

Yujian Li  
College of Computer Science  
Faculty of Information Technology  
Beijing University of Technology  
Beijing, China 100124  
liyujian@bjut.edu.cn

Chuanhui Shan  
College of Computer Science  
Faculty of Information Technology  
Beijing University of Technology  
Beijing, China 100124  
chuanhuishan@emails.bjut.edu.cn

Abstract

Recently, the growth of deep learning has produced a large number of deep neural networks. How to describe these networks unifiedly is becoming an important issue. We first formalize neural networks in a mathematical definition, give their directed graph representations, and prove a generation theorem about the induced networks of connected directed acyclic graphs. Then, using the concept of capsule to extend neural networks, we set up a capsule-unified framework for deep learning, including a mathematical definition of capsules, an induced model for capsule networks and a universal backpropagation algorithm for training them. Finally, we discuss potential applications of the framework to graphical programming with standard graphical symbols of capsules, neurons, and connections.

1 Introduction

Artificial neural networks are mathematical models that are inspired by biological neural networks. As a new era of neural networks, deep learning has become a powerful technology for artificial intelligence. Since presented by Hinton et al. [1], it has made a great amount of successes in image classification, speech recognition, and natural language processing [2-5], influencing on both academia and industry dramatically.

Essentially, deep learning is a collection of various methods for effectively training neural networks with deep structures. A neural network is usually regarded as a hierarchical system composed of many nonlinear computing units (or neurons, nodes). For example, a single-neuron network is the MP model proposed by McCulloch and Pitts in 1943 [6], with the function of performing logical operations. Although the MP model is unable to learn, it started the age of neural networks. In 1949, Hebb first proposed the idea of learning about biological neural networks [7]. In 1958, Rosenblatt invented a model of perceptron and its learning algorithm [8]. Subsequently, Minsky’s criticism of the perceptron brought the study of neural networks to a period of low tide [9], but not stagnating completely. By the 1980s and 1990s, a worldwide research of neural networks came up with the presentation of Hopfield neural network [10], Boltzmann machine [11], multilayer perceptron [12], and so on.

Multilayer perceptron (MLP) was once the most popular model of neural networks. A MLP consists of an input layer, a number of hidden layers and an output layer, as shown in Figure 1. The depth of it is the number of layers excluding the input layer. If the depth is greater than 2, a neural network may be called “deep”. For training MLPs, backpropagation (BP) is certainly the most well-known algorithm in common use [12, 13]. However, a majority of applications using MLPs were implemented with few hidden layers, while gaining little empirical benefit from additional hidden layers. Certain solace might be found in universal approximation theorems [14, 15], stating
that a single-layer perceptron can approximate any multivariate continuous function arbitrarily well with enough hidden units. BP seemed to work only for shallow networks, albeit principally for deep networks. Not until 1991 was this problem on deep learning fully understood.

In 1991, Hochreiter made a milestone of deep learning [16], to formally indicate that typical deep networks suffer from the problem of vanishing or exploding gradients. The problem says, cumulative backpropagated error signals decay or explode exponentially in the number of layers, with consequence of shrinking rapidly or growing out of bounds. This is the major reason why BP is hard to train deep networks. Note that it could also be encountered as the long time lag problem in recurrent neural networks [17].

To overcome the training difficulties in deep neural networks (DNNs), in 2006 Hinton et al. started the new field of deep learning with a two-stage strategy in two landmark papers [1, 18], to demonstrate that unsupervised learning in shallow networks, e.g. contrastive divergence learning in restricted Boltzmann machines, can facilitate supervised learning in DNNs, e.g. BP in deep autoencoders (AEs) and deep MLPs. Furthermore, their pioneering work inspired many important techniques, including max pooling [19], dropout [20], dropconnect [21], batch normalization [22], etc. Additionally, a wealthy of historic accomplishments have been completed in applications such as image classification [2], speech recognition [3, 4], and natural language processing [5]. As a consequence, deep learning brings about a new and striking wave of neural networks in both academia and industry.

Broadly speaking, deep neural networks include feedforward neural networks (FNNs) and recurrent neural networks (RNNs). In this paper, we will focus on FNNs, for example, MLPs. Another kind of FNNs is convolutional neural networks (CNNs) that share connections and weights locally. CNNs were developed on the basis of neocognitrons [23, 24]. In 1998, LeCun et al. combined convolutional layers with downsampling layers to design an early structure of modern CNNs, namely, LeNet [25]. In 2012, Krizhevsky et al. used rectified linear units (ReLUs) and graphics processing units (GPUs) to build a breakthrough model of CNNs, i.e. AlexNet [2], which won the 2012 ImageNet Large Scale Visual Recognition Challenge. Since then, CNNs get into a rapid growth full of brilliant achievements and great contributions in the development of deep learning. They not only take the lead in competitions of image classification and recognition as well as object localization and detection [26-31], but also in a variety of application systems such as deep Q-networks [32], AlphaGo [33], speech recognition [34], and machine translation [5].
Theoretically, a CNN can be regarded as a special MLP. It may consist of an input layer, alternating convolutional and pooling layers, a fully connected layer, and an output layer, as shown in Figure 2. In fact, convolutional layers (or "detection layers"), and pooling layers (or "downsampling layers"), are special hidden layers. A convolutional kernel means the weight of a convolutional layer. Besides LeNet and AlexNet, many variants of CNNs have been presented, such as VGGNet [26], GoogLeNet [29], SqueezeNet [35], SPPNet [36], ResNet [27], DenseNet [37], FCN [38], Faster R-CNN [39], Mask R-CNN [40], YOLO [41], SSD [42], and 3D CNN [43]. There have been so many models of deep neural networks with different structures, even containing shortcut connections, parallel connections, and nested structures. The problem of how to establish a unified framework for DNNs, is becoming a progressively important issue.

In 2017 and 2018, Hinton et al. published two papers on capsule networks [44, 45], to overcome the disadvantages of CNNs. Different from their motivation, we will use capsules to establish a unified framework from a novel point of view. The unified framework has something to do with computational graphs [46]. A computational graph visualizes data dependence relations as an acyclic graph [47]. It may be composed of input vertices, non-input vertices, and dependence edges. Input vertices stand for input variables, non-input vertices stand for operations or transformations. A dependence edge stands for a directed relation between two vertices with one preceding the other. In Figure 3, input vertices are labelled by "x0", "x1" and "x2", non-input vertices are labelled by "+", "−", "×", and "sin". The vertex "×" has two preceding vertices "+" and "−". The dependence edges are all linear relations. For example, the directed edge from "x1" to "+" has a weight of 3, meaning that 3x1 will be input into the vertex "+". It can be seen that x4 = (2x2)/(3x3) is the output of vertex "/", x5 = −x1 − 2x4 is the output of vertex "−", x6 = 3x1 + x2 is the output of vertex "×", x7 = 2x6 × 0.5x5 is the output of vertex "×", and x8 = sin(0.3x7) is the output of vertex "sin". If x1 = 2, x2 = 0 and x3 = 3, we have x4 = 0, x5 = −2, x6 = 6, x7 = −12, x8 = sin(−3.6).

Figure 3: A computational graph that visualizes data dependence relations.

Note that a computational graph may not be a neural network. But a neural network can be viewed as a special computational graph. Like a computational graph, a neural network may also be composed of input vertices, non-input vertices, and dependences edges (or directed connections). However, non-input vertices of a neural network are only chosen from a special set of transformations, which are generally non-linear functions, such as sigmoid, tanh and ReLU. Usually, these transformations are termed activation functions. The input of each activation function (or node) is taken as the weighted sum of the outputs of its preceding nodes and a bias.

This paper is an extension of [48]. The remainder is organized as follows. In Section 2, we propose a mathematical definition to formalize neural networks, give their directed graph representations, and prove a generation theorem about the induced networks of connected directed acyclic graphs. In Section 3, we use the concept of capsule to extend neural networks, define an induced model for capsule networks, and establish a unified framework for deep learning with a universal backpropagation algorithm. In Section 4, we discuss potential applications of the unified framework to graphical programming. Finally, we make conclusions with future work in Section 5.
2 Formalization of Neural networks

2.1 Mathematical definition

A neural network is a computational model composed of neurons (or nodes) and connections. Nodes are divided into input neurons and non-input neurons. Input neurons represent real variables, e.g. $x_1, x_2, \cdots, x_n$. A non-input neuron can receive signals through connections both from input neurons and the outputs of other non-input neurons, and perform a weighted sum of these signals following a transformation termed activation function.

Let $X = \{x_1, x_2, \cdots, x_n\}$ stand for a set of real variables, and $F$ for a set of activation functions. On $X$ and $F$, a neural network can be formally defined as a 4-tuple $\text{net} = (S, H, W, Y)$. The 4-tuple is termed a neural network if it can be recursively generated by the following four rules.

1) **Rule of variable.** For any $z \in X$, let $y_z = z$. Let $S = \{z\}$, $H = \emptyset$, $W = \emptyset$, $Y = \{y_z\}$. Then $\text{net} = (S, H, W, Y)$ is a neural network.

2) **Rule of neuron.** For any nonempty subset $S \subseteq X$, $\forall f \in F$, $\forall b \in \mathbb{R}$, construct a non-input neuron $h \notin X$ that depends on $(f, b)$, select weighting connections $w_{x_i \rightarrow h}(x_i \in S)$, and set $y_h = f(\sum_{x_i \in S} w_{x_i \rightarrow h} x_i + b)$. Let $H = \{h\}$, $W = \{w_{x_i \rightarrow h} | x_i \in S\}$, and $Y = \{y_h\}$. Then, $\text{net} = (S, H, W, Y)$ is a neural network.

3) **Rule of growth.** Suppose $\text{net} = (S, H, W, Y)$ is a neural network. For any nonempty subset $N \subseteq S \cup H$, $\forall f \in F$, $\forall b \in \mathbb{R}$, construct a non-input neuron $h \notin S \cup H$ that depends on $(f, b)$, select weighting connections $w_{z_j \rightarrow h}(z_j \in N)$, and set $y_h = f(\sum_{z_j \in N} w_{z_j \rightarrow h} y_{z_j} + b)$. Let $S' = S \cup \{h\}$, $H' = H \cup \{h\}$, $W' = W \cup \{w_{z_j \rightarrow h} | z_j \in N\}$, and $Y' = Y \cup \{y_h\}$. Then, $\text{net}' = (S', H', W', Y')$ is also a neural network.

4) **Rule of convergence.** Suppose $\text{net}_k = (S_k, H_k, W_k, Y_k)(1 \leq k \leq K)$ are $K$ neural networks, satisfying that $\forall 1 \leq i \neq j \leq K$, $(S_i \cup H_i) \cap (S_j \cup H_j) = \emptyset$. For any nonempty subsets $A_k \subseteq S_k \cup H_k(1 \leq k \leq K)$, $N = \bigcup_{k=1}^{K} A_k$, $\forall f \in F$, $\forall b \in \mathbb{R}$, construct a non-input neuron $h \notin \bigcup_{k=1}^{K} (S_k \cup H_k)$ that depends on $(f, b)$, select weighting connections $w_{z \rightarrow h}(z \in N)$, and set $y_h = f(\sum_{z \in N} w_{z \rightarrow h} y_z + b)$. Let $S = \bigcup_{k=1}^{K} S_k$, $H = \bigcup_{k=1}^{K} H_k \cup \{h\}$, $W = \bigcup_{k=1}^{K} W_k \cup \{w_{z \rightarrow h} | z \in N\}$, and $Y = \bigcup_{k=1}^{K} Y_k \cup \{y_h\}$, then $\text{net} = (S, H, W, Y)$ is also a neural network.

In the above four rules, weighting connection $w_{z \rightarrow h}$ is a data structure that contain the full information of the directed connection $z \rightarrow h$, including its strength, back-end neuron $z$ and front-end neuron $h$. Moreover, if a neuron $h$ depends on $(f, b)$, $f$ is called the activation function of $h$, and $b$ is called the bias of $h$. Additionally, if the 4-tuple $\text{net} = (S, H, W, Y)$ is a neural network, $S$ is called the set of input neurons, $H$ the set of non-input neurons, $W$ the set of weighting connections, and $Y$ the set of outputs. Finally, the rule of neuron can be deduced from the rule of variable and the rule of convergence. In fact, for any nonempty subset $S = \{x_{i_1}, x_{i_2}, \cdots, x_{i_r}\} \subseteq X$, we can use the rule of variable to generate $r$ neural networks $\text{net}_{r'} = (\{x_{r'}\}, \emptyset, \emptyset, \{x_{r'}\}) 1 \leq r' \leq r$. According to the rule of convergence, we can also use the $r$ networks to generate a new neural network $\text{net} = (S, H, W, Y)$, where $S = \bigcup_{r'=1}^{r} S_{r'}$, $H = \{h\}$, $W = \{w_{z \rightarrow h} | z \in S\}$, and $Y = \{y_h\}$. $\text{net}$ is exactly the rule of neuron.

![Diagram](image)

Figure 4: (a) A trivial network; (b) A 1-1 network

2.2 Directed graph representation

Let $X$ be a set of real variables and $F$ be a set of activation functions. For any neural network $\text{net} = (S, H, W, Y)$ on $X$ and $F$, a directed acyclic graph $G_{\text{net}} = (V, E)$ can be constructed with the set of vertices $V = S \cup H$ and the set of directed edges $E = \{z \rightarrow h | w_{z \rightarrow h} \in W\}$. $G_{\text{net}} = (V, E)$ is called the directed graph representation of $\text{net} = (S, H, W, Y)$. How to construct such a graph representation is detailed in the following two cases.
1) The case of $X = \{x_1\}$

For $x_1 \in X$, let $y_{x_1} = x_1$, $S = \{x_1\}$, $H = \emptyset$, $W = \emptyset$, $Y = \{y_{x_1}\}$. According to the rule of variable, $net = (S, H, W, Y)$ is a neural network, as shown in Figure 4(a). This network is called “trivial network”. It has only one input neuron, which does nothing.

Using the rule of growth on the 1-1 network, three different neural networks can be generated next, as shown in Figures 5(a-c). These networks are called “1-2 networks”. Each of them has one input neuron and two non-input neurons.

Using the rule of growth on the three 1-2 networks, twenty-one different neural networks can be totally generated further. They are all 1-3 networks, with seven displayed in Figures 6(a-g). The seven are generated from the network in Figure 5(a).

2) The case of $X = \{x_1, x_2\}$

For $x_1, x_2 \in X$, let $y_{x_1} = x_1$, $y_{x_2} = x_2$, $S_1 = \{x_1\}$, $S_2 = \{x_2\}$, $H_1 = H_2 = \emptyset$, $W_1 = W_2 = \emptyset$, $Y_1 = \{y_{x_1}\}$ and $Y_2 = \{y_{x_2}\}$. Using the rule of variable, $net_1 = (\{x_1\}, \emptyset, \emptyset, \{y_{x_1}\})$ and $net_2 = (\{x_2\}, \emptyset, \emptyset, \{y_{x_2}\})$ are neural networks. Obviously, both of them are trivial networks.
If $S = \{x_1, x_2\}, \forall f \in F, \forall b \in \mathbb{R}$, construct a non-input neuron $h_1 \notin S$ that depends on $(f, b)$, select weighting connections $w_{x_i \rightarrow h_1}(x_i \in S)$, and set $y_{h_1} = f(\sum_{x_i \in S} w_{x_i \rightarrow h_1} x_i + b)$. Let $H = \{h_1\}$, $W = \{w_{x_1 \rightarrow h_1}, w_{x_2 \rightarrow h_1}\}$, and $Y = \{y_{h_1}\}$. According to the rule of neuron, $net = (S, H, W, Y)$ is a neural network. This is a 2-1 network, as depicted in Figure 7. Using the rule of growth on the 2-1 network, seven different 2-2 networks can be generated next, as depicted in Figures 8(a-g).

Using the rule of growth on the seven networks in Figure 8, one hundred and five different neural networks can be totally generated further, with fifteen shown in Figures 9(a-o). The fifteen are all 2-3 networks, generated from the network in Figure 8(a).

Finally, the rule of convergence is necessary. In fact, it cannot generate all neural networks only using the three rules of variable, neuron and growth. An example is the network in Figure 10(c). Without the rule of convergence, this network cannot be generated from the two in Figures 10(a-b).

### 2.3 Induced network and its generation theorem

Suppose $G = (V, E)$ is a connected directed acyclic graph, where $V$ is the set vertices (nodes) and $E$ is the set of directed edges. For any vertex $h \in V$, let $IN_h = \{z|z \in V, z \rightarrow h \in E\}$ be the set of all vertices that precede $h$ adjacenty. Let $OUT_h = \{z|z \in V, h \rightarrow z \in E\}$ be the set of vertices that follow $h$ adjacenty. If $IN_h = \emptyset$, then $h$ is called an input node of $G$. If $OUT_h = \emptyset$, then $h$ is called an output node of $G$. Otherwise, $h$ is called a hidden node of $G$. Let $X$ stand for the set of all input nodes, $O$ for the set of all output nodes, and $M$ for the set of all hidden nodes. Obviously, $V = X \cup M \cup O$, and $M = V - X \cup O$.

Let $y_h$ be the output of node $h$, and $w_{z \rightarrow h}$ be the weighting connection from $z$ to $h$. Then, a computational model of graph $G$ is defined as follows:

1. $\forall z \in X, y_z = z$.
2. $\forall h \in M \cup O$, select $f \in F$ and $b \in \mathbb{R}$ to compute $y_h = f(\sum_{z \in IN_h} w_{z \rightarrow h} y_z + b)$.

Let $S = X \cup H \cup O$, $W = \{w_{z \rightarrow h}|z \rightarrow h \in E\}$, and $Y = \{y_h|h \in V\}$. Then, $net_G = (S, H, W, Y)$ is called an induced network of graph $G$. We have the following generation theorem.

**Generation Theorem:** For any connected directed acyclic graph $G = (V, E)$, its induced network $net_G$ is a neural network that can be recursively generated by the rules of variable, neuron, growth, and convergence.

**Proof:** By induction on $|V|$ (i.e. number of vertices), we prove the theorem as follows.

1. When $|V| = 1$, we have $|X| = 1$ and $|O| = 0$, so the induced network $net_G$ is a neural network
Figure 9: Fifteen 2-3 networks.

2) When $|V| = 2$, we have $|X| = 1$ and $|O| = 1$, so the induced network $net_G$ is a neural network that can be generated directly by the rule of variable.

3) Assume that the theorem holds for $|V| \leq n$. When $|V| = n + 1 \geq 3$, the induced network $net_G$ has at least one output node $h \in O$. Let $E_h = \{ z \to h \in E \}$ denote the set of edges heading to the node $h$. Moreover, let $V' = V - \{ h \}$ and $E' = E - E_h$. Based on the connectedness of $G' = (V', E')$, we have two cases to discuss in the following:

i) If $G' = (V', E')$ is connected, then applying the induction assumption for $|V'| \leq n$, the induced network $net_{G'} = (S', H', W', Y')$ can be recursively generated by the rules of variable, neuron, growth, and convergence. Let $N = IN_h$. In $net_G = (S, H, W, Y)$, we use $f \in F$ and $b \in \mathbb{R}$ to stand for the activation function and bias of node $h$, and $w_{z \to h}(z \in N)$ for the weighting connection from node $z$ to the node $h$. Then, $net_G$ can
be obtained by using the rule of growth on \( \text{net}_{G'} \), to generate the node \( h \) and its output
\[
y_h = f(\sum_{z \in N} w_{z \rightarrow h} y_z + b).
\]

ii) Otherwise, \( G' \) comprises a number of disjoint connected components \( G_k = (V_k, E_k) (1 \leq k \leq K) \). Using the induction assumption for \( |V_k| \leq n (1 \leq k \leq K) \), the induced network \( \text{net}_{G_k} = (S_k, H_k, W_k, Y_k) \) can be recursively generated by the rules of variable, neuron, growth, and convergence. Let \( A_k = (S_k \cup H_k) \cap IN_h \), and \( N = \bigcup_{k=1}^{K} A_k \). In \( \text{net}_{G} = (S, H, W; Y) \), we use \( f \in F \) and \( b \in \mathbb{R} \) to stand for the activation function and bias of the node \( h \), and \( w_{z \rightarrow h} (z \in N) \) for the weighting connection from node \( z \) to node \( h \). Then, \( \text{net}_{G} \) can be obtained by using the rule of convergence on \( \text{net}_{G_k} (1 \leq k \leq K) \), to generate the node \( h \) and its output \( y_h = f(\sum_{z \in N} w_{z \rightarrow h} y_z + b) \).

As a result, the theorem always holds.

Note that in the generation theorem, the rule of neuron can be deleted, because it can be deduced from the rule of variable and the rule of convergence.

3 Capsule framework of Deep learning

3.1 Mathematical definition of capsules

In 2017, Hinton et al. pioneered the idea of capsules and considered a nonlinear "squashing" capsule [45], as shown in Figure 11. The capsule has \( n \) input vectors \( u_1, u_2, \cdots, u_n \), and \( n \) weight matrices \( w_1, w_2, \cdots, w_n \). Let \( \hat{u}_i = w_i u_i (1 \leq i \leq n) \) be prediction vectors. The total input is \( s = \sum_i c_i \hat{u}_i = \sum_i c_i w_i u_i \), where \( c_i \) is a coupling coefficient between low-level capsule \( i \) and the capsule itself. The value of \( c_i \) is determined by a dynamic routing process, satisfying \( \sum_i c_i = 1 \). The output of the capsule \( v \) is a vector computed by the nonlinear squashing function
\[
v = squash(s) = \frac{\|s\|^2 s}{1 + \|s\|^2 \|s\|}.
\]
From the viewpoint of mathematical models, a capsule is essentially an extension of traditional activation functions. A traditional activation function has a scalar input and a scalar output. However, a capsule can have a vector input and a vector output. More generally, a capsule may have a tensor input and a tensor output. As shown in Figure 12, a capsule may have \( n \) input tensors \( X_1, X_2, \ldots, X_n \), \( n \) weight tensors \( W_1, W_2, \ldots, W_n \), and a bias \( B \). In addition, \( \otimes_1, \otimes_2, \ldots, \otimes_n \) are \( n \) weighting operations, which may be taken as "identity transfer", "scalar multiplication", "dot product", "matrix multiplication", "convolution", and so on. Meanwhile, \( W_i \otimes_i X_i (1 \leq i \leq n) \) and \( B \) must be tensors with the same dimension. The total input of the capsule is \( U = \sum W_i \otimes_i X_i + B \), and the output \( Y \) is a tensor computed by a nonlinear capsule function \( \text{cap} \), namely,

\[
Y = \text{cap}(U) = \text{cap}\left(\sum_i W_i \otimes_i X_i + B\right).
\]

According to Eq. (2), a capsule is a generalization of scalar activation function with scalar inputs.

### 3.2 Definition of Capsule Networks

For convenience, we use \( F \) to stand for a nonempty set of capsule functions, and \( T \) for the set of all tensors.

Suppose \( G = (V, E) \) is a connected directed acyclic graph, where \( V \) denotes the set of vertices and \( E \) denotes the set of directed edges. For any vertex \( H \in V \), let \( IN_H \) be the set of all vertices that precede \( H \) adjacently. Let \( OUT_H \) be the set of vertices that follow \( H \) adjacently. If \( IN_H = \emptyset \), then \( H \) is called an input vertex of \( G \). If \( OUT_H = \emptyset \), then \( H \) is called an output vertex of \( G \). Otherwise, \( H \) is called a hidden vertex of \( G \). Let \( \mathcal{X} \) stand for the set of all input vertices, \( \mathcal{O} \) for the set of all output vertices, and \( \mathcal{M} \) for the set of all hidden vertices. Obviously, \( \mathcal{V} = \mathcal{X} \cup \mathcal{M} \cup \mathcal{O} \), and \( \mathcal{M} = \mathcal{V} - \mathcal{X} \cup \mathcal{O} \).

Furthermore, let \( Y_H \) be the output of vertex \( H \), and \( (W_{Z \rightarrow H}, \otimes Z \rightarrow H) \) be the tensor-weighting connection from \( Z \) to \( H \). If \( \forall H \in \mathcal{M} \cup \mathcal{O}, \forall Z \in IN_H, W_{Z \rightarrow H} \otimes Z \rightarrow H \) \( Y_Z \) and \( B \) are tensors with the same dimension, then a tensor-computational model of graph \( G \) is defined as follows:

1) \( \forall Z \in \mathcal{X}, Y_Z = Z \),

2) \( \forall H \in \mathcal{M} \cup \mathcal{O}, \) select \( \text{cap} \in F \) and \( B \in T \) to compute \( Y_H = \text{cap}(\sum_{Z \in IN_H} W_{Z \rightarrow H} \otimes Z \rightarrow H Y_Z + B) \).

Let \( S = \mathcal{X}, \mathcal{H} = \mathcal{M} \cup \mathcal{O}, \mathcal{W} = \{(W_{Z \rightarrow H}, \otimes Z \rightarrow H) | Z \rightarrow H \in \mathcal{E}\} \), and \( \mathcal{Y} = \{Y_H | H \in \mathcal{V}\} \). Then, \( \text{net}_G = (\mathcal{S}, \mathcal{H}, \mathcal{W}, \mathcal{Y}) \) is called a tensor-induced network of graph \( G \). This network is also called a capsule network, where the vertices stand for capsules, and the directed edges for weighting connections. If \( \text{net}_G = (\mathcal{S}, \mathcal{H}, \mathcal{W}, \mathcal{Y}) \) is a capsule network, \( \mathcal{S} \) is called the set of input capsules, \( \mathcal{H} \) the set of non-input capsules, \( \mathcal{W} \) the set of weighting connections, and \( \mathcal{Y} \) the set of output tensors.

Using a capsule network, a MLP can be simplified as a directed acyclic path. For example, the MLP in Figure 1 can be represented as the capsule path in Figure 13. In fact, this MLP has five layers: one input layer, three hidden layers, and one output layer. On the whole, each layer can be thought of as a capsule. Let \( X = (x_1, x_2, \ldots, x_5)^T \) stand for the input capsule, \( H_i = (\text{cap}_i, B_i) (i = 1, 2, 3) \) for the hidden capsules, and \( O = (\text{cap}_4, B_4) \) for the output capsule. The capsule function \( \text{cap}_i \) is defined by the elementwise activation function, and the capsule bias \( B_i \) by the bias vector. If all the weighting operations \( \otimes X \rightarrow H_1, \otimes H_1 \rightarrow H_2, \otimes H_2 \rightarrow H_3, \) and \( \otimes H_3 \rightarrow O \) are all taken as matrix multiplication "\( \times \)" then we are easy to obtain \( W_{X \rightarrow H_1} \otimes X \rightarrow H_1 = ((u_{m,n}^{H_1})_{7 \times 5}, \times) \), \( (W_{H_1 \rightarrow H_2}, \otimes H_1 \rightarrow H_2) = ((u_{m,n}^{H_2})_{7 \times 7}, \times) \), \( (W_{H_2 \rightarrow H_3}, \otimes H_2 \rightarrow H_3) = ((u_{m,n}^{H_3})_{7 \times 7}, \times) \), and \( (W_{H_3 \rightarrow O}, \otimes H_3 \rightarrow O) = ((u_{m,n}^{H_3})_{4 \times 7}, \times) \), which are the tensor-weighting connections from \( H_0 = X \) to \( H_1, H_1 \) to \( H_2, H_2 \) to \( H_3 \) and \( H_3 \) to \( O \). Finally, let \( Y_{H_i} (i = 1, 2, 3) \) stand for the output vector of \( H_i \), and \( Y_O \) for the output vector of \( O \). Setting \( Y_{H_0} = X \) and \( Y_{H_1} = Y_O \), we have \( Y_{H_1} = \text{cap}_1(W_{H_{i-1} \rightarrow H_i} \times Y_{H_{i-1}} + B_i) \) for \( 1 \leq i \leq 4 \). This means that the MLP in Figure 1 can be represented as the capsule path in Figure 13.

![Figure 13: A capsule structure of MLP, with "\( \times \)" standing for matrix multiplication.](image)
Besides MLPs, capsule networks can also be used to simplify the structures of other DNNs. For example, the CNN in Figure 2 can be represented as the capsule path in Figure 14. In fact, this CNN has 7 layers: one input layer, two convolutional layers, two downsampling (pooling) layers, one fully connected layer, and one output layer. On the whole, each of the layers can be thought of as a capsule. Let \( X \) stand for the input capsule, \( H_i = (cap_i, B_i)(i = 1, \cdots, 5) \) for the hidden capsules, and \( O = (cap_6, B_6) \) for the output capsule. The capsule functions \( cap_1 \) and \( cap_3 \) are defined by the elementwise ReLU function. \( cap_2 \) and \( cap_4 \) are defined by down sampling "\( \downarrow \)". \( cap_5 \) is the identity function. \( cap_6 \) is the softmax function. Moreover, the capsule biases \( B_i(i = 1, \cdots, 6) \) are each defined by the bias tensor of the corresponding layer. Let both \( \otimes_{X \rightarrow H_i} \) and \( \otimes_{H_i \rightarrow H_{i+1}} \) be convolution operation "\( \ast \)"; both \( \otimes_{H_i \rightarrow H_{i+1}} \) and \( \otimes_{H_1 \rightarrow H_2} \) be identity transfer "\( \rightarrow \)"; \( \otimes_{H_1 \rightarrow H_2} \) be tensor-reshaping operation "\( \triangleleft \)"; and \( \otimes_{H_i \rightarrow O} \) be matrix multiplication "\( \times \)". Then, \( (W_{X \rightarrow H_1}, \otimes_{X \rightarrow H_1}) = (W_{X \rightarrow H_1}, \ast) \), \( (W_{H_1 \rightarrow H_2}, \otimes_{H_1 \rightarrow H_2}) = (\ast, \rightarrow) \), \( (W_{H_2 \rightarrow H_3}, \otimes_{H_2 \rightarrow H_3}) = (W_{H_2 \rightarrow H_3}, \ast) \), \( (W_{H_3 \rightarrow H_4}, \otimes_{H_3 \rightarrow H_4}) = (\ast, \rightarrow) \), \( (W_{H_4 \rightarrow H_5}, \otimes_{H_4 \rightarrow H_5}) = (\ast, \triangleleft) \), \( (W_{H_5 \rightarrow O}, \otimes_{H_5 \rightarrow O}) = (W_{H_5 \rightarrow O}, \times) \) which are tensor-weighting connections from \( X \) to \( H_1 \), \( H_1 \) to \( H_2 \), \( H_2 \) to \( H_3 \), \( H_3 \) to \( H_4 \), \( H_4 \) to \( H_5 \), and \( H_5 \) to \( O \). Finally, we have

\[
\begin{align*}
Y_{H_1} &= cap_1(W_{X \rightarrow H_1} \ast X + B_1) = ReLU(W_{X \rightarrow H_1} \ast X + B_1), \\
Y_{H_2} &= cap_2(\rightarrow Y_{H_1} + B_2) = \downarrow Y_{H_1} + B_2, \\
Y_{H_3} &= cap_3(W_{H_2 \rightarrow H_3} \ast Y_{H_2} + B_3) = ReLU(W_{H_2 \rightarrow H_3} \ast Y_{H_2} + B_3), \\
Y_{H_4} &= cap_4(\rightarrow Y_{H_3} + B_4) = \downarrow Y_{H_3} + B_4, \\
Y_{H_5} &= cap_5(\triangleleft Y_{H_4} + B_5) = \triangleleft Y_{H_4}, \\
Y_O &= cap_6(W_{H_5 \rightarrow O} \times Y_{H_5} + B_6) = softmax(W_{H_5 \rightarrow O} \times Y_{H_5} + B_6).
\end{align*}
\]

According to Eq. (3), the CNN in Figure 2 can be represented as the capsule path in Figure 14.

**Figure 14:** A Capsule structure of CNN, with "\( \ast \)" standing for convolution operation, "\( \rightarrow \)" for identity transfer, "\( \triangleleft \)" for tensor reshaping, and "\( \times \)" for matrix multiplication.

### 3.3 Types of capsule networks

As mentioned in Section 3.2, a MLP can be simplified as a path structure composed of capsules, so can many CNNs (e.g. LeNet and VGGNet). Note that the path structure is a special case of layered structure. Generally speaking, capsule networks can be divided into two types: layered capsule networks and skip capsule networks. A layer capsule network can only have weighting connections must between two adjacent layers (see Figure 15), whereas a skip capsule network may have weighting connections between any two layers (see Figure 16).

**Figure 15:** A layered capsule network with 5 layers.

Suppose \( G = (\mathcal{V}, \mathcal{E}) \) is a connected directed acyclic graph, and \( net_G = (S, H, V, Y) \) is a tensor-induced network of graph \( G \). We have \( V = S \cup H \) and \( H = M \cup O \). The capsule network \( net_G \) is called "layered" if the set of hidden capsules \( M \) can be partitioned into a number of disjoint subsets \( M_1, M_2, \cdots, M_k \), such that
A capsule network is a tensor-induced network of graph $G$. Accordingly, the total loss function can be computed by

$$\delta = \text{cap}_H(U_H) = \text{cap}_H(\sum_{Z \in IN_H} W_{Z \rightarrow H} \otimes Z \rightarrow H Y_Z + B_H).$$

Let $\delta_H$ denote the backpropagated error signal (or sensitivity) for capsule $H$. By the chain rule, we can express $\delta_H$ as

$$\delta_H = \frac{\partial L}{\partial W_{Z \rightarrow H}} \delta_H = \sum_{P \in OUT_H} \delta_P \cdot \frac{\partial L}{\partial U_H} \cdot \frac{\partial U_H}{\partial W_{Z \rightarrow H}}.$$

Figure 16: A skip capsule network.

1. $M = M_1 \cup M_2 \cup \cdots \cup M_k$, $M_0 = S$, $M_{k+1} = O$,
2. $\forall H \rightarrow H' \in E$, $\exists i \in \{0, 1, \cdots, k\}$, $H \in M_i$ and $H' \in M_{i+1}$,
3. $\forall H, H' \in M_i (i = 0, 1, \cdots, k + 1)$, $H \rightarrow H' \notin E$ and $H' \rightarrow H \notin E$.

If $\text{net}_G = (S, H, W, V)$ is not "layered", it is called "skip".

In Figure 15, we are easy to have a layered structure: $M_0 = \{X_1, X_2\}$, $M_1 = \{H_3, H_4, H_5\}$, $M_2 = \{H_6, H_7\}$, $M_3 = \{H_8, H_9, H_{10}\}$ and $M_4 = \{O_1, O_2, O_3\}$. However, in Figure 16, we cannot have such a layered structure.

### 3.4 Universal backpropagation of capsule networks

A capsule network is a tensor-induced network of graph $G = (V, E)$. It can be denoted as $\text{net}_G = (S, H, W, V)$. Let the set of input capsules $S = X = \{X_1, X_2, \cdots, X_n\}$. Suppose $O = \{O_1, O_2, \cdots, O_m\}$ is the set of output capsules. Then, $H = V - S$ is the set of non-input capsules, and $M = V - X \cup O = \{H_1, H_2, \cdots, H_i\}$ is the set of hidden capsules.

If the total number of capsules $|S \cup H| \geq 2$, then for $\forall H \in H$, we have

$$U_H = \sum_{Z \in IN_H} W_{Z \rightarrow H} \otimes Z \rightarrow H Y_Z + B_H,$$

$$Y_H = \text{cap}_H(U_H) = \text{cap}_H(\sum_{Z \in IN_H} W_{Z \rightarrow H} \otimes Z \rightarrow H Y_Z + B_H).$$

For any output node $H \in O$, let $Y_H$ and $T_H$ be its actual output tensor and expected output tensor respectively for the set of input capsules $S = X$. The loss function between the two tensors is defined as

$$L_H = \text{Loss}(Y_H, T_H).$$

Accordingly, the total loss function can be computed by

$$L = \sum_{H \in O} L_H.$$
Additionally, the capsule framework can be potentially applied to designing a graphical programming platform significantly. Based on a set of standard graphical symbols for capsule networks and plain networks, we can implement deep neural networks by drawing them directly instead of coding. Using this training algorithm on pairs in many iterations, which is detailed in Algorithm 1.

Algorithm 1: One iteration of the universal backpropagation algorithm.

1) Select a learning rate $\eta > 0$.
2) $\forall H \in \mathcal{M} \cup \mathcal{O}$, $\forall Z \in \mathcal{I}_H$, initialize $W_{Z \rightarrow H}$ and $B_H$.
3) $\forall H \in \mathcal{O}$, compute $\delta_H = \frac{\partial \text{Loss}(Y_H, T_H)}{\partial Y_H} \cdot \frac{\partial \text{cap}_H}{\partial U_H}$, $\forall H \in \mathcal{M}$, compute $\delta_H = \sum_{p \in \mathcal{OUT}_H} \delta_p \cdot \frac{\partial \text{cap}_H}{\partial U_H}$.
4) Compute $\Delta W_{Z \rightarrow H} = \delta_H \cdot \frac{\partial U_H}{\partial W_{Z \rightarrow H}}$ and $\Delta B_H = \delta_H$.
5) Compute $\Delta W_{Z \rightarrow H} \leftarrow W_{Z \rightarrow H} - \eta \cdot \Delta W_{Z \rightarrow H}, B_H \leftarrow B_H - \eta \cdot \Delta B_H$.
6) Update $W_{Z \rightarrow H} \leftarrow W_{Z \rightarrow H} - \eta \cdot \Delta W_{Z \rightarrow H}, B_H \leftarrow B_H - \eta \cdot \Delta B_H$.

Algorithm 2: A universal backpropagation algorithm on training pairs in many iterations.

Input: training pairs $(X^k, T^k)(k = 1, \cdots, K)$, Output: $W_{Z \rightarrow H}, \Delta W_{Z \rightarrow H}, B_H, \Delta B_H$.

Select a learning rate $\eta > 0$, $\forall H \in \mathcal{M} \cup \mathcal{O}, \forall Z \in \mathcal{I}_H$, initialize $W_{Z \rightarrow H}$ and $B_H$.

for iter = 1:max_iter
for $\forall H \in \mathcal{O}$, do $\delta_H^{Y_H} = \frac{\partial \text{Loss}(Y_H, T_H)}{\partial Y_H} \cdot \frac{\partial \text{cap}_H}{\partial U_H}$ end for

for $\forall H \in \mathcal{M}$, do $\delta_H^k = \sum_{p \in \mathcal{OUT}_H} \delta_p \cdot \frac{\partial \text{cap}_H}{\partial U_H}$ end for

$\Delta W_{Z \rightarrow H} = \sum_{k=1}^K \delta_H^k \cdot \frac{\partial \text{cap}_H}{\partial W_{Z \rightarrow H}}$ and $\Delta B_H = \sum_{k=1}^K \delta_H^k$.

$W_{Z \rightarrow H} \leftarrow W_{Z \rightarrow H} - \eta \cdot \Delta W_{Z \rightarrow H}, B_H \leftarrow B_H - \eta \cdot \Delta B_H$.
end for

It should be noted that in formulae (7)-(8), the computation of $\frac{\partial \text{cap}_H}{\partial U_H}$ depends on the specific form of capsule function $\text{cap}_H$. For example, when $\text{cap}_H$ is an elementwise sigmoid function, the result is:

$$\frac{\partial \text{cap}_H}{\partial U_H} = \text{sigmoid}(U_H)(1 - \text{sigmoid}(U_H)). (9)$$

Additionally, $\frac{\partial U_H}{\partial W_{Z \rightarrow H}}$ and $\frac{\partial U_H}{\partial Y_H}$ also depend on the specific choice of weighting operation $\otimes_{Z \rightarrow H}$.

Based on formulae (7)-(8), a universal backpropagation algorithm can be designed for capsule networks, with one iteration detailed in Algorithm 1. This algorithm can have many variants from different forms of gradient descent [49].

In practice, we need a training algorithm on pairs $(X^k, T^k)(k = 1, \cdots, K)$, where $X^k = \{X^k_1, X^k_2, \cdots, X^k_n\}$ and $T^k = \{T^k_1, T^k_2, \cdots, T^k_n\}$. For any $H \in \mathcal{O}$, we have the loss between $Y_H$ and $T_H$.

$$L^k_H = \text{Loss}(Y^k_H, T^k_H). (10)$$

and the total loss for the $k$-th pair:

$$L^k = \sum_{H \in \mathcal{O}} L^k_H. (11)$$

Therefore, we can compute the total loss for all training pairs as follows

$$L = \sum_{k=1}^K L^k = \sum_{k=1}^K \sum_{H \in \mathcal{O}} L^k_H. (12)$$

Using gradient descent on formula (12), we can have a universal backpropagation algorithm on training pairs in many iterations, which is detailed in Algorithm 2.

4 Potential Applications to Graphical Programming

The capsule framework can be potentially applied to designing a graphical programming platform based on a set of standard graphical symbols for capsule networks and plain networks. Using this platform, we can implement deep neural networks by drawing them directly instead of coding. The platform is not only expected to make easier deep learning, but also to promote its development significantly.
4.1 Standard graphical symbols for capsule networks

In future applications, the capsule framework will be able to provide a theoretical basis for graphical programming on deep learning. Under the framework, we can design a set of standard graphical symbols to draw capsule networks, mainly including capsule symbols and connection symbols.

Figure 17: Examples of standard capsule symbols: (a) 1D-data capsule, (b) 2D-data capsule, (c) 2D-ReLU capsule, (d) 2D-maximum downsampling capsule, (e) 1D-identical capsule, (f) 1D-ReLU capsule, (g) 1D-softmax capsule.

Some of standard capsule symbols are shown in Figure 17 (a-g), such as 1D-data capsule, 2D-data capsule, 2D-ReLU capsule, 2D-maximum downsampling capsule, 1D-identical capsule, 1D-ReLU capsule, and 1D-softmax capsule. Their types and attributes are listed in Table 1, with more detail given as follows.

1) 1D-data capsule is a structure of vector array for the input of a capsule network. It can be represented as $X = (x_1, \ldots, x_M)$, with 2 basic attributes: dimension $M$ and data type $T$ (e.g. float64).

2) A 2D-data capsule is a structure of matrix array for the input of a capsule network. It can be represented as $X = (X_1, \ldots, X_d)$, with 4 basic attributes: height $M$, width $N$, channel number $d$, and data type $T$. Moreover, each $X_i (1 \leq i \leq d)$ is a matrix of size $M \times N$ and data type $T$.

3) A 2D-ReLU capsule transforms a matrix array input into another matrix array output with elementwise ReLU. It has four basic attributes: height $M$, width $N$, channel number $d$, and data type $T$. Its input is a matrix array $X = (X_1, \ldots, X_d)$, where each $X_i$ is of size $M \times N$ and data type $T$. Its output is also a matrix array $Y = (Y_1, \ldots, Y_d)$, defined as:

$$Y = \text{ReLU}(X) = (\text{ReLU}(X_1), \ldots, \text{ReLU}(X_d)).$$

(13)

4) A 2D-maximum downsampling capsule transforms a matrix array input into another matrix array output with maximum downsampling function $\downarrow_{\lambda, \tau}^{\text{max}}$. It has five basic attributes: height $M$, width $N$, channel number $d$, downsampling window $\lambda \times \tau$, and data type $T$. Its input is a matrix array $X = (X_1, \ldots, X_d)$, where each $X_i$ is of size $M \times N$ and data type $T$. Its output is also a matrix array $Y = (Y_1, \ldots, Y_d)$, defined as:

$$Y = \downarrow_{\lambda, \tau}^{\text{max}}(X) = (\downarrow_{\lambda, \tau}^{\text{max}}(X_1), \ldots, \downarrow_{\lambda, \tau}^{\text{max}}(X_d)),$$

(14)

$$Y_i = \downarrow_{\lambda, \tau}^{\text{max}}(X_i) = (\downarrow_{\lambda, \tau}^{\text{max}}(G_{\lambda, \tau}^A(X_i))).$$

(15)

where $G_{\lambda, \tau}^A$ denotes the non-overlapping block matrix of $A$ divided by $\lambda \times \tau$. If $A$ is a $M \times N$ matrix, then $G_{\lambda, \tau}^A$ is a block matrix that contains $\frac{M}{\lambda}$ rows and $\frac{N}{\tau}$ columns. The $i,j$-th block can be
expressed as
\[ G_{\lambda, \tau}^A(i, j) = (a_{st})_{\lambda \times \tau}, (i - 1) \times \lambda + 1 \leq s \leq i \times \lambda, (j - 1) \times \tau + 1 \leq t \leq j \times \tau. \] (16)

The maximum downsampling of \( G_{\lambda, \tau}^A(i, j) \) is defined as
\[ \downarrow_{\lambda, \tau}^{\text{max}} (G_{\lambda, \tau}^A(i, j)) = \max \{a_{st}| (i - 1) \times \lambda + 1 \leq s \leq i \times \lambda, (j - 1) \times \tau + 1 \leq t \leq j \times \tau\}. \] (17)

The maximum downsampling of \( G_{\lambda, \tau}^A \) is defined as
\[ \downarrow_{\lambda, \tau}^{\text{max}} G_{\lambda, \tau}^A = (\downarrow_{\lambda, \tau}^{\text{max}} (G_{\lambda, \tau}^A(i, j))). \] (18)

5) A 1D-identical capsule transforms a vector input into another vector output with the identical function \( I \). It has two basic attributes: dimension \( M \) and data type \( T \). Its input is a vector \( \mathcal{X} = (X) = X \) of dimension \( M \) and data type \( T \). Its output is also a vector \( \mathcal{Y} = Y \), defined as:
\[ Y = I(X) = X. \] (19)

6) A 1D-ReLU capsule transforms a vector input into another vector output with elementwise ReLU. It has two basic attributes: dimension \( M \) and data type \( T \). Its input is a vector \( \mathcal{X} = X \) of dimension \( M \) and data type \( T \). Its output is a vector \( \mathcal{Y} = Y \), defined as:
\[ Y = \text{ReLU}(X). \] (20)

7) A 1D-softmax capsule transforms a vector input into another vector output with function \( \text{softmax} \). It has two basic attributes: dimension \( M \) and data type \( T \). Its input is a vector \( \mathcal{X} = X \) of dimension \( M \) and data type \( T \). Its output is a vector \( \mathcal{Y} = Y \), defined as:
\[ Y = \text{softmax}(X). \] (21)

Figure 18: Examples of standard connection symbols: (a) convolutional connection, (b) transfer connection, (c) reshaping connection, (d) full connection.

Table 2: Types and attributes of several types of standard connected graphical symbols.

| Connection types          | Attributes                           |
|---------------------------|--------------------------------------|
| Convolutional connection  | (height \( M \), width \( N \), channel number \( d \), data type \( T \)) |
|                           | (kernel number \( k \), height \( m \), width \( n \), channel number \( d \), stride \( s \), data type \( T \)) |
|                           | (height \( M - m + 1 \), width \( N - n + 1 \), channel number \( k \), data type \( T \)) |
| Transfer connection       | (height \( M \), width \( N \), channel number \( d \), data type \( T \)) |
|                           | (height \( M \), width \( M \), data type \( T \)) |
|                           | (height \( M \), width \( N \), channel number \( d \), data type \( T \)) |
| Reshaping connection      | (height \( M \), width \( N \), channel number \( d \), data type \( T \)) |
|                           | (dimension \( M \), channel number \( M \), data type \( T \)) |
|                           | (dimension \( dN \), data type \( T \)) |
| Full connection           | (dimension \( N \), data type \( T \)) |
|                           | (height \( M \), width \( N \), data type \( T \)) |
|                           | (dimension \( N \), data type \( T \)) |

Some of standard connection symbols are shown in Figure 18, such as "convolutional connection", "transfer connection", "reshaping connection", and "full connection". Their types and attributes are listed in Table 2 and further explained as follows.

1) A convolutional connection transforms the back-end capsule into the front-end capsule with convolution operation. It has three attributes: back-end structure, weight structure and front-end
structure. The back-end structure is a matrix array \( \mathcal{X} = (X_1, \cdots, X_d) \), where each \( X_i \) is of size \( M \times N \) and data type \( T \). The weight structure is a \( k \)-kernel tensor array \( \mathcal{W} = (W_1, \cdots, W_k) \) with \( W_i (1 \leq i \leq k) \) representing the \( i \)-th convolutional kernel. Moreover, the tensor \( W_i = (W_{i1}, \cdots, W_{id}) \) is a \( d \)-channel matrix array, where each \( W_{ij} \) is of size \( m \times n \) and data type \( T \). The front-end structure \( \mathcal{Y} = (Y_1, \cdots, Y_d) \) is also a matrix array, defined as:

\[
\mathcal{Y} = \mathcal{W} \ast \mathcal{X} = (W_1 \ast \mathcal{X}, \cdots, W_k \ast \mathcal{X}),
\]

where

\[
Y_i = W_i \ast \mathcal{X} = \sum_{j=1}^{d} W_{ij} \ast X_j.
\]

Note that \( W_{ij} \ast X_j \) is calculated by matrix convolution. If \( A_{m \times n} \) and \( B_{M \times N} \) are two matrices, then their \( s \)-stride convolution \( C = (c_{ij}) = A_{m \times n} * B_{M \times N} \) is a matrix of size \( (\frac{M-m}{s}+1) \times (\frac{N-n}{s}+1) \) and data type \( T \), with \( c_{ij} \) defined as:

\[
c_{ij} = \sum_{u=1}^{m} \sum_{v=1}^{n} a_{uv} \cdot b_{is+u-1,js+v-1}, 1 \leq i \leq \frac{M-m}{s}+1, 1 \leq j \leq \frac{N-n}{s}+1.
\]

\[2\) A transfer connection transforms the back end into the front end with identity operation. It has three attributes: back-end structure, weight structure and front-end structure. The back-end structure is a matrix array \( \mathcal{X} = (X_1, \cdots, X_d) \), where each \( X_i \) is of size \( M \times N \) and data type \( T \). The weight structure \( \mathcal{W} = I \) is the identity matrix of size \( M \times M \) and data type \( T \). The front-end structure \( \mathcal{Y} = (Y_1, \cdots, Y_d) \) is also a matrix array, defined as:

\[
\mathcal{Y} = \mathcal{W} \times \mathcal{X} = (W_1 \times X_1, \cdots, W_d \times X_d) = (I \times X_1, \cdots, I \times X_d) = (X_1, \cdots, X_d) = \mathcal{X},
\]

where \( Y_i = I \times X_i = X_i (1 \leq i \leq d) \).

\[3\) A reshaping connection transforms the back end into the front end with reshaping operation. It has three attributes: back-end structure, weight structure and front-end structure. The back-end structure is a matrix array \( \mathcal{X} = (X_1, \cdots, X_d) \), where each \( X_i \) is of size \( M \times N \) and data type \( T \). The weight structure is a \( d \)-channel vector array \( \mathcal{W} = (W_1, \cdots, W_M) \), where \( W_i = (0, \cdots, 1, 0, \cdots, 0)(1 \leq i \leq M) \) is an \( M \)-dimensional vector. The front-end structure \( \mathcal{Y} \) is an \( NMd \)-dimensional vector, defined as:

\[
\mathcal{Y} = (Y_1, \cdots, Y_{Md}) = (Y_{11}, Y_{21}, \cdots, Y_{M1}, \cdots, Y_{1d}, \cdots, Y_{Md}) = W \times \mathcal{X} = W \times (X_1, \cdots, X_d) = (W \times X_1, \cdots, W \times X_d) = (W_1 \times X_1, \cdots, W_M \times X_d, W_1 \times X_1, \cdots, W_M \times X_d),
\]

where \( Y_{ij} = W_i \times X_j (1 \leq i \leq M, 1 \leq j \leq d) \) is the \( i \)-th row of \( X_j \), and it is an \( N \)-dimensional vector.

\[4\) A full connection transforms the back end into the front end with matrix multiplication. It has three attributes: back-end structure, weight structure and front-end structure. The back-end structure is an \( N \)-dimensional vector \( \mathcal{X} = X \). The weight structure \( \mathcal{W} = W \) is a matrix of size \( M \times N \) and data type \( T \). The front-end structure \( \mathcal{Y} = Y \) is an \( M \)-dimensional vector, defined as:

\[
\mathcal{Y} = \mathcal{W} \times \mathcal{X} = Y = W \times X.
\]

\[4.2 \) Standard graphical symbols for plain networks

As a special case of capsule networks, plain networks can also be implemented by drawing them with standard graphical symbols, such as "data neuron", "ReLU neuron", "identical neuron", "arrow amplifying connection", and "amplifying connection". Some of these graphical symbols are shown in Figure 19(a-e).

A data neuron is a scalar input with data type \( T \). A ReLU neuron transforms a scalar input \( x \) into another scalar output \( y \) with activation function ReLU, defined as:

\[
y = ReLU(x).
\]
Figure 19: Graphical symbols for plain networks: (a) data neuron; (b) ReLU neuron; (c) identical neuron; (d) arrow amplifying connection; (e) amplifying connection.

An identical neuron plays the identical function, namely,
\[ y = I(x) = x. \]  
(29)

An (arrow) amplifying connection transforms the back end into the front end with amplification. It has three attributes: back-end scalar \( x \), weight strength \( w \), and front-end scalar \( y \). The value of \( y \) is computed by:
\[ y = wx. \]  
(30)

In case of no ambiguity, amplifying connection can be in place of arrow amplifying connection.

4.3 Graphical programming

Based on graphical symbols of capsules and their connections, we can design a graphical programming platform to implement deep neural networks. For example, we can implement MLP and LeNet by drawing the capsule graphs in Figures 20-21.

Figure 20: A graphical representation of the capsuled MLP, which is orderly composed of 1D-data capsule (a), 1D-ReLU capsule (b), 1D-ReLU capsule (c), and 1D-identical capsule (d).

Figure 21: A graphical representation of the capsuled LeNet, which is orderly composed of 2D-data capsule (a), 2D-ReLU capsule (b), 2D-ReLU capsule (c), 2D-maximum downsampling capsule (d), 2D-maximum downsampling capsule (e), 1D-identical capsule (f), 1D-ReLU capsule (g), and 1D-softmax capsule (h).

As shown in Figure 20, the capsuled MLP consists of one 1D-data capsule, two 1D-ReLU capsules, and one 1D-identical capsule, together with three full connections. The dimensions of the capsules can be set to 2, 6, 4 and 2, with the same type of "float64". Accordingly, the full connection between module (a) and module (b) must have a back end with dimension=2 and data type = "float64", a weight matrix with height = 6, width = 2 and data type = "float64", and a front end with dimension = 6 and data type = "float64". The full connection between module (b) and module (c) must have a back end with dimension=6 and data type = "float64", a weight matrix with height =4, width =6 and data type = "float64", and a front end with dimension = 4 and data type = "float64". The full connection between module (c) and module (d) must have a back end with dimension=4 and data type = "float64", a weight matrix with height =2, width =4 and data type = "float64", and a front end with dimension = 2 and data type = "float64". Therefore, the capsuled MLP is equivalent to the plain MLP depicted in Figure 22.

As shown in Figure 21, the capsuled LeNet consists of one 2D-data capsule, two 2D-ReLU capsules, two 2D-maximum downsampling capsules, one 1D-identical capsule, one 1D-ReLU capsule and one 1D-softmax capsule, together with two convolutional connections, two transfer connections, one reshaping connection and two full connections. If the LeNet is applied to the MNIST dataset [50], module (a) can be a 2D-data capsule with height=28, weight=28, channel number=1, and data type =
"float64". Module (b) can be a 2D-ReLU capsule with height = 24, width = 24, channel number = 32, and data type = "float64". The convolution connection between module (a) and module (b) can have a back end with height=28, weight=28, channel number=1, and data type = "float64", and a weight structure with kernel number= 32, height = 5, width = 5, channel number = 1, stride = 1, and data type = "float64", and a front end with height = 24, width = 24, channel number = 32, and data type = "float64". The other modules and their connections can be determined compatibly in a similar manner.

Like LeNet, we can implement AlexNet (see Figure 23) by drawing its capsule graph displayed in Figure 24. Using more graphical symbols, we can similarly implement VGGNet, GoogLeNet, ResNet, and so on. Moreover, we can even implement a deep neural network with flexible connections in Figure 25, and a deep capsule network with flexible connections in Figure 26. Obviously, drawing is easier, simpler and more convenient than coding in popular deep learning platforms such as Caffe, TensorFlow, MXNet, and CNTK.

5 Conclusions

We have used capsule networks to establish a unified framework of deep learning. We not only present a strict mathematical definition of neural networks, but also a generation theorem to clarify the intrinsic relationship between feedforward neural networks and connected directed acyclic graphs. As a generalization of neural networks, we obtain two types of capsule networks (i.e. layered and skip) to represent and extend various deep learning models. Additionally, we derive a
universal backpropagation algorithm for capsule networks, and demonstrate its potential applications to graphical programming in combination with standard graphical symbols of plain networks and capsule networks. On a graphical programming platform, we can implement a variety of deep neural networks by drawing them directly, such as MLP, LeNet, AlexNet, and many others. Therefore, this kind of platform will make easier deep learning with beneficial complement to popular deep learning frameworks, such as Caffe, TensorFlow, MXNet and CNTK.

As future work, we will design a sufficient set of standard graphical symbols to describe deep neural networks, and then implement a graphical programming platform to make their construction more convenient and to facilitate their large-scale applications.

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