Machine Learning

Neural Networks 3

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Commonly used neural architectures

- Feed-forward networks, fully-connected layers
  - MLP
  - ReLU networks
- Convolution neural networks
  - LeNet, AlexNet, VGG, ResNet
- Recurrent neural networks
  - RNN, GRU, LSTM
- Sequence-to-sequence models
- Transformers

Building blocks

- Affine transformation
- Nonlinearity (also known as activation functions)
- Normalization
- Convolution
- Pooling
- Skip connection
- Gating
- Attention

Affine transformation

- The operation

$$f(x) = Wx + b \tag{1}$$

  is called affine transformation, where W and b are trainable parameters.

- In pytorch, this is unfortunately called `torch.nn.Linear`.

Nonlinearity: Sigmoid function

- The operation

$$\sigma(x) = \begin{bmatrix} \frac{1}{1+\exp(-x_1)} \\ \frac{1}{1+\exp(-x_2)} \\ \vdots \\ \frac{1}{1+\exp(-x_d)} \end{bmatrix} \tag{2}$$

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Nonlinearity: hyperbolic tangent

- The operation

$$f(x) = \begin{bmatrix} \tanh(x_1) \\ \tanh(x_2) \\ \vdots \\ \tanh(x_d) \end{bmatrix} \tag{3}$$

  is called the hyperbolic tangent nonlinearity, where

$$\tanh(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}. \tag{4}$$

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Feed-forward networks

- A neural network of the form

$$F(x) = W_\ell(\cdots \sigma(W_2 \sigma(W_1 x + b_1) + b_2)) + b_\ell \tag{6}$$

  is called a multi-layer perceptron (MLP).
- A neural network of the form

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  is called a ReLU network.
- They are unfortunately often called feed-forward networks (FFNs).
- An affine transformationn with a nonlinearity is unfortunately often called a fully-connected layer (FC layer).

Normalization: Batch normalization

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- Batch normalization (Ioffe and Szegedy, 2015) is defined as

$$f(x) = \frac{x - \mu}{\sqrt{\sigma^2}} \quad \text{where} \quad \mu = \frac{1}{B}\sum_{i=1}^{B} x_i, \quad \sigma^2 = \frac{1}{B}\sum_{i=1}^{B} x_i^2 - \mu^2 \tag{8}$$

where x_i is the i-th sample in a batch of size B.

Normalization: Layer normalization

- Layer normalization (Ba *et al.*, 2016) is defined as

$$f(x) = \begin{bmatrix} \frac{[x]_1 - \mu}{\sqrt{\sigma^2}} \\ \frac{[x]_2 - \mu}{\sqrt{\sigma^2}} \\ \vdots \\ \frac{[x]_d - \mu}{\sqrt{\sigma^2}} \end{bmatrix} \quad \text{where} \quad \mu = \frac{1}{d}\sum_{i=1}^{d}[x]_i, \quad \sigma^2 = \frac{1}{d}\sum_{i=1}^{d}[x]_i^2 - \mu^2 \tag{9}$$

where $[x]_i$ is the i-th coordinate of the vector x.

Convolution

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$$y_t = \sum_{i=1}^{d} x_i w_{t-i}, \tag{10}$$

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- The 1D cross correlation of x and w is defined as

$$y_t = \sum_{i=1}^{d} x_i w_{t+i}. \tag{11}$$

Convolution

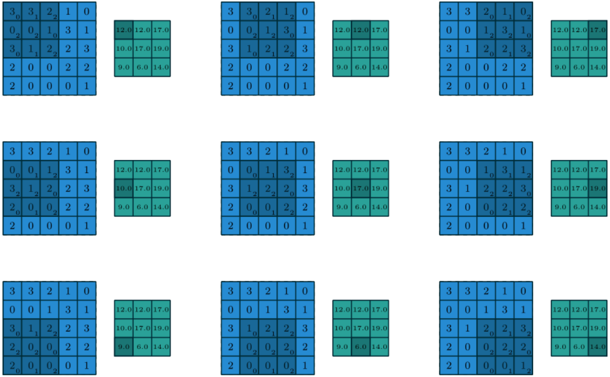

Figure 1.1: Computing the output values of a discrete convolution.

(Dumoulin and Visin, 2018)

Convolution

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- In pytorch, convolution (e.g., `torch.nn.Conv1d`) is unfortunately implemented with as cross correlation and with affine transformation.

Pooling

- Max pooling

$$y_t = \max_{i=1,\dots,d} x_{t+i}. \tag{12}$$

- Mean pooling

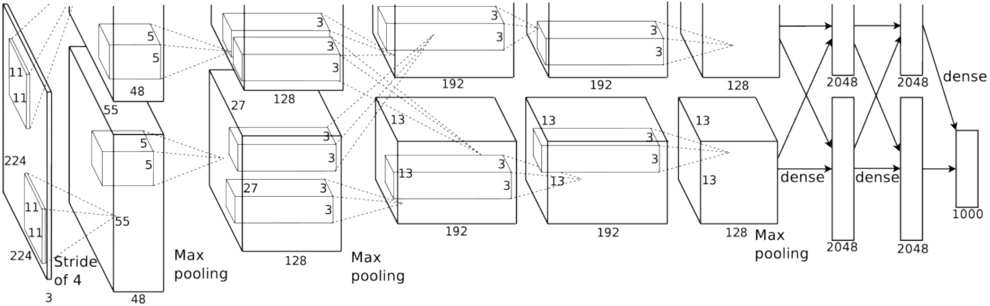
$$y_t = \frac{1}{d} \sum_{i=1}^{d} x_{t+i}. \tag{13}$$

- Pooling is useful for learning whether there exists something.

Convolutional neural networks (CNNs)

- A convolutional neural network is a stack of convolutions and ReLUs.
- Depending on the task, there might also be max pooling.

Convolutional neural networks (CNNs)



(Krizhevsky *et al.*, 2012)

Skip connections

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$$f(x) = x + T(x) \tag{14}$$

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- Since $T(x) = f(x) - x$, the transformation T whatever there is other than the identity x. A skip connection is also called a residual connection.

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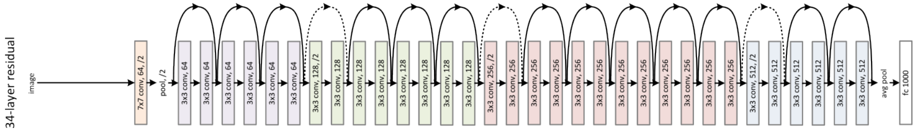

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Gating

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- For example, the gated linear unit (Dauphin *et al.*, 2017) is defined as

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- We can also have a softer skip connection

$$f(x) = (1 - \alpha)x + \alpha T(x) \quad \text{where} \quad \alpha = \sigma(Wx + b) \tag{17}$$

  for some other transformation T.

Recurrent neural networks (RNNs)

- Some data, e.g., text and speech, comes in varying lengths.
- The input is a sequence $x_1, \dots, x_T$ and the output is a sequence $y_1, \dots, y_T$.

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- An Elman network (Elman, 1990) has the form

$$h_t = \sigma(Vh_{t-1} + Ux_t + b_1) \tag{18}$$

$$y_t = Wh_t + b_2 \tag{19}$$

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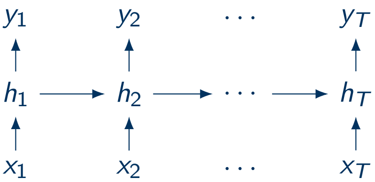
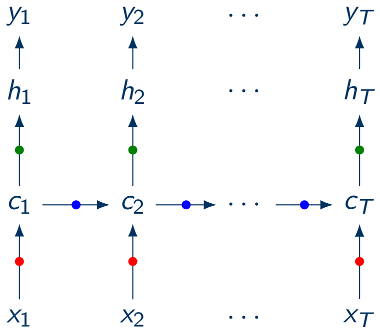


Recurrent neural networks (RNNs)

- The recurrence is gated in long short-term memory networks (LSTMs) (Hochreiter and Schmidhuber, 1997).
  - input gate (red dot)
  - forget gate (blue dot)
  - output gate (green dot)



Attention mechanism

- Given a query q, keys $k_1, \ldots, k_T$, and values $v_1, \ldots, v_T$, the attention mechanism (Bahdanau *et al.*, 2015) is defined as

$$f(q, k_1, \ldots, k_T, v_1, \ldots, v_T) = \sum_{i=1}^{T} \frac{\exp(k_i^\top q)}{\sum_{j=1}^{T} \exp(k_j^\top q)} v_i \tag{20}$$

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\begin{aligned}
f(q, k_1, \ldots, k_T, v_1, \ldots, v_T) &= \sum_{i=1}^{T} \frac{\exp(k_i^\top q)}{\sum_{j=1}^{T} \exp(k_j^\top q)} v_i && (20) \\
&= \mathrm{softmax}(qK^\top)V, && (21)
\end{aligned}
$$

where

$$
K = \begin{bmatrix} — & k_1 & — \\ — & k_2 & — \\ & \vdots & \\ — & k_T & — \end{bmatrix} \quad V = \begin{bmatrix} — & v_1 & — \\ — & v_2 & — \\ & \vdots & \\ — & v_T & — \end{bmatrix}. \qquad (22)
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$k_1 \quad k_2 \quad \cdots \quad k_T$

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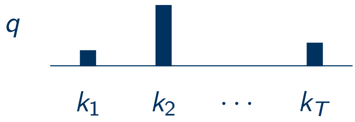

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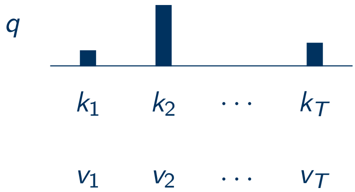

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- A seq2seq is often equipped with an attention mechanism and the loop becomes

$$q_i = \text{update}(q_{i-1}, y_{i-1}) \tag{25}$$

$$z_i = \text{attend}(q_i, h_1, \dots, h_T, h_1, \dots, h_T) \tag{26}$$

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  where $h_1, \ldots, h_T = \text{encode}(x_1, \ldots, x_T)$.
- The loop is often refer to as the decoder, and seq2seq is unfortunately often called a encoder-decoder model.

Self-attention

- When applying attention on

$$q_t = W_1 x_t + b_1 \tag{28}$$
$$k_t = W_2 x_t + b_2 \tag{29}$$
$$v_t = W_3 x_t + b_3 \tag{30}$$

  we are using the transformation of the input to attend to itself; hence the name self-attention (Vaswani *et al.*, 2017).

- To contrast with self-attention, regular attention is often called cross attention.

Transformer

- A Transformer block is defined as

$$\mathrm{FC}(\mathrm{FC}(H)) + H \tag{31}$$

where $H = \mathrm{attend}(W_1 X, W_2 X, W_3 X) + X$.

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- A Transformer (Vaswani *et al.*, 2017) is a seq2seq where both the encoder and the decoder consist of a sequence of Transformer blocks.

Questions to think about

- If a simple MLP is already an universal approximator, why do we need convolution, recurrence, and attention?
- Even though some layers have intuitions attached, after training, are they learning what is intended?
- If we want to solve a new problem, how do we know what layer types to use?
- If there are differences among different layers, why are people using Transformers more than other model architectures these days?
- Are there things that are easy to learn for one layer type but hard to learn for another?