Neural Network Basics

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Outline

Deep Learning in NLP

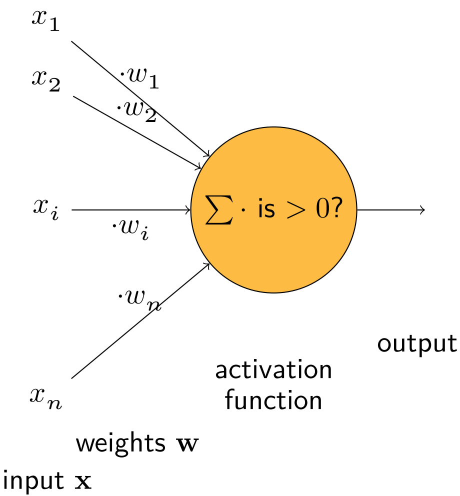
- NLP tasks learn end-to-end using deep learning — the number-one approach in current research
- State of the art in POS tagging, parsing, named-entity recognition, machine translation, ...
- Good news: training without almost any linguistic insight
- Bad news: requires enormous amount of training data and really big computational power

What is deep learning?

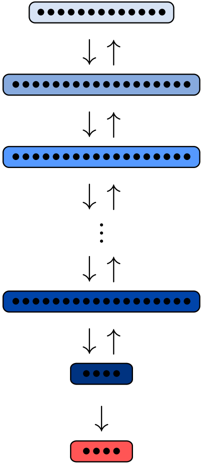
- Buzzword for machine learning using neural networks with many layers using back-propagation
- Learning of a real-valued function with millions of parameters that solves a particular problem
- Learning more and more abstract representation of the input data until we reach such a suitable representation for our problem

Neural Networks Basics

Single Neuron



Neural Network



$$x$$

$$\downarrow$$

$$h_1 = f(W_1 x + b_1)$$

$$\downarrow$$

$$h_2 = f(W_2 h_1 + b_2)$$

$$\downarrow$$

$$\vdots$$

$$\downarrow$$

$$h_n = f(W_n h_{n-1} + b_n)$$

$$\downarrow$$

$$o = g(W_o h_n + b_o)$$

$$\downarrow$$

$$E = e(o, t) \quad \rightarrow \quad \frac{\partial E}{\partial o}$$

$$\uparrow$$

$$\frac{\partial E}{\partial W_o} = \frac{\partial E}{\partial o} \cdot \frac{\partial o}{\partial W_o}$$

$$\uparrow$$

$$\uparrow$$

$$\uparrow$$

$$\uparrow$$

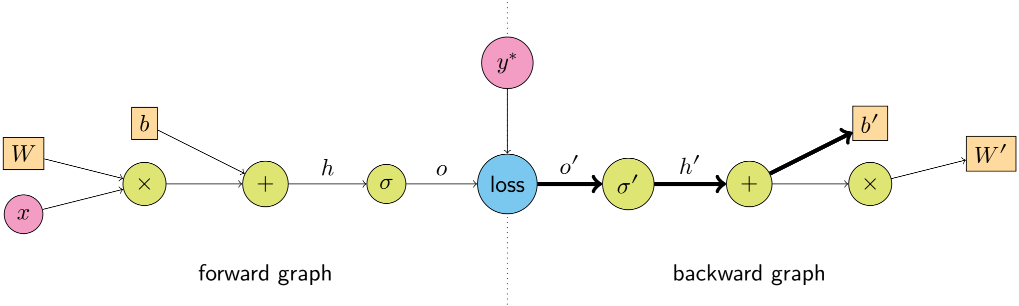
$$\uparrow$$

Implementation

Logistic regression:

$$y = \sigma\left(Wx + b\right) \tag{1}$$

Computation graph:



Representing Words

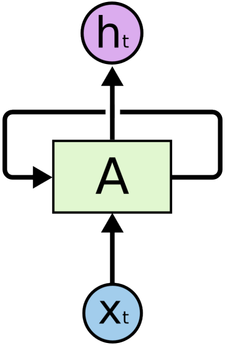
Discrete vs. Continous

Representing Sequences

Representing Sequences

Recurrent Networks

…the default choice for sequence labeling

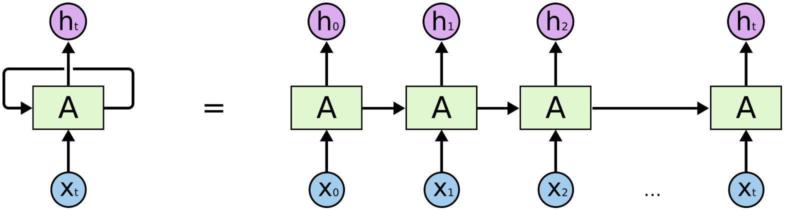


- inputs: $x_{,} \ldots, x_T$
- initial state $h_0 = \mathbf{0}$, a result of previous computation, trainable parameter
- recurrent computation: $h_t = A(h_{t-1}, x_t)$

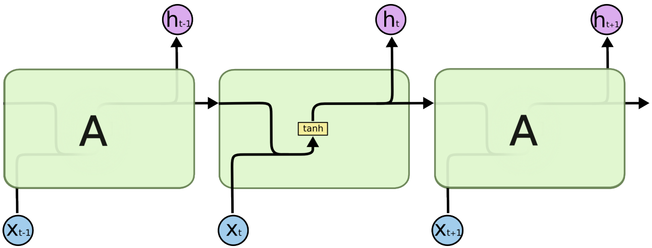
RNN as Imperative Code

```
def rnn(initial_state, inputs):
  prev_state = initial_state
  for x in inputs:
    new_state, output = rnn_cell(x, prev_state)
    prev_state = new_state
    yield output
```

RNN as a Fancy Image



Vanilla RNN



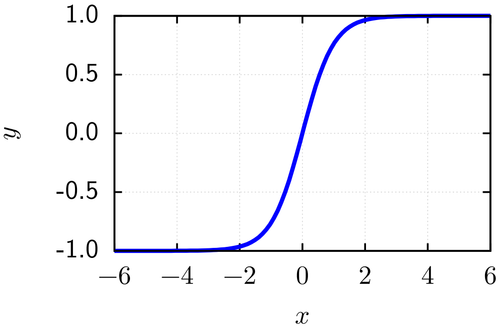
$$h_t = \tanh\left(W[h_{t-1}; x_t] + b\right)$$

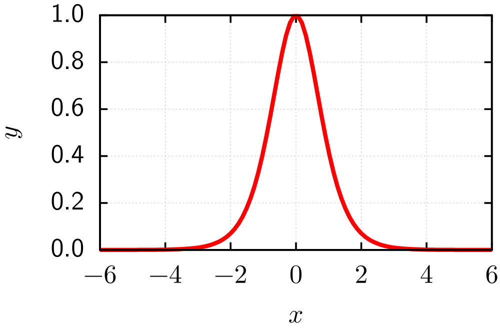
- cannot propagate long-distance relations
- vanishing gradient problem

Vanishing Gradient Problem (1)

$$\tanh x = \frac{1 - e^{-2x}}{1 + e^{-2x}}$$

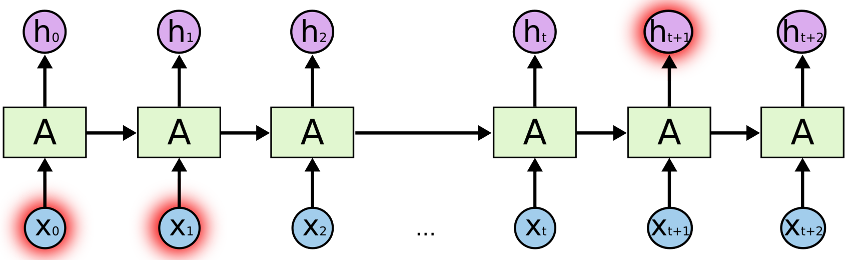
$$\frac{\mathrm{d} \tanh x}{\mathrm{d}x} = 1 - \tanh^2 x \in (0, 1]$$





Weight initialized $\sim \mathcal{N}(0, 1)$ to have gradients further from zero.

Vanishing Gradient Problem (2)

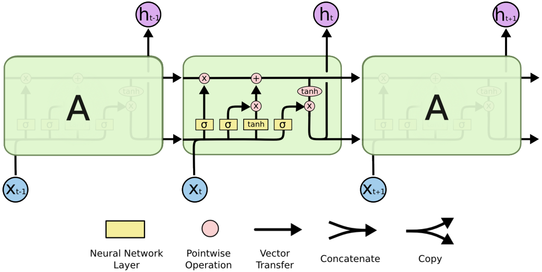


$$\frac{\partial E_{t+1}}{\partial b} = \frac{\partial E_{t+1}}{\partial h_{t+1}} \cdot \frac{\partial h_{t+1}}{\partial b} \quad \text{(chain rule)}$$

$$
\begin{aligned}
\frac{\partial h_t}{\partial b} &= \frac{\partial \tanh \overbrace{(W_h h_{t-1} + W_x x_t + b)}^{=z_t \text{ (activation)}}}{\partial b} \qquad (\tanh' \text{ is derivative of } \tanh) \\
&= \tanh'(z_t) \cdot \left(\frac{\partial W_h h_{t-1}}{\partial b} + \underbrace{\frac{\partial W_x x_t}{\partial b}}_{=0} + \underbrace{\frac{\partial b}{\partial b}}_{=1} \right) \\
&= \underbrace{W_h}_{\sim \mathcal{N}(0,1)} \underbrace{\tanh'(z_t)}_{\in (0;1]} \frac{\partial h_{t-1}}{\partial b} + \tanh'(z_t)
\end{aligned}
$$

Long Short-Term Memory Networks

LSTM = Long short-term memory

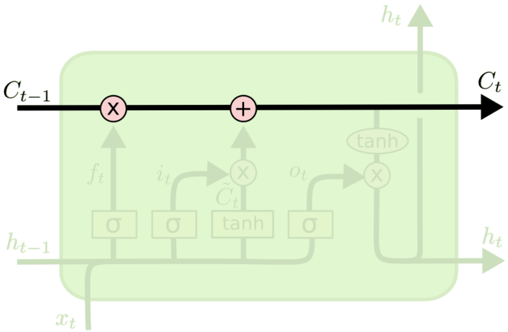


Control the gradient flow by explicitly gating:

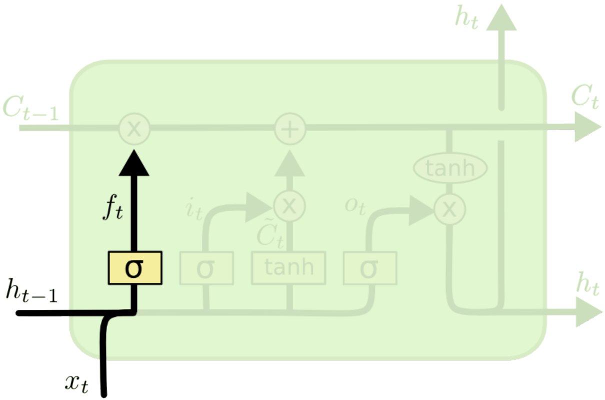
- what to use from input,
- what to use from hidden state,
- what to put on output

LMST: Hidden State

- two types of hidden states
- h_t — "public" hidden state, used an output
- c_t — "private" memory, no non-linearities on the way
- direct flow of gradients (without multiplying by ≤ 1 derivatives)



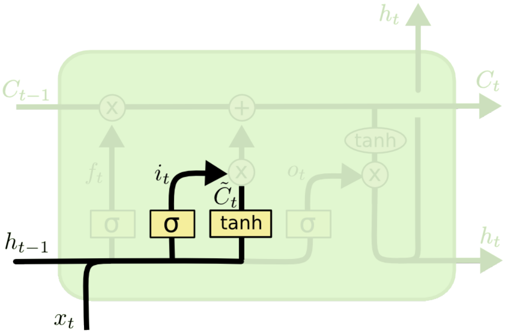
LSTM: Forget Gate



$$f_t = \sigma\left(W_f[h_{t-1}; x_t] + b_f\right)$$

- based on input and previous state, decide what to forget from the memory

LSTM: Input Gate

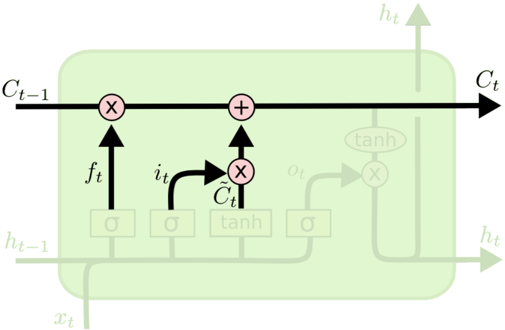


$$i_t = \sigma\left(W_i \cdot [h_{t-1}; x_t] + b_i\right)$$

$$\tilde{C}_t = \tanh\left(W_c \cdot [h_{t-1}; x_t] + b_C\right)$$

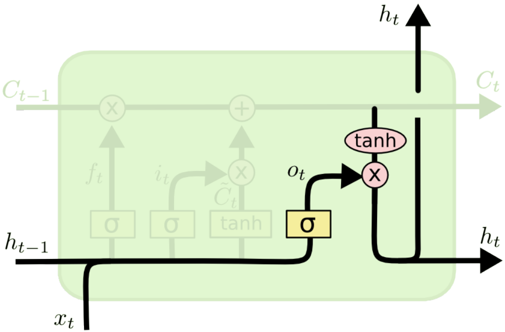
- $\tilde{C}$ — candidate what may want to add to the memory
- i_t — decide how much of the information we want to store

LMST: Cell State Update



$$C_t = f_t \odot C_{t-1} + i_t \odot \tilde{C}_t$$

LSTM: Output Gate



$$o_t = \sigma\left(W_o \cdot [h_{t-1}; x_t] + b_o\right)$$

$$h_t = o_t \odot \tanh C_t$$

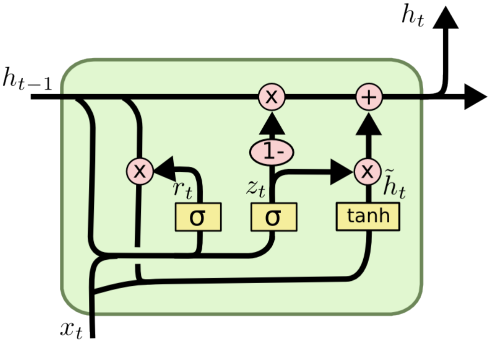
Here we are, LSTM!

$$
\begin{aligned}
f_t &= \sigma\left(W_f[h_{t-1}; x_t] + b_f\right) \\
i_t &= \sigma\left(W_i \cdot [h_{t-1}; x_t] + b_i\right) \\
o_t &= \sigma\left(W_o \cdot [h_{t-1}; x_t] + b_o\right) \\
\tilde{C}_t &= \tanh\left(W_c \cdot [h_{t-1}; x_t] + b_C\right) \\
C_t &= f_t \odot C_{t-1} + i_t \odot \tilde{C}_t \\
h_t &= o_t \odot \tanh C_t
\end{aligned}
$$

Question How would you implement it efficiently?
Compute all gates in a single matrix multiplication.

Gated Recurrent Units

update gate	$z_t = \sigma(x_t W_z + h_{t-1} U_z + b_z) \in (0,1)$
remember gate	$r_t = \sigma(x_t W_r + h_{t-1} U_r + b_r) \in (0,1)$
candidate hidden state	$\tilde{h}_t = \tanh\left(x_t W_h + (r_t \odot h_{t-1}) U_h\right) \in (-1,1)$
hidden state	$h_t = (1 - z_t) \odot h_{t-1} + z_t \cdot \tilde{h}_t$



LSTM vs. GRU

- GRU is smaller and therefore faster
- performance similar, task dependent
- theoretical limitation: GRU accepts regular languages, LSTM can simulate counter machine

;

RNN in PyTorch

```
rnn = nn.LSTM(input_dim, hidden_dim=512, num_layers=1,
    bidirectional=True, dropout=0.8)
output, (hidden, cell) = self.rnn(x)
```

https://pytorch.org/docs/stable/nn.html?highlight=lstm#torch.nn.LSTM

RNN in TensorFlow

```
inputs = ... # float tf.Tensor of shape [batch, length, dim]
lengths = ... # int tf.Tensor of shape [batch]

# Cell objects are templates
fw_cell = tf.nn.rnn_cell.LSTMCell(512, name="fw_cell")
bw_cell = tf.nn.rnn_cell.LSTMCell(512, name="bw_cell")

outputs, states = tf.nn.bidirectional_dynamic_rnn(
    cell_fw, cell_bw, inputs, sequence_length=lengths)
```

https://www.tensorflow.org/api_docs/python/tf/nn/bidirectional_dynamic_rnn

Bidirectional Networks

- simple trick to improve performance
- run one RNN forward, second one backward and concatenate outputs

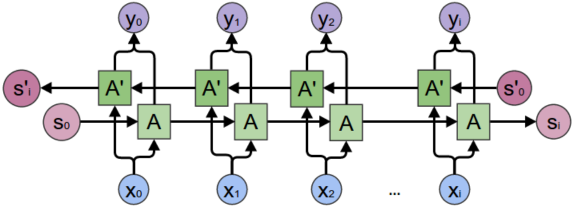


Image from: `http://colah.github.io/posts/2015-09-NN-Types-FP/`

- state of the art in tagging, crucial for neural machine translation

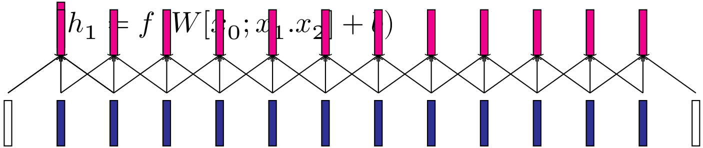
Representing Sequences

Convolutional Networks

1-D Convolution

≈ sliding window over the sequence

$$h_i = f\left(W\left[x_{i-1}; x_i; x_{i+1}\right] + b\right)$$



$x_0 = \vec{0}$ embeddings $\mathbf{x} = (x_1, \ldots, x_N)$ $x_N = \vec{0}$

pad with 0s if we want to keep sequence length

1-D Convolution: Pseudocode

```
xs = ... # input sequnce

kernel_size = 3 # window size
filters = 300 # output dimensions
strides=1     # step size

W = trained_parameter(xs.shape[2] * kernel_size, filters)
b = trained_parameter(filters)
window = kernel_size // 2

outputs = []
for i in range(window, xs.shape[1] - window):
    h = np.mul(W, xs[i - window:i + window]) + b
    outputs.append(h)
return np.array(h)
```

1-D Convolution: Frameworks

TensorFlow

```
h = tf.layers.conv1d(x, filters=300 kernel_size=3,
                     strides=1, padding='same')
```

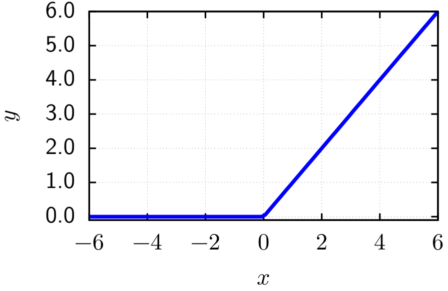
https://www.tensorflow.org/api_docs/python/tf/layers/conv1d

PyTorch

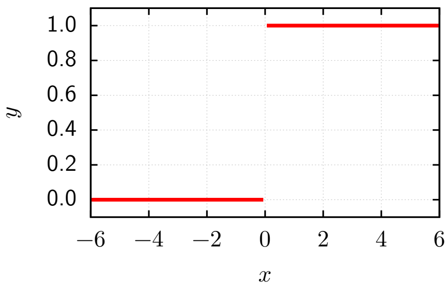
```
conv = nn.Conv1d(in_channels, out_channels=300, kernel_size=3, stride=1,
                 padding=0, dilation=1, groups=1, bias=True)
h = conv(x)
```

https://pytorch.org/docs/stable/nn.html#torch.nn.Conv1d

ReLU:



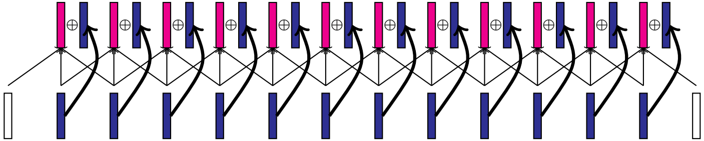
Derivative of ReLU:



faster, suffer less with vanishing gradient

Residual Connections

$$h_i = f\left(W\left[x_{i-1}; x_i; x_{i+1}\right] + b\right) + x_i$$



$x_0 = \vec{0}$ embeddings $\mathbf{x} = (x_1, \ldots, x_N)$ $x_N = \vec{0}$

Allows training deeper networks.

Why do you it helps?

Better gradient flow – the same as in RNNs.

Residual Connections: Numerical Stability

Numerically unstable, we need activation to be in similar scale $\Rightarrow$ layer normalization.
Activation before non-linearity is normalized:

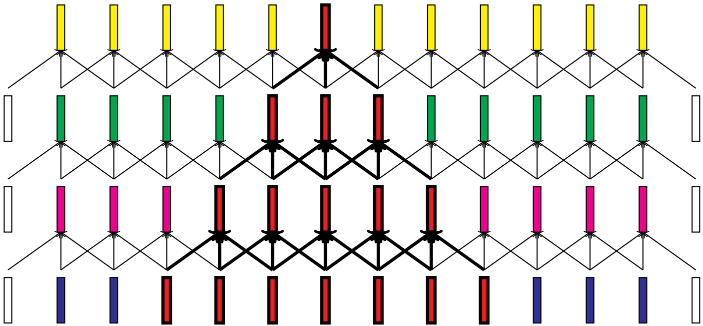
$$\bar{a}_i = \frac{g_i}{\sigma_i}(a_i - \mu_i)$$

...g is a trainable parameter, μ, σ estimated from data.

$$\mu = \frac{1}{H}\sum_{i=1}^{H} a_i$$

$$\sigma = \sqrt{\frac{1}{H}\sum_{i=1}^{H}(a_i - \mu)^2}$$

Receptive Field



$x_0 = \vec{0}$ embeddings $\mathbf{x} = (x_1, \ldots, x_N)$ $x_N = \vec{0}$

Can be enlarged by dilated convolutions.

Convolutional architectures

$+$

- extremely computationally efficient

$-$

- limited context
- by default no aware of n-gram order

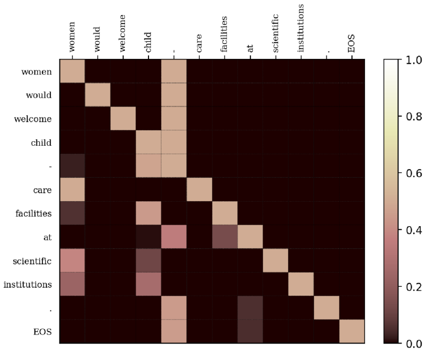
- max-pooling over the hidden states $=$ element-wise maximum over sequence
- can be understood as an $\exists$ operator over the feature extractors

Representing Sequences

Self-attentive Networks

Self-attentive Networks

- In some layers: states are linear combination of previous layer states
- Originally for the Transformer model for machine translation



- similarity matrix between all pairs of states
- $O(n^2)$ memory, $O(1)$ time (when paralelized)
- next layer: sum by rows

Multi-headed scaled dot-product attention

Single-head setup

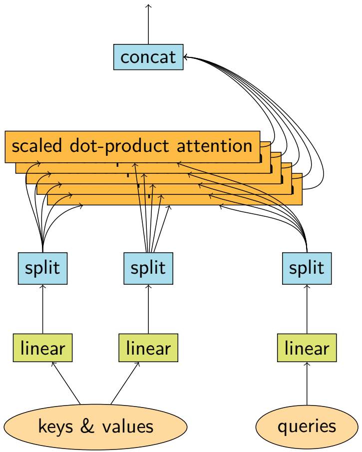
$$\mathrm{Attn}(Q, K, V) = \mathrm{softmax}\left(\frac{QK^\top}{\sqrt{d}}\right)V$$

$$h_{i+1} = \sum \mathrm{softmax}\left(\frac{h_i h_i^\top}{\sqrt{d}}\right)$$

Multihead-head setup

$$\mathrm{Multihead}(Q, V) = (H_1 \oplus \cdots \oplus H_h)W^O$$

$$H_i = \mathrm{Attn}(QW_i^Q, VW_i^K, VW_i^V)$$



Dot-Product Attention in PyTorch

```
def attention(query, key, value, mask=None):
    d_k = query.size(-1)
    scores = torch.matmul(query, key.transpose(-2, -1)) \
             / math.sqrt(d_k)
    p_attn = F.softmax(scores, dim = -1)
    return torch.matmul(p_attn, value), p_attn
```

Dot-Product Attention in TensorFlow

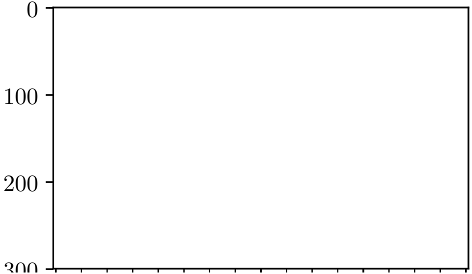
```
def scaled_dot_product(self, queries, keys, values):
    o1 = tf.matmul(queries, keys, transpose_b=True)
    o2 = o1 / (dim**0.5)

    o3 = tf.nn.softmax(o2)
    return tf.matmul(o3, values)
```

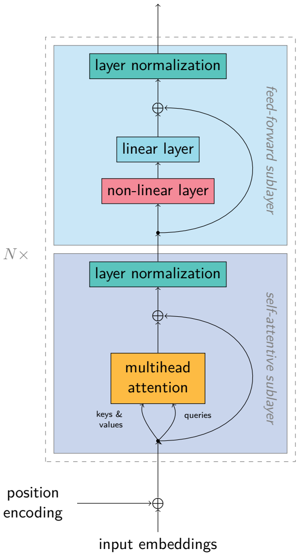
Position Encoding

Model cannot be aware of the position in the sequence.

$$\mathrm{pos}(i) = \begin{cases} \sin\left(\frac{t}{10^4}^{\frac{i}{d}}\right), & \text{if } i \mod 2 = 0 \\ \cos\left(\frac{t}{10^4}^{\frac{i-1}{d}}\right), & \text{otherwise} \end{cases}$$



Stacking self-attentive Layers



- several layers (original paper 6)
- each layer: 2 sub-layers: self-attention and feed-forward layer
- everything inter-connected with residual connections

Architectures Comparison

	computation	sequential operations	memory
Recurrent	$O(n \cdot d^2)$	$O(n)$	$O(n \cdot d)$
Convolutional	$O(k \cdot n \cdot d^2)$	$O(1)$	$O(n \cdot d)$
Self-attentive	$O(n^2 \cdot d)$	$O(1)$	$O(n^2 \cdot d)$

d model dimension, n sequence length, k convolutional kernel

Summary

1. Discrete symbols $\rightarrow$ continuous representation with trained embeddings
2. Architectures to get suitable representation: recurrent, convolutional, self-attentive
3. Output: classification, sequence labeling, autoregressive decoding …next time