CS 784: Computational Linguistics Lecture 9: Neural Networks II (for Text Classification)

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Check out https://pytorch.org/tutorials/intermediate/nlp_from_scratch_index.html if you aren't familiar with this topic!

Recap: Unified View of Text Classification

$$\mathsf{classify}(\mathit{s}) = \arg\max_{\mathit{y}} \mathit{score}(\mathit{s}, \mathit{y}; \Theta)$$

s: input text, y: class label, Θ : model parameters.

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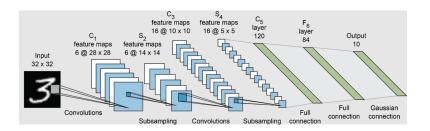
Model $score(s, y; \Theta)$ using a neural network.

Last lecture: represent s as a fixed-dimensional vector \mathbf{x} using bag-of-word embeddings.

This lecture: extract more powerful features \mathbf{x} of \mathbf{s} using advanced neural network architectures.



Convolutional Neural Networks



Introduced in the context of computer vision, but also used for text classification.

The Convolutional Kernel

x _{1,5}	x _{2,5}	x _{3,5}	X4,5	<i>x</i> 5,5
×1,4	×2,4	x _{3,4}	×4,4	x _{5,4}
x _{1,3}	x _{2,3}	x _{3,3}	x _{4,3}	x _{5,3}
x _{1,2}	x _{2,2}	x _{3,2}	×4,2	<i>x</i> 5,2
x _{1,1}	x _{2,1}	x _{3,1}	x _{4,1}	x _{5,1}

$$\mathbf{O} = \mathbf{X} * \mathbf{W} \qquad \mathbf{X} \in \mathbb{R}^{n \times m}, \mathbf{W} \in \mathbb{R}^{k \times \ell}, \mathbf{O} \in \mathbb{R}^{(n-k+1) \times (m-\ell+1)}$$

$$o_{i,j} = \sum_{p=1}^{k} \sum_{q=1}^{\ell} x_{i+p-1,j+q-1} \cdot w_{p,q}$$

• A kernel is a small matrix (e.g., 2×2) that slides over the input. At each position, kernel computes element-wise multiplication and sum of the input and kernel.

CNNs

The Convolutional Kernel

x _{1,5}	x _{2,5}	<i>x</i> _{3,5}	x4,5	x _{5,5}					
x _{1,4}	x _{2,4}	x _{3,4}	X4,4	<i>x</i> _{5,4}	$\mathbf{W} \in \mathbb{R}^{2 imes 2}$	01,4	02,4	03,4	0,
x _{1,3}	x _{2,3}	x _{3,3}	×4,3	x _{5,3}		01,3	02,3	03,3	04
x _{1,2}	x _{2,2}	x _{3,2}	x _{4,2}	<i>x</i> _{5,2}		01,2	02,2	03,2	04
x _{1,1}	×2,1	×3,1	×4,1	x _{5,1}		01,1	02,1	03,1	04

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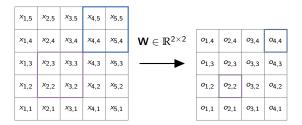
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$$o_{i,j} = \sum_{p=1}^{k} \sum_{q=1}^{\ell} x_{i+p-1,j+q-1} \cdot w_{p,q}$$

- A kernel is a small matrix (e.g., 2×2) that slides over the input. At each position, kernel computes element-wise multiplication and sum of the input and kernel.
- (Outdated) convention: rotate the kernel by 180 degrees.

Convolutional Neural Networks: Characteristics



• A convolutional kernel can be thought of as weighted sum over a local region of the input.

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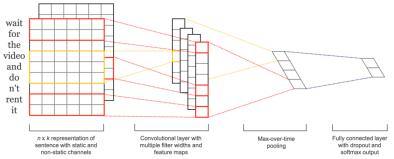
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- The weights are learnable from data to optimize for downstream task.

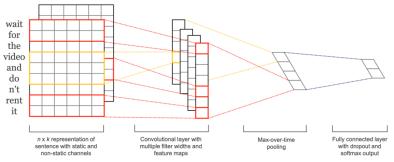
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- A convolutional kernel can be thought of as weighted sum over a local region of the input.
- The weights are learnable from data to optimize for downstream task.
- Therefore, a learned kernel is a local feature extractor (e.g., color patterns, edge with a specific shape).

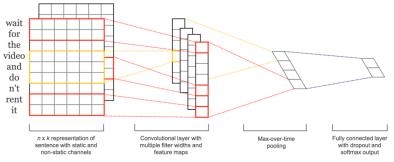


[Source: Kim, 2014]



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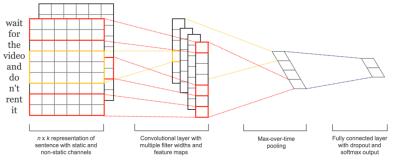
• Input $\mathbf{X} \in \mathbb{R}^{n \times d}$. n: number of token, d: embedding dimension.



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- Kernels $\in \mathbb{R}^{h \times d}$ (kernel size h << n). Any thoughts on why the second dimension is always d?





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- Input X ∈ ℝ^{n×d}.
 n: number of token, d: embedding dimension.
- Kernels $\in \mathbb{R}^{h \times d}$ (kernel size h << n). Any thoughts on why the second dimension is always d?
- Output $\mathbf{O} \in \mathbb{R}^{(n-h+1)\times 1}$:

$$o_i = \sum_{i=1}^h \sum_{k=1}^d x_{i+j-1,k} \cdot w_{j,k}$$

For a convolutional kernel

$$\mathbf{O} = \mathbf{X} * \mathbf{W} \qquad (\in \mathbb{R}^{(n-h+1)\times 1})$$

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Solution: **pooling** – make the one with variable length fixed! In this case, we will convert $\mathbf{O} \in \mathbb{R}^{(n-h+1)\times 1}$ to a single scalar.

$$\mathtt{pooling}: \mathbb{R}^* \to \mathbb{R}$$

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$$\texttt{pooling}: \mathbb{R}^* \to \mathbb{R}$$

Stacking scalars from a fixed number of kernels yields a fixed-dimensional feature vector.

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More generally, pooling removes one dimension from a tensor.

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More generally, pooling removes one dimension from a **tensor**.

Consider the tensor $\mathbf{O} \in \mathbb{R}^{a \times b \times c \times d}$, and we would like to remove the third (c) dimension.

• Max pooling: take the maximum from the output of each kernel.

$$\mathtt{maxpool}(\mathbf{O})_{i,j,k} = \max_{p=1}^{c} \mathbf{O}_{i,j,p,k}$$

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Mean pooling: take the average value from the output of each kernel.

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$$\mathbf{O}$$
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 Attention pooling: take a weighted average of the output of each kernel.

$$\mathtt{attnpool}(\mathbf{O})_{i,j,k} = \sum_{p=1}^{c} \alpha_{p} \mathbf{O}_{i,j,p,k},$$

CNNs as MLPs

The basic form of a 2-layer perceptron:

$$\begin{split} \mathbf{z}^{(1)} &= g\left(\mathbf{W}^{(1)}\mathbf{x} + \mathbf{b}^{(1)}\right) \\ \mathbf{z}^{(2)} &= \mathbf{W}^{(2)}\mathbf{z}^{(1)} + \mathbf{b}^{(2)} \end{split}$$

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The application of one kernel at one position can be expressed as

$$o = \mathbf{W}\mathbf{x}$$
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where $\mathbf{W} \in \mathbb{R}^{1 \times (h \times d)}$ is the kernel and $\mathbf{x} \in \mathbb{R}^{(h \times d) \times 1}$ is the input.

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This corresponds to the first layer without the bias term and activation function—in fact, it is a linear transformation.

Recurrent Neural Networks

Elman (1990), a computational psycholinguist, proposed the simple recurrent neural network (RNN) architecture.

Recurrent Neural Networks

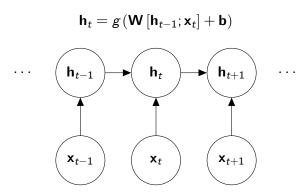
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Suppose h_T is passed to the classifier as the fixed-dimensional feature vector.

We can easily calculate $\frac{\partial loss}{\partial \mathbf{h}_{\tau}}$, as well as $\frac{\partial \mathbf{h}_{t}}{\partial \mathbf{h}_{t-1}}$ and $\frac{\partial \mathbf{h}_{t}}{\partial \mathbf{W}}$ for each t.

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$$\mathbf{h}_t = g(\mathbf{W}[\mathbf{h}_{t-1}; \mathbf{x}_t] + \mathbf{b})$$

Suppose $\mathbf{h}_{t+1} = \mathbf{W}[\mathbf{h}_t; \mathbf{x}_{t+1}] + \mathbf{b} = \alpha \mathbf{h}_t (\alpha \neq 1)$. What will happen if t goes to $+\infty$?

An Important Issue of Simple RNNs

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The norm of \mathbf{h}_t will either explode (if $\alpha > 1$) or vanish (if $\alpha < 1$) as t increases.

This motivates the development of more advanced RNN architectures.

Forget gate
$$\mathbf{f}_t = \sigma\left(\mathbf{W}_f[\mathbf{h}_{t-1}; \mathbf{x}_t] + \mathbf{b}_f\right)$$

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Forget gate
$$\begin{aligned} \mathbf{f}_t &= \sigma\left(\mathbf{W}_f[\mathbf{h}_{t-1}; \mathbf{x}_t] + \mathbf{b}_f\right) \\ \text{Input gate} & \mathbf{i}_t &= \sigma\left(\mathbf{W}_i[\mathbf{h}_{t-1}; \mathbf{x}_t] + \mathbf{b}_i\right) \\ \text{Cell} & \tilde{\mathbf{c}}_t &= \tanh\left(\mathbf{W}_c[\mathbf{h}_{t-1}; \mathbf{x}_t] + \mathbf{b}_c\right) \end{aligned}$$

Hochreiter & Schmidhuber (1997) proposed the LSTM architecture to address the vanishing/exploding gradient problem.

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⊙: element-wise multiplication.

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⊙: element-wise multiplication.

Key idea: keep entries in $\tilde{\mathbf{c}}_t$ and \mathbf{h}_t in the range [-1, 1].

Update gate
$$\mathbf{z}_t = \sigma(\mathbf{W}_z[\mathbf{h}_{t-1}; \mathbf{x}_t] + \mathbf{b}_z)$$

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Update rule \mathbf{h}_t = (1 - \mathbf{z}_t) \odot \mathbf{h}_{t-1}

+ \mathbf{z}_t \odot \tanh\left(\mathbf{W}_h\left[\mathbf{r}_t \odot \mathbf{h}_{t-1}; \mathbf{x}_t\right] + \mathbf{b}_h\right)
```

GRUs (Cho et al., 2014) can be viewed as simplified LSTMs from a practical perspective.

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Works well with fewer parameters and less computation.

Even with LSTM and GRU architectures, RNNs usually require **gradient clipping** to stabilize training.

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To obtain the fixed-dimensional output as RNN features for classification, we may use the hidden states at the last time step, or pooling over all hidden states (Lin et al., 2017).

Pretrained RNNs

In earlier years, people pretrained RNNs on large corpora! Peters et al. (2018). Deep contextualized word representations. (Also known as ELMo; Embeddings from Language Models)

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ELMo trains a bidirectional LSTM on a large corpus, and use the hidden states as text features.

The hidden states are also referred to as **contextualized word embeddings**.

Recursive Neural Networks

Generalized RNNs that support tree-structured computation graph.

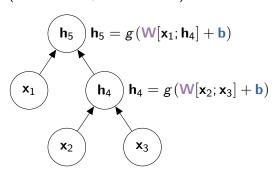
$$\mathbf{h}_t = g(\mathbf{W}[\mathbf{h}_{t-1}; \mathbf{x}_t] + \mathbf{b})$$

Run constituency parser on sentence and construct vector recursively (Socher et al., 2011 & 2013).

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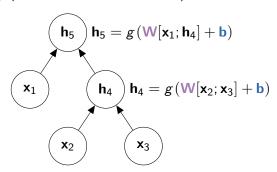


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We may use complicated cells (e.g., LSTMs) to compute \mathbf{h}_i (Zhu et al., 2015, Tai et al. 2015).

From LSTMs to Tree LSTMs

$$\begin{split} \mathbf{f}_t &= \sigma\left(\mathbf{W}_f\big[\mathbf{h}_{t-1};\mathbf{x}_t\big] + \mathbf{b}_f\right) & \mathbf{I}_n &= \sigma\left(\mathbf{W}_\ell\big[\mathbf{h}_\ell;\mathbf{h}_r\big] + \mathbf{b}_\ell\right) \\ \mathbf{i}_t &= \sigma\left(\mathbf{W}_i\big[\mathbf{h}_{t-1};\mathbf{x}_t\big] + \mathbf{b}_i\right) & \mathbf{r}_n &= \sigma\left(\mathbf{W}_r\big[\mathbf{h}_\ell;\mathbf{h}_r\big] + \mathbf{b}_r\right) \\ \mathbf{\tilde{c}}_t &= \tanh\left(\mathbf{W}_c\big[\mathbf{h}_{t-1};\mathbf{x}_t\big] + \mathbf{b}_c\right) & \mathbf{\tilde{c}}_n &= \tanh\left(\mathbf{W}_c\big[\mathbf{h}_I;\mathbf{h}_r\big] + \mathbf{b}_c\right) \\ \mathbf{c}_t &= \mathbf{f}_t \odot \mathbf{c}_{t-1} + \mathbf{i}_t \odot \tilde{\mathbf{c}}_t & \mathbf{c}_n &= \mathbf{I}_n \odot \mathbf{c}_I + \mathbf{r}_n \odot \mathbf{c}_r + \tilde{\mathbf{c}}_n \\ \mathbf{o}_t &= \sigma\left(\mathbf{W}_o\big[\mathbf{h}_{t-1};\mathbf{x}_t\big] + \mathbf{b}_o\right) & \mathbf{o}_n &= \sigma\left(\mathbf{W}_o\big[\mathbf{h}_I;\mathbf{h}_r\big] + \mathbf{b}_o\right) \\ \mathbf{h}_t &= \mathbf{o}_t \odot \tanh(\mathbf{c}_t) & \mathbf{h}_n &= \mathbf{o}_n \odot \tanh(\mathbf{c}_n) \end{split}$$

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Recursive networks with left-branching trees shares a lot in common with RNNs.

Transformers 00000000000

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Recursive networks with left-branching trees shares a lot in common with RNNs.

Syntactically meaningful parse trees are not necessary for good representations: instead, size balanced trees work well for most tasks (Shi et al., 2018).

RNNs and RvNNs as MI Ps

All the gates in advanced RNN architectures are linear transformations followed by an activation function.

Taking LSTMs as an example,

Forget gate
$$\mathbf{f}_t = \sigma\left(\mathbf{W}_f\big[\mathbf{h}_{t-1}; \mathbf{x}_t\big] + \mathbf{b}_f\right)$$
 Input gate
$$\mathbf{i}_t = \sigma\left(\mathbf{W}_i\big[\mathbf{h}_{t-1}; \mathbf{x}_t\big] + \mathbf{b}_i\right)$$
 Cell
$$\mathbf{\tilde{c}}_t = \tanh\left(\mathbf{W}_c\big[\mathbf{h}_{t-1}; \mathbf{x}_t\big] + \mathbf{b}_c\right)$$
 Output gate
$$\mathbf{o}_t = \sigma\left(\mathbf{W}_o\big[\mathbf{h}_{t-1}; \mathbf{x}_t\big] + \mathbf{b}_o\right)$$
 Update
$$\mathbf{c}_t = \mathbf{f}_t \odot \mathbf{c}_{t-1} + \mathbf{i}_t \odot \mathbf{\tilde{c}}_t$$
 Hidden state
$$\mathbf{h}_t = \mathbf{o}_t \odot \tanh(\mathbf{c}_t)$$

Gates are combined linearly to form intermediate results.

Removing the third dimension of a tensor using a weighted average:

$$\mathtt{attnpool}(\mathbf{O})_{i,j,k} = \sum_{p=1}^{c} \alpha_p \mathbf{O}_{i,j,p,k}$$

Recap: Attention Pooling

Removing the third dimension of a tensor using a weighted average:

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where \mathbf{v}_p is the (stretched) vector of $\mathbf{O}_{*,*,p,*}$.

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We may calculate **s** with more complicated neural architectures.

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We may calculate **s** with more complicated neural architectures.

In (most) machine learning context, attention is just weighted sum!

Vaswani et al. (2017). Attention is All You Need.

Attention Is All You Need

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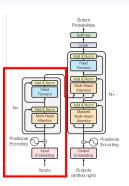
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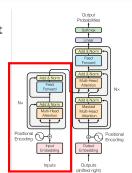
Transformers

 Introduced for sequence-to-sequence tasks, but could be more accessible understood as a feature extractor.



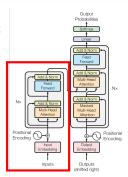
Transformers

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- Key idea: every token has attention to every other token. In slightly more CS/math words, after passing through one transformer layer, the representation of one token should contain information from all context tokens.



Transformers

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For sentence with tokens w_i, \ldots, w_n , a transformer computes

$$\mathbf{E} = \mathtt{Embedding}(w_i, \dots, w_n) \in \mathbb{R}^{d_1 imes n}$$

$$K = W_k E$$
 $W_k \in \mathbb{R}^{d_2 \times d_1}$ $K \in \mathbb{R}^{d_2 \times n}$

$$\mathbf{Q} = \mathbf{W}_a \mathbf{E}$$
 $\mathbf{W}_a \in \mathbb{R}^{d_2 \times d_1}$ $\mathbf{Q} \in \mathbb{R}^{d_2 \times n}$

$$\mathbf{V} = \mathbf{W}_{v}\mathbf{E} \qquad \mathbf{W}_{\mathbf{v}} \in \mathbb{R}^{d_{3} \times d_{1}} \qquad \mathbf{V} \in \mathbb{R}^{d_{3} \times n}$$

Transformer Encoder

$$\begin{split} \mathbf{E} &= \texttt{Embedding}(w_i, \dots, w_n) \in \mathbb{R}^{d_1 \times n} \\ \mathbf{K} &= \mathbf{W}_k \mathbf{E} \qquad \mathbf{W}_k \in \mathbb{R}^{d_2 \times d_1} \qquad \mathbf{K} \in \mathbb{R}^{d_2 \times n} \\ \mathbf{Q} &= \mathbf{W}_q \mathbf{E} \qquad \mathbf{W}_q \in \mathbb{R}^{d_2 \times d_1} \qquad \mathbf{Q} \in \mathbb{R}^{d_2 \times n} \\ \mathbf{V} &= \mathbf{W}_v \mathbf{E} \qquad \mathbf{W}_v \in \mathbb{R}^{d_3 \times d_1} \qquad \mathbf{V} \in \mathbb{R}^{d_3 \times n} \end{split}$$

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The next layer representations are given by

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Consider the dot product between vectors \mathbf{a} and \mathbf{b} : if each entry in both vector is drawn from a distribution with zero mean and unit variance, what happens if the dimensionality grows?

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The variance of the dot product grows **linearly** with the dimensionality.

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Recall:

$$\begin{split} & \texttt{softmax}\left([1,-1]\right) = [0.88,0.12] \\ & \texttt{softmax}\left([10,-10]\right) \approx [1,2.0612 \times 10^{-9}] \end{split}$$

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The scaling factor $\sqrt{d_2}$ stabilizes the variance of the dot product. See also Xavier initialization (Glorot & Bengio, 2010).

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This formulation isn't so different from weighted bag of words.

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$$p_{i,2j} = \sin\left(\frac{i}{10000^{2j/d_1}}\right)$$
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Despite the arbitrary choice of the constant 10,000, the theoretical motivation is to make the add- δ relation in position encoding representable by a linear transformation.

$$\forall \delta \in \mathbb{N}_+, \exists \mathbf{M}_{\delta} s.t. \forall i, \mathbf{p}_{i+\delta} = \mathbf{M}_{\delta} \mathbf{p}_i$$

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Key idea: add position encoding **p** to the input embeddings.

$$p_{i,2j} = \sin\left(\frac{i}{10000^{2j/d_1}}\right)$$
 $p_{i,2j+1} = \cos\left(\frac{i}{10000^{2j/d_1}}\right)$

Despite the arbitrary choice of the constant 10,000, the theoretical motivation is to make the add- δ relation in position encoding representable by a linear transformation.

$$\forall \delta \in \mathbb{N}_+, \exists \mathbf{M}_{\delta} s.t. \forall i, \mathbf{p}_{i+\delta} = \mathbf{M}_{\delta} \mathbf{p}_i$$

Now: learnable position encoding (Shaweet al., 2018, inter alia) 2018, inter alia

Multi-Head Attention

$$\begin{split} \mathbf{E} &= \texttt{Embedding}(w_i, \dots, w_n) \in \mathbb{R}^{d_1 \times n} \\ \mathbf{K} &= \mathbf{W}_k \mathbf{E} \qquad \mathbf{W}_k \in \mathbb{R}^{d_2 \times d_1} \qquad \mathbf{K} \in \mathbb{R}^{d_2 \times n} \\ \mathbf{Q} &= \mathbf{W}_q \mathbf{E} \qquad \mathbf{W}_q \in \mathbb{R}^{d_2 \times d_1} \qquad \mathbf{Q} \in \mathbb{R}^{d_2 \times n} \\ \mathbf{V} &= \mathbf{W}_v \mathbf{E} \qquad \mathbf{W}_v \in \mathbb{R}^{d_3 \times d_1} \qquad \mathbf{V} \in \mathbb{R}^{d_3 \times n} \end{split}$$

The equation above is called one **head** of attention.

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To capture different aspects of the input, we concatenate multiple heads to form the feature.

Remember these heads should be initialized differently.

Stacking Multiple Layers of Transformers

$$\begin{split} \mathbf{E} &= \texttt{Embedding}(w_i, \dots, w_n) \in \mathbb{R}^{d_1 \times n} \\ \mathbf{K} &= \mathbf{W}_k \mathbf{E} \qquad \mathbf{W}_k \in \mathbb{R}^{d_2 \times d_1} \qquad \mathbf{K} \in \mathbb{R}^{d_2 \times n} \\ \mathbf{Q} &= \mathbf{W}_q \mathbf{E} \qquad \mathbf{W}_q \in \mathbb{R}^{d_2 \times d_1} \qquad \mathbf{Q} \in \mathbb{R}^{d_2 \times n} \\ \mathbf{V} &= \mathbf{W}_\nu \mathbf{E} \qquad \mathbf{W}_\nu \in \mathbb{R}^{d_3 \times d_1} \qquad \mathbf{V} \in \mathbb{R}^{d_3 \times n} \\ \tilde{\mathbf{E}} &= \mathbf{V} \text{softmax} \left(\frac{\mathbf{K}^T \mathbf{Q}}{\sqrt{d_2}} \right) \in \mathbb{R}^{d_3 \times n} \end{split}$$

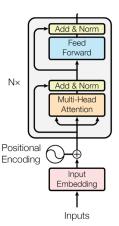
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The output of one transformer layer $\tilde{\mathbf{E}}$ is fed into the next layer as the input \mathbf{E} .

The Residual Connections in Transformers

After processing in each transformer component, the output is added to the input.

$$\mathbf{x} \leftarrow \mathbf{x} + \mathcal{F}(\mathbf{x})$$



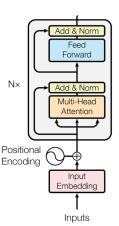
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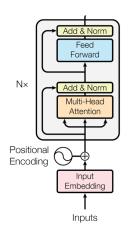
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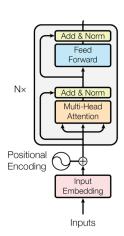
Another interpretation: the residual connection is the main flow of information, while other results are added to the main flow.



Transformers as MLPs

$$\mathbf{E} = ext{Embedding}(w_i, \dots, w_n) \in \mathbb{R}^{d_1 \times n}$$
 $\mathbf{K} = \mathbf{W}_k \mathbf{E} \qquad \mathbf{W}_k \in \mathbb{R}^{d_2 \times d_1}$
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 $\tilde{\mathbf{E}} = \mathbf{V} ext{softmax}\left(\frac{\mathbf{K}^T \mathbf{Q}}{\sqrt{d_2}}\right) \in \mathbb{R}^{d_3 \times n}$

All above are generalized linear operations, coupled with a some real MLP in each Transformer layer.



Suppose $\mathbf{H} \in \mathbb{R}^{n \times d}$ is the final hidden state of a transformer. If we calculate attention weights α on \mathbf{H} , does it mean that the model is attending to the corresponding tokens?

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∂loss For input-based explanation, compute

Simonyan et al. 2013. Deep Inside Convolutional Networks: Visualising Image Classification Models and Saliency Maps

What's Not Covered (Much) in the Lecture

 Initialization and normalization techniques for stabilizing training.

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- Initialization and normalization techniques for stabilizing training.
 - https://pytorch.org/docs/stable/nn.init.html Ba et al. (2016). Layer Normalization.
- Dropout (Srivastava et al., 2014): a simple regularization technique that randomly sets some the input units (of a neural layer) to zero at each update during training. Remember to turn off dropout during evaluation!

Next

Language Modeling