

Advanced Natural Language Processing

Lecture 7: Transformer



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Content



- Transformer modules
- Code example

Transformer: Is Attention All We Need?



- Proposed by Google brain in 2017
- Nearly applied in every state-of-the-art NLP model today
 - Even CV models and protein/music/audio models

Attention Is All You Need

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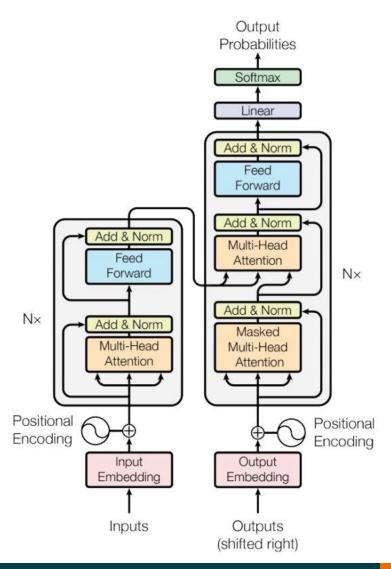
Illia Polosukhin* † illia.polosukhin@gmail.com



Courtesy of Paramount Pictures

Transformer

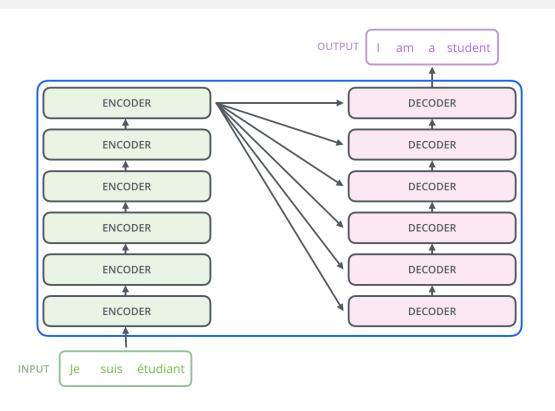


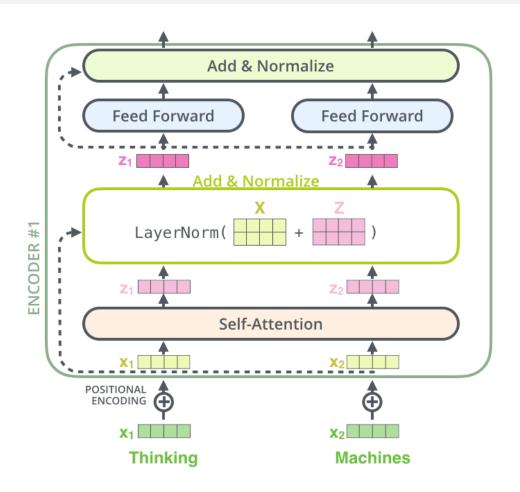


- Purely rely on attention mechanism
 - No CNN or RNN
- Stacked encoder and decoder layers
- Self-attention and cross-attention
- Feed forward layers
- Layer normalization
- Residual connection

Transformer

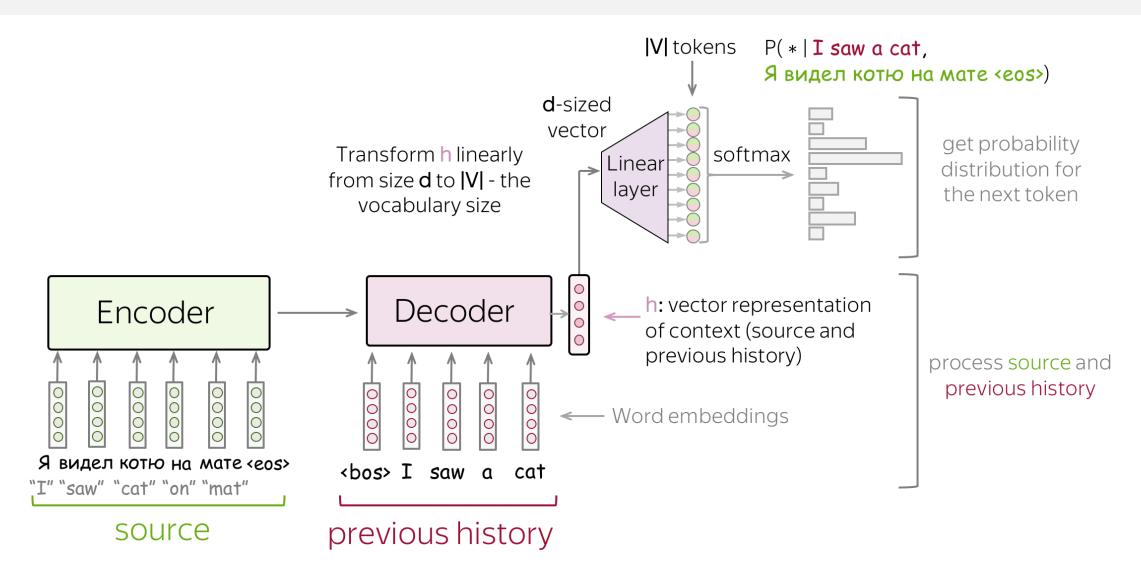






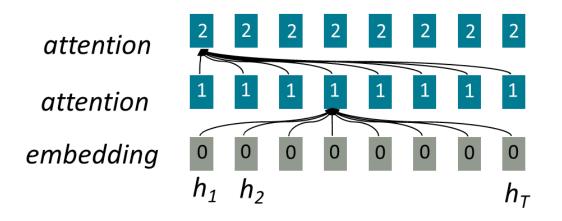
Transformer





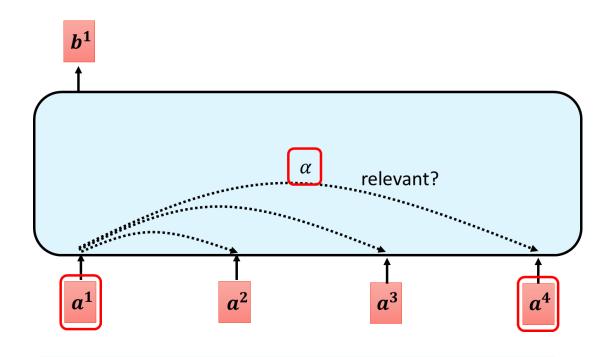


- Attention treats each word's representation as a query to access and incorporate information from a set of values.
- Self-attention is encoder-encoder (or decoder-decoder) attention where each word attends to each other word within the input (or output).

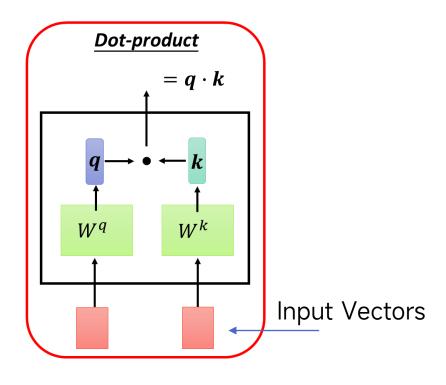


All words attend to all words in previous layer; most arrows here are omitted



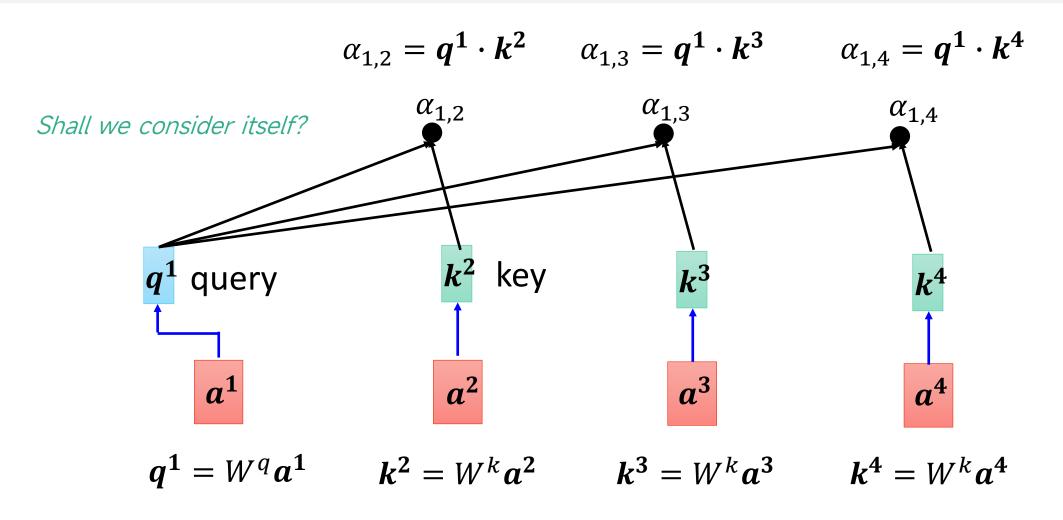


- query asking for information;
- key saying that it has some information;
- value giving the information.
- (key-value) storage

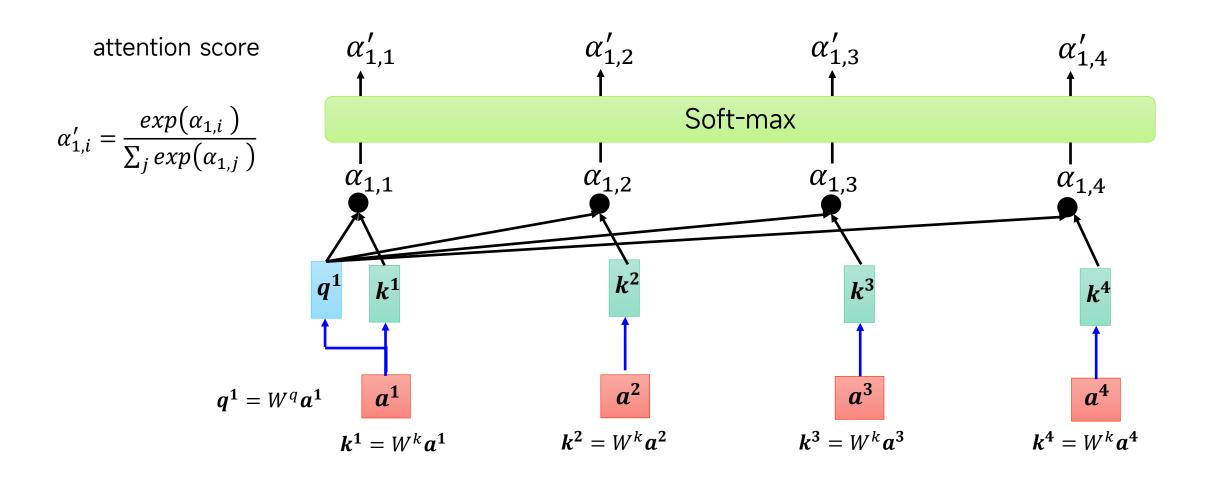


Find the relevant vectors in a sequence





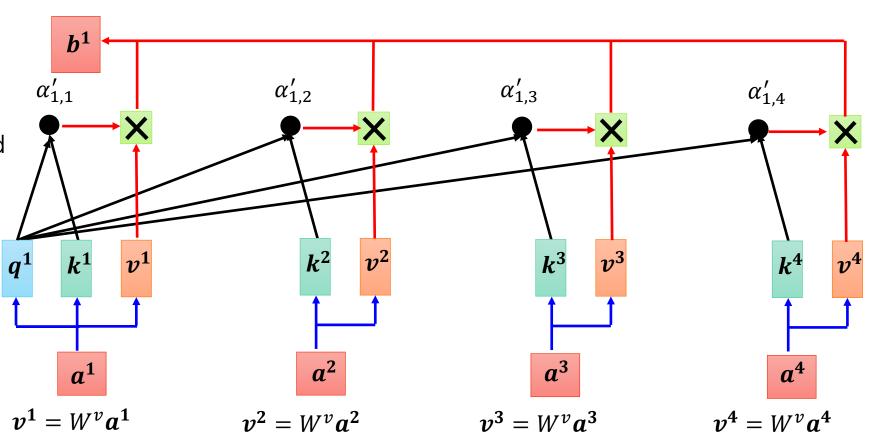




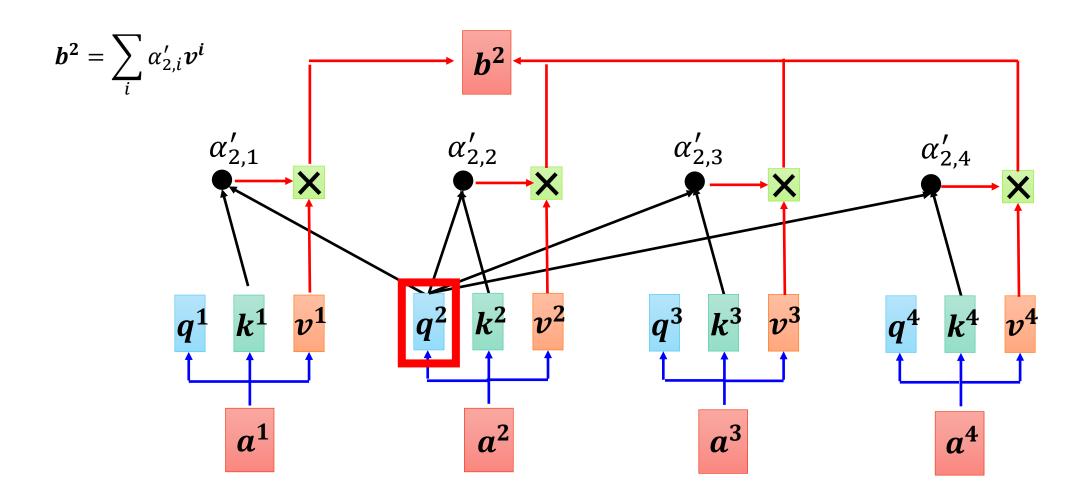


$$\boldsymbol{b^1} = \sum_i \alpha'_{1,i} \boldsymbol{v^i}$$

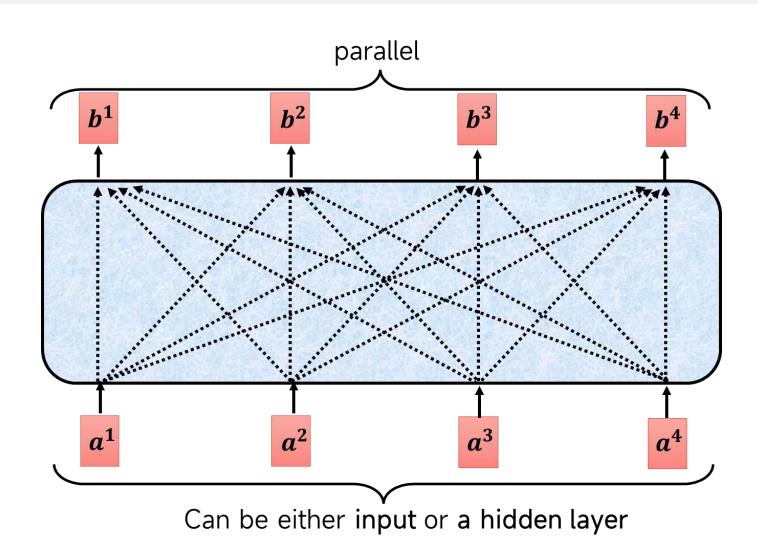
- Extract information based on attention scores
- Weighted sum of input vectors





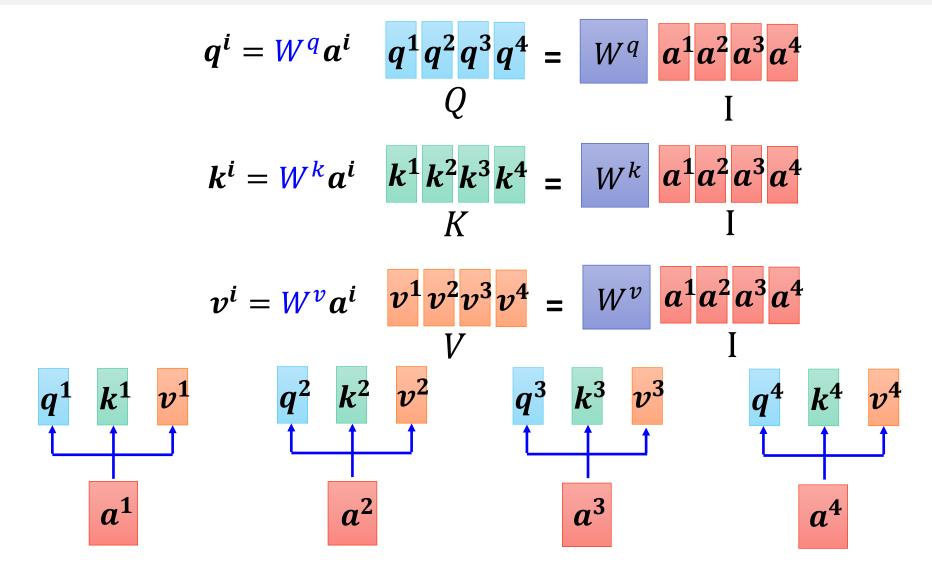




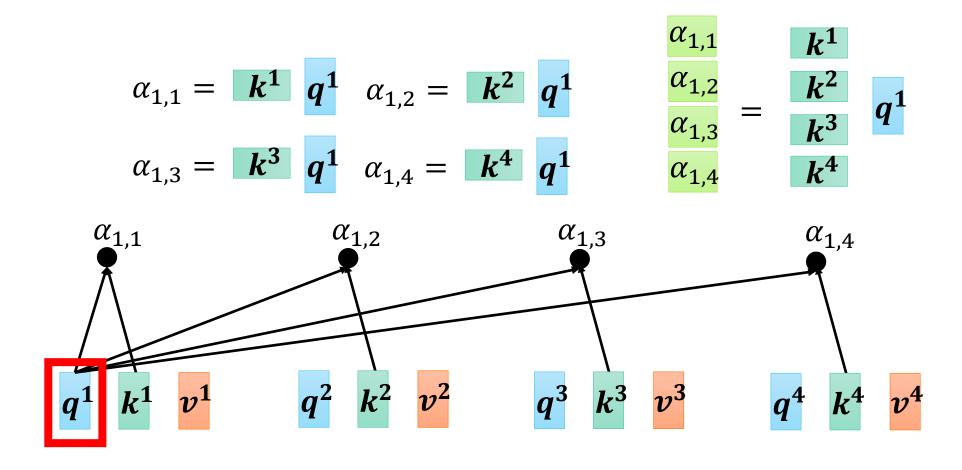


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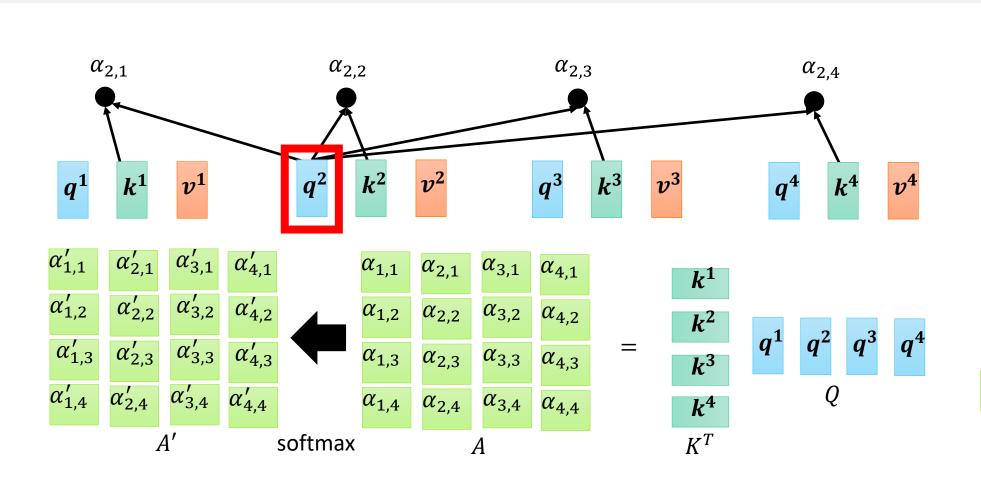


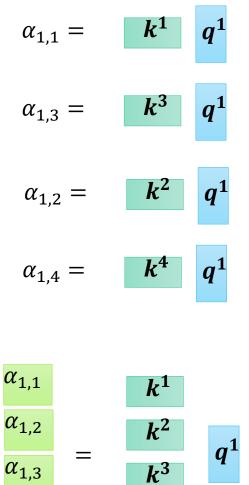








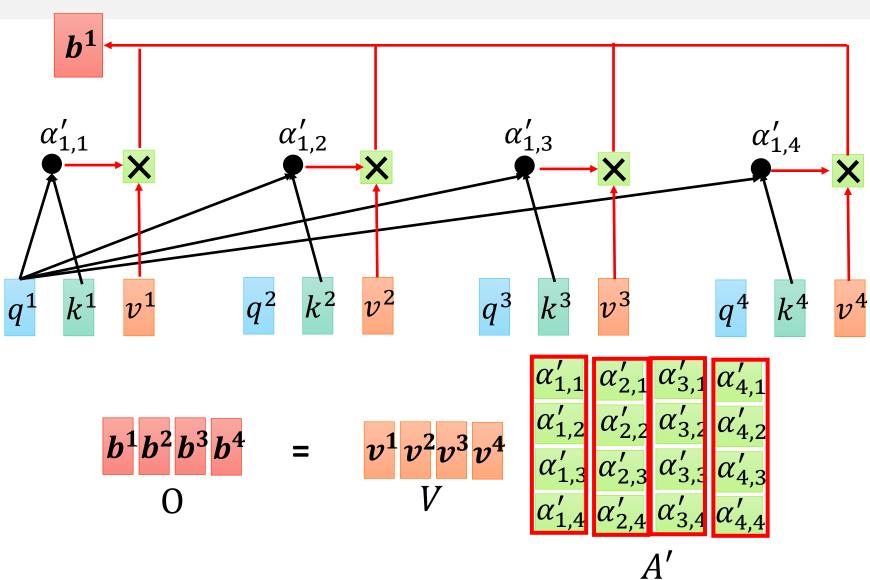




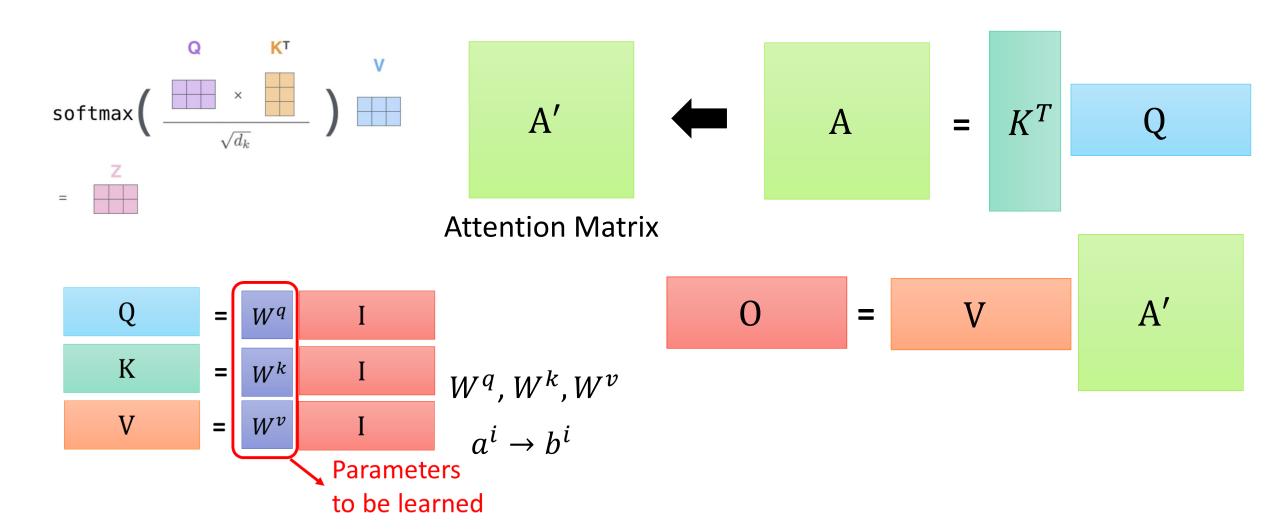
 k^4

 $\alpha_{1,4}$

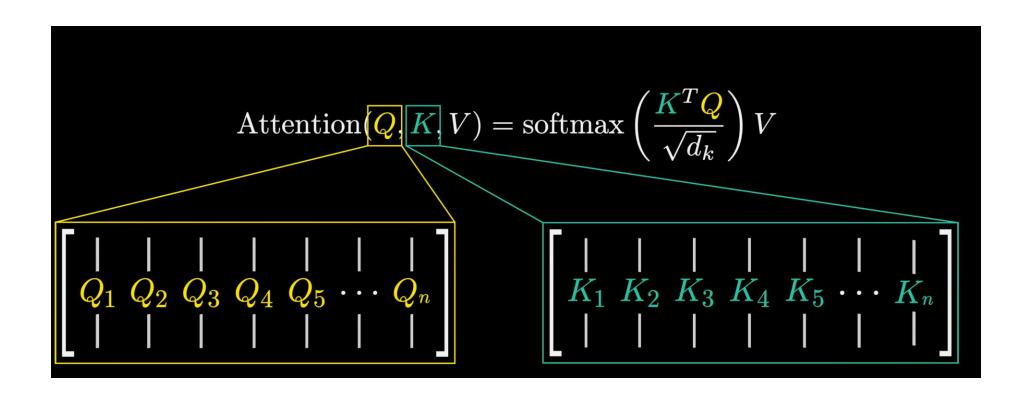












Attention in transformers, step-by-step | Deep Learning Chapter 6

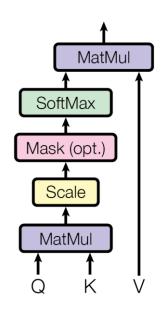


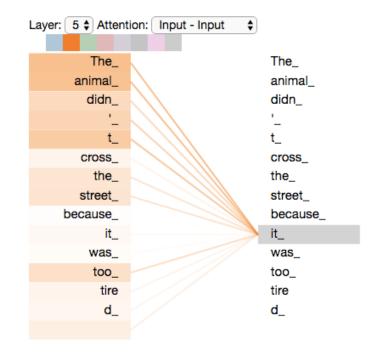
- The input hidden states $X = [x_1, x_2, ..., x_S]^T$
 - For position i, hidden state is x_i
- The key and value input are X
 - $K = W^K X, V = W^V X$
- For position i, the query input is x_i
 - $Q_i = W^Q x_i$
- The self-attention output is calculated as

$$y_i = \operatorname{softmax}(\frac{K^T Q_i}{\sqrt{d_k}})V$$

Put the weighted sum in a matrix form,

$$y = \operatorname{softmax}\left(\frac{K^T Q}{\sqrt{d_k}}\right) V$$







• To illustrate why the dot products get large, assume that the components of q and k are independent random variables with mean 0 and variance 1. Then their dot product,

$$q \cdot k = \sum_{i=1}^{d_k} q_i k_i$$

has mean 0 and variance d_k .

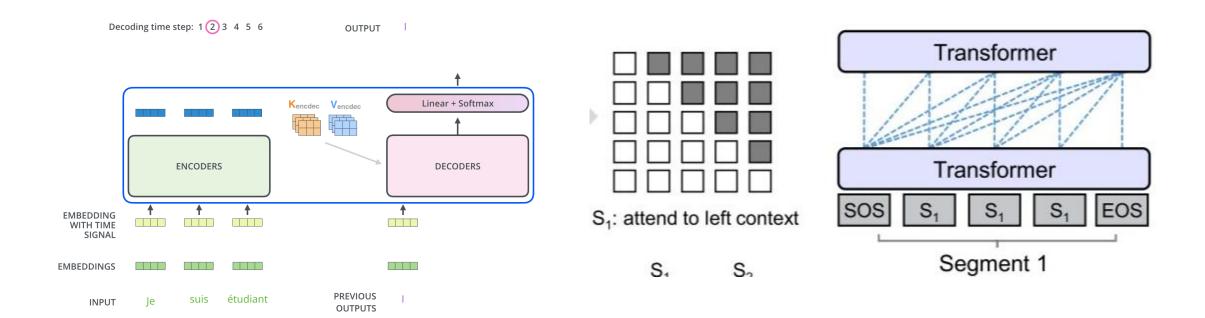
从熵不变性看Attention的Scale操作 - 科学空间

⁴To illustrate why the dot products get large, assume that the components of q and k are independent random variables with mean 0 and variance 1. Then their dot product, $q \cdot k = \sum_{i=1}^{d_k} q_i k_i$, has mean 0 and variance d_k .

Masked Self-Attention



• Many models generate texts in an auto-regressive manner, from left to right

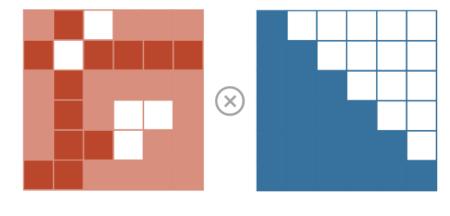


Masked Self-Attention



Efficient implementation: compute attention as we normally do, mask out attention to future words by setting attention scores to $-\infty$

$$\alpha = \operatorname{softmax}(\frac{QK^T}{\sqrt{d_k}})$$



raw attention weights

Missing $\sqrt{d_k}$

mask

```
dot = torch.bmm(queries, keys.transpose(1, 2))
indices = torch.triu_indices(t, t, offset=1)
dot[:, indices[0], indices[1]] = float('-inf')

dot = F.softmax(dot, dim=2)
```

http://peterbloem.nl/blog/transformers

Multi-head Self-Attention



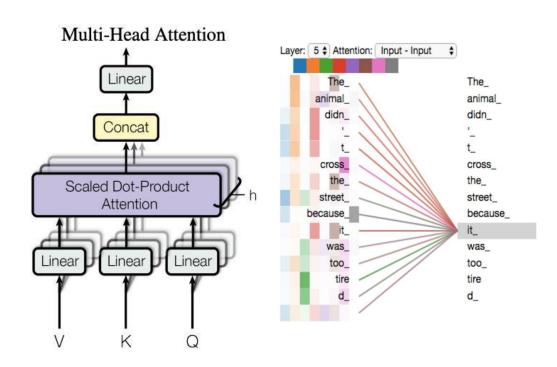
- Linearly project the queries, keys and values h times with different, learned linear projections

 MultiHead $(X, X, X) = \text{Concat}(\text{head}_1, ..., \text{head}_h)W^O$
- Where,

head_i = Attention
$$(XW_i^Q, XW_i^K, XW_i^V)$$

= softmax $((XW_i^Q)(XW_i^K)^T)(XW_i^V)W_i^O$
 $W_i^K \in R^{d_m \times d_k}, d_k = \frac{d_m}{h}$

- It expands the model's ability to focus on different positions
- It gives the attention layer multiple representation subspaces



Multi-head Self-Attention

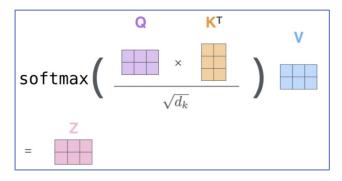


1) This is our input sentence*

2) We embed each word*

3) Split into 8 heads. We multiply X or R with weight matrices 4) Calculate attention using the resulting Q/K/V matrices

5) Concatenate the resulting Z matrices, then multiply with weight matrix W° to produce the output of the layer

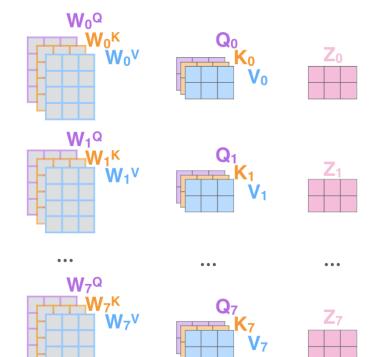


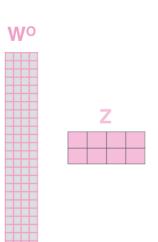
Thinking Machines



* In all encoders other than #0, we don't need embedding. We start directly with the output of the encoder right below this one

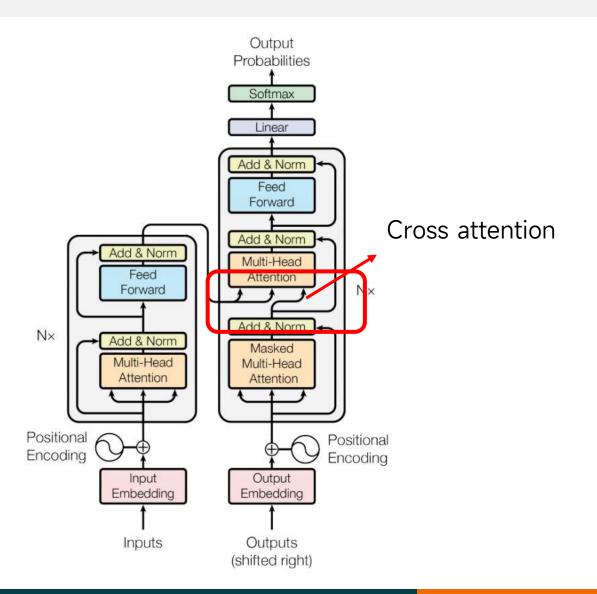






Cross-Attention



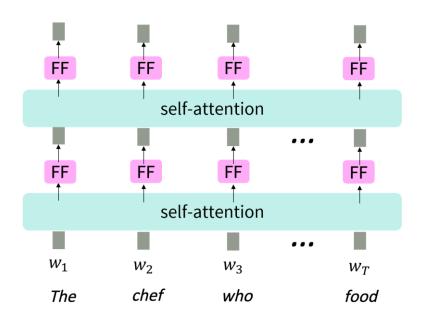


- The key/value vectors are from encoder output
- The query vectors are from last block in the decoder

Feed Forward Layer



- Apply a feedforward layer to the output of attention, providing non-linear activation (and additional expressive power)
- Feature expansion and compression $(4 \cdot d_m)$
- Store knowledge and act as a memory
- Consists of two linear layers [<u>link</u>]



$$FFN(\mathbf{x}_i) = ReLU(\mathbf{x}_i \mathbf{W}_1 + \mathbf{b}_1) \mathbf{W}_2 + \mathbf{b}_2$$
$$\mathbf{W}_1 \in \mathbb{R}^{d \times d_{ff}}, \mathbf{b}_1 \in \mathbb{R}^{d_{ff}}$$
$$\mathbf{W}_2 \in \mathbb{R}^{d_{ff} \times d}, \mathbf{b}_2 \in \mathbb{R}^d$$

In practice, they use $d_{ff} = 4d$

[2012.14913] Transformer Feed-Forward Layers Are Key-Value Memories



- Estimates the normalization statistics from the inputs within a hidden layer
- Reduce uninformative variation by normalizing to zero mean and standard deviation of one within each layer
- All the hidden units in a layer share the same trainable parameter γ , β

$$y = \frac{x - E[x]}{\sqrt{\text{Var}[x] + \epsilon}} \gamma + \beta$$

• Each token share the same normalization term E[x], Var[x]

```
# features: (bsz, max len, hidden dim)
class LayerNorm(nn.Module):
   def init (self, features, eps=1e-6):
        super(LayerNorm, self).__init__()
       self.a 2 = nn.Parameter(torch.ones(features))
        self.b_2 = nn.Parameter(torch.zeros(features))
        self.eps = eps
   def forward(self, x):
       mean = x.mean(-1, keepdim=True) # mean: [bsz,
max len, 1]
        std = x.std(-1, keepdim=True) # std: [bsz,
max len, 1]
       return self.a_2 * (x - mean) / (std + self.eps)
+ self.b 2
```



- Why layer normalization for Transformer?
 - Stabilize training by reducing the network sensitivity to the scale of input features, leading to faster convergence and improved performance
 - Address internal covariate shift problem, a phenomenon where the distribution of inputs to a given layer changes during training as the model parameters are updated
 - Enhance gradient flow and address challenges like exploding or vanishing gradients

<u>Understanding Layer Normalization - by Daniel Kleine</u>



• Layer normalization is <u>different</u> in the context of CNN and Transformer

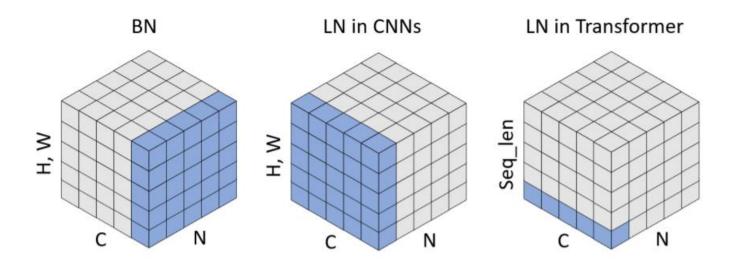
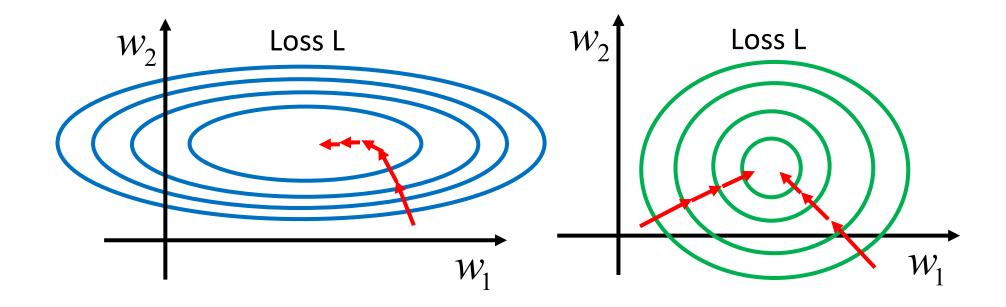


Figure 1: An illustration of **normalization methods**. Each subplot represents a feature map tensor, with B as the batch axis, C as the channel axis, and (H, W) or Seq_len as the spatial axes. The elements in blue are normalized by the same mean and variance, computed by aggregating the values of these elements.



• Improves convergence stability and sometimes even quality.



Positional Embedding



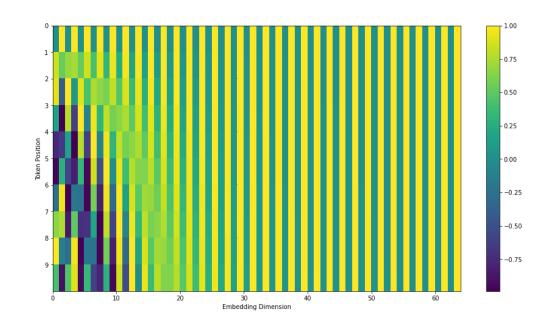
 Help the model determine the position of each word, or the distance between different words in the sequence

$$PE(pos, 2i) = sin(\frac{pos}{10000^{\frac{2i}{d_m}}})$$

$$PE(pos, 2i + 1) = cos(\frac{pos}{10000^{\frac{2i}{d_m}}})$$

$$10000^{\frac{2i}{d_m}}$$

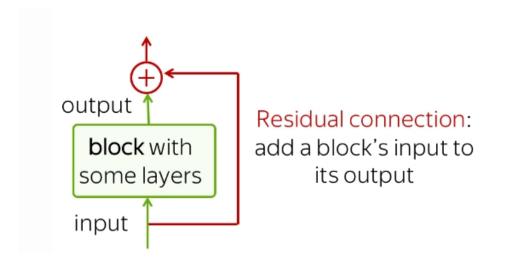
- pos is the position, i is the dimension, d_m is the model hidden state dimension
- Relative position embedding [ALiBi, RoPE]
 - In future class

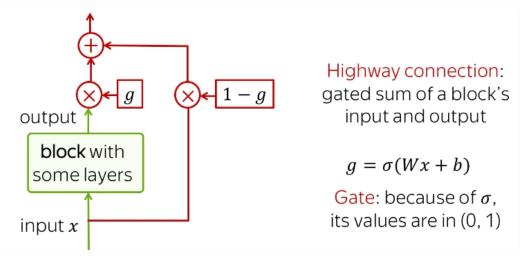


Residual Connection



- Residual connection $x^{l} = \operatorname{block}(x^{l-1}) + x^{l-1}$
- Used after each attention and FFN block
- Mitigate the gradient vanishing problem
- Ease the gradient flow through a network and allow stacking a lot of layers.





[1505.00387] Highway Networks (arxiv.org)

Dropout



- During training, randomly zeroes some of the elements of the input tensor with probability p using samples from a Bernoulli distribution
- Compare model.train(), vs. model.eval(), vs. torch.no_grads()

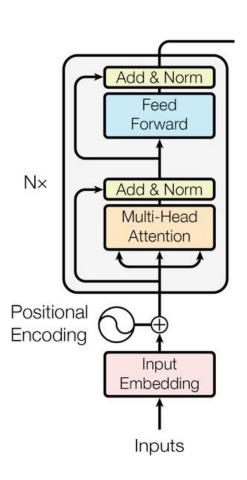
```
def forward(self, hidden_states: torch.Tensor, input_tensor: torch.Tensor)
   hidden_states = self.dense(hidden_states)
   hidden_states = self.dropout(hidden_states)
   hidden_states = self.LayerNorm(hidden_states + input_tensor)
   return hidden_states
```

<u>Illustrated Guide to Transformers Neural Network</u>

Srivastava, N., Hinton, G., Krizhevsky, A., Sutskever, I., & Salakhutdinov, R. (2014). Dropout: a simple way to prevent neural networks from overfitting. The Journal of Machine Learning Research, 15(1), 1929-1958.

Transformer Encoder





From the bottom to the top:

- Input embedding
- Positional encoding
- A stack of Transformer encoder layers

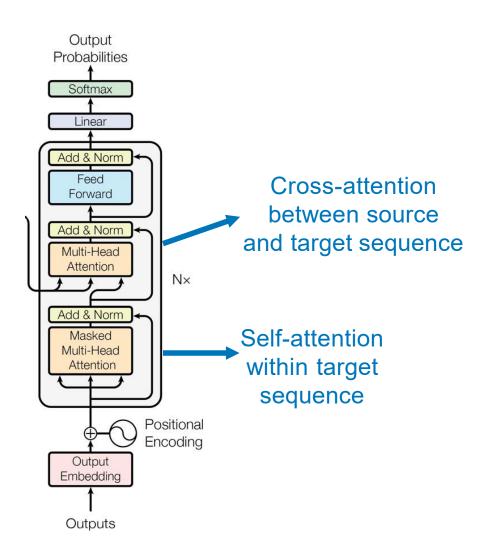
Transformer encoder is a stack of *N* layers, which consists of two sub-layers:

- Multi-head attention layer
- Feed-forward layer

$$\mathbf{x}_1, \dots, \mathbf{x}_n \in \mathbb{R}^{d_1} \longrightarrow \mathbf{h}_1, \dots, \mathbf{h}_n \in \mathbb{R}^{d_2}$$

Transformer Decoder





From the bottom to the top:

- Output embedding
- Positional encoding
- A stack of Transformer decoder layers
- Linear + softmax

Transformer decoder is a stack of *N* layers, which consists of three sub-layers:

- Masked multi-head attention
- Multi-head cross-attention
- Feed-forward layer
- (W/ Add & Norm between sub-layers)

Count the Model Parameters



- Suppose hidden state h, layer number L, head number n_h ,
- Total model parameters = embedding params. + layer params. \times layer numbers
- Embedding layer
 - Token embedding $|V| \cdot d$
 - Position embedding (learned or not): $l_c \cdot d$
 - l_c : Max. sentence length

Use code:

sum(p.numel() for p in model.parameters())

Count the Model Parameters



- Suppose hidden state h, encoder/decoder layer number L, head number n_h , then head hidden state $h_d = \frac{h}{n_h}$
 - Self-attention / cross-attention
 - For all heads, W_q , W_k , W_v , W_o each has $d \cdot n_h \cdot h_d = d^2$ parameters
 - Feedforward sublayer
 - Two matrices of $d \cdot (d \cdot 4)$ has $8d^2$ params. in total
 - Layer Norm $2 \cdot (d + d) = 4d$ (each encoder layer has two LNs)
- For each encoder layer, $4d^2 + 8d^2 + 4d = 12d^2 + 4d$ params.
- For each decoder layer, $4d^2 + 4d^2 + 8d^2 + 6d = 16d^2 + 6d$ params.
- Total parameters count is $(|V| + l_c)d + (28d^2 + 10d) \cdot L$.
 - When tie the input and output embeddings

Transformer Deep Dive: Parameter Counting

Count the Model Parameters



Example: suppose a model has 61M parameters

- If all weights are stored with 32-bit numbers, total storage will be about
 - 61M × 4 Bytes (32 bits) = 232.7 MB (244 × 10⁶ Bytes)
- If all weights are stored with 8-bit numbers, total storage will be about
 - 61M × 1 Byte (8 bits) = 58.2 MB
 - Bit (比特/位) vs. bytes (字节), 1B = 8b
 - MB vs. MiB → 1MiB = 1024KB
 - Usually, MB = MiB
 - WLAN 1000M → 1000 Mbps (megabits per second)
 - Hard drive 1MB = 1000 KB

Transformer Architecture Specifications



■ d_{model}

	N	d_{model}	$d_{ m ff}$	h	d_k	d_v
base	6	512	2048	8	64	64

From Vaswani et al.

Model Name	$n_{ m params}$	$n_{ m layers}$	$d_{ m model}$	$n_{ m heads}$	$d_{ m head}$
GPT-3 Small	125M	12	768	12	64
GPT-3 Medium	350M	24	1024	16	64
GPT-3 Large	760M	24	1536	16	96
GPT-3 XL	1.3B	24	2048	24	128
GPT-3 2.7B	2.7B	32	2560	32	80
GPT-3 6.7B	6.7B	32	4096	32	128
GPT-3 13B	13.0B	40	5140	40	128
GPT-3 175B or "GPT-3"	175.0B	96	12288	96	128

Add & Norm

Feed
Forward

Add & Norm

Multi-Head
Attention

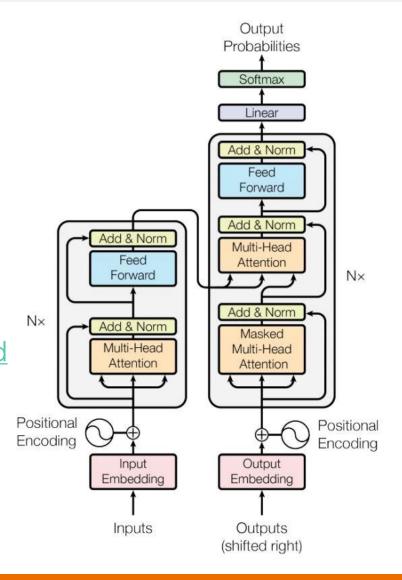
Add & Norm

From GPT-3; d_{head} is our d_k

Further Reading



- The Illustrated Transformer
- The Annotated Transformer
- Transformer论文逐段精读 李沐
- Transformer models: an introduction and catalog
- Formal Algorithms for Transformers [arxiv]
- Transformers from scratch | peterbloem.nl
- LLM Visualization
- Transformer Explainer: LLM Transformer Model Visually Explained
- huggingface/transformers
- karpathy/nanoGPT



Configure the Coding Environment



- Windows, Linux, Mac OS
- Environment management
 - Conda [<u>Documentation</u>]
 - uv [Documentation]
- Command line tool
 - For windows, use git
- Coding IDE
 - VSCode, PyCharm
 - Remote SSH development
 - Plugins (e.g., github Copilot, Jupyter Notebook)

配置pvthon开发环境-参考1 参考2

conda create -n sta python=3.11.* # create a conda env named 'sta'
conda activate sta # activate the sta env and enter in
pip install torch transformers pdbpp # when you are in the 'sta'
env, install python packages using pip
conda deactivate sta # deactivate and exit from the env

Coding Tools



- Linux and shell scripts
 - User SSH to connect a remote server

```
mkdir -p ~/data
cd ~/data
wget -c https://dl.fbaipublicfiles.com/flores101/dataset/flores101_dataset.tar.gz -O mydata.tar.gz
tar -zxf mydata.tar.gz

for fname in flores101_dataset/dev/*; do
    lang=$(basename $fname '.dev')
    echo $lang
    mkdir -p results/$lang
    head -n 10 flores101_dataset/dev/$lang.dev > results/${lang}/${lang}-copy.txt
done
```

Coding Tools



Schedule

- 1/13/20: Course overview + the shell
- 1/14/20: Shell Tools and Scripting
- 1/15/20: Editors (Vim)
- **1/16/20**: <u>Data Wrangling</u>
- 1/21/20: Command-line Environment
- 1/22/20: <u>Version Control (Git)</u>
- 1/23/20: Debugging and Profiling
- 1/27/20: <u>Metaprogramming</u>
- 1/28/20: Security and Cryptography
- 1/29/20: Potpourri
- 1/30/20: <u>Q&A</u>

The Missing Semester of Your CS Education

- Python debug
 - Read the error message
 - Read the official documentation
 - Read the code/package examples
 - Read tutorials
 - Narrow down the bug by toy samples
 - Learn the code style [Google Python Style Guide]
- Play with the python code

Example of LLM Training



```
from datasets import load dataset
from trl import SFTConfig, SFTTrainer
import torch
# Set device
device = "cuda" if torch.cuda.is available() else "cpu"
# Load dataset
dataset = load dataset("HuggingFaceTB/smoltalk", "all")
# Configure model and tokenizer
model name = "HuggingFaceTB/SmolLM2-135M"
model =
AutoModelForCausalLM.from pretrained(pretrained model name o
r path=model name).to(
    device
tokenizer =
AutoTokenizer.from pretrained(pretrained model name or path=
model name)
# Setup chat template
model, tokenizer = setup chat format(model=model,
tokenizer=tokenizer)
```

```
# Configure trainer
training_args = SFTConfig(
    output dir="./sft output",
    max steps=1000,
    per device train batch size=4,
    learning rate=5e-5,
    logging steps=10,
    save steps=100,
    eval_strategy="steps",
    eval steps=50,
# Initialize trainer
trainer = SFTTrainer(
   model=model,
    args=training_args,
    train dataset=dataset["train"],
    eval dataset=dataset["test"],
    processing class=tokenizer,
# Start training
trainer.train()
```

<u>Supervised Fine-Tuning - Hugging Face LLM Course</u>

More Examples



karpathy/nanoGPT.

```
Config/
                         249
                                  # training loop
                         250
                                  X, Y = get batch('train') # fetch the very first batch
  Model.py
                                  t0 = time.time()
                          251
                         252
                                  local iter num = 0 # number of iterations in the lifetime of this process
  Train.py
                                  raw model = model.module if ddp else model # unwrap DDP container if needed
                         253

    Sample.py

                         254
                                  running mfu = -1.0
                         255
                                  while True:
   Bench.py
                          256
                                      # determine and set the learning rate for this iteration
                         257
                                      lr = get lr(iter num) if decay lr else learning rate
                         258
                                      for param group in optimizer.param groups:
                          259
                                          param group['lr'] = lr
                          260
                         261
                         262
                                      # evaluate the loss on train/val sets and write checkpoints
                         263
                                      if iter num % eval interval == 0 and master process:
                                          losses = estimate_loss()
                          264
```

print(f"step {iter_num}: train loss {losses['train']:.4f}, val loss {losses['val']:.4f}")

265

Further Reading



- Python-For-Beginners Book
- Pytorch tutorial
- [★] CS224N-pytorch tutorial
- [★] Deep Learning Tuning Playbook
- Bash-handbook github repo
- Bash scripting cheatsheet
- AutoDL帮助文档
- 文档中心 · 魔搭社区

Decoding Algorithm



• Generate target sentences

$$Y = \underset{(y_1, y_2, ..., y_L)}{\operatorname{argmax}} \prod_{i=1}^{L} p(y_i | y_{< i}, X; \theta)$$

Exhaustive search is very expensive

Greedy search

Beam search

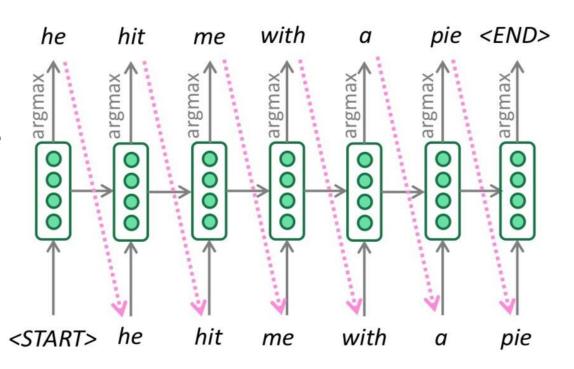
Top-k sampling

Top-p sampling

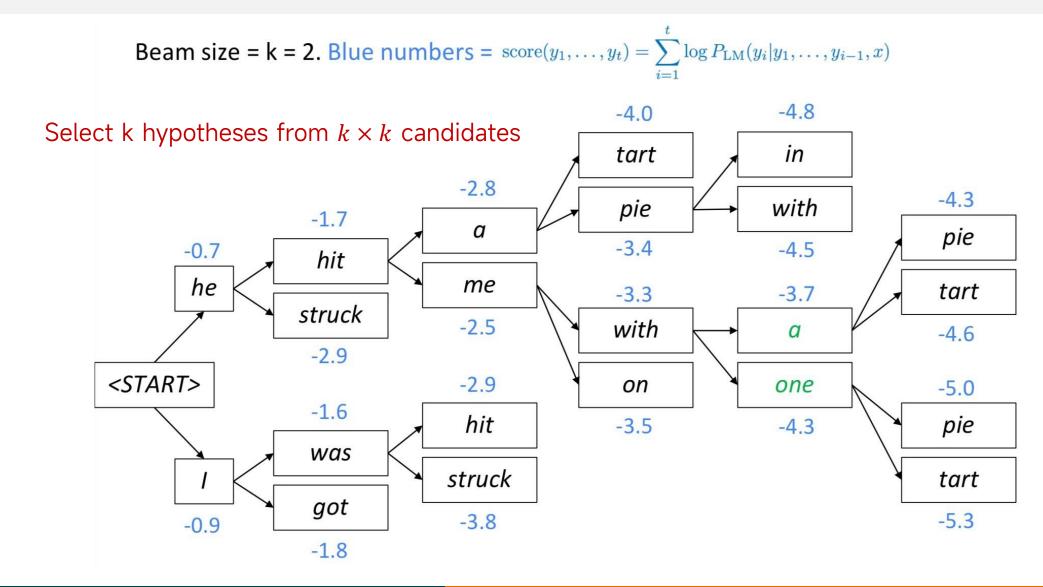
Greedy Search



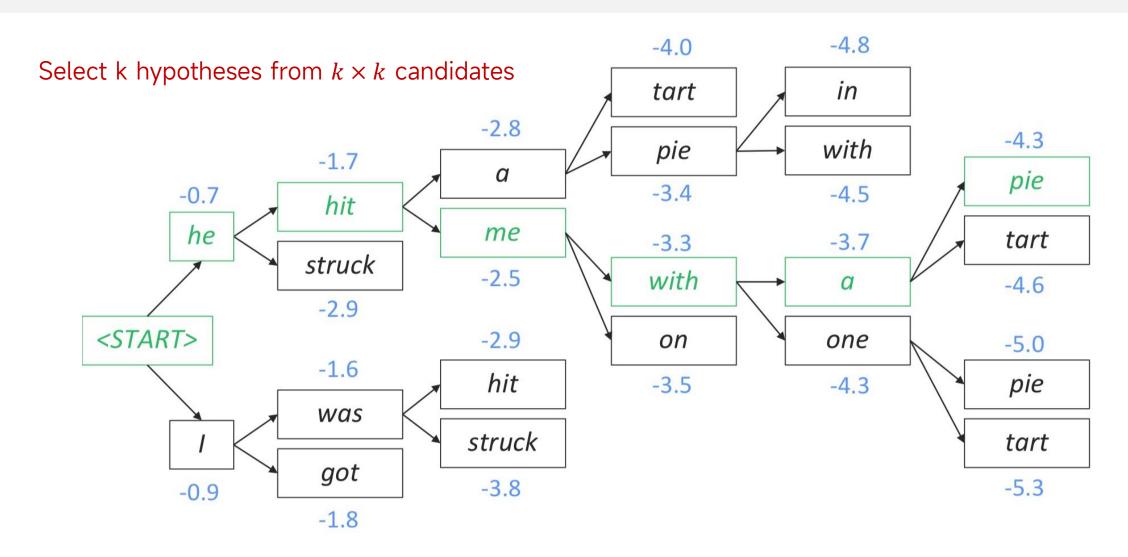
- Compute argmax at every step of decoder to generate word y_i
- Problems:
 - Will often generate the "easy" words first
 - Will prefer multiple common words to one rare word
 - May return a poor sentence that has low probabilities of words at the end.













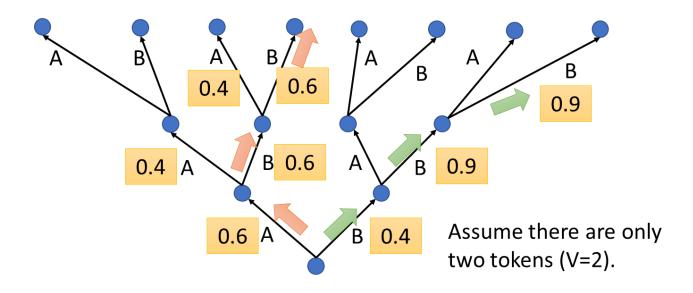
- Different hypotheses may produce <eos> token at different time steps
 - When a hypothesis produces <eos>, save it along with its score, stop expanding it and place it aside
 - Keep expanding the remaining best hypotheses
- Continue beam search until:
 - All k hypotheses produce <eos>, or
 - Hit max decoding length limit T
- Select top hypotheses using the normalized likelihood score

$$S_{norm} = \frac{1}{T} \sum_{i=1}^{t} \log p(y_i | y_{\leq i}, X; \theta)$$

• Otherwise, shorter hypotheses have higher scores



Code for beam search



The red path is greedy decoding. The green path is the best one.

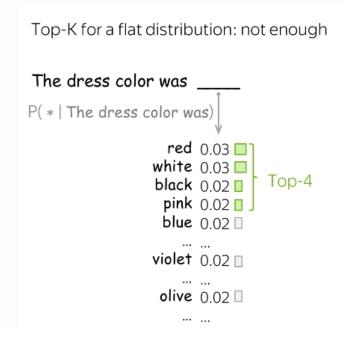
束搜索 - 动手学深度学习

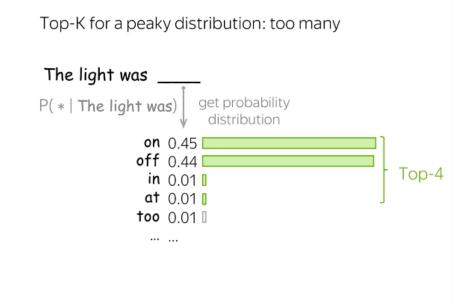
Top-k Sampling



- Always sample from top-K most likely tokens
 - Instead of selecting with scores in beam search
- When k=3, first select the top-3 tokens that have highest probabilities
- Renormalize the token distribution and sample the next token accordingly

```
# set top_k to 50
sample_output = model.generate(
    **model_inputs,
    max_new_tokens=40,
    do_sample=True,
    top_k=50
)
```





Top-k Sampling



Renormalize the token distribution and sample the next token accordingly

```
# sample

probs = nn.functional.softmax(next_token_scores, dim=-1)

next_tokens = torch.multinomial(probs, num_samples=1).squeeze(1)

2812
```

<u>Code for sampling-based decoding algorithm</u>, and <u>top-K logits wrapper</u>

Code of decoding algorithms in Transformers

Top-p Sampling



Nucleus sampling

ullet Select the smallest number of top tokens such that their cumulative probability is at least p

We propose a new stochastic decoding method: Nucleus Sampling. The key idea is to use the shape of the probability distribution to determine the set of tokens to be sampled from. Given a distribution $P(x|x_{1:i-1})$, we define its top-p vocabulary $V^{(p)} \subset V$ as the smallest set such that

$$\sum_{x \in V^{(p)}} P(x|x_{1:i-1}) \ge p. \tag{2}$$

Top-p Sampling



- The number of tokens we sample from is dynamic and depends on the properties of the distribution
- Renormalize the token distribution and sample the next token accordingly

```
sample_output = model.generate(
    **model_inputs,
    max_new_tokens=40,
    do_sample=True,
    top_p=0.92,
    top_k=0
)
```

Code for Top-p logits wrapper

<u>Top-p and Top-k sampling code</u>

How to generate text: using different decoding methods for language generation with Transformers

Temperature-based Sampling



• Define logits as $l = \{l_i\}_{i \in |V|}$, we use softmax function to get the probabilities

$$p(v_k) = \frac{e^{l_k/\tau}}{\sum_j e^{l_j/\tau}}$$

- Here, τ is the decoding temperature
 - A low temperature results a more deterministic response, keeps the model focused on the most likely response
 - A high temperature makes the model explore a wider range of responses, resulting in a more creative response

Code for temperature-based sampling

The Effect of Sampling Temperature on Problem Solving in Large Language Models - ACL Anthology



Thank you