

Deep Learning for Vision (DLV)

Classification - part II

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2023-2024



Knowledge

- What is attention, how it works
- What is Transformer:
 - main components: multi-head self/cross attention, positional encoding, encoder vs decoder
 - advantages and drawbacks

Skills and know-how

- Choose between fully-connected, convolution and attention layers given context
- Choose/adapt architecture according to constraints
- Propose ways to deal with few labeled data given context

1 The Transformer revolution

- Attention mechanism: why and how?
- The Transformer architecture
- The Vision Transformer

2 Dealing with few annotated data

The Transformer was proposed for Neural Machine Translation (NMT) task

This is known as a sequence-to-sequence problem.

Input: a sequence of tokens. Output: a sequence of tokens

Let's assume we want to translate French sentences to English.

We are working at character level (*i.e.*, each token corresponds to a character).

We use a simple character set common for both English and French and made up of 26 letters.

Propose a way to encode each character on a vector of d dimensions.

This is known as input embedding.

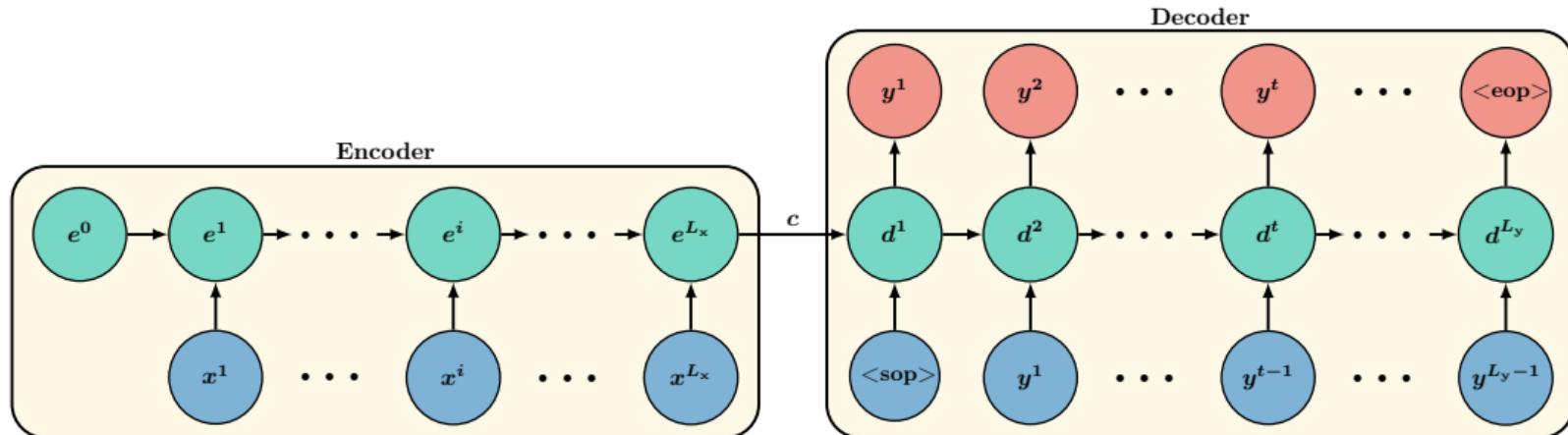
- ① if $d \geq 26$
- ② if $d < 26$

Neural Machine Translation (NMT)

A sequence-to-sequence task

x : a sequence of input tokens representing some text.

y : a sequence of output tokens representing the translated text.



For instance, encoder and decoder can be LSTM/GRU.

Limitation

- The whole input sequence is compressed into a fixed-size context vector c .

Idea: attention mechanism

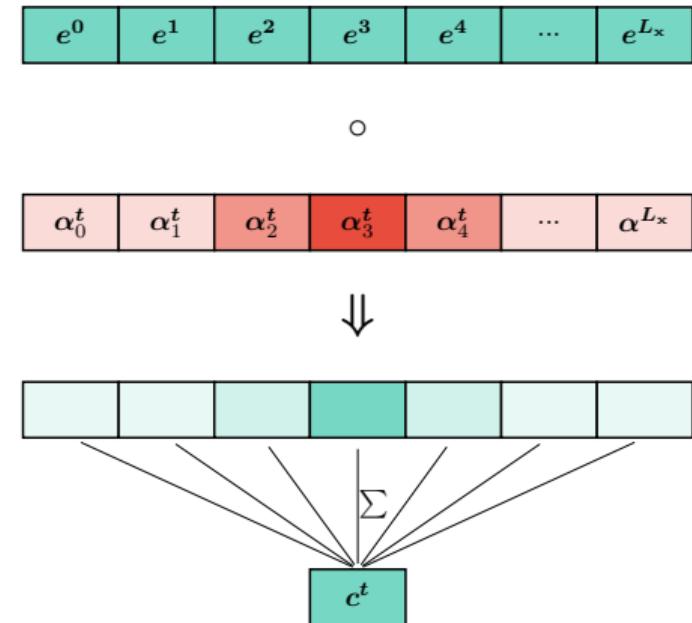
From a static context vector:

$$c = f(x)$$

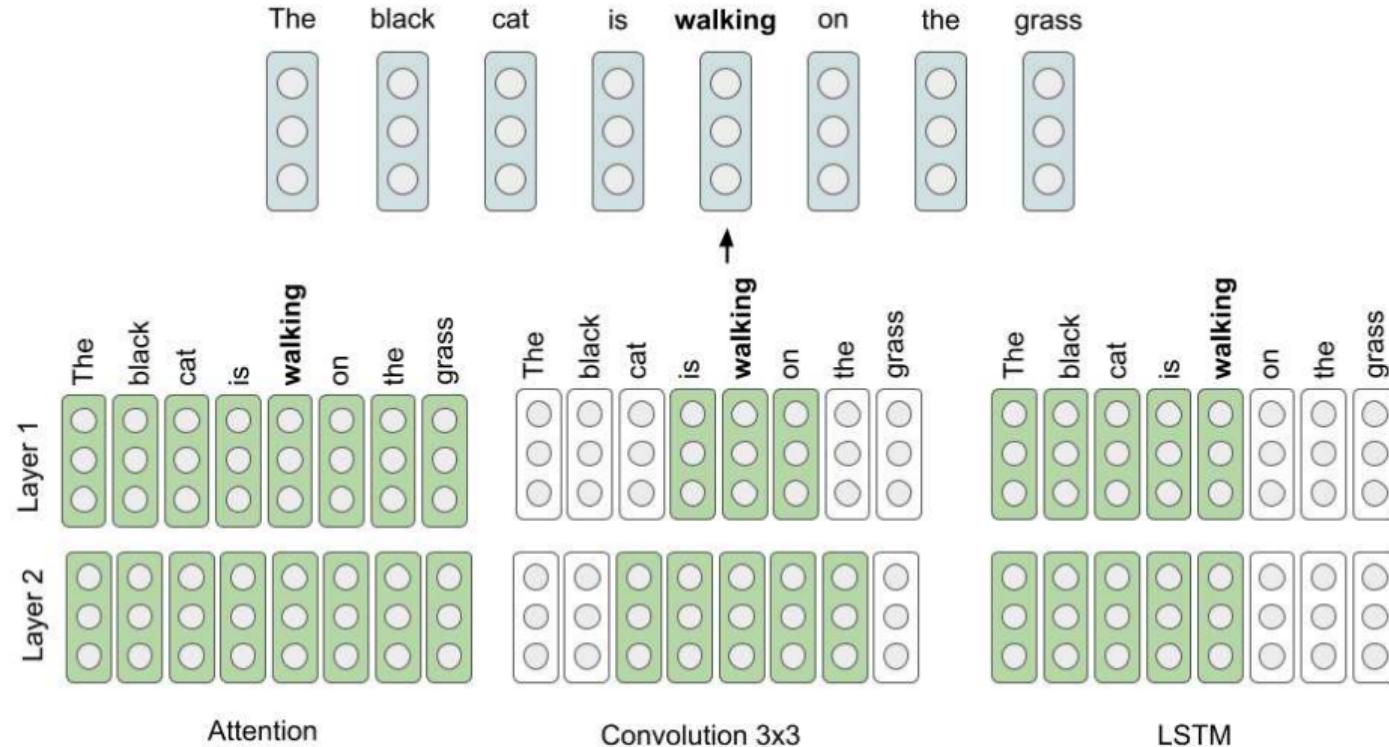
to a dynamic context vector:

$$c^t = \sum_{i=1}^{L_x} \alpha_i^t e^i$$

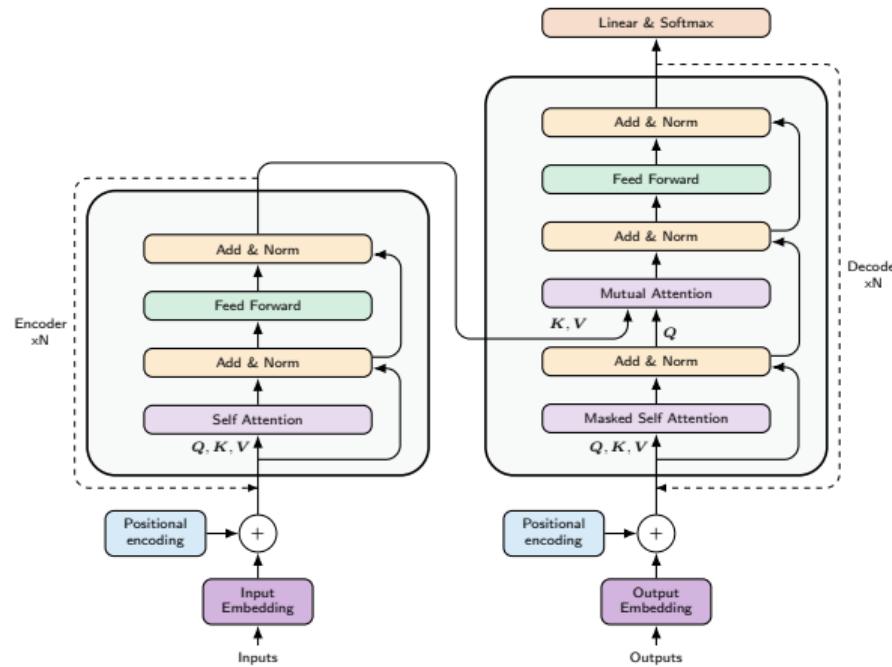
with: $\sum_i \alpha_i = 1$.



Context modeling comparison



Attention is all you need: Transformer (2017) [1]



Two main blocks:

- Transformer encoder
- Transformer decoder

One-shot encoding

$$\mathbf{f} = \text{encoder}(\mathbf{x} + \text{PE})$$

Iterative decoding

$$\mathbf{c}^t = \text{decoder}(\mathbf{f}, \{\hat{\mathbf{y}}^0, \dots, \hat{\mathbf{y}}^{t-1}\} + \text{PE})$$

$$\hat{\mathbf{y}}^t = \arg \max(\mathbf{W} \mathbf{c}^t)$$

- Mainly relies on the Query-Key-Value attention paradigm

Concept

Goal: retrieve the useful information among a collection of data

Inputs: a *query* and a set of data

Approach

- Compute a similarity score between the query and all the data
 - Generate an answer based on the most relevant data
- Two representations of the data are used: *keys* for comparison with the query, and *values* for the answer

Analogy with library search engine

Query: keywords; Keys: book titles; Values: book contents

Issue

Gradient propagation for hard attention (select only the most relevant item)

► Soft attention (weighted sum of items)

Scaled Dot-Product Attention

$q \in \mathbb{R}^d$: a query vector

$K \in \mathbb{R}^{L \times d}$: a matrix gathering key vectors for each available item

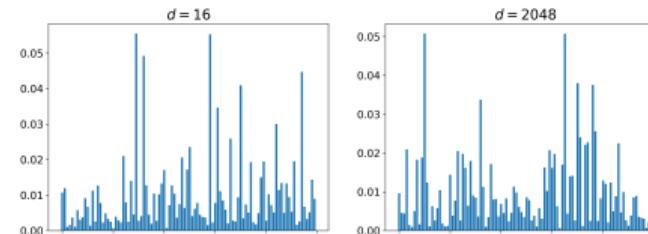
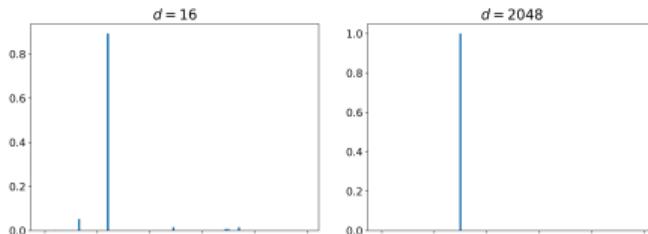
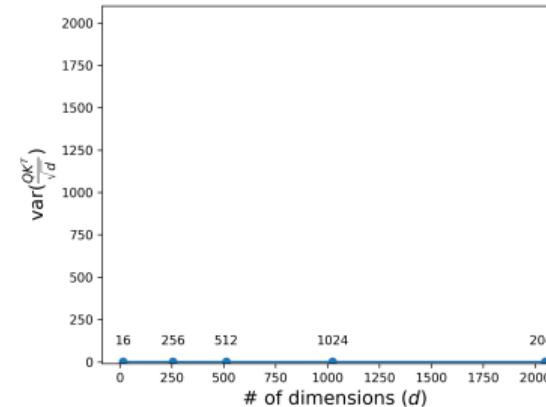
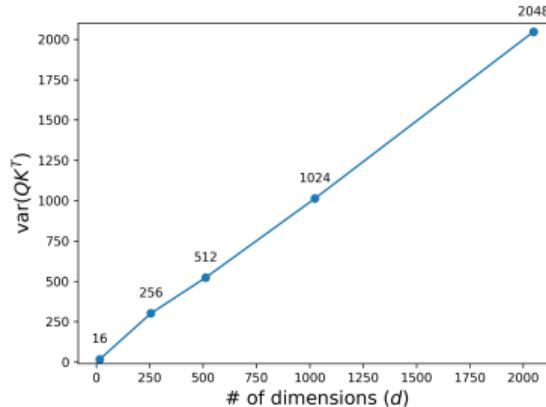
$V \in \mathbb{R}^{L \times d}$: a matrix gathering values vectors for each available item

$$\text{Attention}(q, K, V) = \underbrace{\text{softmax}\left(\frac{qK^T}{\sqrt{d}}\right)}_{\alpha} V = c \quad (\in \mathbb{R}^d)$$

► Dot product as distance function

Why scaling by $\frac{1}{\sqrt{d}}$?

For 1 query and 10,000 keys (from normal distribution):



- Queries, Keys and Values are from the same source

Query-key-value for feature extraction

\mathbf{X} : the latent representation of an input sequence.

$$\mathbf{Q} = \mathbf{X}\mathbf{W}^Q (\in \mathbb{R}^{L_x \times d})$$

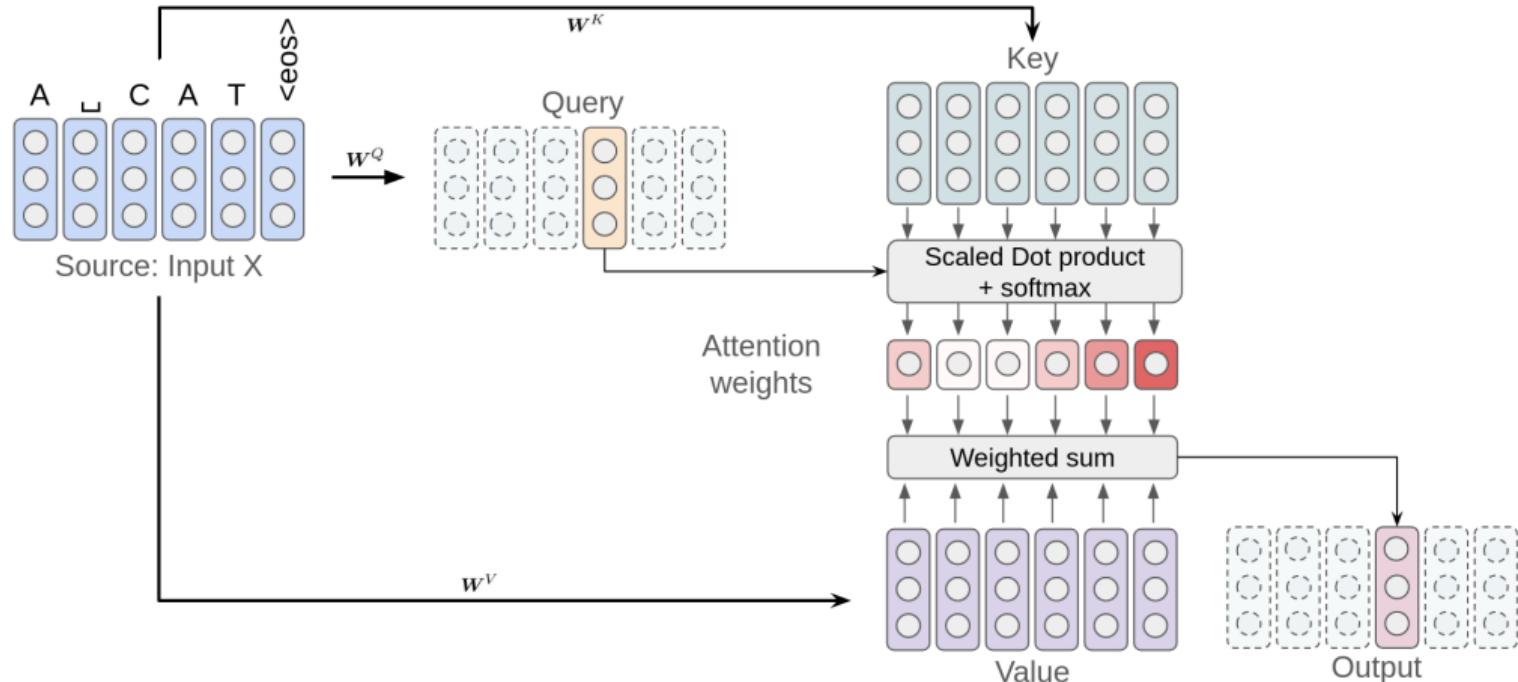
$$\mathbf{K} = \mathbf{X}\mathbf{W}^K (\in \mathbb{R}^{L_x \times d})$$

$$\mathbf{V} = \mathbf{X}\mathbf{W}^V (\in \mathbb{R}^{L_x \times d})$$

$$\mathbf{Y} = \text{softmax} \left(\frac{\mathbf{Q}\mathbf{K}^T}{\sqrt{d}} \right) \mathbf{V}$$

\mathbf{W}^Q , \mathbf{W}^K and \mathbf{W}^V are matrices of trainable weights (fully-connected layers)

Self-attention



- Output can be computed in parallel through matrix multiplications
- Output length = Query length (= Key length = Value length)

Multi-head self-attention (MSA)

h self-attention in parallel

$$\mathbf{Q}_1 = \mathbf{X} \mathbf{W}_1^Q \quad \dots \quad \mathbf{Q}_h = \mathbf{X} \mathbf{W}_h^Q$$

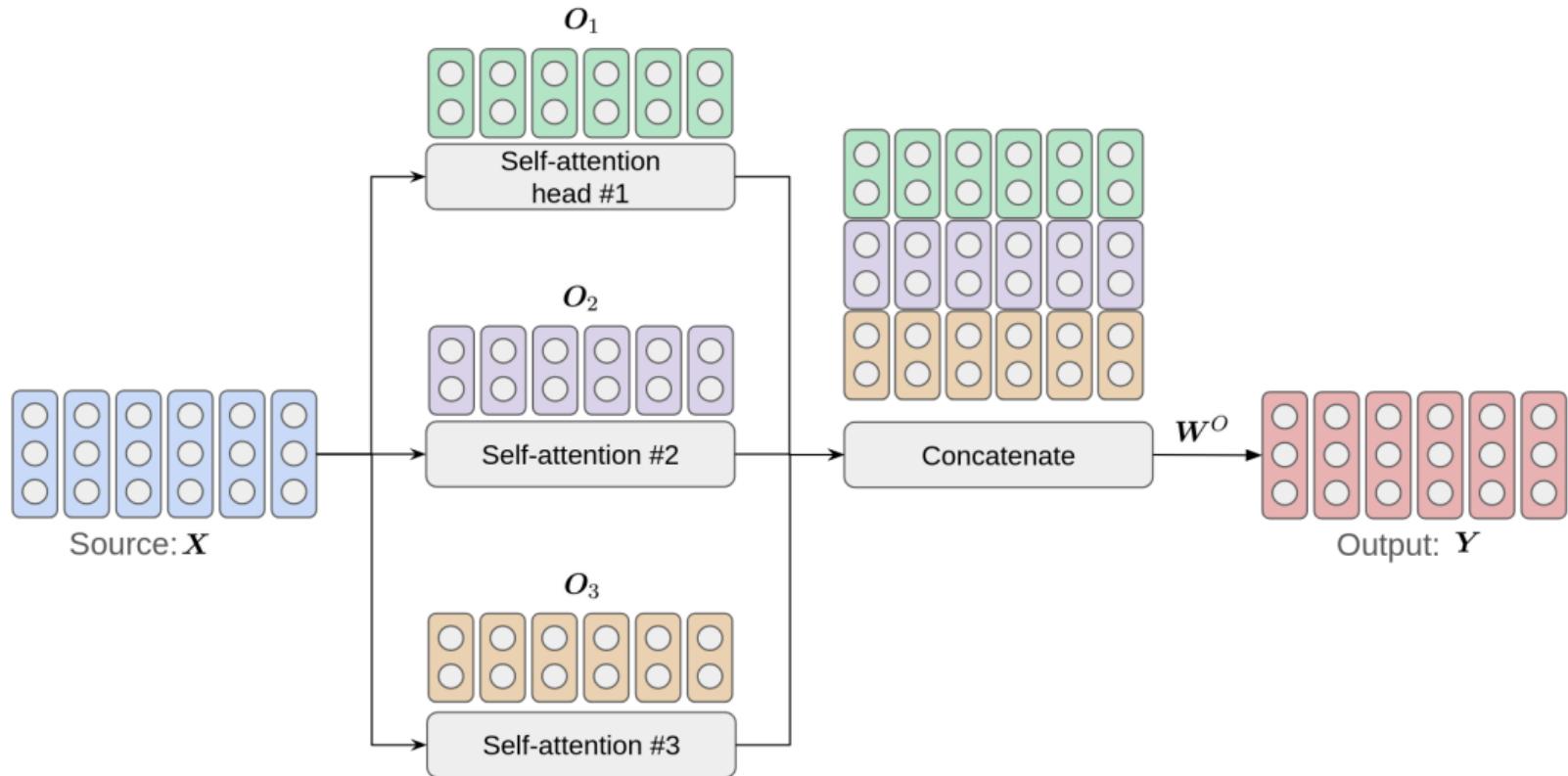
$$\mathbf{K}_1 = \mathbf{X} \mathbf{W}_1^K \quad \dots \quad \mathbf{K}_h = \mathbf{X} \mathbf{W}_h^K$$

$$\mathbf{V}_1 = \mathbf{X} \mathbf{W}_1^V \quad \dots \quad \mathbf{V}_h = \mathbf{X} \mathbf{W}_h^V$$

$$\mathbf{O}_1 = \text{softmax} \left(\frac{\mathbf{Q}_1 \mathbf{K}_1^T}{\sqrt{d}} \right) \mathbf{V}_1 \quad \dots \quad \mathbf{O}_h = \text{softmax} \left(\frac{\mathbf{Q}_h \mathbf{K}_h^T}{\sqrt{d}} \right) \mathbf{V}_h$$

$$\mathbf{Y} = \text{concat}(\mathbf{O}_1, \dots, \mathbf{O}_h) \mathbf{W}^O$$

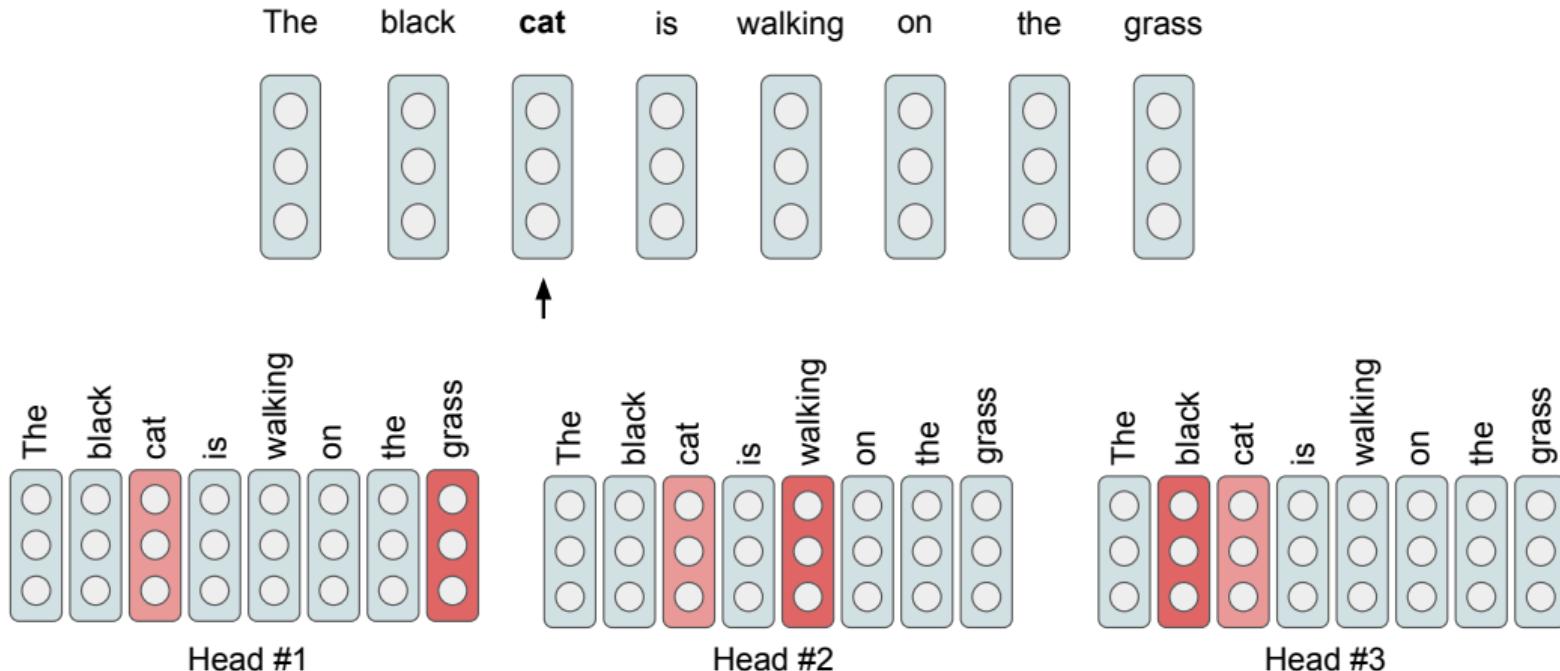
Multi-head Self-Attention (MSA)



Multi-head Self-Attention (MSA)

Intuition

Each head is specialized for a specific query (e.g., action, location, description)



Issue with Multi-head Self Attention (MSA)

Self-attention is invariant to input permutation:

$$\text{MSA}([\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3]) = [\mathbf{y}_1, \mathbf{y}_2, \mathbf{y}_3] \Rightarrow \text{MSA}([\mathbf{x}_2, \mathbf{x}_1, \mathbf{x}_3]) = [\mathbf{y}_2, \mathbf{y}_1, \mathbf{y}_3]$$

The position information is lost whereas it is crucial

- A word/sentence is a sequence of characters, not a set of characters

Goal

Inject positional information to preserve the sequentiality

Solution

Additive positional encoding:

- Input of transformer encoder: $\mathbf{I} = \mathbf{X} + \text{PE}$

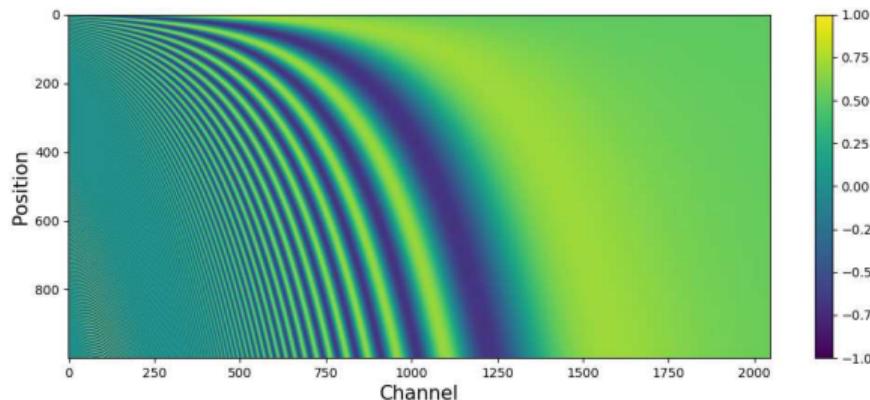
A combination of sines and cosines

$\text{PE}(p, k)$: k^{th} value of positional embedding vector for position p .

$$\text{PE}(p, 2k) = \sin(w_k \cdot p)$$

$$\text{PE}(p, 2k + 1) = \cos(w_k \cdot p)$$

$\forall k \in [0, d/2]$, with $w_k = 1/10000^{2k/d}$



Advantages

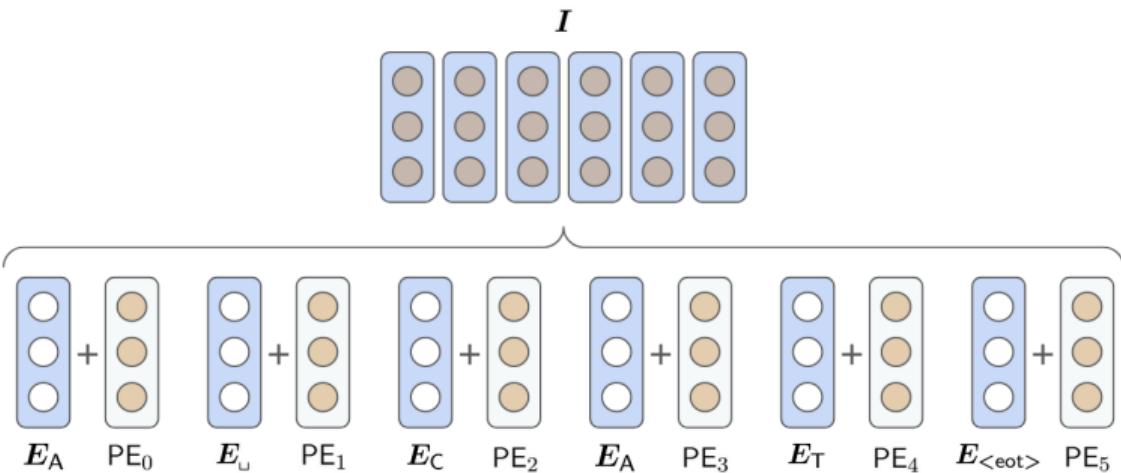
- Does not depend on the input length
- Encoding unique for each position
- Periodicity of sine/cosine could help to adapt to unseen position
- Bonus: no additional trainable parameters



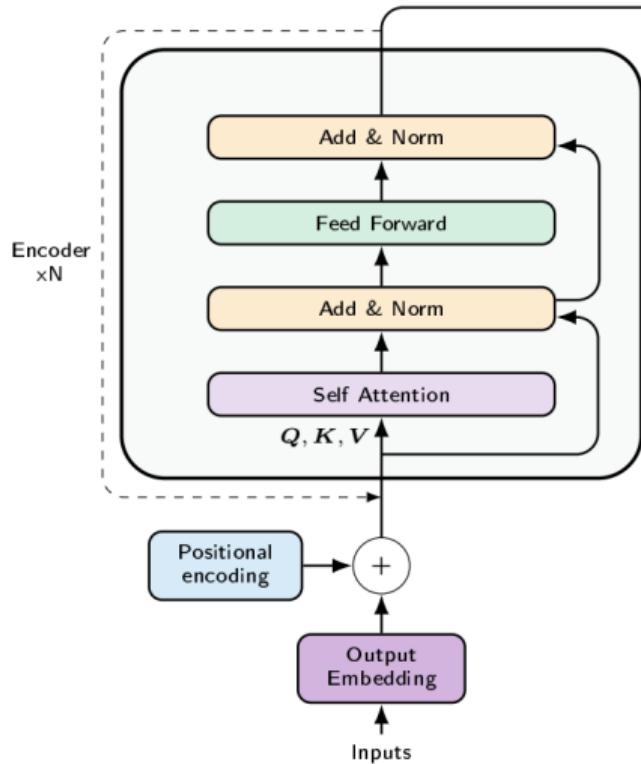
Raw text



Raw position



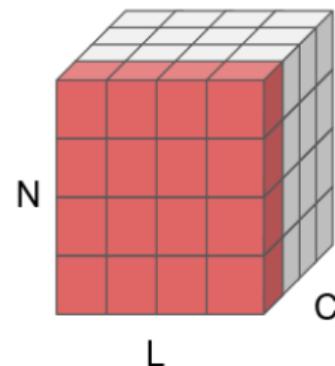
Transformer encoder



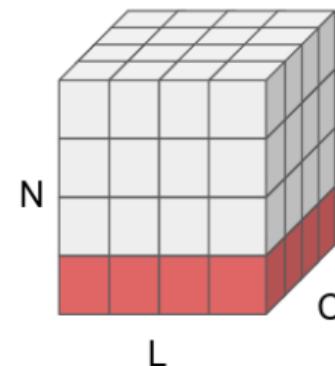
A stack of 6 transformer encoder layers

- Multi-head Self Attention
 - Global context modeling
- Add: residual connections
 - Multi-scale representation
 - Reinforce identity
- Norm: layer normalization
 - Stabilize training (range of values)
- Feed Forward: 2 fully-connected layers
 - Local projection

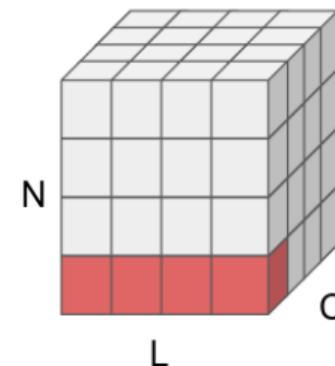
- Normalization approaches differ on how data is segmented to perform normalization



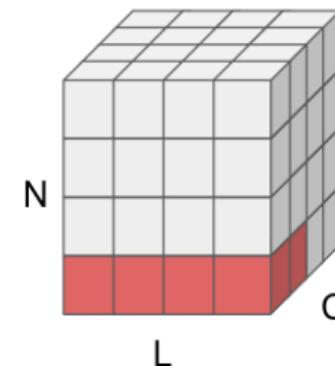
Batch Normalization



Layer Normalization



Instance Normalization



Group Normalization

$$\hat{x} = \frac{x - \mu_x}{\sqrt{\sigma_x^2 + \epsilon}}$$

N: batch dimension (one sample)
L: length dimension (one character, or pixel)
C: channel dimension (one feature)

Transformer encoder layer

Input sequence of L token embedding: \mathbf{X} of shape $L \times d$

Expressed as a function of L , d and n , the number of parameters, the number of floating point operations and the output shape (biases are ignored)

- ➊ for a succession of two fully-connected layers: $\mathbf{Y} = (\mathbf{X}\mathbf{W}^1)\mathbf{W}^2$
(applied on the channel axis, same weights for all tokens)
The first one is made up of n neurons, the second one of d neurons
- ➋ for the simplified self-attention layer: $\mathbf{Y} = (\mathbf{X}\mathbf{W}^Q)(\mathbf{X}\mathbf{W}^K)^T(\mathbf{X}\mathbf{W}^V)\mathbf{W}^O$
We keep d dimensions through the attention process

In both cases, compute those metrics for $d = 1024$, $n = 2048$ and

- ➊ $L = 50$
- ➋ $L = 784$
- ➌ $L = 1,048,576$

Mutual attention (also known as cross attention)

- Queries from target domain, and keys and values from source domain

General case

Inputs: \mathbf{X} : the features from the encoded input sequence (source domain),
 $\tilde{\mathbf{z}}$: the query sequence (e.g., a question)
 \mathbf{z} : the query vector ($\mathbf{z} = g(\tilde{\mathbf{z}})$).

$$\mathbf{q} = \mathbf{z}\mathbf{W}^Q (\in \mathbb{R}^d)$$

$$\mathbf{K} = \mathbf{X}\mathbf{W}^K (\in \mathbb{R}^{L_x \times d})$$

$$\mathbf{V} = \mathbf{X}\mathbf{W}^V (\in \mathbb{R}^{L_x \times d})$$

$$\mathbf{c} = \text{Attention}(\mathbf{q}, \mathbf{K}, \mathbf{V}) = \underbrace{\text{softmax} \left(\frac{\mathbf{q}\mathbf{K}^T}{\sqrt{d}} \right)}_{\alpha} \mathbf{V}$$

Prediction: $\hat{\mathbf{y}} = h(\mathbf{c})$, with g and h parametric functions

Mutual attention (also known as cross attention)

- Queries from target domain, and keys and values from source domain

The iterative decoding process case

Inputs: \mathbf{X} : the features from the encoded input sequence (source domain),
 $\tilde{\mathbf{z}} = \hat{\mathbf{y}}^{0:t-1}$: an output sequence (target domain)
 \mathbf{z}^t : a query vector at iteration t ($\mathbf{z}^t = g(\hat{\mathbf{y}}^0, \dots, \hat{\mathbf{y}}^{t-1})$).

$$\mathbf{q}^t = \mathbf{z}^t \mathbf{W}^Q (\in \mathbb{R}^d)$$

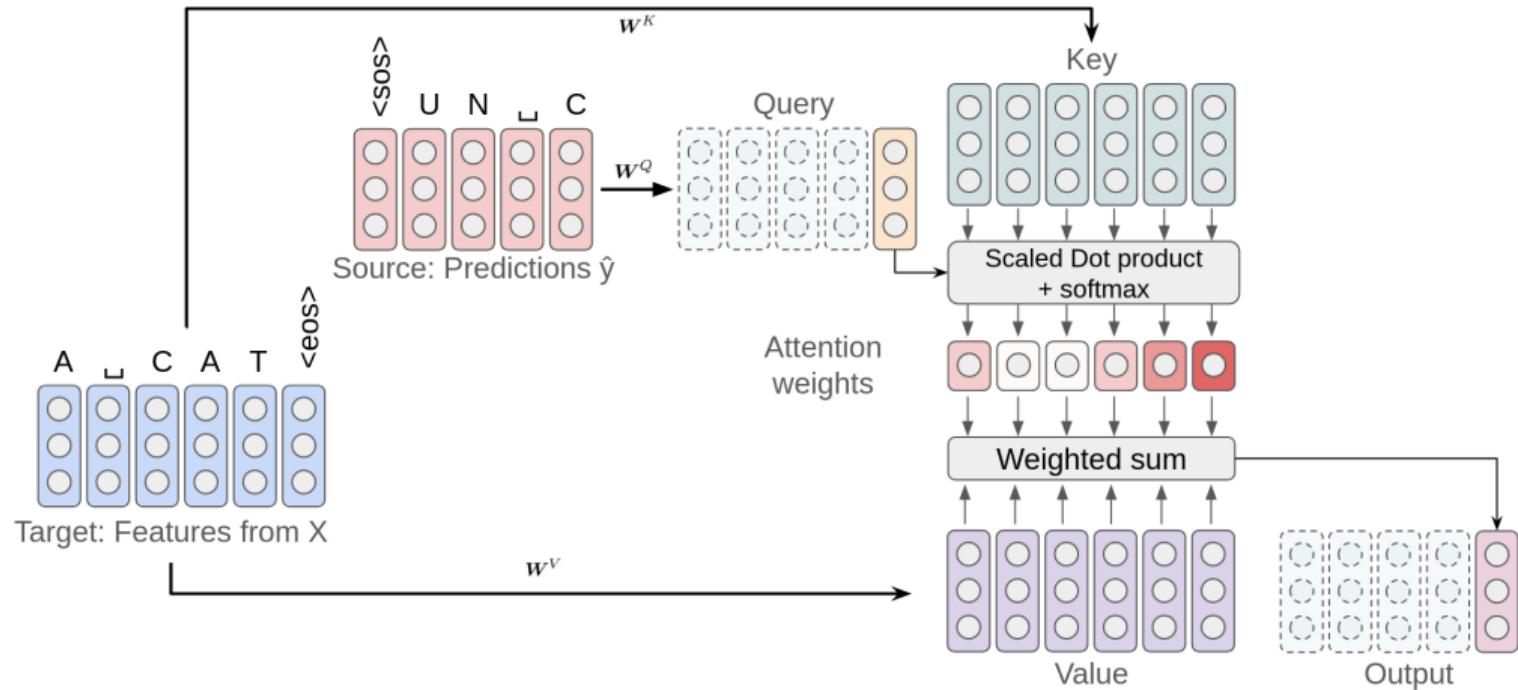
$$\mathbf{K} = \mathbf{X} \mathbf{W}^K (\in \mathbb{R}^{L_x \times d})$$

$$\mathbf{V} = \mathbf{X} \mathbf{W}^V (\in \mathbb{R}^{L_x \times d})$$

$$\mathbf{c}^t = \text{Attention}(\mathbf{q}^t, \mathbf{K}, \mathbf{V}) = \underbrace{\text{softmax}\left(\frac{\mathbf{q}^t \mathbf{K}^T}{\sqrt{d}}\right)}_{\alpha^t} \mathbf{V}$$

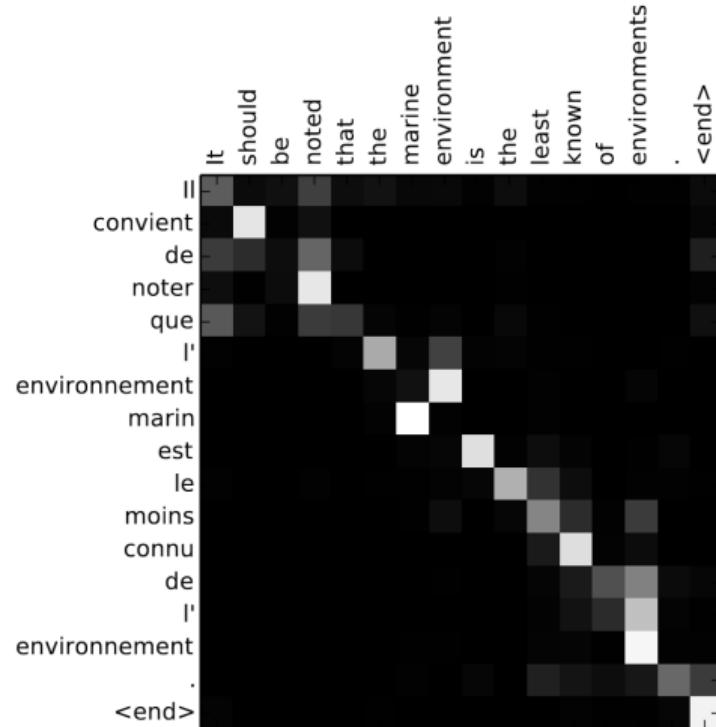
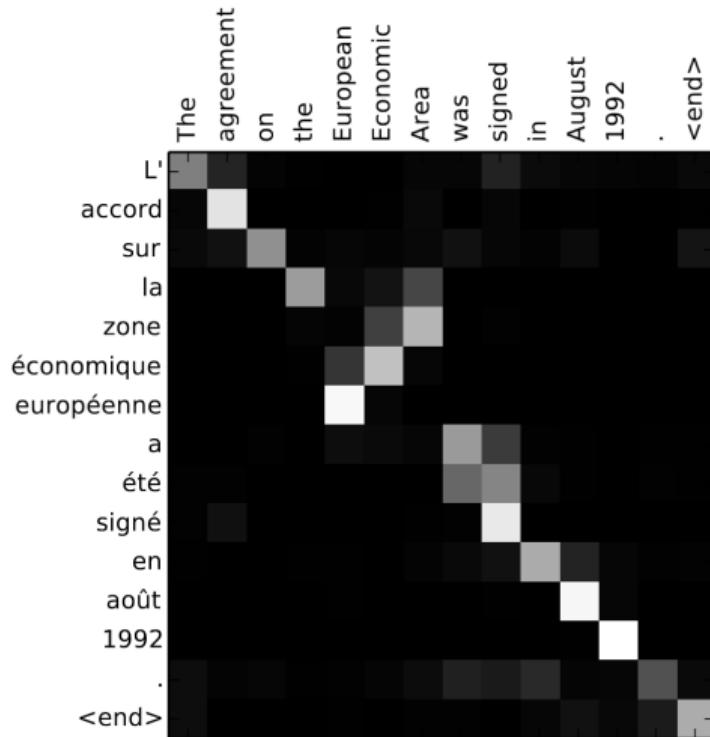
New prediction: $\hat{\mathbf{y}}^t = h(\mathbf{c}^t)$, with g and h parametric functions

Mutual attention



► Output length = Query length (\neq Key length = Value length)

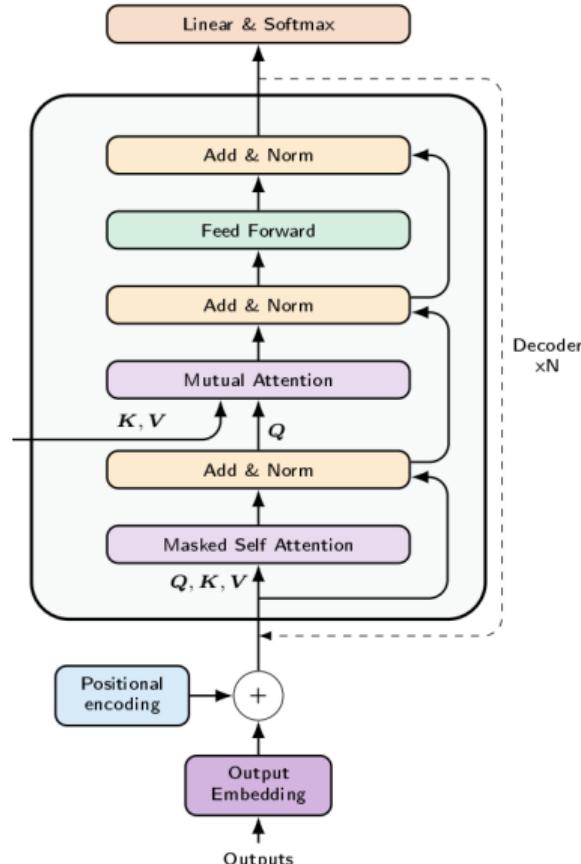
Mutual attention: attention map



Images from [2]

► Size: target sequence length × source sequence length

Transformer decoder

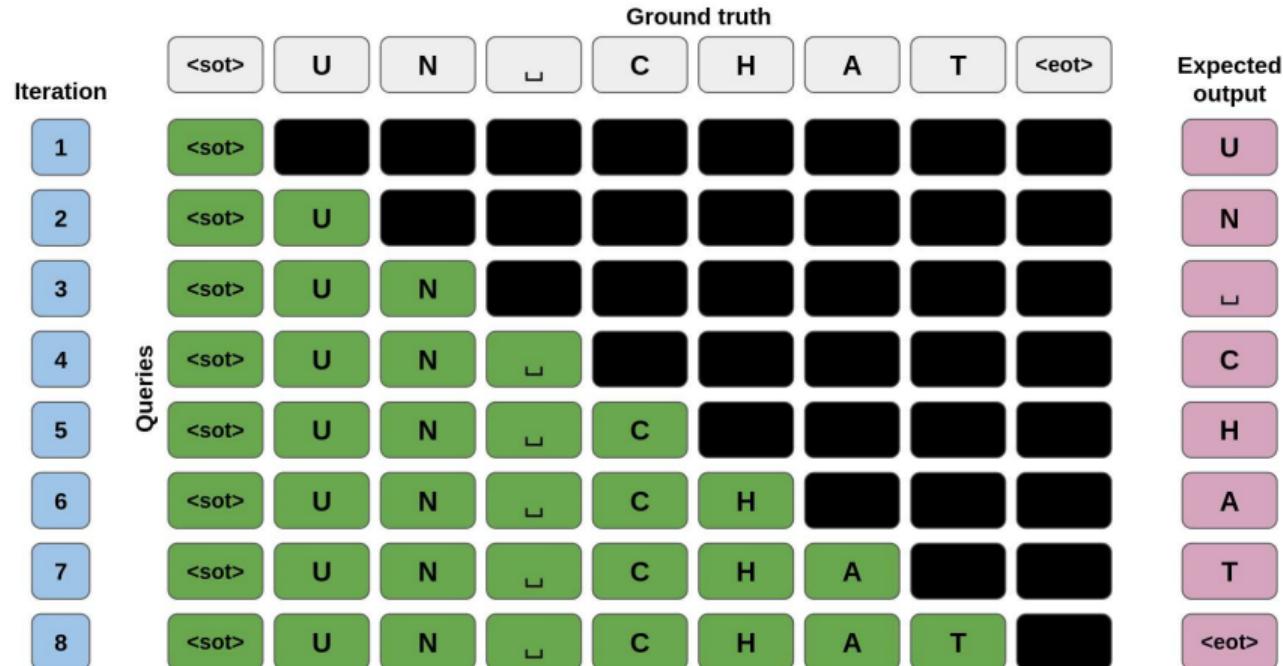


A stack of 6 transformer decoder layers

- Multi-head Masked Self Attention
 - Global query modeling
- Add: residual connections
 - Multi-scale representation
 - Reinforce identity
- Norm: layer normalization
 - Stabilize training (range of values)
- Multi-head mutual attention
 - Look for relevant information from source
- Feed Forward: 2 fully-connected layers
 - Local projection

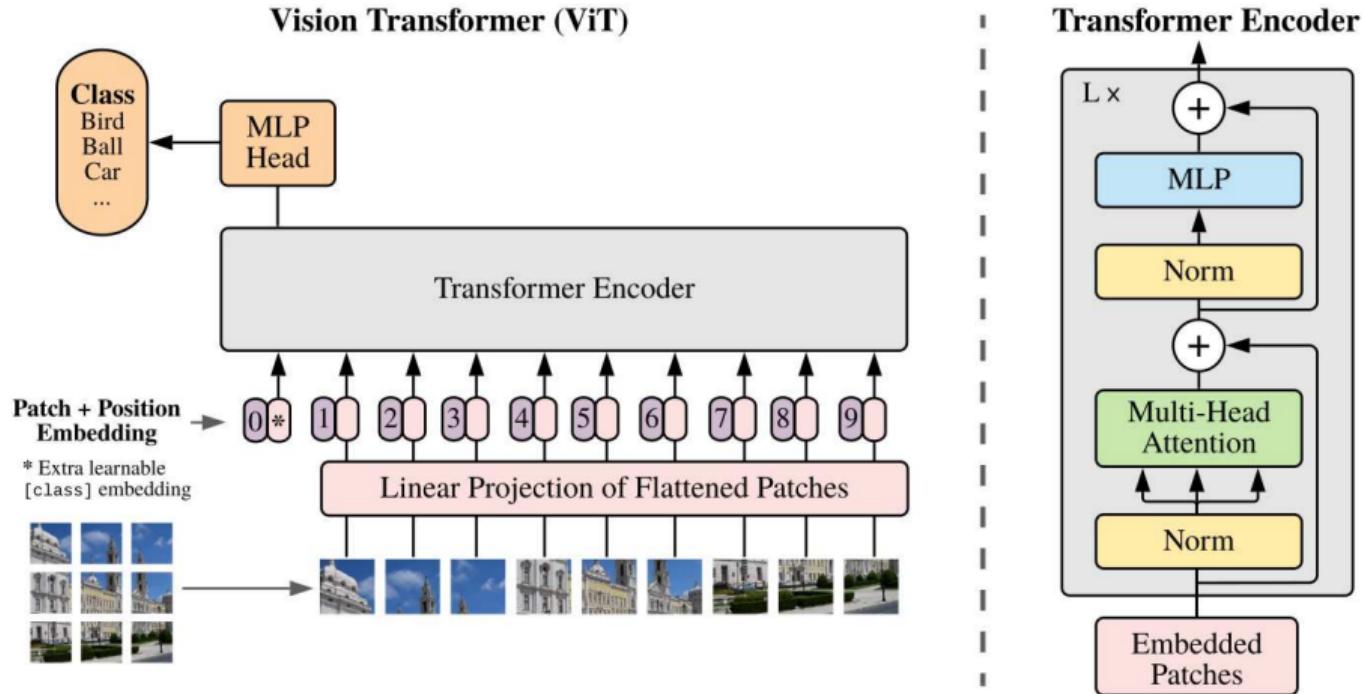
Masked self attention and teacher forcing

- Parallelize decoding process at training time using ground truth



Conclusion

- A modular approach: expressivity can be enhanced by adding more encoder/decoder layers
 - But slower training/inference and more required data
- Self attention: a way to model global context without sequential computations (at each layer, each token can attend to all the other tokens)
 - But a quadratic complexity
- Parameter-free additive positional encoding
 - But the relation between positions must be learned through training
- Defined for Natural Language Processing: SOTA architecture
 - How to adapt it for computer vision?



Input image: 224×224 , patch size: $16 \times 16 \Rightarrow 196$ patches

Architecture	Top-1 accuracy (%) on ImageNet	# params (M)
ResNet-50	79.26	26
ResNet-101	80.13	45
ResNet-152	80.62	60
ViT-B/16	77.91	86
ViT-B/32	73.38	86
ViT-L/16	76.53	307
ViT-L/32	71.16	307

Attention-based architectures require more data to exploit their full potential:

- Spatial relations between patches must be learned from scratch
- What to do when there is not enough labeled data?

1 The Transformer revolution

2 Dealing with few annotated data

- Create artificial data
- Use annotation from other datasets
- Benefit from unlabeled data

Create artificial examples

- Data augmentation
- Synthetic data

Benefit from other annotated datasets

- Transfer learning
- Fine-tuning

Benefit from unlabeled data

- Semi-supervised learning
- Self-supervised learning

Data augmentation

► Deformation function applied on labeled data



(a) Original



(b) Crop and resize



(c) Crop, resize (and flip)



(d) Color distort. (drop)



(e) Color distort. (jitter)



(f) Rotate $\{90^\circ, 180^\circ, 270^\circ\}$



(g) Cutout



(h) Gaussian noise



(i) Gaussian blur



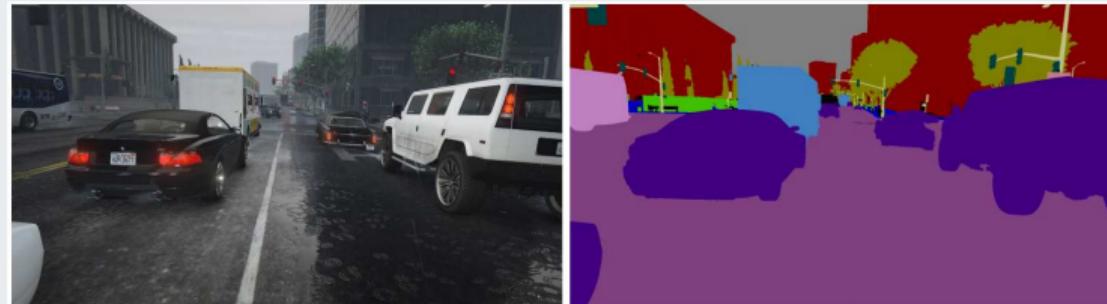
(j) Sobel filtering

⚠ Must preserve the information of interest (should not modify the associated ground truth)

Synthetic data

- Create new couples (input, ground truth) from scratch

Video games as simulation engines



GTA V for semantic segmentation [4]

Digital fonts for handwritten text recognition

This is an artificial text line image

Transfer learning

Idea

The knowledge learned from task A can be helpful for task B

- Benefit from annotated data of another task/dataset

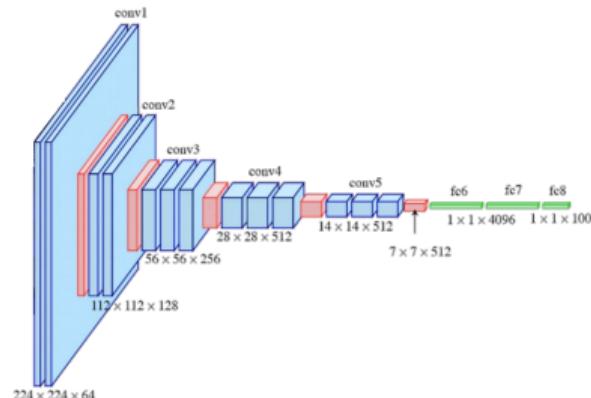
First step: pre-training

Train on a source task/dataset
e.g., classification on ImageNet

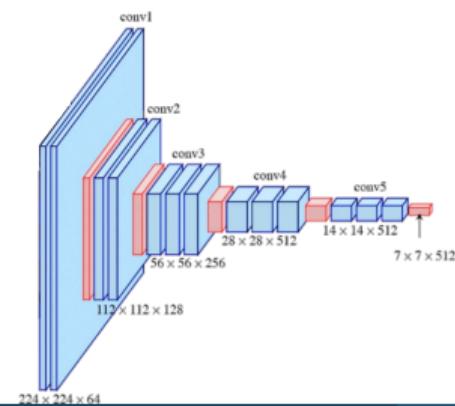
ImageNet



train



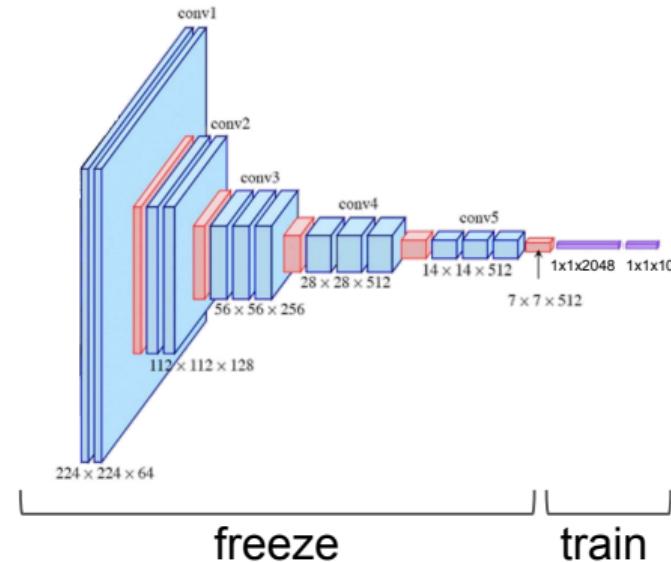
keep
layers



Adaptation to target dataset

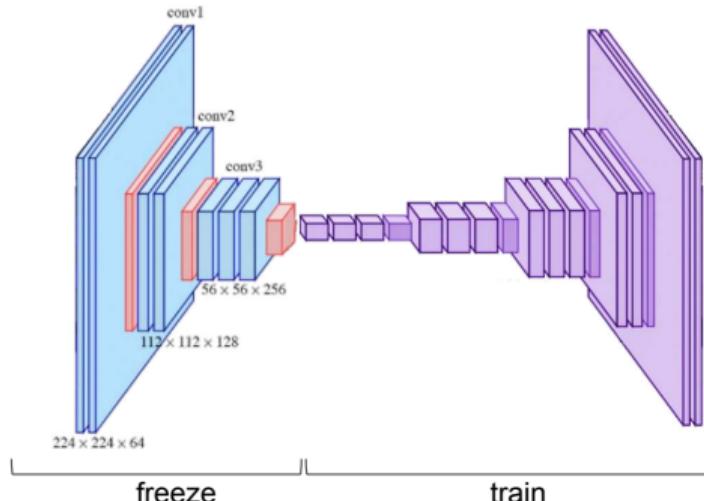
e.g., classification on CIFAR 10

- Classes different: change projection head
- Semantically similar: preserve top layers

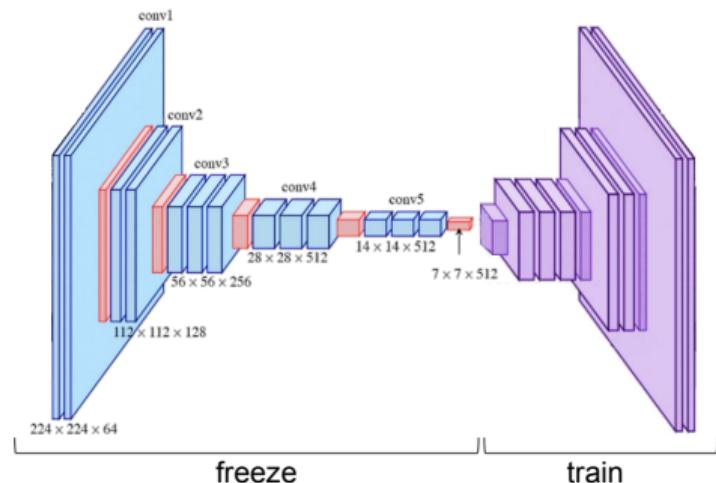


Adaptation to target task

e.g., segmentation



semantically far
much data

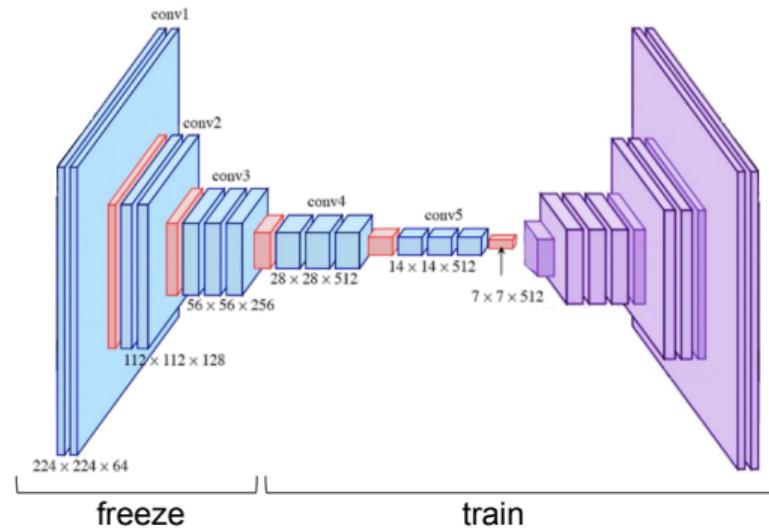


semantically close
few data

If enough target data: fine-tuning

Additional training step

- Training the transferred part of the architecture (either completely or top layers only), with low learning rate

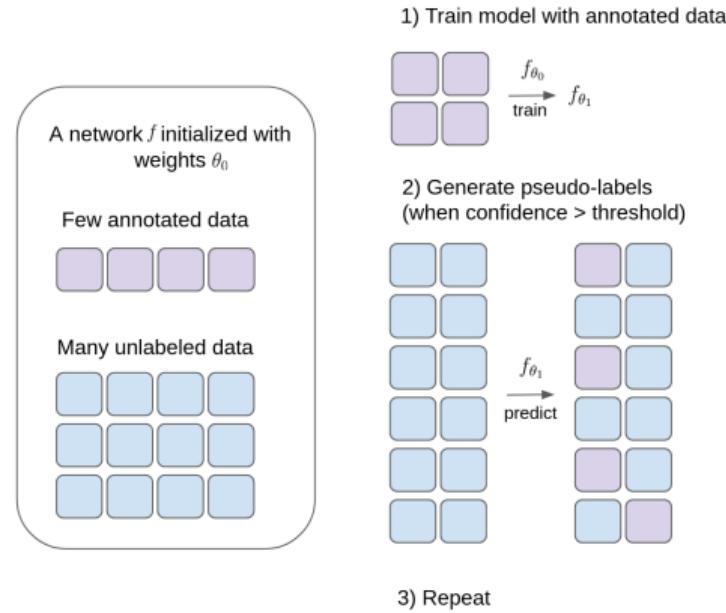


Performance on ImageNet (fine-tuning included)

Architecture	Top-1 accuracy (%) on ImageNet	
	Pre-trained on ImageNet	Pre-trained on JFT-300M
ResNet-50	79.26	✗
ResNet-101	80.13	✗
ResNet-152	80.62	✗
ViT-B/16	77.91	84.15
ViT-B/32	73.38	80.73
ViT-L/16	76.53	87.12
ViT-L/32	71.16	84.37
ViT-H/14	✗	88.04

Idea: use prediction as ground truth

- Use trained model to generate pseudo-labels from unlabeled data
- Further train the model with both annotated data and pseudo-labels



Idea: Learn from unlabeled data

Two main approaches

Generative architecture

The goal is to solve a pretext task

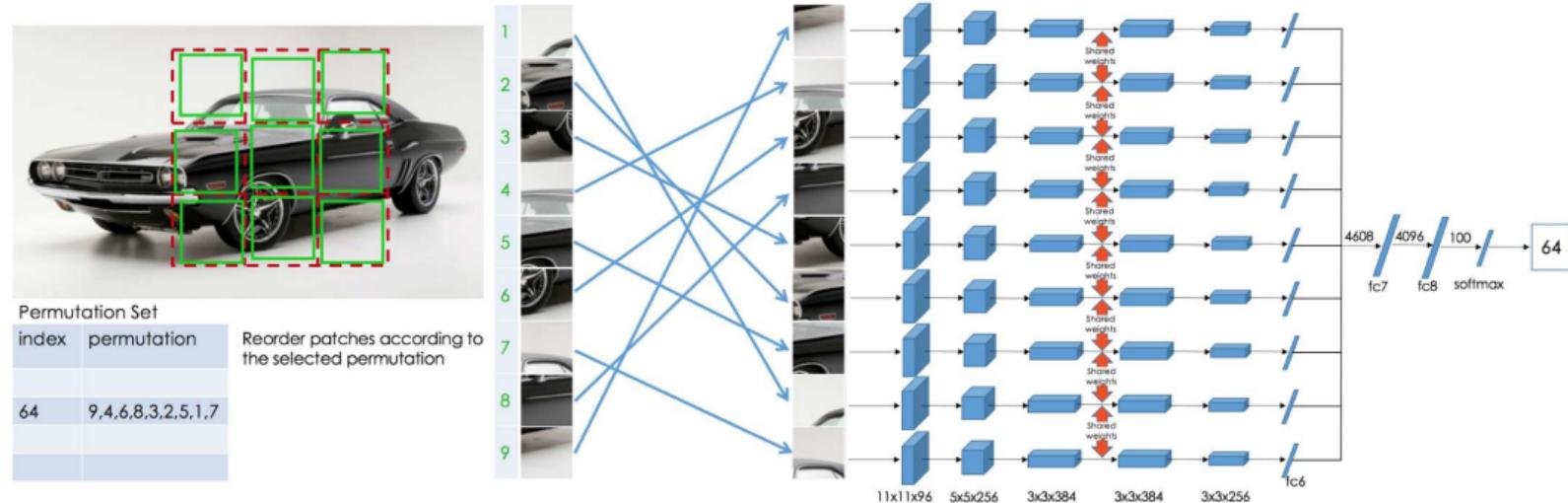
- Solve Jigsaw puzzles
- Reconstruct the input image:
(Variational) Auto-encoders, Masked auto-encoders

Joint Embedding Architecture

- Contrastive learning: SimCLR
Learning from positive and negative samples
- Non-contrastive learning: DINO
Learning from different representations of the same input

Jigsaw puzzle (2016) [5]

► Find the right permutation: classification formulation

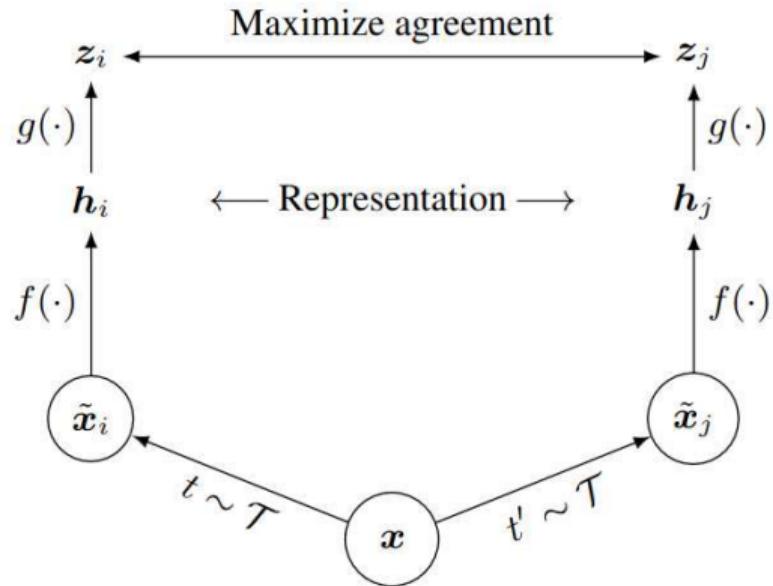


Contrastive learning: SimCLR (2020) [6]

- Idea: generate two views for each input (= positive pair). Bring latent representations of positives closer and keep latent representations of negatives away
- Siamese networks: same architecture with same weights used on different inputs while comparing outputs

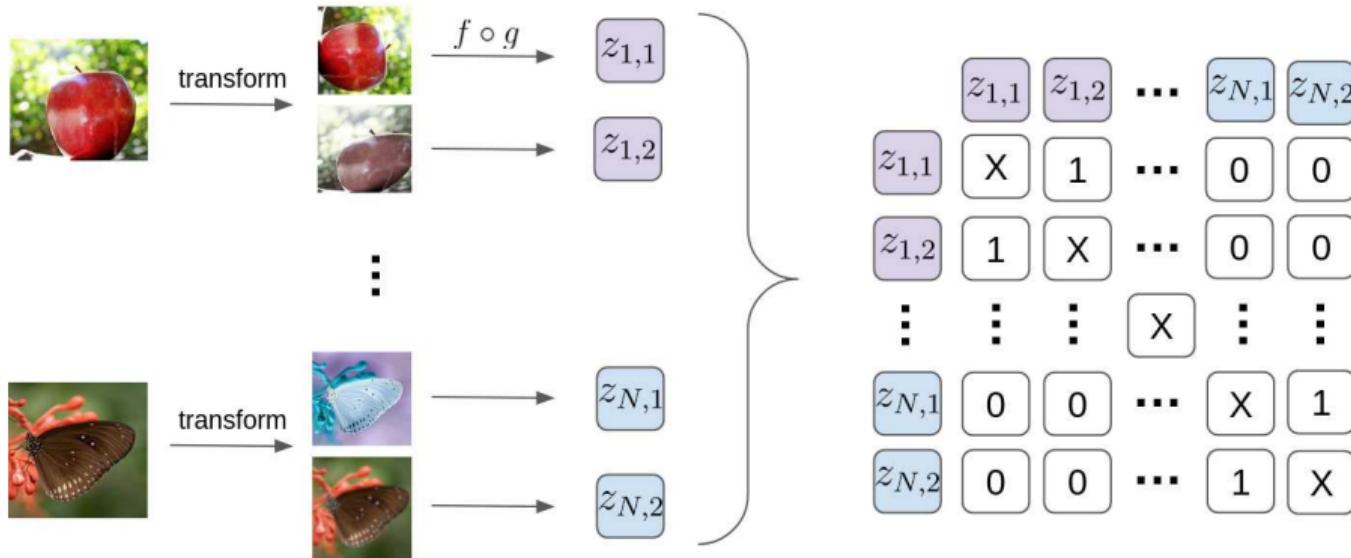
Algorithm 1 SimCLR's main learning algorithm.

```
input: batch size  $N$ , constant  $\tau$ , structure of  $f, g, \mathcal{T}$ .  
for sampled minibatch  $\{\mathbf{x}_k\}_{k=1}^N$  do  
  for all  $k \in \{1, \dots, N\}$  do  
    draw two augmentation functions  $t \sim \mathcal{T}, t' \sim \mathcal{T}$   
    # the first augmentation  
     $\tilde{\mathbf{x}}_{2k-1} = t(\mathbf{x}_k)$   
     $h_{2k-1} = f(\tilde{\mathbf{x}}_{2k-1})$  # representation  
     $z_{2k-1} = g(h_{2k-1})$  # projection  
    # the second augmentation  
     $\tilde{\mathbf{x}}_{2k} = t'(\mathbf{x}_k)$   
     $h_{2k} = f(\tilde{\mathbf{x}}_{2k})$  # representation  
     $z_{2k} = g(h_{2k})$  # projection  
  end for  
  for all  $i \in \{1, \dots, 2N\}$  and  $j \in \{1, \dots, 2N\}$  do  
     $s_{i,j} = \mathbf{z}_i^\top \mathbf{z}_j / (\|\mathbf{z}_i\| \|\mathbf{z}_j\|)$  # pairwise similarity  
  end for  
  define  $\ell(i, j)$  as  $\ell(i, j) = -\log \frac{\exp(s_{i,j}/\tau)}{\sum_{k=1}^{2N} \mathbb{1}_{[k \neq i]} \exp(s_{i,k}/\tau)}$   
   $\mathcal{L} = \frac{1}{2N} \sum_{k=1}^N [\ell(2k-1, 2k) + \ell(2k, 2k-1)]$   
  update networks  $f$  and  $g$  to minimize  $\mathcal{L}$   
end for  
return encoder network  $f(\cdot)$ , and throw away  $g(\cdot)$ 
```



Contrastive learning: SimCLR (2020) [6]

- Find the matching pairs
- Cosine similarity as distance metric



- Efficiency depends on mini-batch size

Classification performance (Top-1 accuracy) with ResNet architecture

	Food	CIFAR10	CIFAR100	Birdsnap	SUN397	Cars	Aircraft	VOC2007	DTD	Pets	Caltech-101	Flowers
<i>Linear evaluation:</i>												
SimCLR (ours)	68.4	90.6	71.6	37.4	58.8	50.3	50.3	80.5	74.5	83.6	90.3	91.2
Supervised	72.3	93.6	78.3	53.7	61.9	66.7	61.0	82.8	74.9	91.5	94.5	94.7
<i>Fine-tuned:</i>												
SimCLR (ours)	88.2	97.7	85.9	75.9	63.5	91.3	88.1	84.1	73.2	89.2	92.1	97.0
Supervised	88.3	97.5	86.4	75.8	64.3	92.1	86.0	85.0	74.6	92.1	93.3	97.6
Random init	86.9	95.9	80.2	76.1	53.6	91.4	85.9	67.3	64.8	81.5	72.6	92.0

Pre-training on ImageNet

Backbone either frozen (linear evaluation=transfer learning) or trained (fine-tuning)

► Self-distillation through teacher-student paradigm

Algorithm 1 DINO PyTorch pseudocode w/o multi-crop.

```

# gs, gt: student and teacher networks
# C: center (K)
# tps, tpt: student and teacher temperatures
# l, m: network and center momentum rates
gt.params = gs.params
for x in loader: # load a minibatch x with n samples
    x1, x2 = augment(x), augment(x) # random views

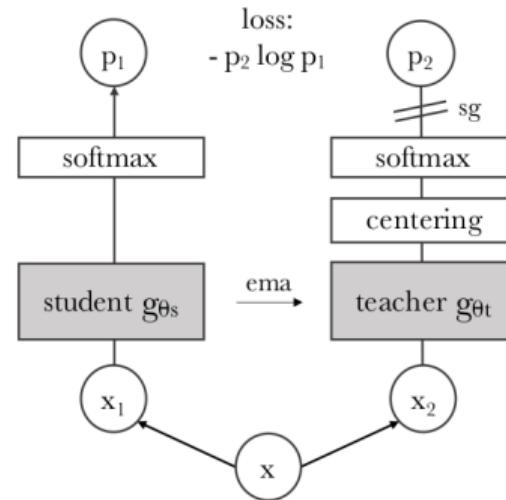
    s1, s2 = gs(x1), gs(x2) # student output n-by-K
    t1, t2 = gt(x1), gt(x2) # teacher output n-by-K

    loss = H(t1, s2)/2 + H(t2, s1)/2
    loss.backward() # back-propagate

    # student, teacher and center updates
    update(gs) # SGD
    gt.params = l*gt.params + (l-1)*gs.params
    C = m*C + (1-m)*cat([t1, t2]).mean(dim=0)

def H(t, s):
    t = t.detach() # stop gradient
    s = softmax(s / tps, dim=1)
    t = softmax((t - C) / tpt, dim=1) # center + sharpen
    return - (t * log(s)).sum(dim=1).mean()

```



x_1, x_2 are two augmentations of an image x (crop vs whole image).

Student trained to output same distribution as teacher with cross-entropy loss (H)

Stop-gradient (sg): only the student is trained through gradient descent.

Exponential moving average (ema): $\theta_t = \lambda\theta_t + (1 - \lambda)\theta_s \quad \lambda \in [0.996, 1]$

► Keywords

Knowledge distillation / teacher-student paradigm

Transferring knowledge from one network to another (generally for compression purposes). e.g., a small network (student) is trained to mimick the output of a bigger network (teacher).

Self-distillation

Teacher and student share the same architecture (but not the same weights: these are not siamese network)

Teacher weights are not updated through gradient descent but with EMA from student weights.

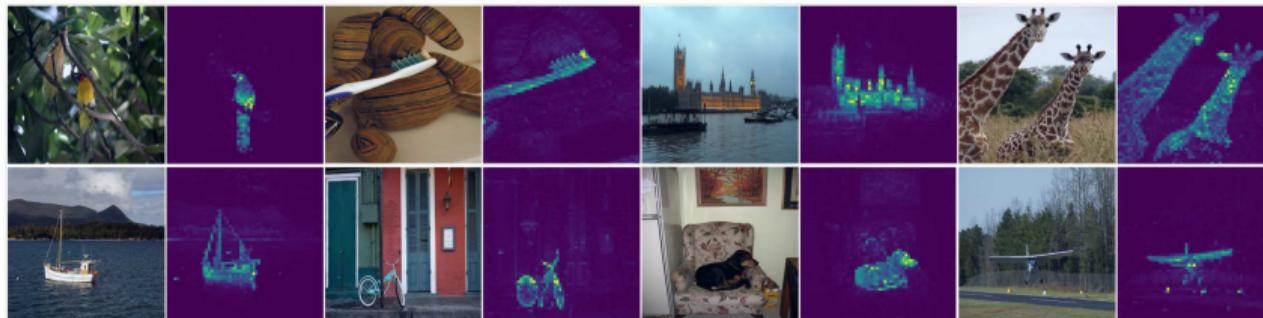
Failing modes

One dimension dominates, no matter the input:

- Centering: $t \leftarrow t - C$ with $C \leftarrow mC + (1 - m) \frac{1}{B} \sum_{i=1}^B g_{\theta_t}(x_i)$

Uniform distribution, no matter the input:

- Sharpening: $t \leftarrow t/\tau_t$



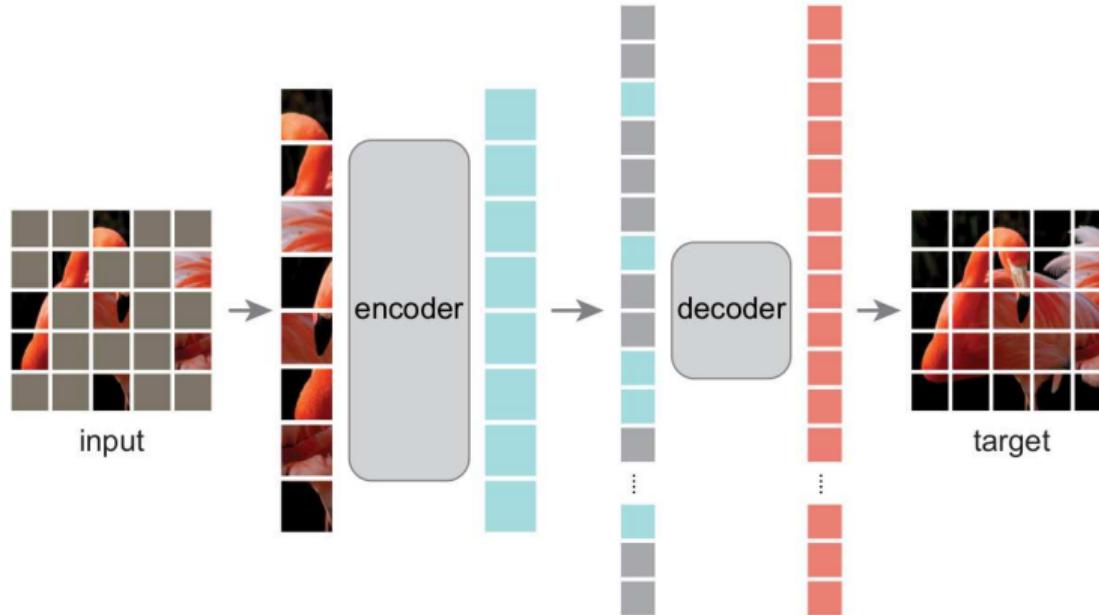
Attention maps: self-attention for CLS token

Classification performance (Top-1 accuracy) with ViT architecture

	Cifar ₁₀	Cifar ₁₀₀	INat ₁₈	INat ₁₉	Flwrs	Cars	INet
<i>ViT-S/16</i>							
Sup. [69]	99.0	89.5	70.7	76.6	98.2	92.1	79.9
DINO	99.0	90.5	72.0	78.2	98.5	93.0	81.5
<i>ViT-B/16</i>							
Sup. [69]	99.0	90.8	73.2	77.7	98.4	92.1	81.8
DINO	99.1	91.7	72.6	78.6	98.8	93.0	82.8

Pre-training on ImageNet

- Reconstruct the missing parts (pixel-level MSE loss)



- Vision Transformer architecture

► Classification performance (Top-1 accuracy) with ViT architectures, pre-trained and evaluated on ImageNet

Approach	ViT-B	ViT-L	ViT-H	ViT-H ₄₈₈
Supervised	82.3	82.6	83.1	\times
DINO	82.8	\times	\times	\times
MAE	83.6	85.9	86.9	87.8



Left: masked input, Middle: reconstructed image, Right: ground truth

Architecture is not everything, be careful with benchmarks!

- Training time, number of epochs/iterations, mini-batch size
- Weight initialization, optimizer, initial learning rate, learning rate scheduler
- Dropout, normalization, activation functions
- Pre-processing, post-processing
- **Pre-training, transfer learning, data augmentation, synthetic data**

► Really difficult to fairly compare approaches

Architectures

- Deeper and deeper → more efficient but requires more data
- Powerful attention mechanism → requires even more data

Data is crucial

- There are many ways to deal with few labeled data
- But still an active field of research (e.g., medical data)

Classification

- Performance constantly increasing but still not perfect
- Task limited (one instance per image, no location information)

► Next time: Practical Session!

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