Deep Learning for Vision (DLV)
Classification - part II

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2024-2025

Goals of this course

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

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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.

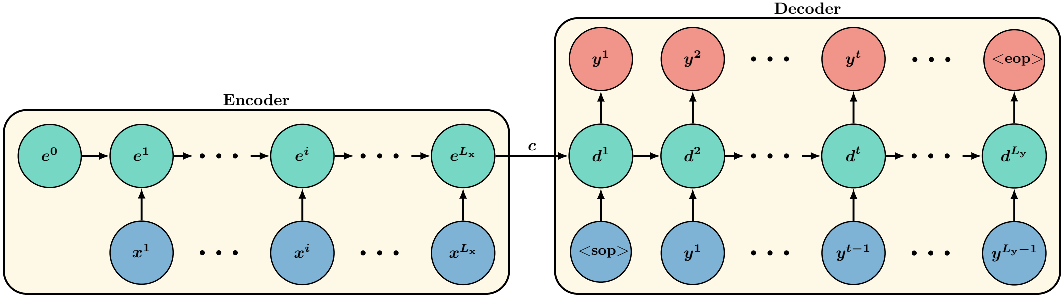
1. if $d \geq 26$
2. if $d < 26$

Neural Machine Translation (NMT)

A sequence-to-sequence task

$\boldsymbol{x}$: a sequence of input tokens representing some text.

$\boldsymbol{y}$: a sequence of output tokens representing the translated text.



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

Context

Limitation

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

Idea: attention mechanism

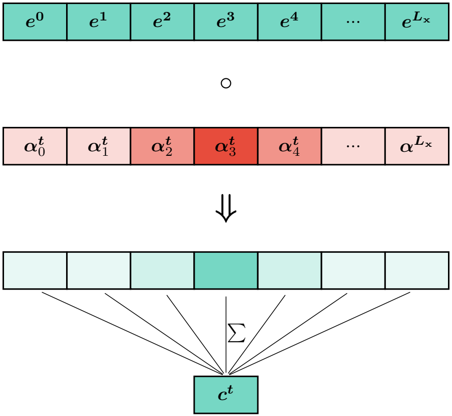
From a static context vector:

$$\boldsymbol{c} = f(\boldsymbol{x})$$

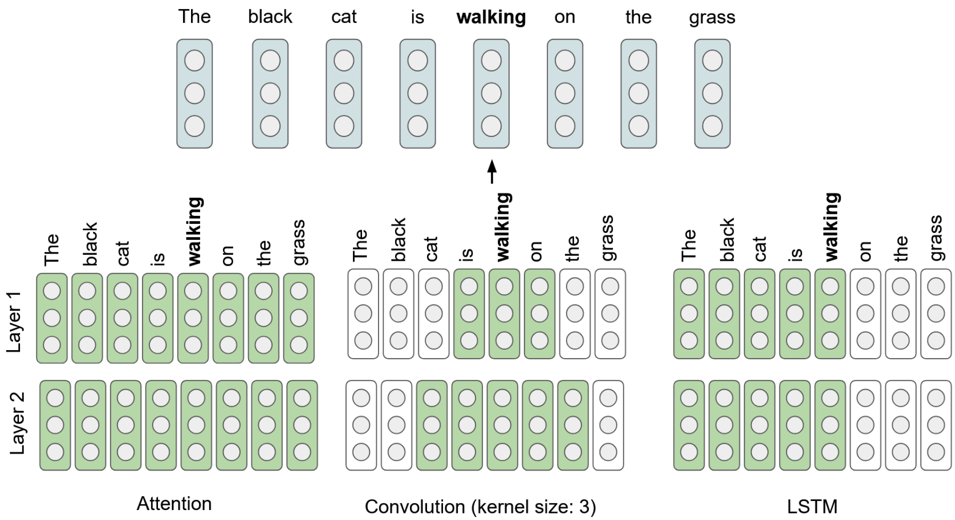
to a dynamic context vector:

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

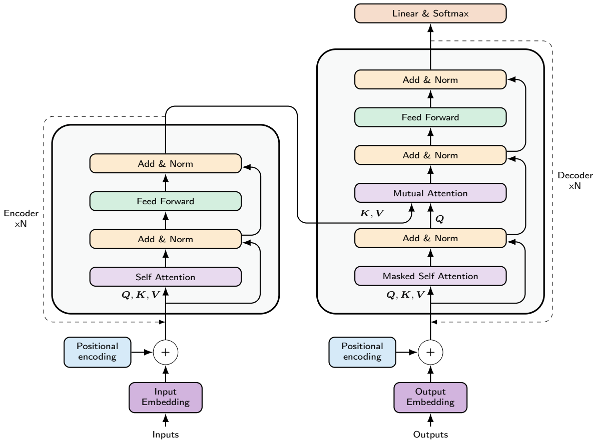
with: $\sum_i \alpha_i = 1$.



Context modeling comparison



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



Two main blocks:

- Transformer encoder
- Transformer decoder

One-shot encoding

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

Iterative decoding

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

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

➤ 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)

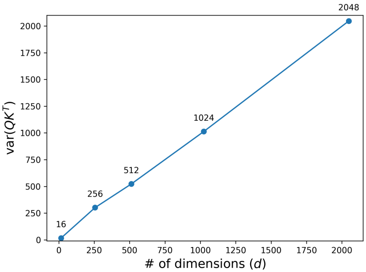
Scaled Dot-Product Attention

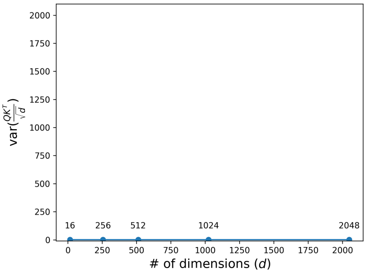
$\boldsymbol{q} \in \mathbb{R}^d$: a query vector
$\boldsymbol{K} \in \mathbb{R}^{L\times d}$: a matrix gathering key vectors for each available item
$\boldsymbol{V} \in \mathbb{R}^{L\times d}$: a matrix gathering values vectors for each available item

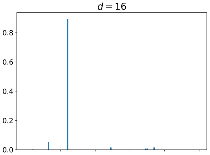
$$\mathrm{Attention}(\boldsymbol{q}, \boldsymbol{K}, \boldsymbol{V}) = \underbrace{\text{softmax}\left(\frac{\boldsymbol{q}\boldsymbol{K}^T}{\sqrt{d}}\right)}_{\alpha} \boldsymbol{V} = \boldsymbol{c} \quad (\in \mathbb{R}^d)$$

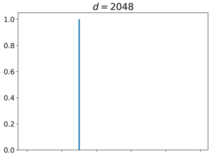
➤ Dot product as distance function

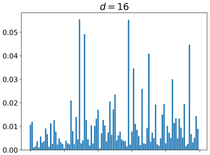
For 1 query and 10,000 keys (from normal distribution):

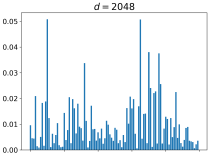












- Queries, Keys and Values are from the same source

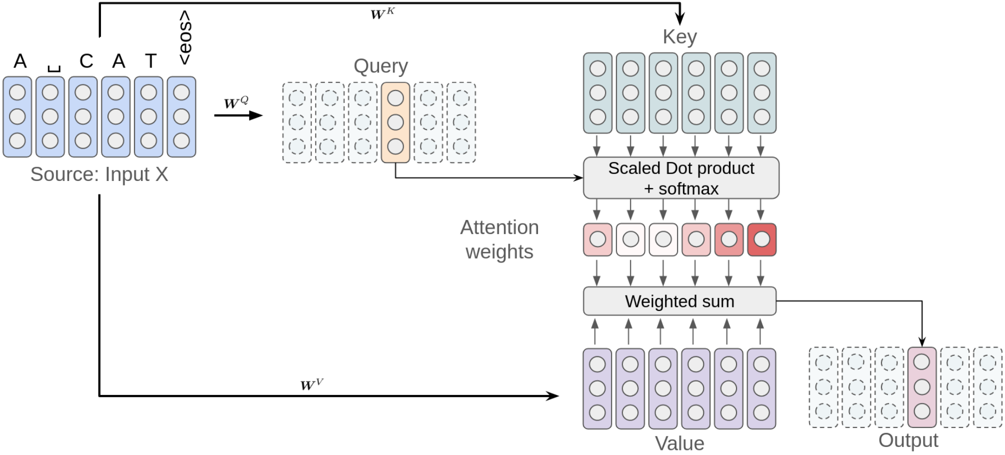
Query-key-value for feature extraction

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

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

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

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



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

Multi-head self-attention (MSA)

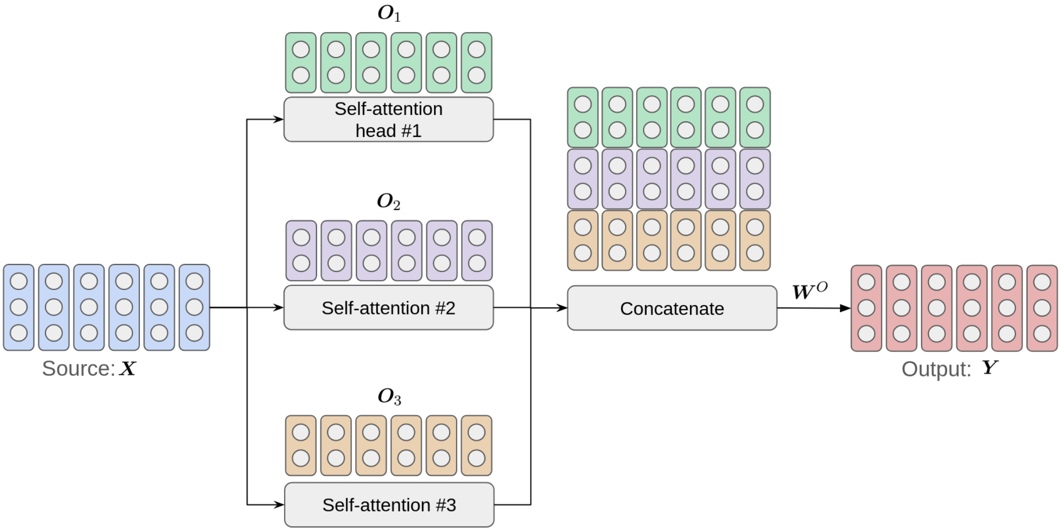
h self-attention in parallel

$$\boldsymbol{Q}_1 = \boldsymbol{X}\boldsymbol{W}_1^Q \quad \ldots \quad \boldsymbol{Q}_h = \boldsymbol{X}\boldsymbol{W}_h^Q$$
$$\boldsymbol{K}_1 = \boldsymbol{X}\boldsymbol{W}_1^K \quad \ldots \quad \boldsymbol{K}_h = \boldsymbol{X}\boldsymbol{W}_h^K$$
$$\boldsymbol{V}_1 = \boldsymbol{X}\boldsymbol{W}_1^V \quad \ldots \quad \boldsymbol{V}_h = \boldsymbol{X}\boldsymbol{W}_h^V$$

$$\boldsymbol{O}_1 = \mathsf{softmax}\left(\frac{\boldsymbol{Q}_1\boldsymbol{K}_1^T}{\sqrt{d}}\right)\boldsymbol{V}_1 \quad \ldots \quad \boldsymbol{O}_h = \mathsf{softmax}\left(\frac{\boldsymbol{Q}_h\boldsymbol{K}_h^T}{\sqrt{d}}\right)\boldsymbol{V}_h$$

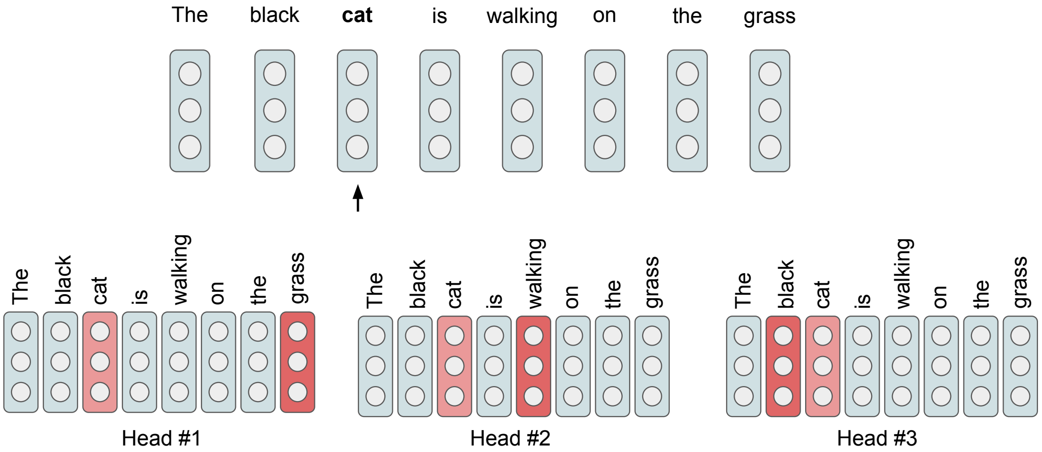
$$\boldsymbol{Y} = \mathsf{concat}(\boldsymbol{O}_1, \ldots, \boldsymbol{O}_h)\boldsymbol{W}^O$$

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

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

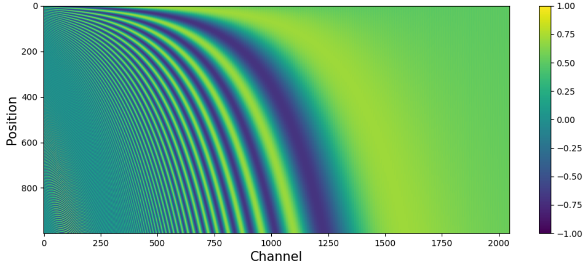
Additive positional encoding:
➤ Input of transformer encoder: $\boldsymbol{I} = \boldsymbol{X} + \text{PE}$

A combination of sines and cosines

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

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

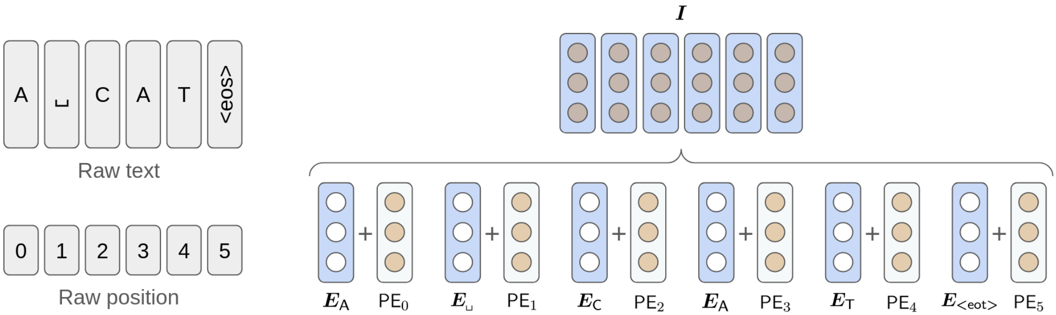
$\forall k \in [0, d/2]$, with $w_k = 1/10000^{2k/d}$

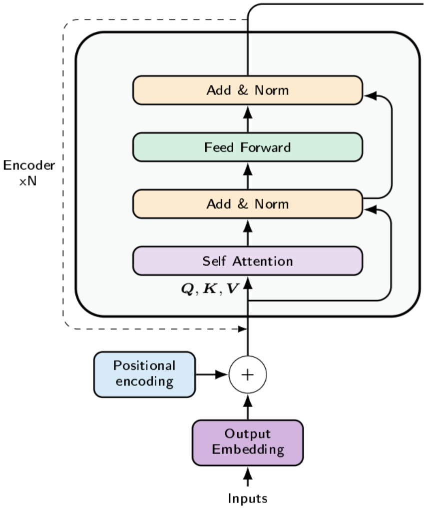


Positional encoding

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

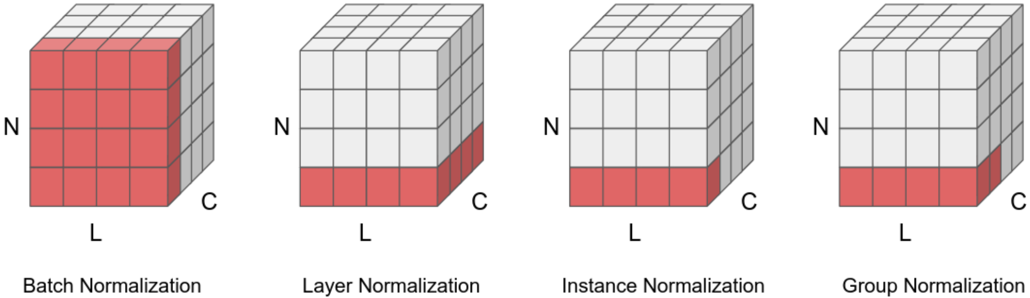




A stack of 6 transformer encoder layers

- 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 differs on how data is segmented to perform 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: $\boldsymbol{X}$ of shape $L \times d$

Express 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)

1. for a succession of two fully-connected layers: $\boldsymbol{Y} = (\boldsymbol{X}\boldsymbol{W}^1)\boldsymbol{W}^2$
   (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
2. for the simplified self-attention layer: $\boldsymbol{Y} = (\boldsymbol{X}\boldsymbol{W}^{\mathsf{Q}})(\boldsymbol{X}\boldsymbol{W}^{\mathsf{K}})^T(\boldsymbol{X}\boldsymbol{W}^{\mathsf{V}})\boldsymbol{W}^{\mathsf{O}}$
   We keep d dimensions through the attention process

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

1. $L = 50$
2. $L = 784$
3. $L = 1,048,576$

Mutual attention (also known as cross attention)

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

General case

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

$$\boldsymbol{q} = \boldsymbol{z}\boldsymbol{W}^Q (\in \mathbb{R}^d)$$
$$\boldsymbol{K} = \boldsymbol{X}\boldsymbol{W}^K (\in \mathbb{R}^{L_x \times d})$$
$$\boldsymbol{V} = \boldsymbol{X}\boldsymbol{W}^V (\in \mathbb{R}^{L_x \times d})$$

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

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

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

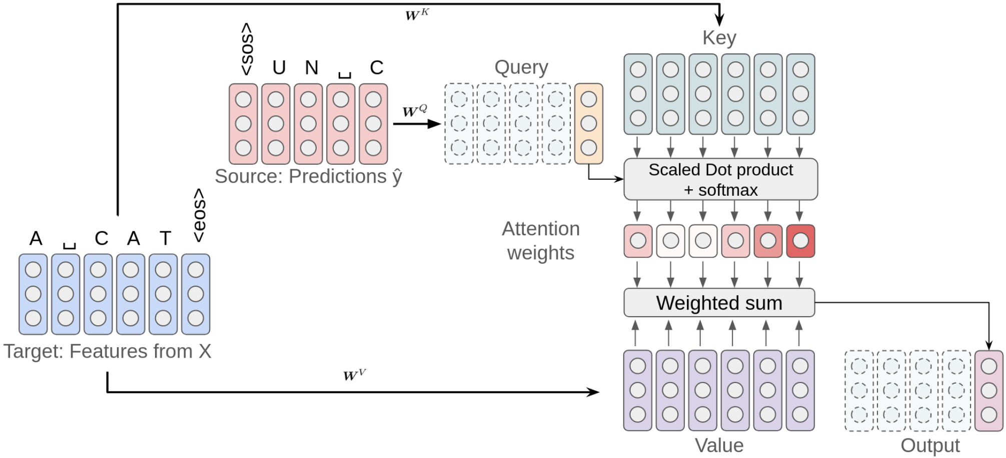
The iterative decoding process case

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

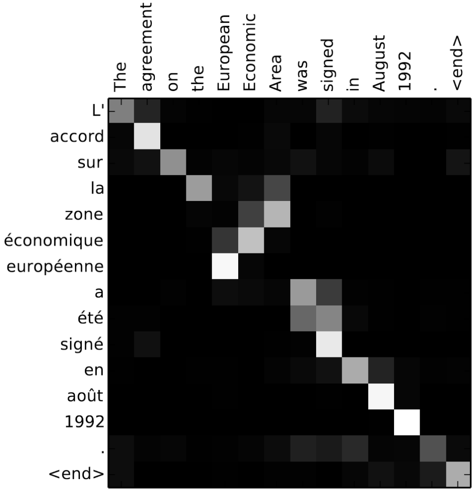
$$\begin{aligned}
\boldsymbol{q}^t &= \boldsymbol{z}^t \boldsymbol{W}^Q (\in \mathbb{R}^d) \\
\boldsymbol{K} &= \boldsymbol{X} \boldsymbol{W}^K (\in \mathbb{R}^{L_x \times d}) \\
\boldsymbol{V} &= \boldsymbol{X} \boldsymbol{W}^V (\in \mathbb{R}^{L_x \times d})
\end{aligned}$$

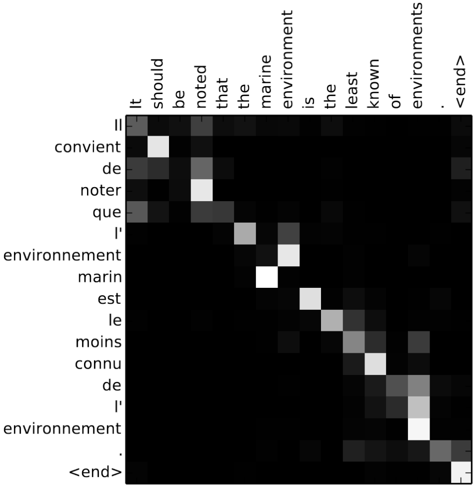
$$\boldsymbol{c}^t = \mathrm{Attention}(\boldsymbol{q}^t, \boldsymbol{K}, \boldsymbol{V}) = \underbrace{\text{softmax}\left(\frac{\boldsymbol{q}^t \boldsymbol{K}^T}{\sqrt{d}}\right)}_{\alpha^t} \boldsymbol{V}$$

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



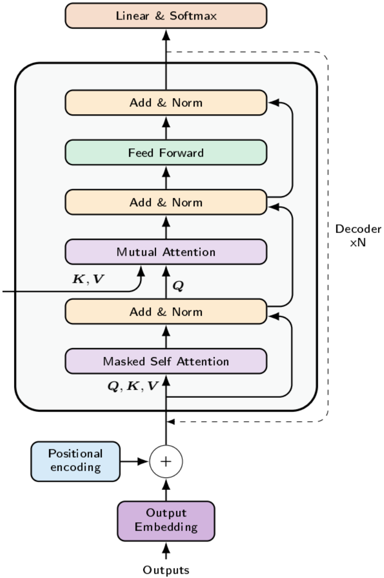
➤ Output length = Query length ($\neq$ Key length = Value length)





Images from [2]

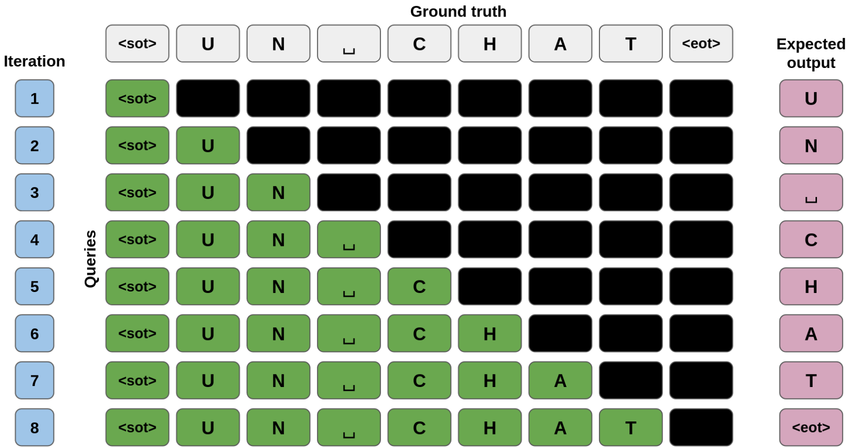
- Size: target sequence length × source sequence length



A stack of 6 transformer decoder layers

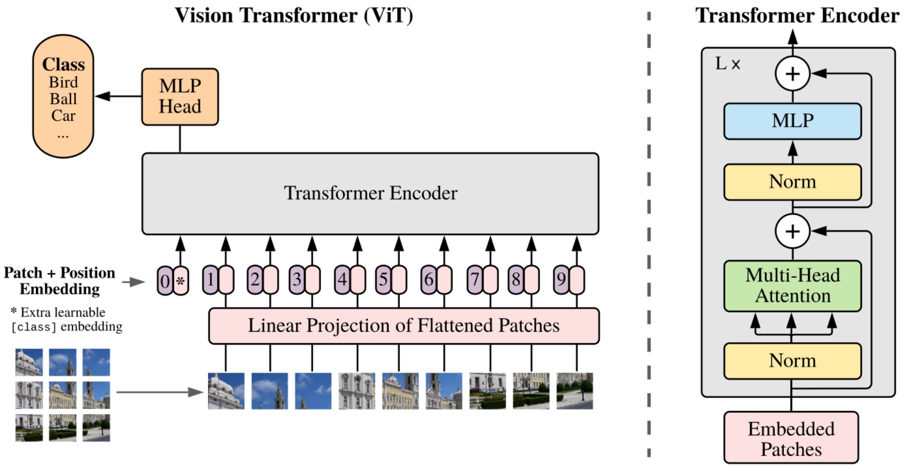
- Multi-head Masked Self Attention
  - ➤ Global query modeling
- Add: residual connections
  - ➤ Multi-scale representation
  - ➤ Reinforce identity
- Norm: layer normalization
  - ➤ Stabilize training (range of values)
- Multi-head mutual attention
  - ➤ Look for relevant information from source
- Feed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

- 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?

Dealing with few annotated data

Create artificial examples

- Data augmentation
- Synthetic data

Benefit from other annotated datasets

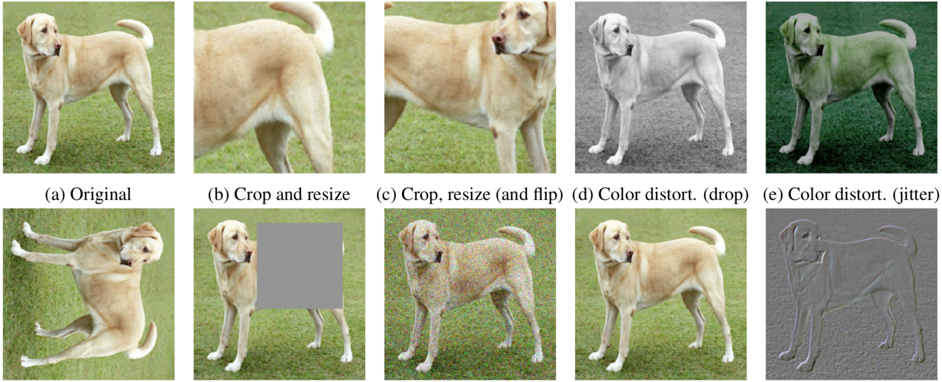
- Transfer learning
- Fine-tuning

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)

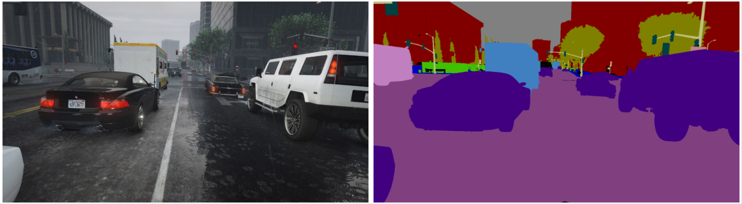
(f) Rotate $\{90°, 180°, 270°\}$ (g) Cutout (h) Gaussian noise (i) Gaussian blur (j) Sobel filtering

⚠ 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

Idea

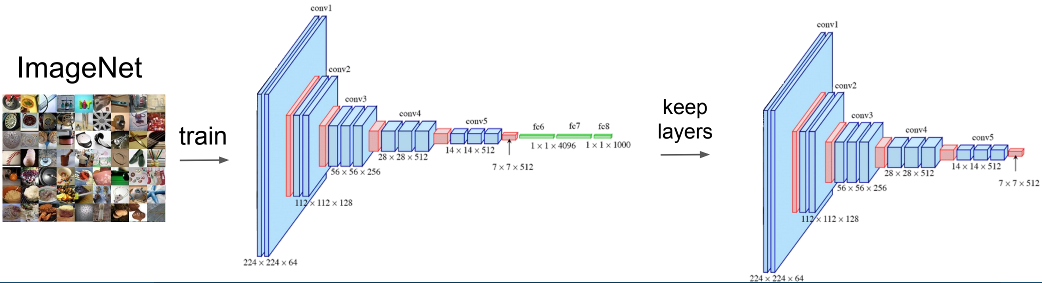
The knowledge learned from task A can be helpful for task B

➤ Benefit from annotated data of another task/dataset

First step: pre-training

Train on a source task/dataset

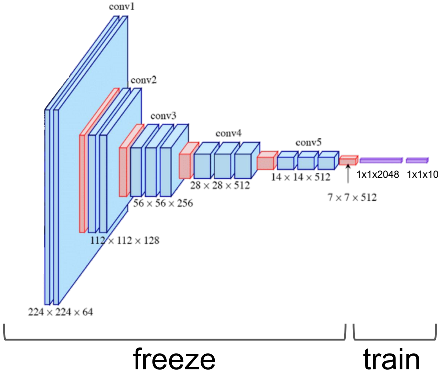
e.g., classification on ImageNet



Adaptation to target dataset

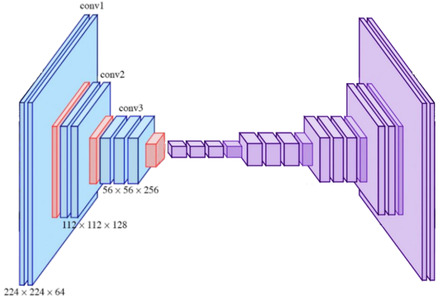
e.g., classification on CIFAR 10

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



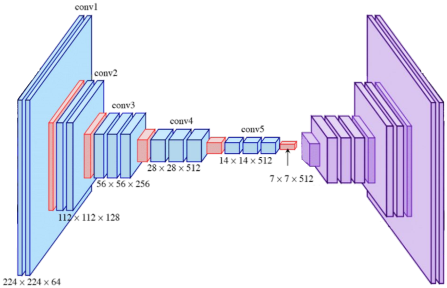
Adaptation to target task

e.g., segmentation



freeze | train

semantically far
much data



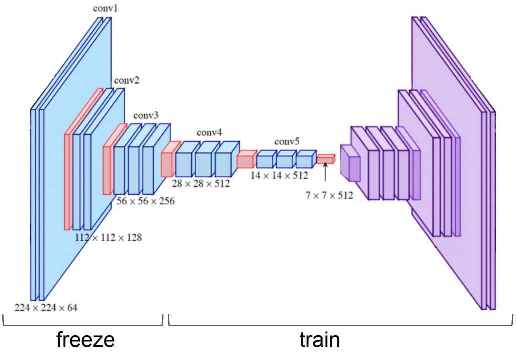
freeze | train

semantically close
few data

If enough target data: fine-tuning

Additional training step

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

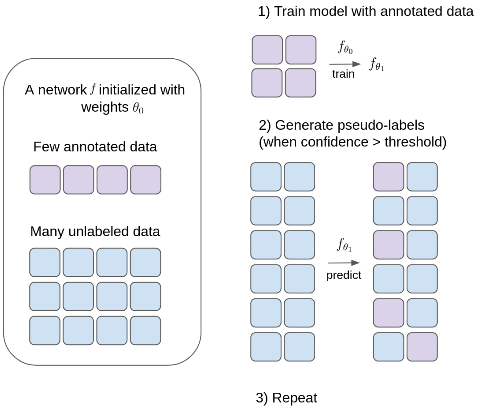


Performance on ImageNet (fine-tuning included)

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

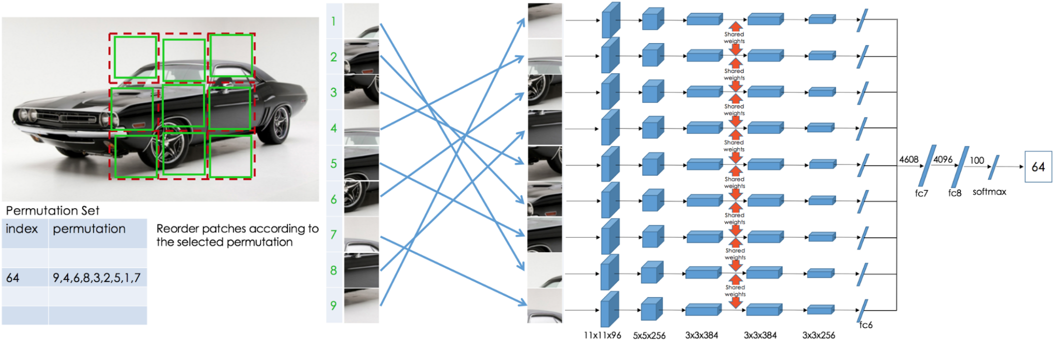
The goal is to solve a pretext task

- 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

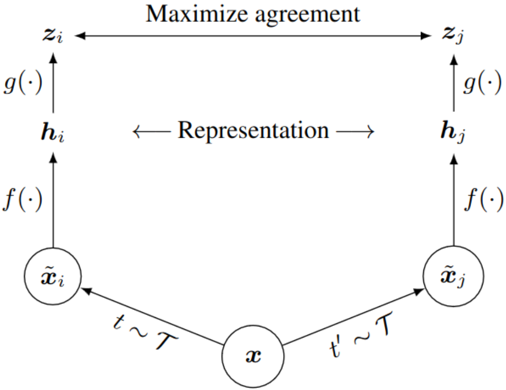
- Find the right permutation: classification formulation



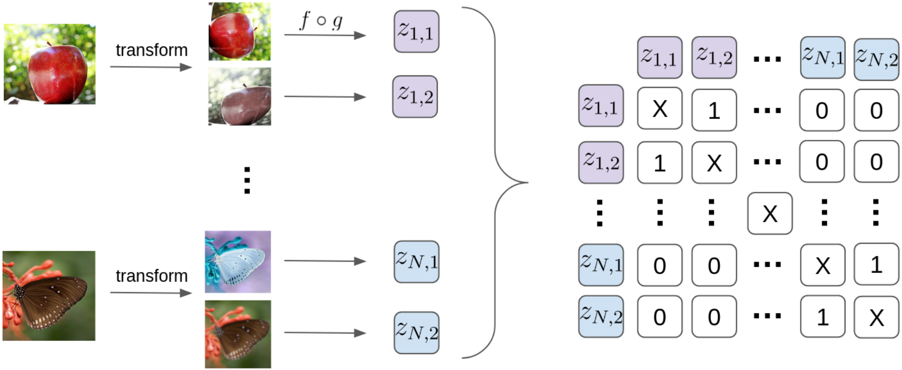
- Idea: generate two views for each input (= positive pair). Bring latent representations of positives closer and keep latent representations of negatives away
- Siamese networks: same architecture with same weights used on different inputs while comparing outputs

Algorithm 1 SimCLR's main learning algorithm.

input: batch size N, constant τ, structure of f, g, $\mathcal{T}$.
for sampled minibatch $\{\boldsymbol{x}_k\}_{k=1}^{N}$ **do**
  for all $k \in \{1, \dots, N\}$ **do**
    draw two augmentation functions $t \sim \mathcal{T}$, $t' \sim \mathcal{T}$
    # the first augmentation
    $\tilde{\boldsymbol{x}}_{2k-1} = t(\boldsymbol{x}_k)$
    $\boldsymbol{h}_{2k-1} = f(\tilde{\boldsymbol{x}}_{2k-1})$ # representation
    $\boldsymbol{z}_{2k-1} = g(\boldsymbol{h}_{2k-1})$ # projection
    # the second augmentation
    $\tilde{\boldsymbol{x}}_{2k} = t'(\boldsymbol{x}_k)$
    $\boldsymbol{h}_{2k} = f(\tilde{\boldsymbol{x}}_{2k})$ # representation
    $\boldsymbol{z}_{2k} = g(\boldsymbol{h}_{2k})$ # projection
  end for
  for all $i \in \{1, \dots, 2N\}$ and $j \in \{1, \dots, 2N\}$ **do**
    $s_{i,j} = \boldsymbol{z}_i^\top \boldsymbol{z}_j / (\|\boldsymbol{z}_i\| \|\boldsymbol{z}_j\|)$ # 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 $g(\cdot)$



- 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
Linear evaluation:												
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**
Fine-tuned:												
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)

DINO (self-DIstillation with NO labels, 2021) [7]

➤ Self-distillation through teacher-student paradigm

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

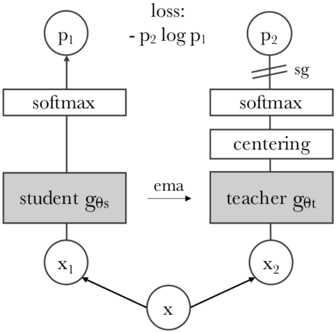
```
# gs, gt: student and teacher networks
# C: center (K)
# tps, tpt: student and teacher temperatures
# l, m: network and center momentum rates
gt.params = gs.params
for x in loader: # load a minibatch x with n samples
    x1, x2 = augment(x), augment(x) # random views

    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 + (1-l)*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): $\theta_t = \lambda\theta_t + (1-\lambda)\theta_s \quad \lambda \in [0.996, 1]$

DINO (self-DIstillation with NO labels, 2021) [7]

- Keywords

Knowledge distillation / teacher-student paradigm

Transfering 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.

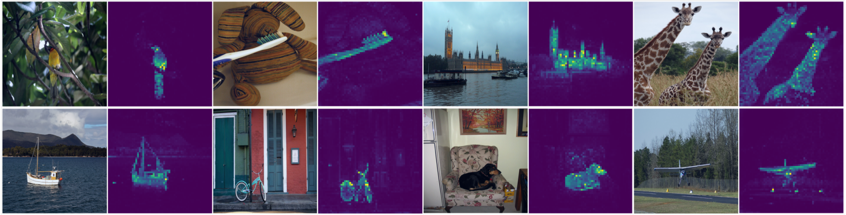
Failing modes

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: $t \leftarrow t/\tau_t$



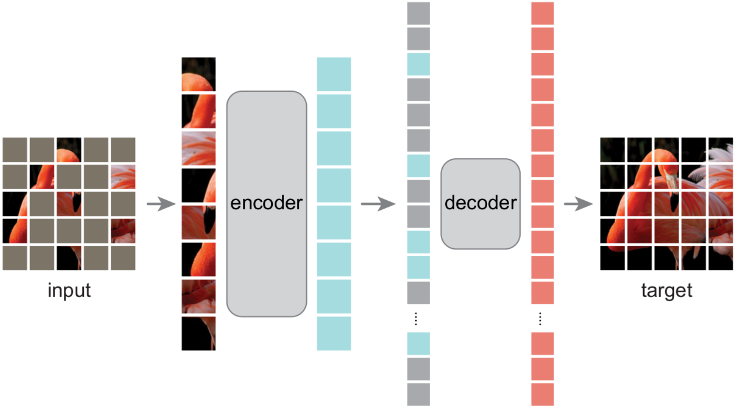
Attention maps: self-attention for CLS token

Classification performance (Top-1 accuracy) with ViT architecture

	Cifar_{10}	Cifar_{100}	INat_{18}	INat_{19}	Flwrs	Cars	INet
ViT-S/16							
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**
ViT-B/16							
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

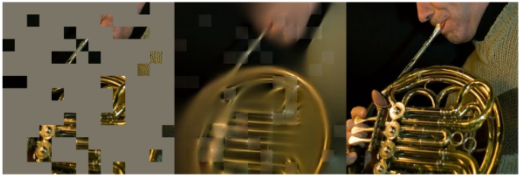
➤ Reconstruct the missing parts (pixel-level MSE loss)



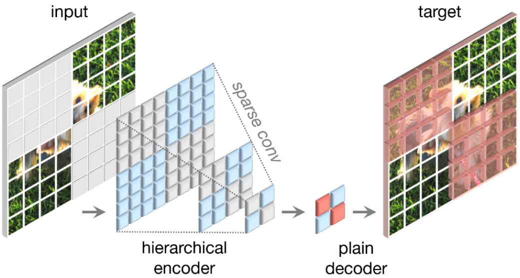
➤ Vision Transformer architecture

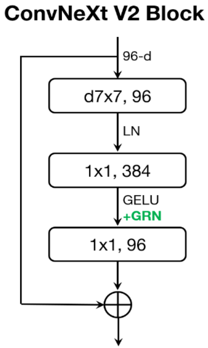
➤ Classification performance (Top-1 accuracy) with ViT architectures, pre-trained and evaluated on ImageNet

Approach	ViT-B	ViT-L	ViT-H	ViT-H_{488}
Supervised	82.3	82.6	83.1	✗
DINO	82.8	✗	✗	✗
MAE	83.6	85.9	86.9	**87.8**




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





- 88.9% top-1 accuracy on ImageNet (659M params)

Be careful with benchmarks V2

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

Conclusion

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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