Deep learning

13.3. Transformer Networks

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https://fleuret.org/dlc/



Vaswani et al. (2017) proposed to go one step further: instead of using attention mechanisms as a supplement to standard convolutional and recurrent operations, they designed a model composed of attention layers only.

They designed this "transformer" for a sequence-to-sequence translation task, but it is currently key to state-of-the-art approaches across NLP tasks.

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The standard practice is to train a transformer in a non-supervised manner on large unlabeled datasets such as Wikipedia—or re-use a pre-trained transformer—and then fine tune it in a supervised manner for tasks which require a ground truth such as sentiment analysis.

They first introduce a multi-head attention module.



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The "scaled dot-product attention" (left) is very close to the attention module we saw in lecture 13.2. "Attention Mechanisms", with the addition of an optional masking (in pink). This may be useful when such a module is used for a generative auto-regressive operation and the attention should be causal, looking only to the past.

The attention is a function of the keys, queries, and values. The only difference with what was seen in the previous course is that the attention matrix is rescaled with the dimension of the embedding, which matters quite a lot.

In the multi-head attention, each head h has its own processing of the input keys, queries, and values through respectively W_i^K , W_i^Q , and W_i^V . And there is one final processing W^O applied on the concatenated results of the multiple heads. Their complete Transformer model is composed of:

- An encoder that combines N = 6 modules, each composed of a multi-head attention sub-module, and a [per-token] one hidden-layer MLP, with residual pass-through and layer normalization.
- A **decoder** with a similar structure, but with causal attention layers to allow for regression training, and additional attention layers that attend to the encoder final keys and values.

Positional information is provided through an **additive** positional encoding of same dimension d_{model} as the internal representation, and is of the form

$$\begin{aligned} & \textit{PE}_{t,2i} = \sin\left(\frac{t}{10,000^{\frac{2i}{d_{model}}}}\right) \\ & \textit{PE}_{t,2i+1} = \cos\left(\frac{t}{10,000^{\frac{2i+1}{d_{model}}}}\right). \end{aligned}$$

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Contrary to what we previously saw with the concatenated binary positional encoding, here the position is provided as additive encoding, where t is the position in the sequence, and 2i and 2i + 1 the dimension.



"Original" Transformer (Vaswani et al., 2017).

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This is a depiction of the standard transformer architecture for sequence-to-sequence translation. It consists of an encoder (left part) and a decoder (right part). Both are a stack of N = 6 modules. Each token (subword) of the input sequence is encoded with a look-up table to get its embedding of dimension d, so that the input is a tensor of size $T \times d$. Then the positional encoding of same size is added to it.

Each of the N modules of the encoder is composed of a multi-head self-attention operation followed by a "feed forward" operation that applies a one hidden layer perceptron at every position of the sequence separately. This can be

implemented with 1×1 convolutions. Both the self-attention and the feed-forward are combined with residual pass-through.

The decoder is an auto-regressive model, and each of its module has a multi-head self-attention operation, then an attention that attends to the encoder, and a feed-forward operation. The selfattention is masked to make it causal, i.e. it takes into account only the part of the sequence already generated. The attention to the encoder is not masked but its keys and values are functions of the outputs of the corresponding module in the encoding stack. The architecture is tested on English-to-German and English-to-French translation using the standard WMT2014 datasets.

- English-to-German: 4.5M sentence pairs, 37k tokens vocabulary.
- English-to-French: 36M sentence pairs, 32k tokens vocabulary.
- 8 P100 GPUs (150 TFlops FP16), 0.5 day for the small model, 3.5 days for the large one.

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Table 2: The Transformer achieves better BLEU scores than previous state-of-the-art models on the English-to-German and English-to-French newstest2014 tests at a fraction of the training cost.

Madal	BL	EU	Training Cost (FLOPs)			
Woder	EN-DE	EN-FR	EN-DE	EN-FR		
ByteNet [18]	23.75					
Deep-Att + PosUnk [39]		39.2		$1.0 \cdot 10^{20}$		
GNMT + RL [38]	24.6	39.92	$2.3\cdot10^{19}$	$1.4\cdot10^{20}$		
ConvS2S [9]	25.16	40.46	$9.6\cdot10^{18}$	$1.5\cdot10^{20}$		
MoE [32]	26.03	40.56	$2.0\cdot10^{19}$	$1.2\cdot 10^{20}$		
Deep-Att + PosUnk Ensemble [39]		40.4		$8.0 \cdot 10^{20}$		
GNMT + RL Ensemble [38]	26.30	41.16	$1.8\cdot10^{20}$	$1.1\cdot10^{21}$		
ConvS2S Ensemble [9]	26.36	41.29	$7.7\cdot 10^{19}$	$1.2 \cdot 10^{21}$		
Transformer (base model)	27.3	38.1	3.3 ·	10^{18}		
Transformer (big)	28.4	41.8	2.3	10^{19}		

(Vaswani et al., 2017)

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The standard metric in natural language processing is the Bilingual Evaluation Understudy Score (BLEU) score which aims at evaluating a generated sequence to a reference sentence. The BLEU score ranges between 0 (perfect mismatch) and 1 (perfect match).



(Vaswani et al., 2017)

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On the left is a visualization of the attention as computed by one head of the layer 5 of the encoder $% \left({{\left[{{{\rm{T}}_{\rm{T}}} \right]}_{\rm{T}}} \right)$

On the right the attention given by the word "its" for two different heads is on "law" and "application" which provides help for gender and grammatical issues.



(Vaswani et al., 2017)

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Two other heads also in layer 5.

Standard transformers now combine differently the residual connection and the normalization (Wang et al., 2019).



(b) pre-norm residual unit

Figure 1: Examples of pre-norm residual unit and postnorm residual unit. \mathcal{F} = sub-layer, and LN = layer normalization.

(Wang et al., 2019)

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Transformer self-training and fine-tuning for NLP

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The transformer networks were introduced for translation, and trained with a supervised procedure, from pairs of sentences.

However, as for word embeddings, they can be trained in an unsupervised manner, for auto-regression or as denoising auto-encoders, from very large data-sets, and fine-tuned on supervised tasks with small data-sets.

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A transformer [pre-]trained in a unsupervised manner for the task of predicting a token: for autoregression, the input is the sentence up to the token to predict, for mask language modeling, the input is a full sentence with some tokens replaced by a "mask" token. No ground truth is required for those tasks.

As for word embedding, training a transformer model like this allows to capture statistical structures in the text and provide an extremely good representation for more sophisticated tasks which can only be trained in a supervised manner with only small datasets available. BERT (Bidirectional Encoder Representation from Transformers, Devlin et al., 2018) is an encoder of a transformer pre-trained with:

- Masked Language Model (MLM), that consists in predicting [15% of] words which have been replaced with a "MASK" token.
- Next Sentence Prediction (NSP), which consists in predicting if a certain sentence follows the current one.

It is then fine-tuned on multiple NLP tasks.

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BERT (Devlin et al., 2018)

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Figure 1: Overall pre-training and fine-tuning procedures for BERT. Apart from output layers, the same architectures are used in both pre-training and fine-tuning. The same pre-trained model parameters are used to initialize models for different down-stream tasks. During fine-tuning, all parameters are fine-tuned. [CLS] is a special symbol added in front of every input example, and [SEP] is a special separator token (e.g. separating questions/answers).

(Devlin et al., 2018)

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BERT is trained in an unsupervised manner to do two tasks at the same time: predicting missing words and predicting whether two sentences follow each other in the corpus.





Class Label



Single Sentence

0

T_N

E_N

 $\hat{\mathbf{U}}$

Tok N





B-PER

T₂

 E_2

î

Tok 2

T

Single Sentence

BERT

0

Τ,

Е,

Tok 1

с

EICLS

[CLS]



Paragraph

(c) Question Answering Tasks: SQuAD v1.1

Question



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(Devlin et al., 2018)



(Clark et al., 2019)

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Once again, visualizing the attention matrices show that it connects a word with other words that help to get its meaning. Large Language Models

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GPT (Generative Pre-Training, Radford, 2018) is a decoder of a transformer trained for auto-regressive text generation.



(Radford, 2018)

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Note that GPT model is inherently causal, so only carries information forward, and consists of 12 modules as opposed to 6 for the original transformer.

The tasks GPT can be fine-tuned on are:

- Classification: for instance for sentiment analysis, when the input is a comment, and the task is to predict whether it is positive or negative.
- Entailment: given a premise and a hypothesis, the task is to predict whether the hypothesis is implied by the premise.
- Similarity: the task is to predict if two pieces of text have the same meaning.
- Multiple choice: the task is to predict the correct answer.



GPT (Radford, 2018)

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"GPT-2 is a large transformer-based language model with 1.5 billion parameters, trained on a dataset of 8 million web pages. GPT-2 is trained with a simple objective: predict the next word, given all of the previous words within some text. The diversity of the dataset causes this simple goal to contain naturally occurring demonstrations of many tasks across diverse domains. GPT-2 is a direct scale-up of GPT, with more than 10X the parameters and trained on more than 10X the amount of data."

(Radford et al., 2019)

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We can use HuggingFace's pre-trained models (https://huggingface.co/).

```
import torch
from transformers import GPT2Tokenizer, GPT2LMHeadModel
tokenizer = GPT2Tokenizer.from_pretrained('gpt2')
model = GPT2LMHeadModel.from_pretrained('gpt2')
model.eval()
tokens = tokenizer.encode('Studying Deep-Learning is')
for k in range(100): # no more than 100 tokens
outputs = model(torch.tensor([tokens])).logits
next_token = torch.argmax(outputs[0, -1])
tokens.append(next_token)
if tokenizer.decode([next_token]) == '.': break
print(tokenizer.decode(tokens))
```

prints

Studying Deep-Learning is a great way to learn about the world around you.

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HugginFace is a company that develops and distributes open-source implementations of language models. The transformers can be installed using the pipe of the nearly that the pipe of th

model and generates the end of a sentence given "Studying Deep-Learning is" as beginning.

tokenizer can take as input a sequence of strings to produce a sequence of token, or the opposite, take as input a sequence of tokens and produces the corresponding sequence of words.

In this example, the generative procedure picks at each iteration the word with the maximum probability, but stochastic sampling could also be used.

The generated sentence could make sense in other situations (e.g. replacing "Deep-Learning" with another topic of studies), but is grammatically correct and consistent with "studying".

Large GPT have been shown to exhibit some "few shot learning" capabilities when they are properly "primed" (Brown et al., 2020).

For instance using Hugging Face's gpt2 model with 120M parameters, we can get these sentence completions, where the generated parts are in bold:

I: I love apples, O: positive, I: music is my passion, O: positive, I: my job is boring, O: negative, I: frozen pizzas are awesome, O: **positive**,

I: I love apples, O: positive, I: music is my passion, O: positive, I: my job is boring, O: negative, I: frozen pizzas taste like cardboard, O: **negative**,

I: water boils at 100 degrees, O: physics, I: the square root of two is irrational, O: mathematics, I: the set of prime numbers is infinite, O: mathematics, I: gravity is proportional to the mass, O: **physics**,

I: water boils at 100 degrees, O: physics, I: the square root of two is irrational, O: mathematics, I: the set of prime numbers is infinite, O: mathematics, I: squares are rectangles, O: **mathematics**,

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(Brown et al., 2020)

The GPT-3 model has 175B parameters and is trained on 300B tokens from various sources (Brown et al., 2020). The Pathways Language Model (PaLM) has 540B parameters and is trained on 780B tokens (Chowdhery et al., 2022).

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$\texttt{Context} \rightarrow$	Q: What is 98 plus 45? A:
$\texttt{Completion} \rightarrow$	143

Figure G.44: Evaluation example for Arithmetic 2D+

$\texttt{Context} \ \rightarrow$	Q: What is 95 times 45? A:
$\texttt{Completion} \ \rightarrow$	4275

Figure G.45: Evaluation example for Arithmetic 2Dx

$\texttt{Context} \ \rightarrow$	Q: What is 509 minus 488? A:
$\texttt{Completion} \ \rightarrow$	21

Figure G.46: Evaluation example for Arithmetic 3D-

Setting	2D+	2D-	3D+	3D-	4D+	4D-	5D+	5D-	2Dx	1DC
GPT-3 Zero-shot	76.9	58.0	34.2	48.3	4.0	7.5	0.7	0.8	19.8	9.8
GPT-3 One-shot	99.6	86.4	65.5	78.7	14.0	14.0	3.5	3.8	27.4	14.3
GPT-3 Few-shot	100.0	98.9	80.4	94.2	25.5	26.8	9.3	9.9	29.2	21.3

(Brown et al., 2020)

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 ${\sf OpenAI}/{\sf Github's}\ {\sf Copilot}$

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Explaining a Joke

I will explain these jokes: (1) The problem with kleptomaniacs is that they always take things literal Explanation: This joke is wordplay. Someone who "takes things literally" i But the definition of kleptomania is someone who literally takes things. (2) Always borrow money from a pessimist. They'll never expect it back. Explanation: Most people expect you to pay them back when you borrow money them, they will expect that you won't pay them back anyways.	lly. is someone who doesn't fully understand social cues and context, which is a negative trait. 7, however a pessimist is someone who always assumes the worst, so if you borrow money from
<pre>Input: I was supposed to start writing the paper at 5:00 PM. But th started playing with this cool new language model for 10 minutes. minutes later, it's suddenly 9:30 PM! Model Output: This joke is about how time flies when you're having The person was supposed to start writing a paper at 5:00 PM, but th started playing with a language model instead. They thought they with only playing with it for 10 minutes, but it was actually 4.5 hours "On great, your step dad's poetry reading is that night!" So now 1 flying in on April 7th. Model Output: The joke is that the speaker's mother is trying to them to go to their step dad's poetry reading, but the speaker dow want to go, so they are changing their flight to the day after the poetry reading.</pre>	<pre>hen I 10 10 10 1 [get excited when I smell food and become super alert when the 10 10 10 10 1 [get excited when I smell food and become super alert when the 10 10 10 10 10 10 10 10 10 10 10 10 10</pre>
Input: Reading "War and Peace" doesn't scare me. I once had to revi CL for my intern's whole project on his final day! ModelOutput: 'War and Peace' is a very long book, so reading it daunting task. However, the speaker is saying they had to review t code for their intern's project on their final day, which is even daunting.	<pre>iew the is a is a the more</pre> Input: What's the difference between a zebra and an umbrella? One is a striped animal related to horses, another is a device you use to stop the rain from falling on you. Model Output: This joke is an anti-joke. The joke is that the answer is obvious, and the joke is that you were expecting a funny answer.

(Chowdhery et al., 2022)

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Inference Chaining

I will explain how to make logical inferences: (1) John wakes to the sound of his children giggling outside the door. They bust in and say "Happy Father's Dayl" with a plate full of food. 2022 has been a great year. Can we infer that John is a father because of "his children". We can infer that the current year is 2022. Barack Obama was inaugurated in 2009, so it has been about 13 years since Obama was inaugurated. John's children" we can infer that the current year is 2022. Barack Obama was inaugurated in 2009, so it has been about 13 years since Obama was inaugurated. John's children are old enough to speak, so if John were born after Obama's inauguration, he would have been younger than 10 when he had children. So, we can infer that John was born before Obama's inauguration. The answer is "yes". (2) Sam sees a piano in the subway stations. Laughing, his friends prod him to play, saying "Remember how amazing your rendition of Chopsticks was at the Christmas party?" Can we infer that John majored in piano at Juilliand? Answer: Juilliard is a top school for music, so someone who majored in piano at Juilliard would be an expert pianist. "Chopsticks" is a very simple song to play on the piano. His friends were therefore likely being sarcastic when they told him to play, which would imply that Sam was not an expert piano player. So it is unlikely that Sam majored in piano at Juilliard. The answer is "no". Input: Guido was writing a Python program. He keeps getting confused by Input: When I found out my grandma was in the hospital I felt a variable scope and looking it up on StackOverflow. Is it possible that particular color. When someone cut me off in traffic I felt a different color. What is the most likely color I would see if I the Guido in the prompt refers to Guido van Rossum? Model Output: Guido van Rossum is the creator of Python. He would not combined these two colors? need to look up variable scope on StackOverflow. The answer is "no". Model Output: The color that I felt when I found out my grandma was in the hospital was likely a sad color, like blue. The color that I felt when someone cut me off in traffic was likely an angry color, like Input: Trevor has wanted to see the mountain with all of the heads on it red. If I combined these two colors, I would likely see purple. The for a long time, so he finally drove out to see it. What is the capital answer is "purple". of the state that is directly east of the state that Trevor is currently in? Model Output: The mountain with all of the heads on it is Mount Input: Michael is at that really famous museum in France looking at Rushmore. Mount Rushmore is in South Dakota. The state directly east of South Dakota is Minnesota. The capital of Minnesota is St. Paul. The its most famous painting. However, the artist who made this painting just makes Michael think of his favorite cartoon character from his answer is "St. Paul". childhood. What was the country of origin of the thing that the cartoon character usually holds in his hand? Model Output: The most famous painting in the Louvre is the M Input: Jennifer looked out her window and sees a really cool cloud below Lisa. The artist who made the Mona Lisa is Leonardo da Vinci. Leonardo her. She unbuckles her seatbelt and heads to the bathroom. Is Jennifer da Vinci is also the name of the main character in the cartoon Teenage probably traveling more than 300 miles per hour relative to the earth? Mutant Ninja Turtles. Leonardo da Vinci is from Italy. The thing that ModelOutput: 300 miles per hour is about 480 km/h. This is about the Leonardo da Vinci usually holds in his hand is a katana. The country speed of a commercial airplane. Clouds are usually below airplanes, so Jennifer is probably on an airplane. The answer is "yes". of origin of the katana is Japan. The answer is "Japan".

(Chowdhery et al., 2022)

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Summary:

- The original Transformer (Vaswani et al., 2017) combines an encoder composed of blocks each made of a self-attention layer, and a per-token MLP, and a decoder composed of blocks each made of a causal self-attention layer, a cross attention layer, and a per-token MLP.
- BERT (Devlin et al., 2018) has the structure of the Transformer's encoder.
- GPT (Radford, 2018; Radford et al., 2019) has the structure of the Transformer's decoder without cross-attention.
- A model can be self-trained to predict masked words (BERT), or for auto-regression (GPT), and fine-tuned on downstream tasks.
- Special tokens can separate parts of inputs (e.g. question / answer) or indicate the output token used for prediction (e.g. sentiment analysis).
- These models scale extremely well to 100s of billions of tokens and parameters (Kaplan et al., 2020)
- Auto-regressive language models can be primed to solve with remarkable accuracy zero-shot learning tasks (Brown et al., 2020; Chowdhery et al., 2022).

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Vision Transformers

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As in NLP, attention mechanisms in vision allow models to leverage long-term dependencies that would require many convolutional layers, e.g. for Self-Attention Generative Adversarial Networks (SAGANs):



"The self-attention module is complementary to convolutions and helps with modeling long range, multi-level dependencies across image regions. Armed with self-attention, the generator can draw images in which fine details at every location are carefully coordinated with fine details in distant portions of the image."

(Zhang et al., 2018)

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The Vision Transformer (ViT, Dosovitskiy et al. 2020) is a very simple architecture for image classification.

"Inspired by the Transformer scaling successes in NLP, we experiment with applying a standard Transformer directly to images, with the fewest possible modifications. To do so, we split an image into patches and provide the sequence of linear embeddings of these patches as an input to a Transformer. Image patches are treated the same way as tokens (words) in an NLP application. We train the model on image classification in supervised fashion."

(Dosovitskiy et al., 2020)

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Model	Layers	Hidden size D	MLP size	Heads	Params
ViT-Base	12	768	3072	12	86M
ViT-Large	24	1024	4096	16	307M
ViT-Huge	32	1280	5120	16	632M

Table 1: Details of Vision Transformer model variants.



(Dosovitskiy et al., 2020)

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With large pre-training, Vision Transformers (ViT) performs better than Resnets adapted to "Big Transfer" (BiT).



1 exaFLOPs \simeq 1h RTX 3090

(Dosovitskiy et al., 2020)

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RGB embedding filters (first 28 principal components) Image: State of the state of



(Dosovitskiy et al., 2020)

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The left figure shows filters learned to encode the patches. They exhibit the expected structure of an image linear basis.

The right image shows for every one of the 7×7 patch positions the similarity of its positional encoding with the positional encodings of all other patches. The learned encodings reflect the rows and columns, and more generally the 2d structure of the image lattice.



⁽Dosovitskiy et al., 2020)

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This scatter plot shows for every layer and every head the average distance in pixels between a patch and the patches it attends too.

Early layers have very diverse "attention distances", while the last one tend to have long distance attention only.



(Dosovitskiy et al., 2020)

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This picture is obtained by looking at the attention of the output token and then going backward through layers, multiplying by the attention averaged across heads for each. The Swin Transformer (Liu et al., 2021) improves the ViT architectures through the use of hierarchical representation with local attention in shifting windows.



(Liu et al., 2021)

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The DETR algorithm (Carion et al., 2020) combines a CNN and a transformer for object detection.



(Carion et al., 2020)

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A CNN converts the original image into a tensor of 1/32 the size, which is flatten as a sequence of tokens.

The sequence if then fed into a Transformer with a non-causal feed-forward decoder (as opposed to the standard auto-regressive one). The maximum number of detections is specified by the number initial "object queries" given to the decoder.

The final read-out is done with a per-token MLP that maps the internal feature dimension to the box coordinates, and a linear layer that maps the internal feature representation to the class (+ "background") logits.

The loss is computed for an optimal matching σ computed with the Hungarian algorithm between the ground truth and the *N* predicted detections.

•							
Model	GFLOPS/FPS $\#$	^L params AP	AP_{50}	AP_{75}	AP_{S}	AP_{M}	AP_{L}
Faster RCNN-DC5 Faster RCNN-FPN Faster RCNN-R101-FPN	320/16 180/26 246/20	166M39.042M40.260M42.0	$ \begin{array}{r} 60.5 \\ 61.0 \\ 62.5 \end{array} $	42.3 43.8 45.9	$21.4 \\ 24.2 \\ 25.2$	$43.5 \\ 43.5 \\ 45.6$	$52.5 \\ 52.0 \\ 54.6$
Faster RCNN-DC5+ Faster RCNN-FPN+ Faster RCNN-R101-FPN+	320/16 180/26 246/20	166M41.142M42.060M44.0	$61.4 \\ 62.1 \\ 63.9$	44.3 45.5 47.8	22.9 26.6 27.2	$45.9 \\ 45.4 \\ 48.1$	$55.0 \\ 53.4 \\ 56.0$
DETR DETR-DC5 DETR-R101 DETR-DC5-R101	86/28 187/12 152/20 253/10	41M42.041M43.360M43.560M44.9	62.4 63.1 63.8 64.7	44.2 45.9 46.4 47.7	20.5 22.5 21.9 23.7	45.8 47.3 48.0 49.5	61.1 61.1 61.8 62.3

(Carion et al., 2020)

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