Machine Learning Course - CS-433

Self-supervised Learning

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EPFL

Self-supervised Learning

$\{(x, \cancel{y})\}_{i=1}^{n}$

Problem: Labelled data for supervised learning is often limited and expensive to acquire.

Transfer learning: Fine-tune an existing model trained on a related task giving it a good internal representation of the input data. This can allow us to achieve high performance on the downstream task with significantly fewer labels. However, we still need supervision (labels) for the base task.

Self-Supervised Learning: Use the input itself to generate supervisory signals. The base task is an artificial pretext task that requires learning useful features and structure in the input data.

fake task

In the pretext task we want to learn a model f:

$$f : \mathbf{x}_{\text{in}} \mapsto \mathbf{x}_{\text{out}}$$

Where we use a transformation $g : \mathbf{x} \mapsto (\mathbf{x}_{\text{in}}, \mathbf{x}_{\text{out}})$ to create an input and a target from an (unlabelled) datapoint $\mathbf{x} \in \mathcal{X}$. Note that g often involves some randomness.

Example Pretext Tasks

Examples of self-supervised learning for text:

- Masked Language Modelling BERT
- Next Token Prediction (as in previous LLM lecture)

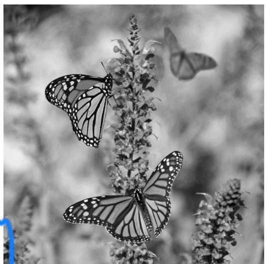
... for images:

Predicting Image Rotation:

90°

$\{0°, 90°, 180°, 270°\}$

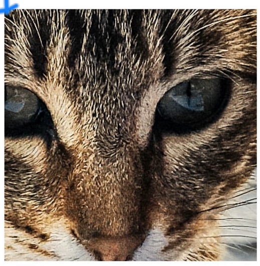
Image Colorization:



N NE

Predicting Relative Patch Placement:

W



Second patch
is above and
left of the first

She/it   She didn't fit in the car because [MASK] was too ~~small~~ big

Masked Language Modelling (MLM)

Learn to predict masked (hidden) words for example:

`She [MASK] her coffee` $\mapsto$ `She drank her coffee`

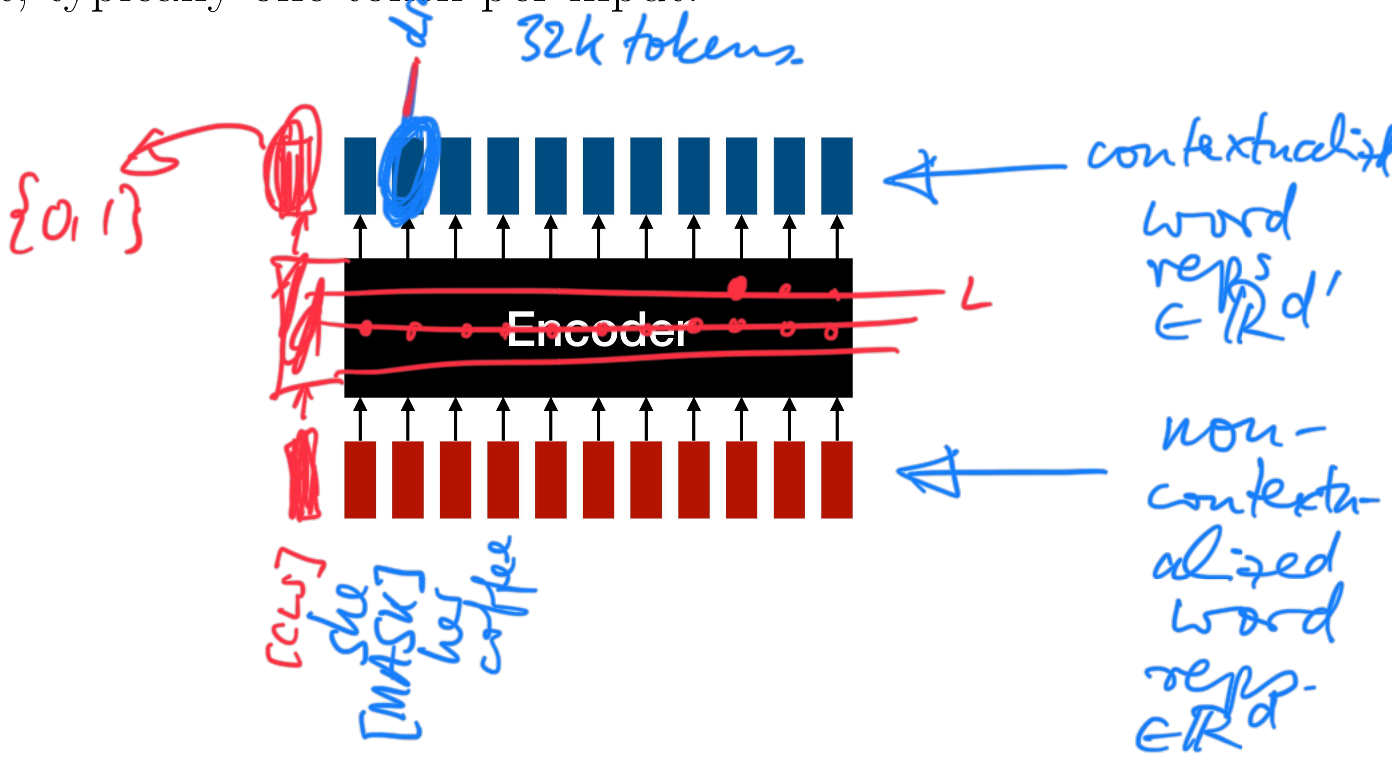
Forces the model to learn a comprehensive representation of the language that is very useful for many downstream tasks. Can train on huge corpora of text (books, Wikipedia, etc) without any labelling.

BERT

2018 Google

Bidirectional **E**ncoder **R**epresentations from **T**ransformers is a well known family of language models based on the encoder-only transformer architecture and trained on masked language modelling.

Encoder: Sees the whole sequence at once, every token can generally attend to every other token (both previous and later ones, hence bidirectional). Generates a fixed sized output, typically one token per input.



predict {0,1}

Training Inputs: BERT is trained on input sequences consisting of two sentences and special tokens, for example:

classification

```
[CLS] The cat is sleeping.
[SEP] It's on the sofa. [SEP]
```

separator

Where [CLS] is a special classification token and [SEP] is used to separate the two sentences. Around 15% of the standard tokens are selected to be replaced by [MASK]. Occasionally the selected tokens are replaced by a random word or not replaced to reduce distribution shift for downstream tasks that do not have [MASK]. Positional and segment encodings are added to the token embeddings.

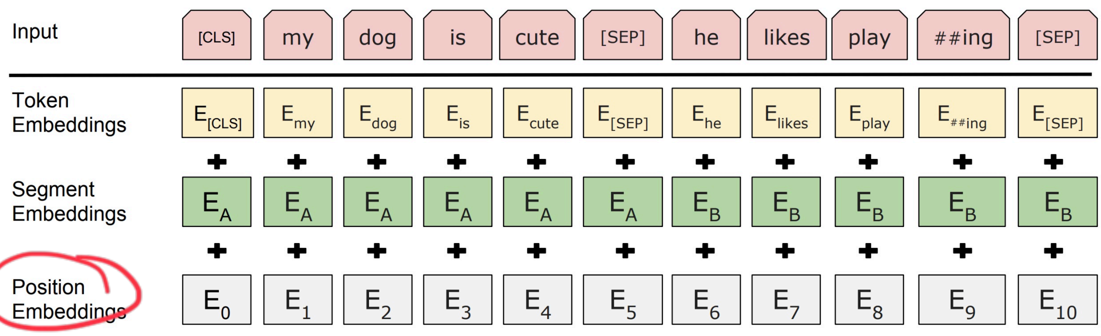


Figure from the original BERT paper: https://arxiv.org/abs/1810.04805

Training Objective:

- For each selected (replaced / masked) token: Predict the original token. Softmax cross-entropy loss over all possible tokens.
- For the [CLS] token: Predict whether the second sentence immediately follows the first sentence or not (binary classification).

$$a+b=b+a$$

$$(a,1)+(b,2) \neq (b,1)+(a,2)$$

Downstream tasks: The structure of the BERT training task allows fine-tuning for a variety of downstream tasks.

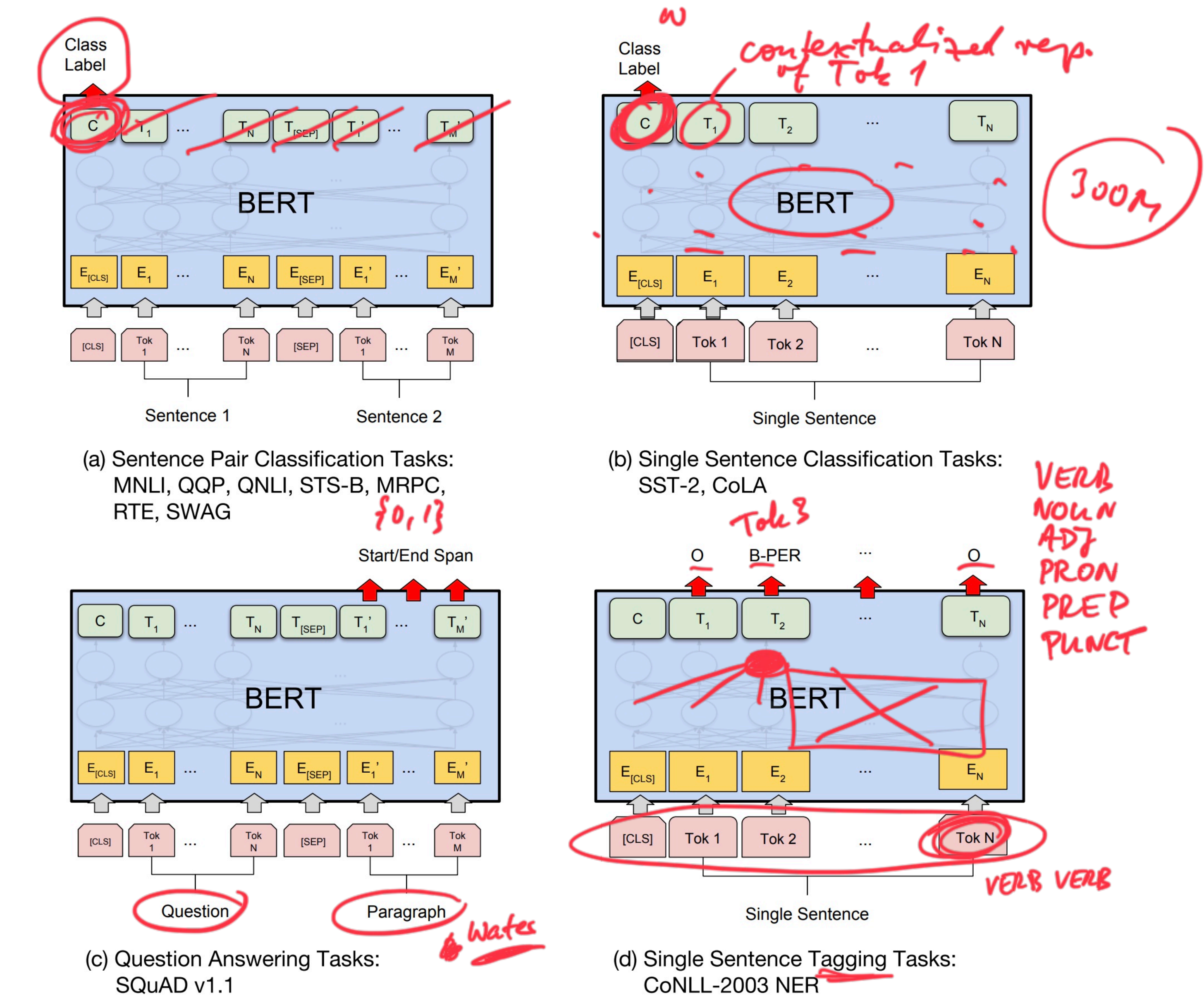


Figure from the original BERT paper: https://arxiv.org/abs/1810.04805

- Classifying sentences or pairs (e.g. sentiment analysis): Use the `[CLS]` token.
- Word level classification (e.g. named entity recognition): Use the output for each token.
- Extracting a relevant passage (e.g. search): Use the individual outputs to define a span.

Next Token Prediction, LLMs

Predict the next token given previous tokens, e.g.:
`She drank her` $\mapsto$ `coffee`

Similar to Masked Language Modelling but is causal (auto-regressive), we can only see previous words, not later ones.

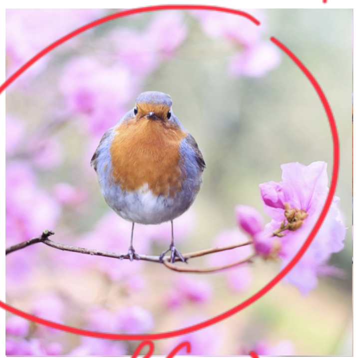
This makes it better suited for generating arbitrary length responses. In line with common use-cases of LLMs, such as prompting, in-context learning.

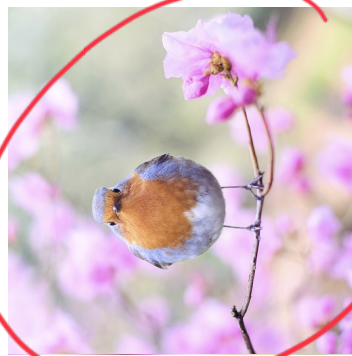
(See previous lecture)

Joint Embedding Methods

Learn an encoder invariant to certain transformations on the data, e.g., to rotation:

x_1 x_2





$f(x_1) \approx f(x_2)$

Rather than learning a model $f : \mathbf{x}_{\text{in}} \mapsto \mathbf{x}_{\text{out}}$, learn $f : \mathcal{X} \to \mathbb{R}^d$ s.t.

$$f(\mathbf{x}_1) \approx f(\mathbf{x}_2)$$

where $g : \mathbf{x} \mapsto (\mathbf{x}_1, \mathbf{x}_2)$ is a transformation that creates two views from the same input datapoint $\mathbf{x} \in \mathcal{X}$.

g is usually a random function that applies multiple data augmentations, each with certain probability.

Problem: constant f is a trivial encoder that is invariant!

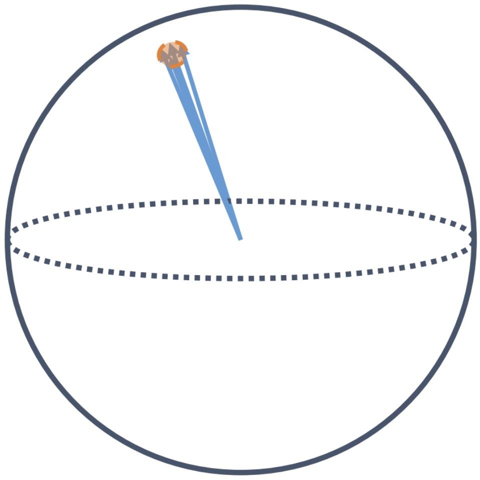


Figure from https://arxiv.org/abs/2110.09348

Bootstrap your own latent

Solved by contrastive learning (next!) or non-contrastive methods with regularization, e.g.,

new f

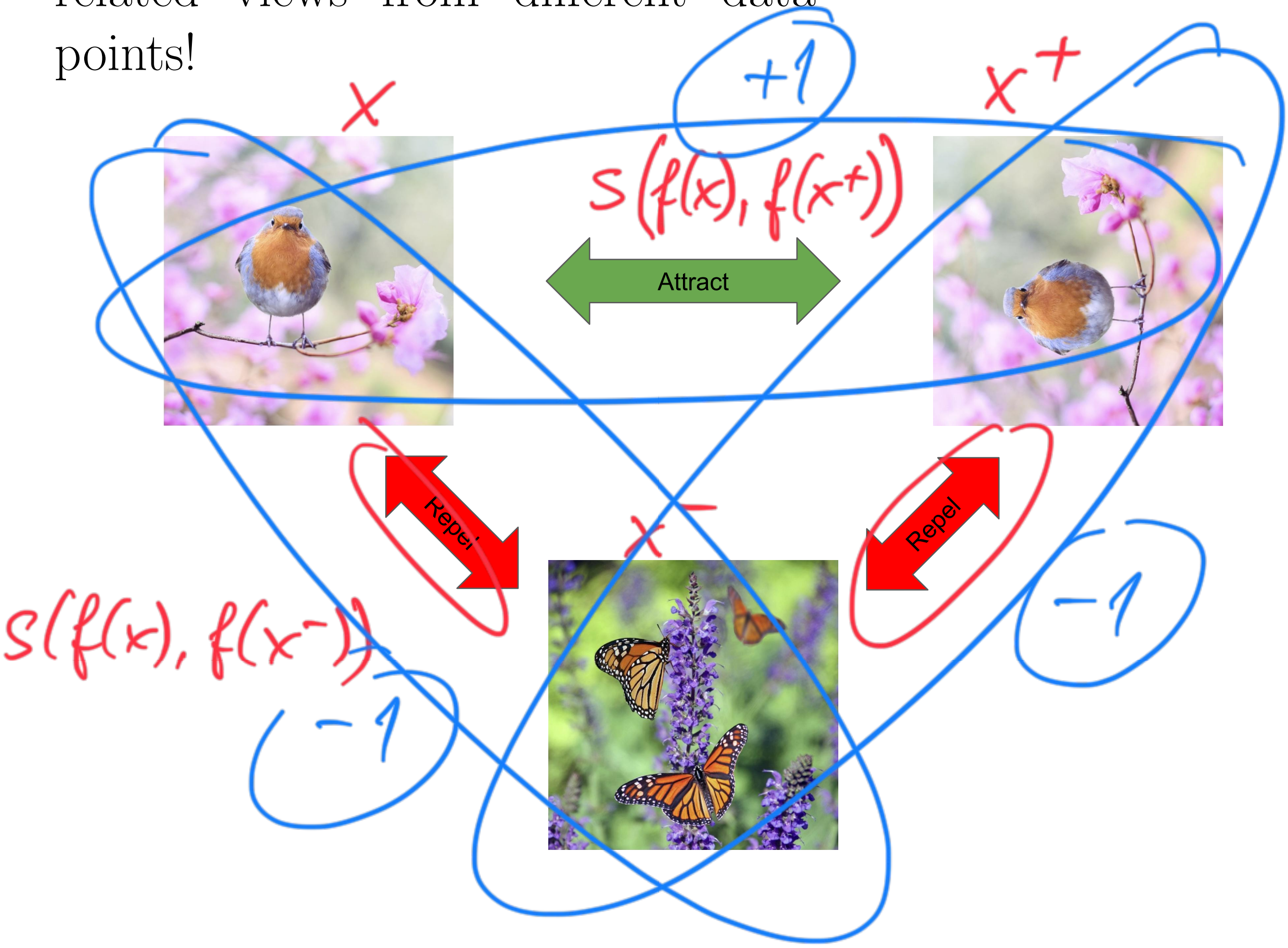
- BYOL: use two encoders f_1, f_2 where f_2 is the exponential moving average of f_1 and force

$$\underline{f_1}(\mathbf{x}_1) \approx \underline{f_2}(\mathbf{x}_2).$$

old f

Contrastive learning

Push away representations of unrelated views from different data points!



Objective: given a positive pair $\mathbf{x}, \mathbf{x}^+$ from the datapoint $\mathbf{x}$, and a negative view $\mathbf{x}^-$ from a different datapoint $\mathbf{x}' \neq \mathbf{x}$,

?

$$\mathrm{s}\left(f(\mathbf{x}), f(\mathbf{x}^+)\right) > \mathrm{s}\left(f(\mathbf{x}), f(\mathbf{x}^-)\right),$$

where the s function quantifies the similarity of two embeddings.

SimCLR

A contrastive learning framework with optimized choices.

Pr. of correct pred.

1. classification objective with N negative samples:

min f

$$L(\mathbf{x}) = -\mathbb{E}\left[\log \frac{e^{\mathrm{s}\left(f(\mathbf{x}),f(\mathbf{x}^+)\right)}}{e^{\mathrm{s}(f(\mathbf{x}),f(\mathbf{x}^+))} + \sum_{i=1}^{N} e^{\mathrm{s}\left(f(\mathbf{x}),f(\mathbf{x}_i^-)\right)}}\right].$$

softmax

- maximize the score between $\mathbf{x}$ and $\mathbf{x}^+$,
- minimize the score between $\mathbf{x}$ and all $\mathbf{x}_i^-$.

2. use an additional projector to map the encoder output to the similarity (possibly lower-dimensional) space:

$$f(\mathbf{x}) = \underbrace{f_2}_{\text{projector}} \circ \underbrace{f_1}_{\text{encoder}}(\mathbf{x})$$

last layer — everything before

- learn f_1 and f_2 jointly in an end-to-end fashion,
- use only f_1 for downstream tasks.

3. use cosine similarity with temperature scaling τ:

$$\mathrm{s}\left(\mathbf{e}_1, \mathbf{e}_2\right) = \frac{\langle \mathbf{e}_1, \mathbf{e}_2 \rangle}{\|\mathbf{e}_1\|_2 \|\mathbf{e}_2\|_2} / \tau.$$

4. generate views with data augmentation:

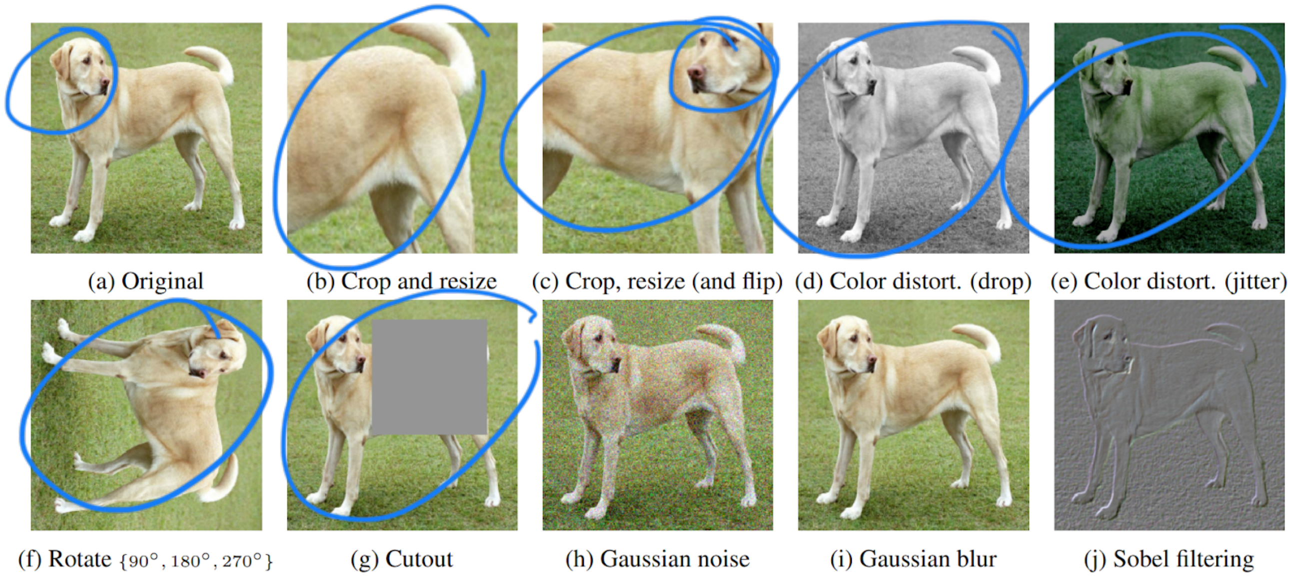


Figure from the SimCLR paper: https://arxiv.org/abs/2002.05709

- stronger data augmentations than those used in supervised learning,
- random crop creates global to local ($B \to A$) views or adjacent view ($D \to C$) prediction tasks.

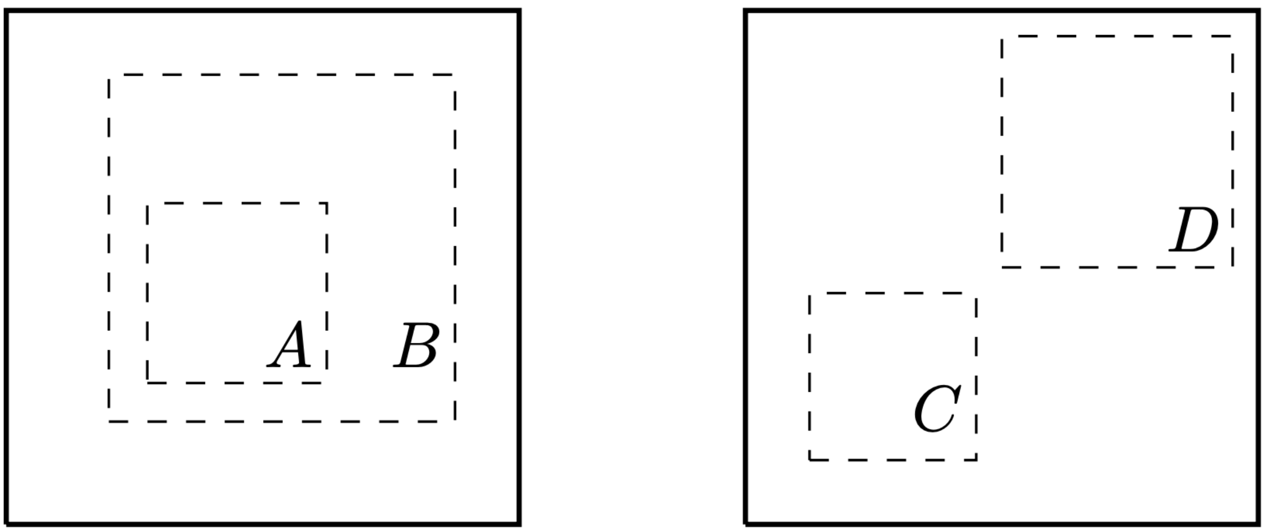


Figure from the SimCLR paper: https://arxiv.org/abs/2002.05709

CLIP

OpenAI

contrastive learning of image repres.

Use captioned images to learn a joint multimodal embedding space.

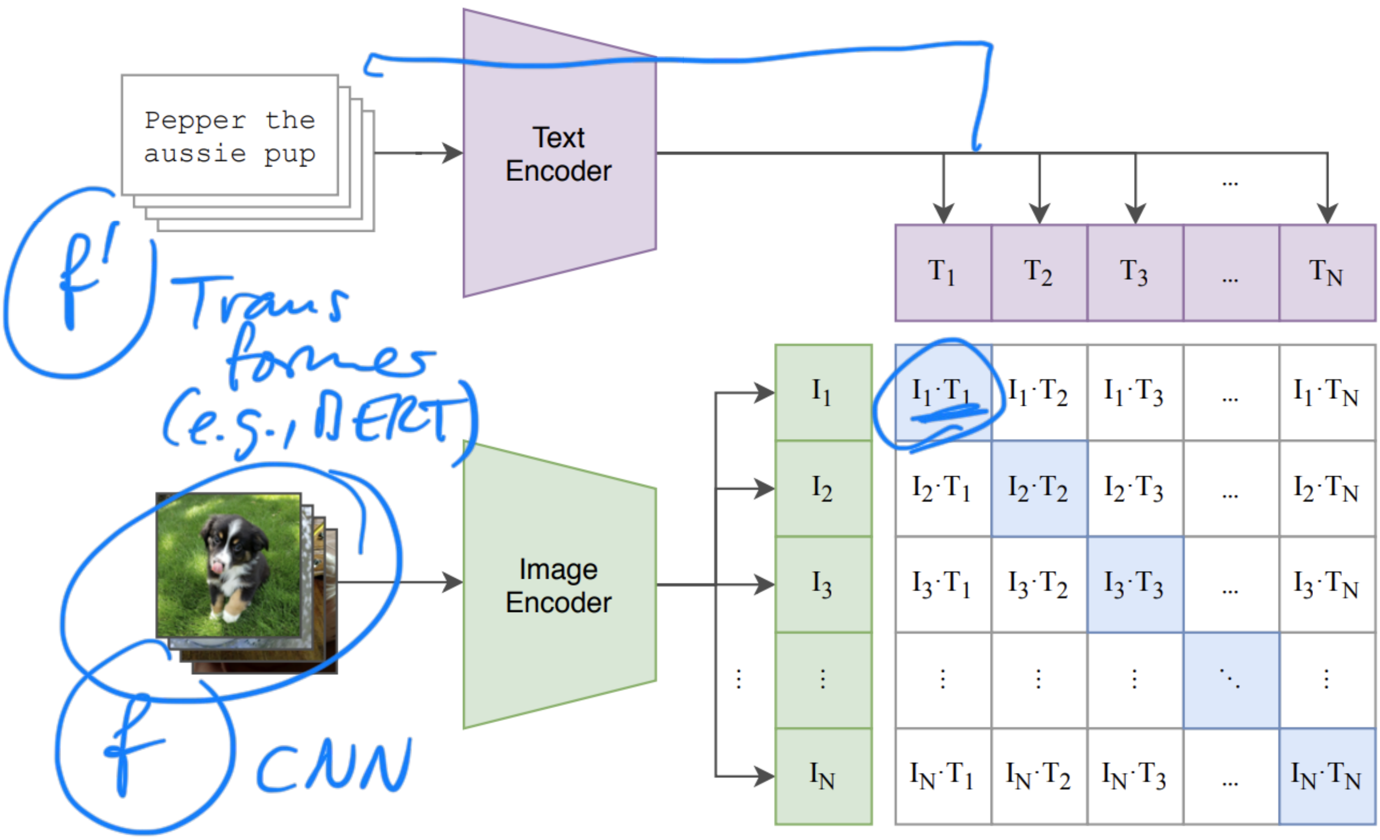


Figure from the CLIP paper: https://arxiv.org/abs/2103.00020

Objective: Maximize cosine similarity of caption and image embeddings while minimizing unrelated pairs.

Few-shot learning: learn to classify new classes with only a few labelled examples. CLIP is able to zero-shot classify with the following text input: "A photo of [class]".