Unsupervised pre-training for few-shot learning, vol. 2: reconstruction-based methods

CS 330

Logistics

Project proposal due **TODAY!**

Homework 2 due **Wednesday**

Make sure you have set-up Azure!

(well ***before*** the HW deadline)

Plan for Today

Recap

- Problem formulation
- Contrastive learning

Reconstruction-based unsupervised pre-training

- Why reconstruction?
- Autoencoders
- *Masked* autoencoders: BERT, MAE
- Autoregressive models: GPT, Flamingo

} Topic of Homework 3!

Goals for by the end of lecture:

- Familiarize you with widely-used methods for unsupervised pre-training
- Introduce methods for efficient fine-tuning of pre-trained models
- Prepare you for HW3

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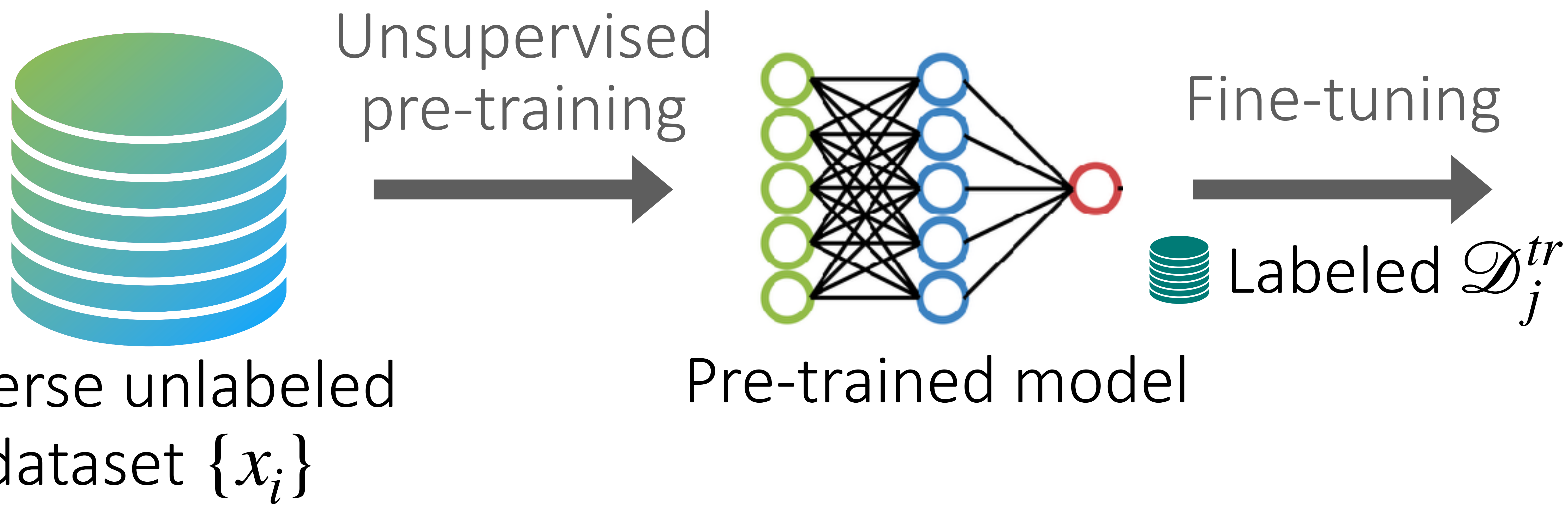
Unsupervised Pre-Training Set-Up



Goal: Get predictor for task $\mathscr{T}_j$

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Key Idea of Contrastive Learning

Similar examples should have **similar representations**

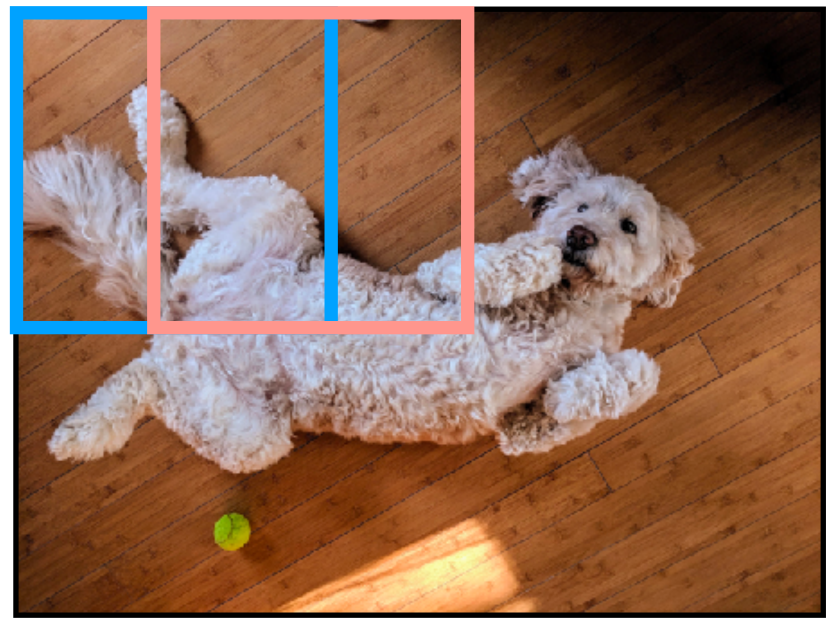
Examples with the same class label

(Requires labels, related to Siamese nets, ProtoNets)

Augmented versions of the example

(flip & crop)

Nearby image patches



Nearby video frames

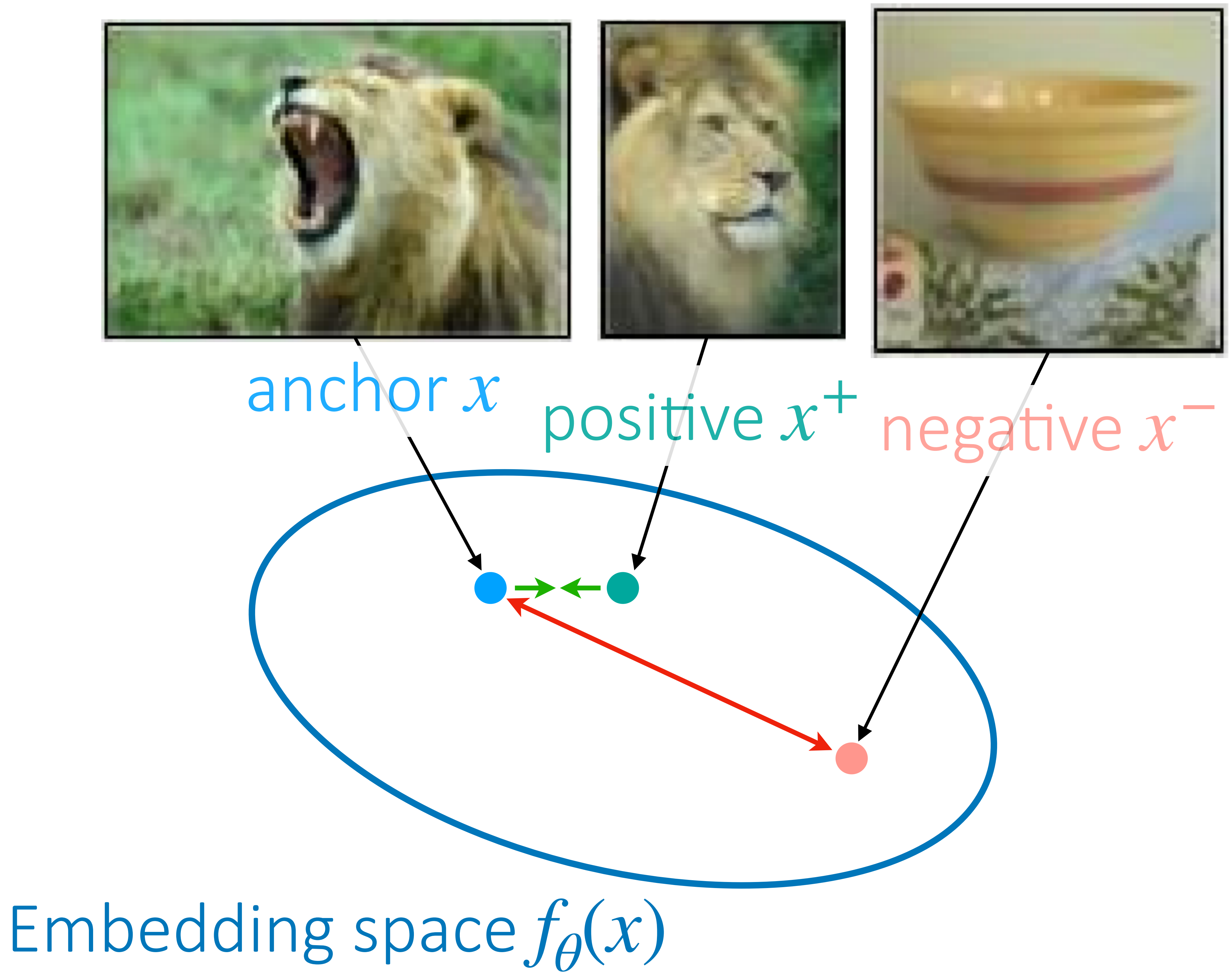
Dog credit to Maggie & Luke

van den Oord, Li, Vinyals. CPC. 2018; Chen, Kornblith, Norouzi, Hinton. SimCLR. ICML 2020

Contrastive Learning Implementation

Similar examples should have **similar representations**

Need to both **compare** & ***contrast***!



V1. Triplet loss:

$$\min_{\theta} \sum_{(x,x^+,x^-)} \max\left(0, \|f_\theta(x) - f_\theta(x^+)\|^2 - \|f_\theta(x) - f_\theta(x^-)\|^2 + \epsilon\right)$$

Schroff, Kalenichenko, Philbin. CVPR 2015

Contrastive Learning Implementation

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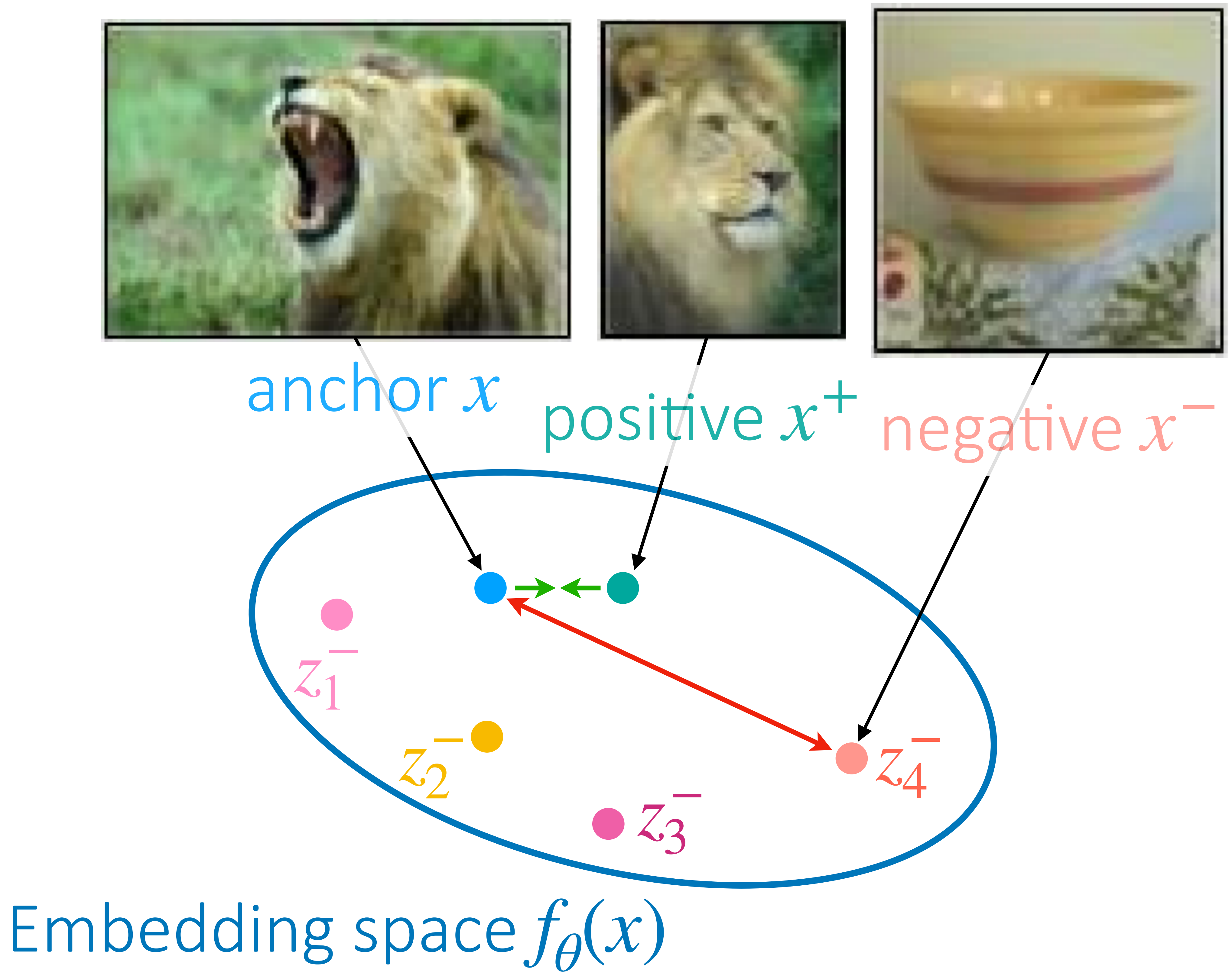

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$$\min_\theta \sum_{(x,x^+,x^-)} \max\left(0,\ \|f_\theta(x) - f_\theta(x^+)\|^2 - \|f_\theta(x) - f_\theta(x^-)\|^2 + \epsilon\right)$$

V2. From binary to N-way classification (aka **SimCLR***):

$$\mathcal{L}_{\text{N-way}}(\theta) = -\sum_z \log \frac{\exp(-d(z, z^+))}{\exp(-d(z, z^+)) + \sum_i \exp(-d(z, z_i^-))}$$

Loss read as "*classification loss when discriminating positive pair from negatives*"

*also known as the **NT-Xent** loss, when $d(\cdot\,,\cdot)$ is **scaled cosine similarity**

Sohn. N-Pair Loss Objective. NIPS 2016; Chen, Kornblith, Norouzi, Hinton. SimCLR. ICML 2020

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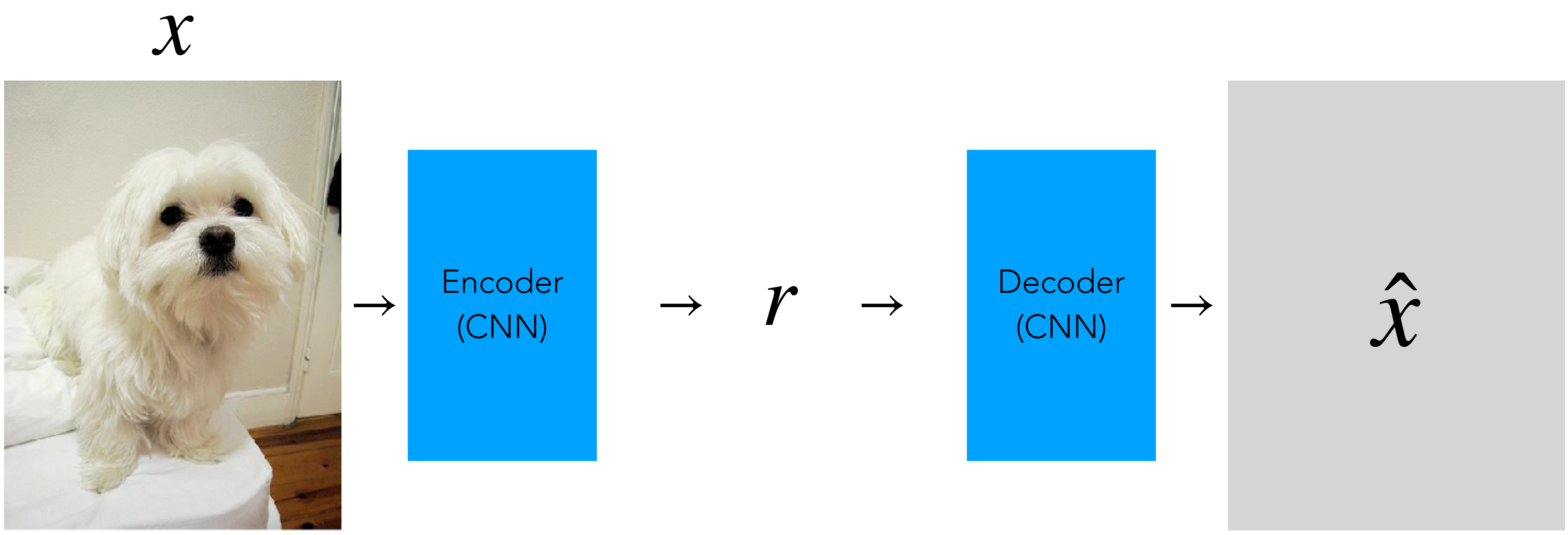
- **Why reconstruction?**
- Autoencoders
- *Masked* autoencoders: BERT, MAE
- Autoregressive models: GPT, Flamingo
- Emergent behaviors in large models

Why reconstruction?

Simple intuition: a good representation of an input should be sufficient to **reconstruct** it

Bonus: *no need to worry about pesky things like* ***sampling negatives*** *or* ***large batch sizes!***



Input image, sentence, audio signal, etc.

Reconstruction of input image

If the encoder is producing a "good" representation, a reasonably-sized decoder should be able to produce **reconstruction** $\hat{x}$ very close to **input** x from **representation** r

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Autoencoders: a first attempt

Simple intuition: a good representation lets us **reconstruct** the input

x

$\rightarrow$ Encoder (CNN) $\rightarrow$ r $\rightarrow$ Decoder (CNN) $\rightarrow$ $\hat{x}$

$$\mathcal{L} = d(x, \hat{x})$$

Loss function is reconstruction error, e.g. L2 distance:

$$d(x, \hat{x}) = \|x - \hat{x}\|^2$$

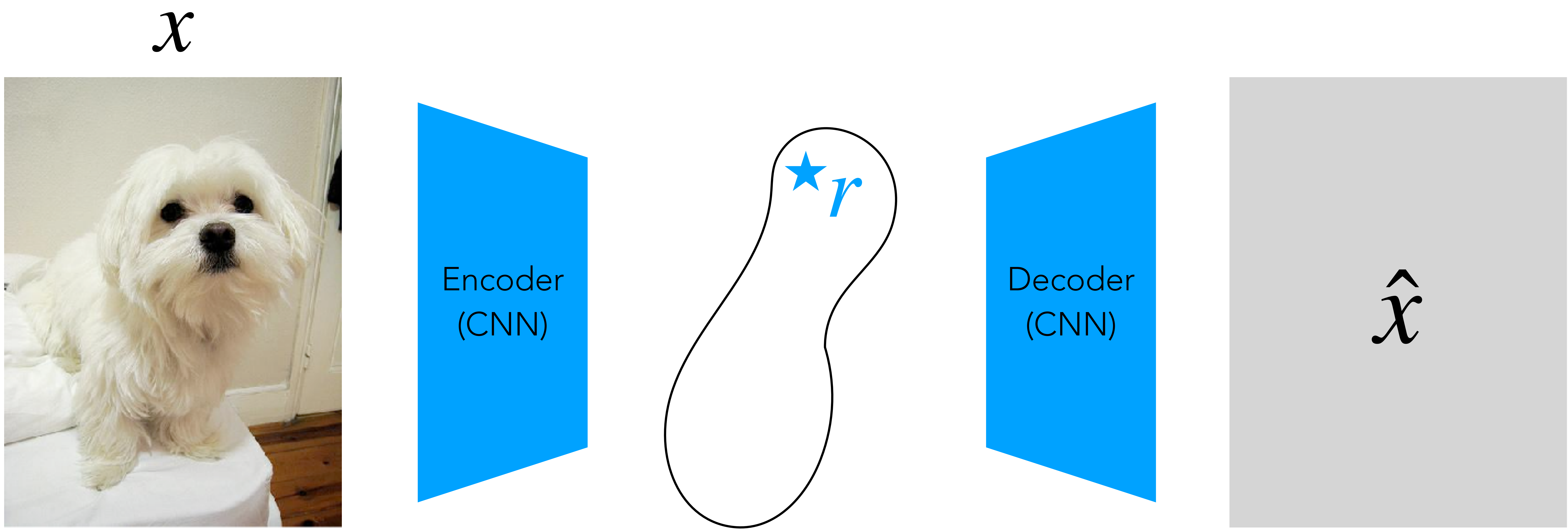
Input image, sentence, audio signal, etc.

Reconstruction of input image

What can go wrong here?

Is the **identity function** a good encoder/decoder?

Autoencoders: adding a bottleneck



Input image, sentence, audio signal, etc.

Compact, latent representation of input image

Reconstruction of input image

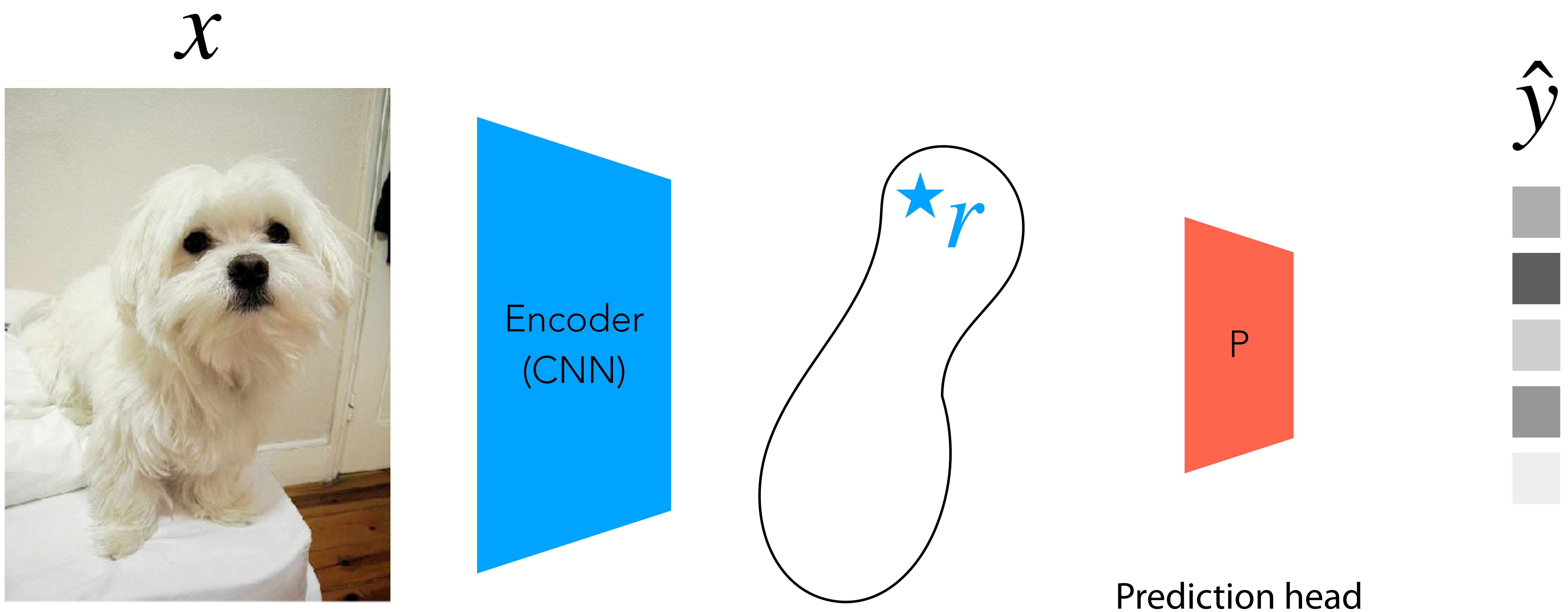
$$\mathcal{L} = d(x, \hat{x})$$

Loss function is reconstruction error, e.g. L2 distance:

$$d(x, \hat{x}) = \|x - \hat{x}\|^2$$

Key idea: latent representation is **bottlenecked**, e.g., **lower-dimensional** than the input → *Hope:* latent dimensions are forced to represent **high-level** concepts that **generalize** to other tasks

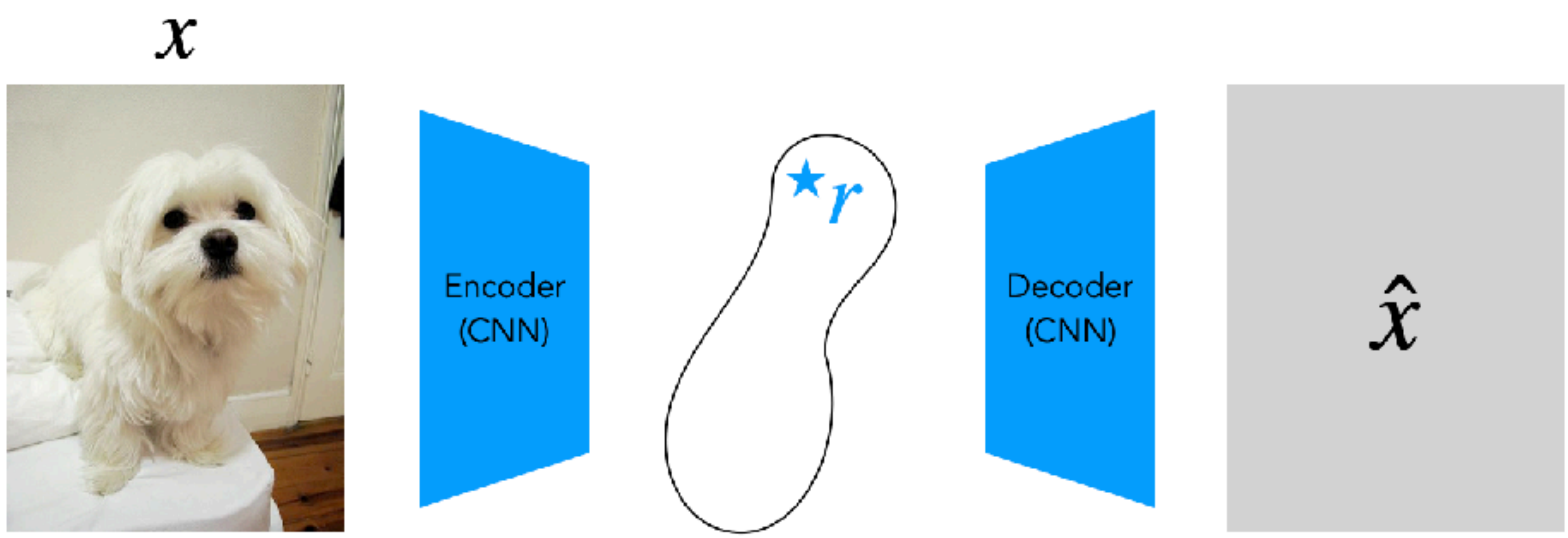
Autoencoders: few-shot learning



Prediction head mapping r to output space

Few-shot learning recipe: freeze encoder, fine-tune prediction head using our few-shot data (e.g., a linear layer)

Autoencoders



Pros:

- Simple, general
- Just need to pick $d(x, \hat{x})$
- No need to select positive/negative pairs

Cons:

- Need to design a bottlenecking mechanism
- Relatively poor few-shot performance

Why?

r is just **memorizing** details of x needed to minimize pixel-level reconstruction loss → r is more like a **hash** of x than a **conceptual summary**

How do we encourage the encoder to extract high-level features?

One strategy is **other types of bottlenecks**:

- **information** bottlenecks (adding noise)
- **sparsity** bottlenecks (zero most dimensions)
- **capacity** bottlenecks (weak decoder)

In practice,** we'll stop worrying about designing bottlenecks and just make the task a little **harder

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- ***Masked* autoencoders**: BERT, MAE
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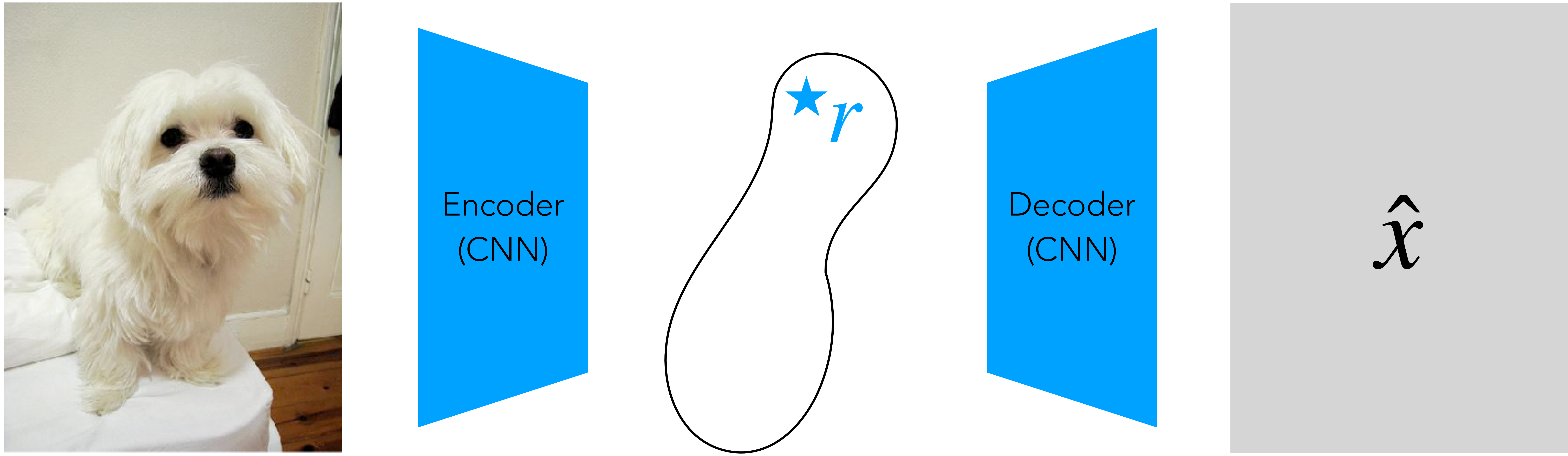
Beyond the bottleneck: ***masked* autoencoders**

<u>*Ultimately*</u>, **regular** autoencoders are trying to predict x from… x (through r)

We bottleneck z to avoid **totally degenerate** solutions, but what if the task is just "too easy", admitting unhelpful solutions?

Masked autoencoders use a **more difficult** learning task to encourage the encoder to extract more meaningful features

x



Input image, sentence, audio signal, etc.

Compact, latent representation of input image

Reconstruction of input image

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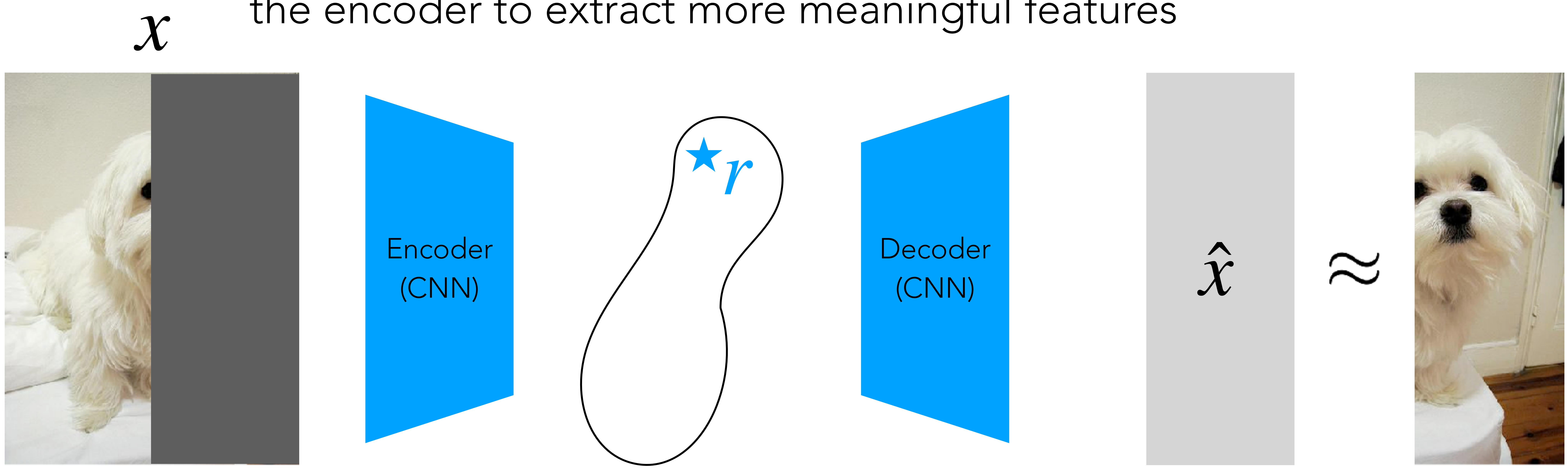


Masked input image

Latent representation

Reconstruction of **masked portion** (or **entire**) input image

Beyond the bottleneck: ***masked* autoencoders**

*<u>General recipe</u> for **pre-training** masked autoencoder f_θ:*

1. Choose **distance function** $d(\,\cdot\,,\,\cdot\,) \to \mathbb{R}$
2. For **train batch** examples x_i :

These pieces are our design choices/control knobs

A. Sample $\tilde{x}_i,\, y_i \sim$ `mask(` x_i `)`

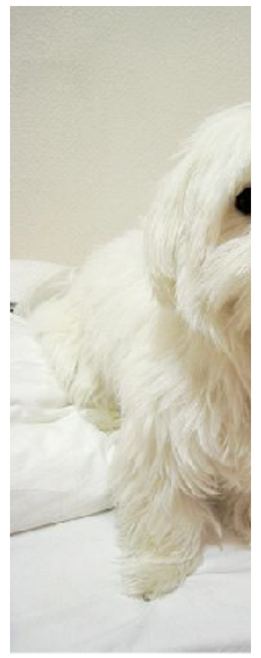
*$\tilde{x}_i,\, y_i$ are typically two **disjoint** sub-regions of x_i*

B. Make prediction $\hat{y}_i = f_\theta(\tilde{x}_i)$

C. Compute loss $\mathcal{L}_i = d(y_i, \hat{y}_i)$

in some cases, the target y_i may be all of x_i

x_i $\quad$ $\tilde{x}_i$ $\quad$ y_i

`mask(`  `)` =  , 

f_θ : CNN or **Transformer** (stay tuned)

$d(y, \hat{y}) = \|y - \hat{y}\|^2$

x_i

`mask(` *Joe Biden is the US president* `)` =

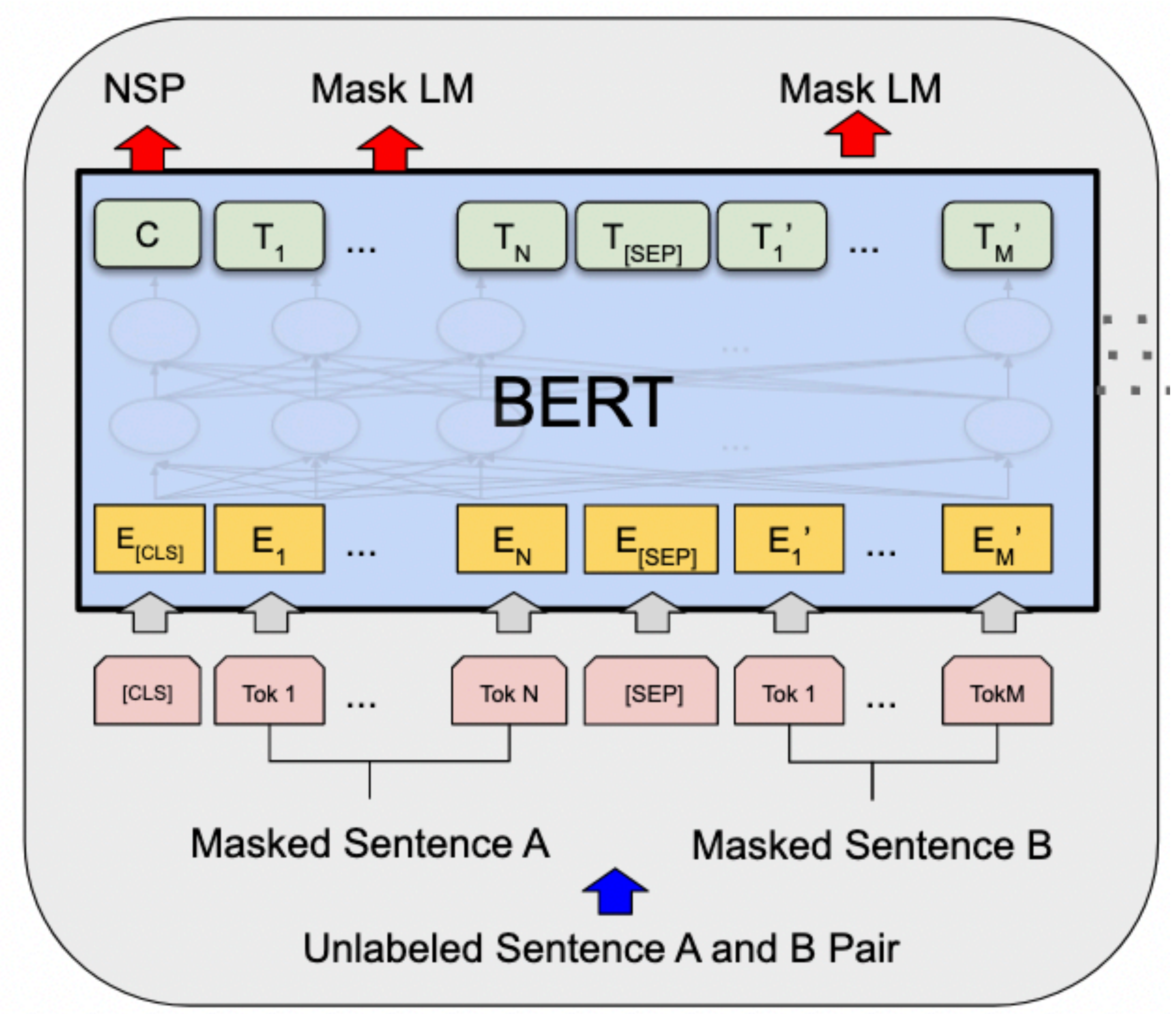
$\tilde{x}_i$ $\quad$ y_i

Joe <mask> is the US <mask>, $\quad$ *{ Biden; president }*

f_θ **: Transformer** (e.g., **BERT**; stay tuned**)**

$d(y, \hat{y}) = \mathrm{KL}\left(y \| \hat{y}\right)$

Masked autoencoders for language: **BERT** (Devlin et al, 2017)

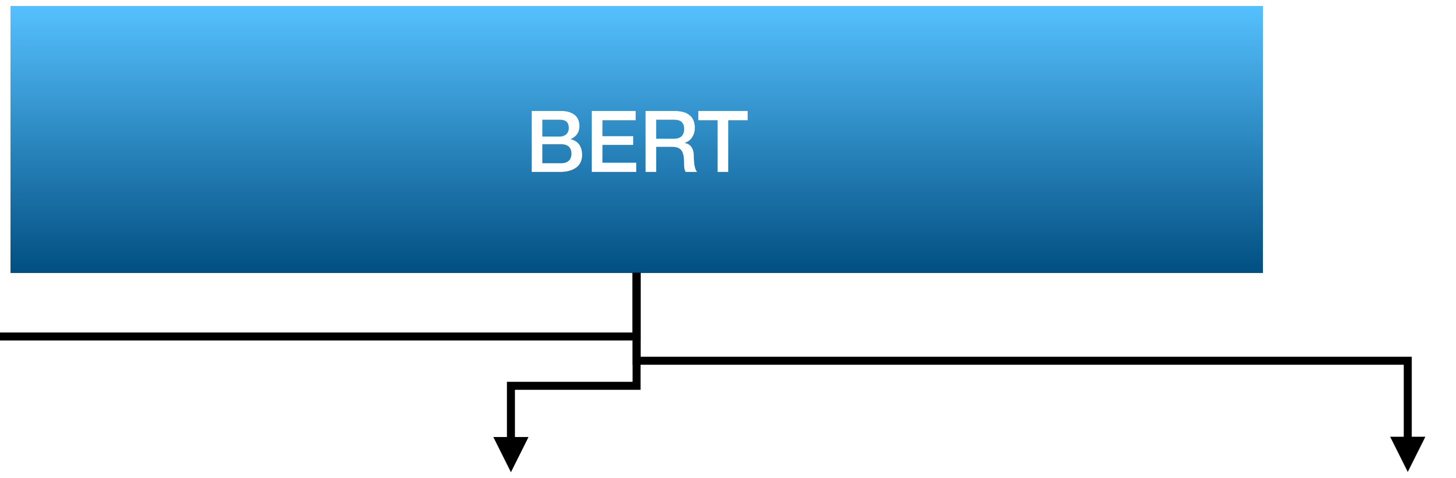


Case study: **BERT** as a masked autoencoder

x : **[CLS] Joe Biden is the US president. [SEP] He was inaugurated on January…**

t : 0 1 2 3 4 5 6 7 8 9 10 11 12

$\tilde{x}$: **[CLS] Joe <mask> is the US <mask>. [SEP] He <mask> inaugurated on January…**



$p_\theta^2(\cdot \mid \tilde{x})$ $\quad$ $p_\theta^6(\cdot \mid \tilde{x})$ $\quad$ $p_\theta^9(\cdot \mid \tilde{x})$

__Probability distribution__ over possible words at each masked index j

$y_2 =$ **Biden**

$y_6 =$ **president**

$y_9 =$ **was**

__Target word__ for each masked index

$$d(y, \hat{y}) = \sum_j \mathrm{KL}(y_j \,\|\, \hat{y}_j) = -\log p_\theta^2(\textbf{Biden} \mid \tilde{x}) - \log p_\theta^6(\textbf{president} \mid \tilde{x}) - \log p_\theta^9(\textbf{was} \mid \tilde{x})$$

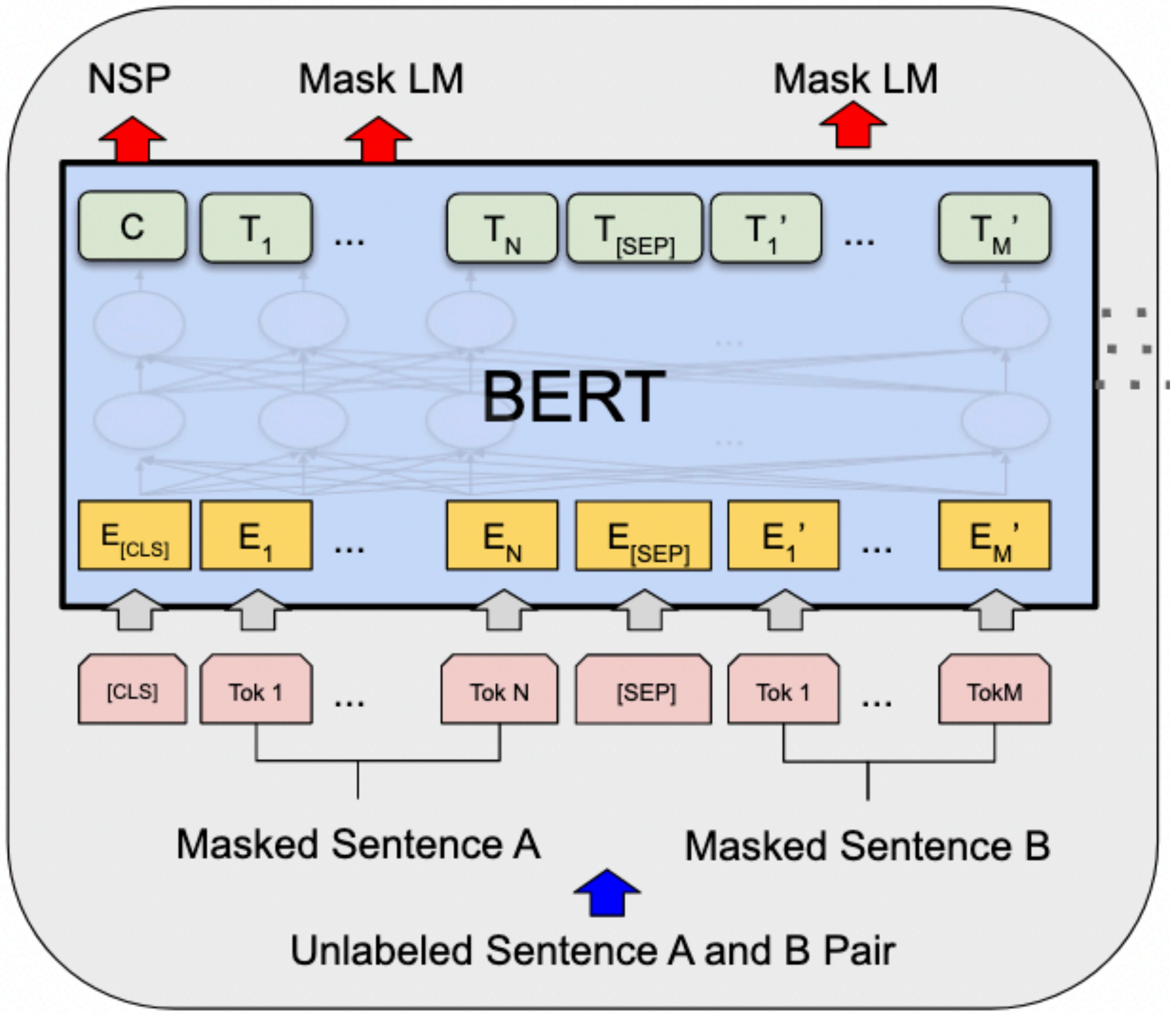
Details of BERT masking:

1. Choose **random 15%*** of input timesteps
2. Of these, **80%** are replaced with <mask> token
3. Replace **other 20%** with a **random** token

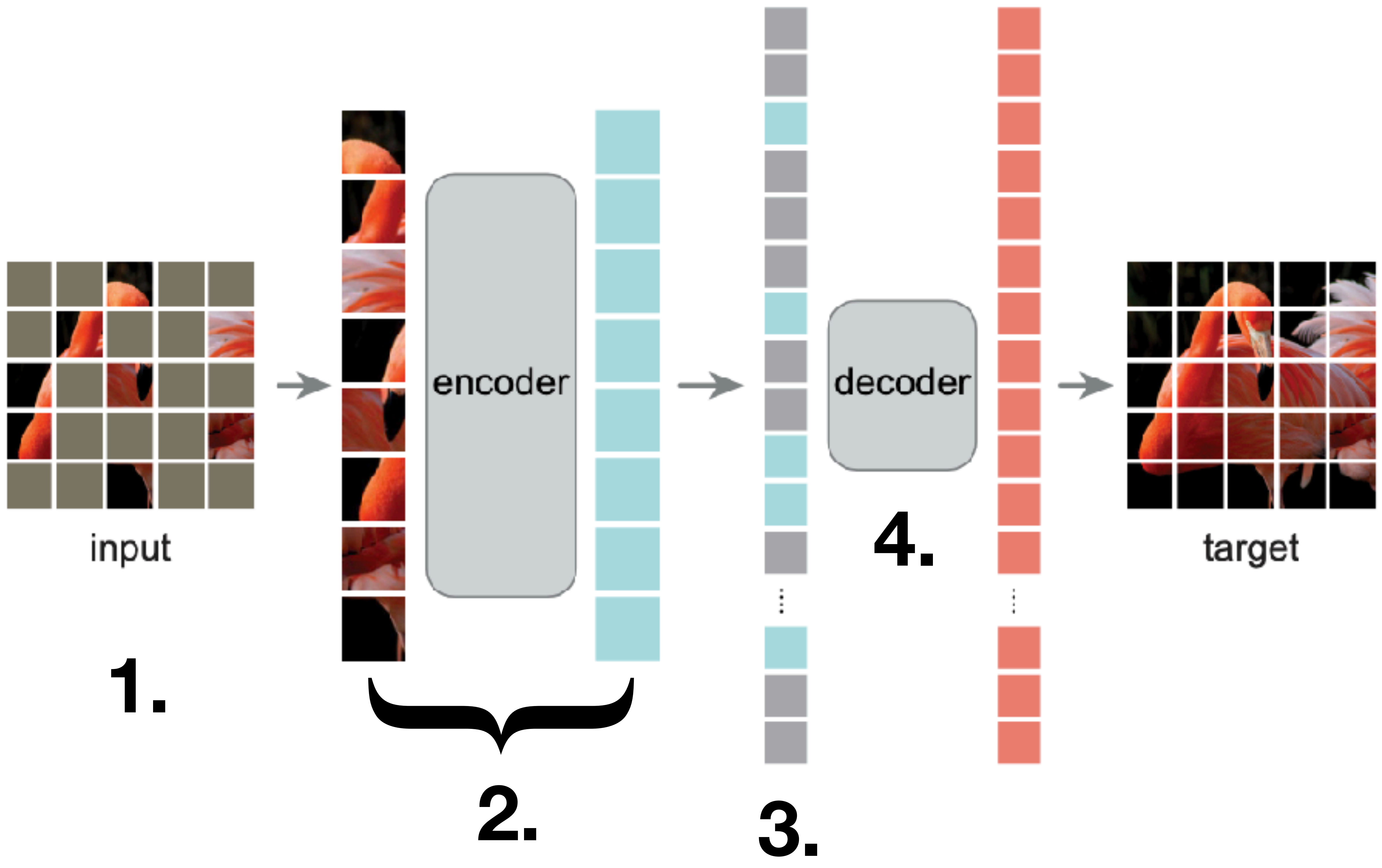
*It's possible we can do better than just picking **random** timesteps:

- Mask **longer** spans of text
- Selecting for **information-dense** spans

Masked autoencoders for language:
BERT (Devlin et al, 2017)



For **images**:
MAE (He et al, 2021)



Instead of words, we have a sequence of ***image patches***

1. Mask **~75%** of image patches
2. Compute representations of **only** unmasked patches
3. Insert **placeholder** patches at masked locations
4. Decode back into original image

Fine-tune on top of the output of ***step 2***

Masked AEs give state-of-the-art **few-shot image classification** performance (with unsup. pre-training)

*The unsupervised masked autoencoding recipe works better than pre-training **with labels** on the **same data!***

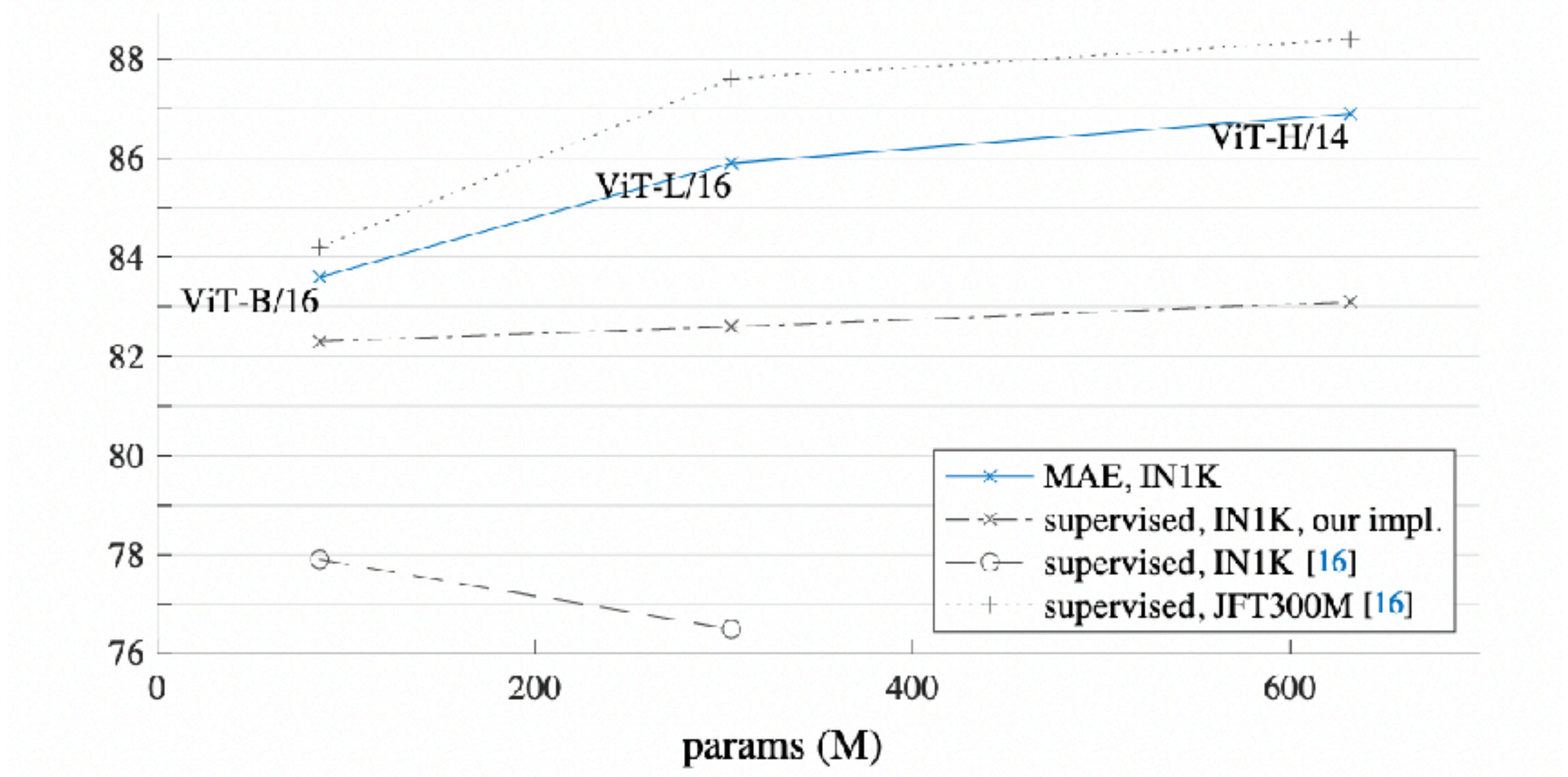


Figure 8. **MAE pre-training *vs.* supervised pre-training**, evaluated by fine-tuning in ImageNet-1K (224 size). We compare with the original ViT results [16] trained in IN1K or JFT300M.

*When **fine-tuning** (not just **linear probing** on frozen pre-trained model), better than **contrastive learning**!*

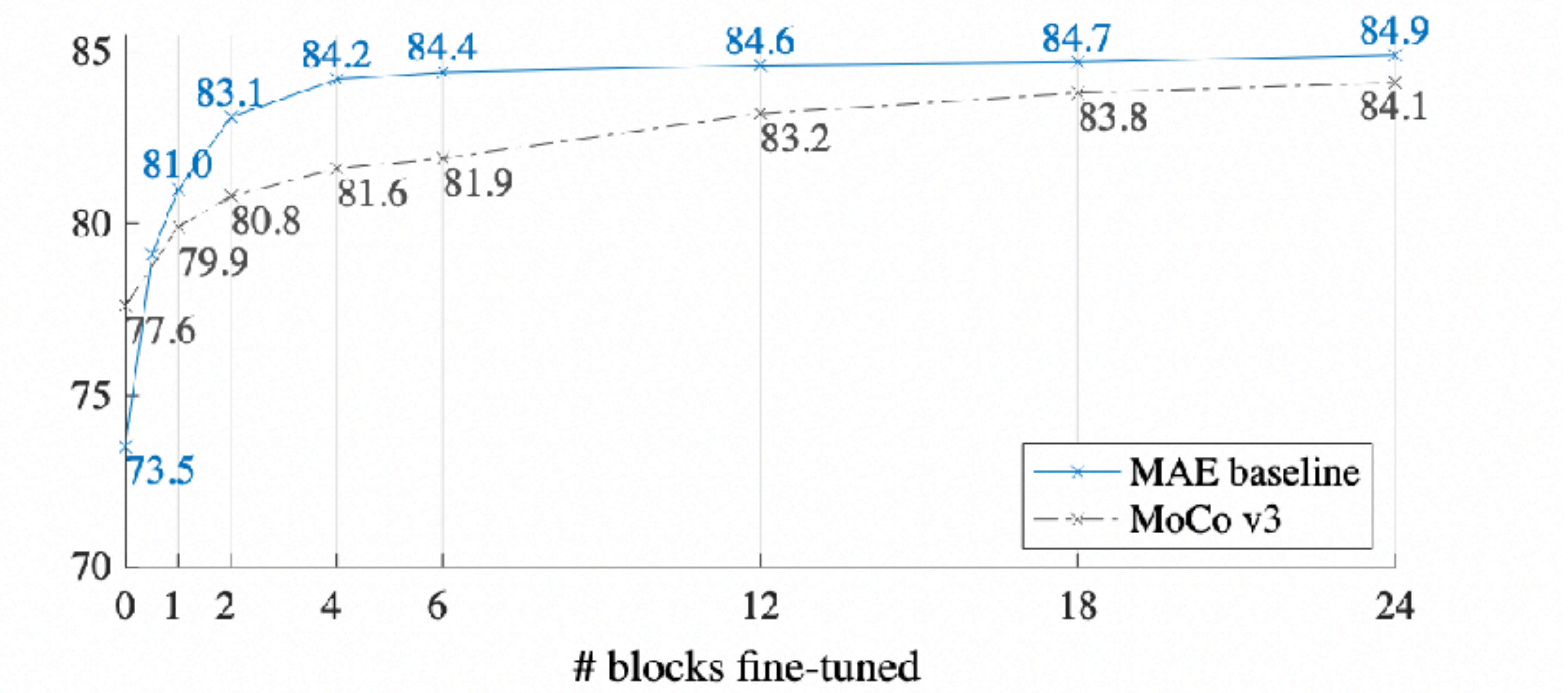


Figure 9. **Partial fine-tuning** results of ViT-L w.r.t. the number of fine-tuned Transformer blocks under the default settings from Table 1. Tuning 0 blocks is linear probing; 24 is full fine-tuning. Our MAE representations are less linearly separable, but are consistently better than MoCo v3 if one or more blocks are tuned.

He et al, 2021

A (very quick) overview of Transformers

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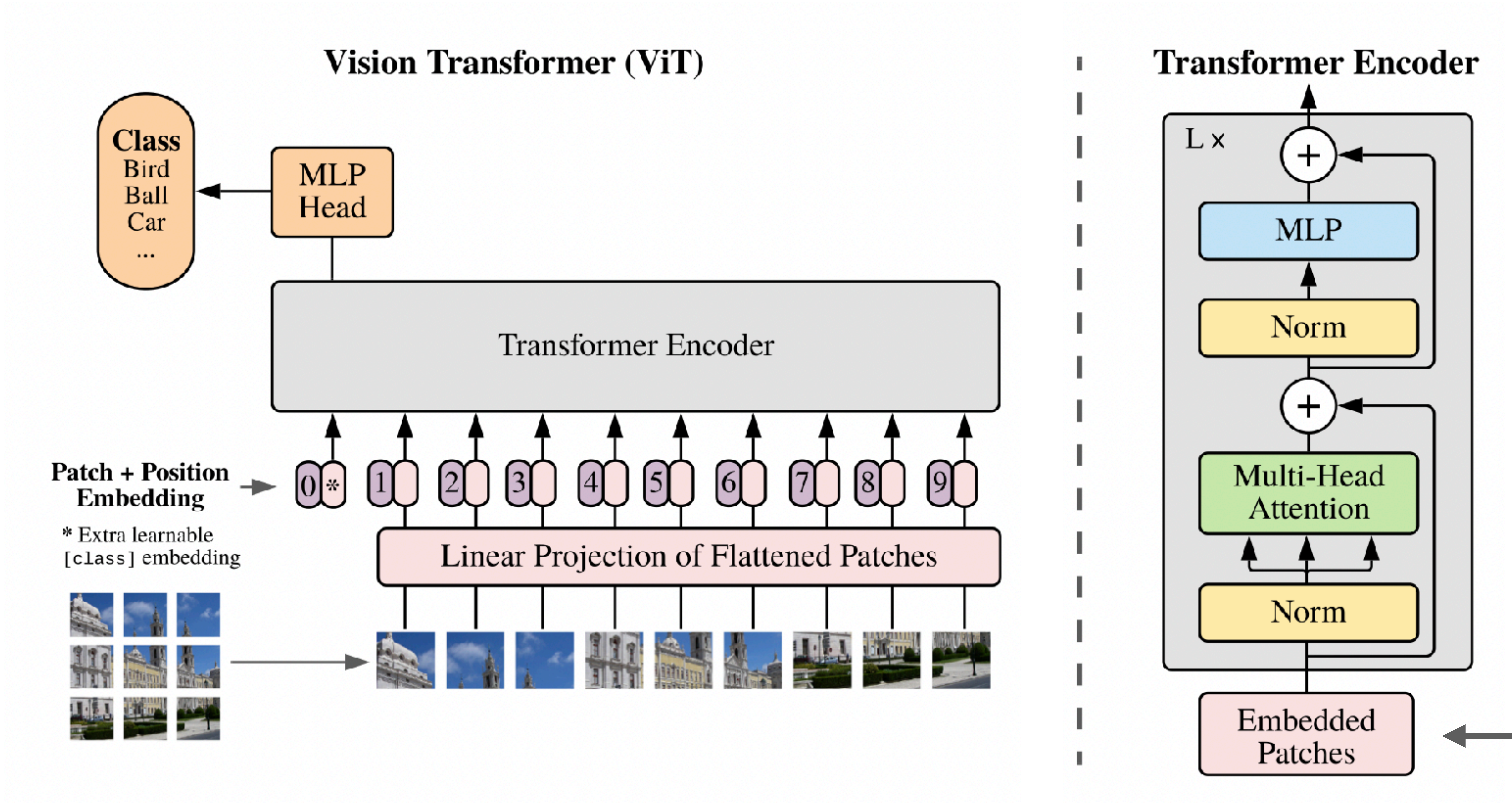

The ~**only difference** between Transformers for vision/language/RL/molecules/etc. is what we do for this initial **embedding step**

ViT; Dosovitskiy, Beyer, Kolesnikov, et al. (2021)

Transformers in a bit more detail

So… how do we ~~pre-train~~ fine-tune Transformers?

Extra token prepended to beginning of sequence

[CLS]
Joe
Biden
is
the
US
President

take representation of [CLS]

Fine-tune new prediction head on top of [CLS] rep.

What should we do with the parameters of **this guy** during fine-tuning?

Options:

1. **Freeze** them
2. **Fine-tune** them
3. **Something** else???
   a. Fine-tune **some** of them?
   b. Freeze and inject **new** parameters?

LoRA: Low-rank adaptation of language models (Hu et al., 2021)

What if we just want to fine-tune our model… "a little bit"?

What does "a little bit" even mean? <discuss>

1. *Preserve the **knowledge** in the **pre-trained model** (to avoid overfitting)*
2. *Avoid needing to store a **new version** of **every single** parameter in the model (to save space)*

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Associative *[key-value]* memory view of linear transform **(Kohonen, 1972)**

Consider the **linear transform**, the building block of NNs & Transformers

1. *Preserve the* ***knowledge*** *in the* ***pre-trained model*** *(to avoid overfitting)*
2. *Avoid needing to store a* ***new version*** *of* ***every single*** *parameter in the model (to save space)*

$$W = \sum_r v_r u_r^\top$$

For rank-r matrix, we have this decomposition (with orthogonal u_r by SVD)

Therefore, $$Wx = \left(\sum_r v_r u_r^\top \right) x = \sum_r v_r \left(u_r^\top x \right) \rightarrow$$

Wx produces a sum over the **'memories'** v_r weighted by the **relevance** $u_r^\top x$ (each u_r is a **'key'**)

"A little bit" means ***only add a few memories*** *→ only make a* ***low-rank*** *change to W*

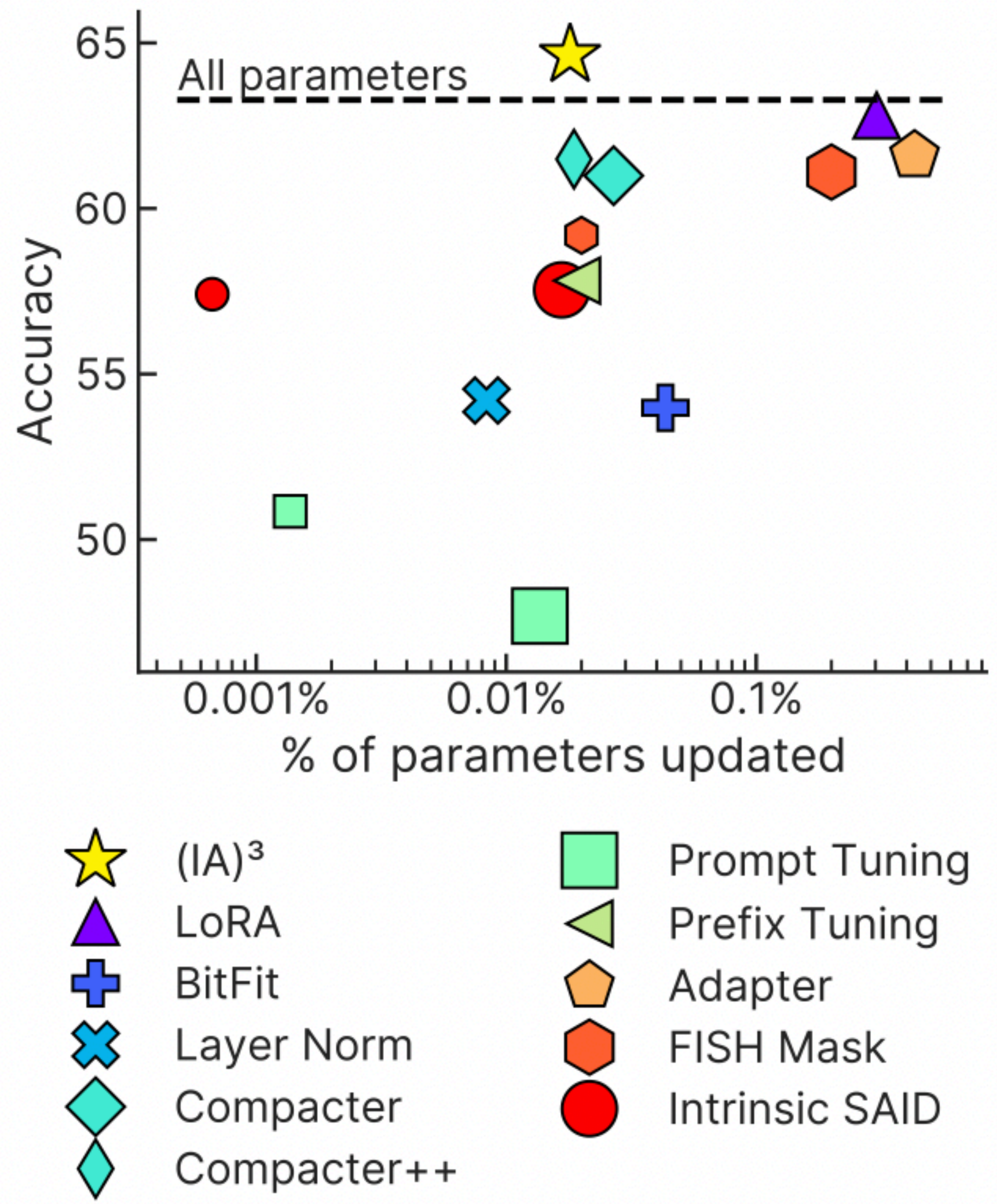
LoRA: $$W_{ft} = W_0 + AB^\top, \quad A, B \in \mathbb{R}^{d \times p} \quad p < d$$

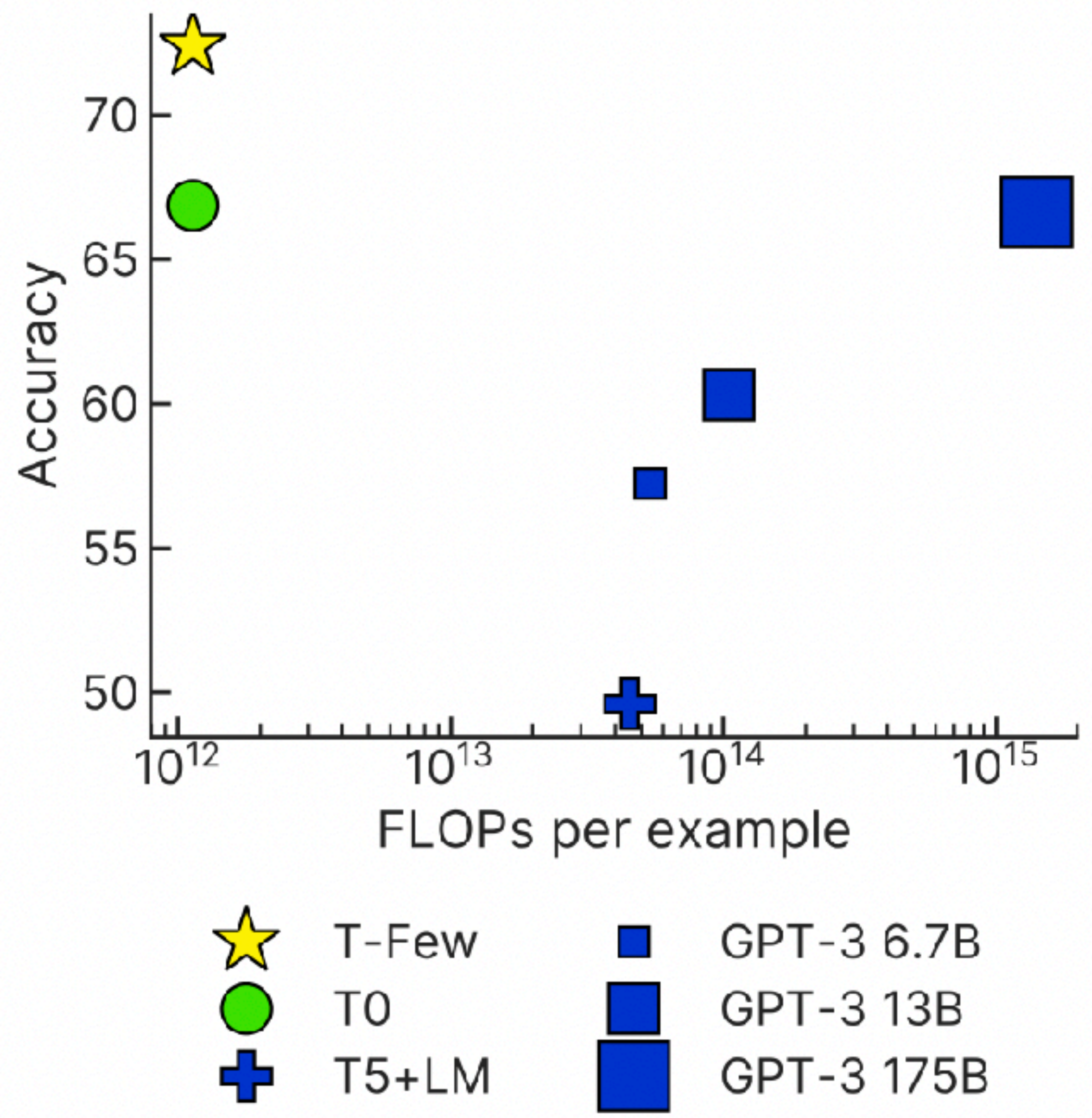
pre-trained dxd weights **(frozen)**

new **low-rank residual (fine-tuned)**

$AB^\top$ should be **zero-initialized (how?)**

(Many) other approaches to "lightweight" fine-tuning





*When "few-shot" means **~20-70,** lightweight fine-tuning (**T-Few**) can outperform in-context learning in **much** larger models!*

T-Few; Lu, Tam, Muqeeth, et al. (2022)

You will compare fine-tuning and in-context learning in HW3!

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Striving for simplicity: **autoregressive models**

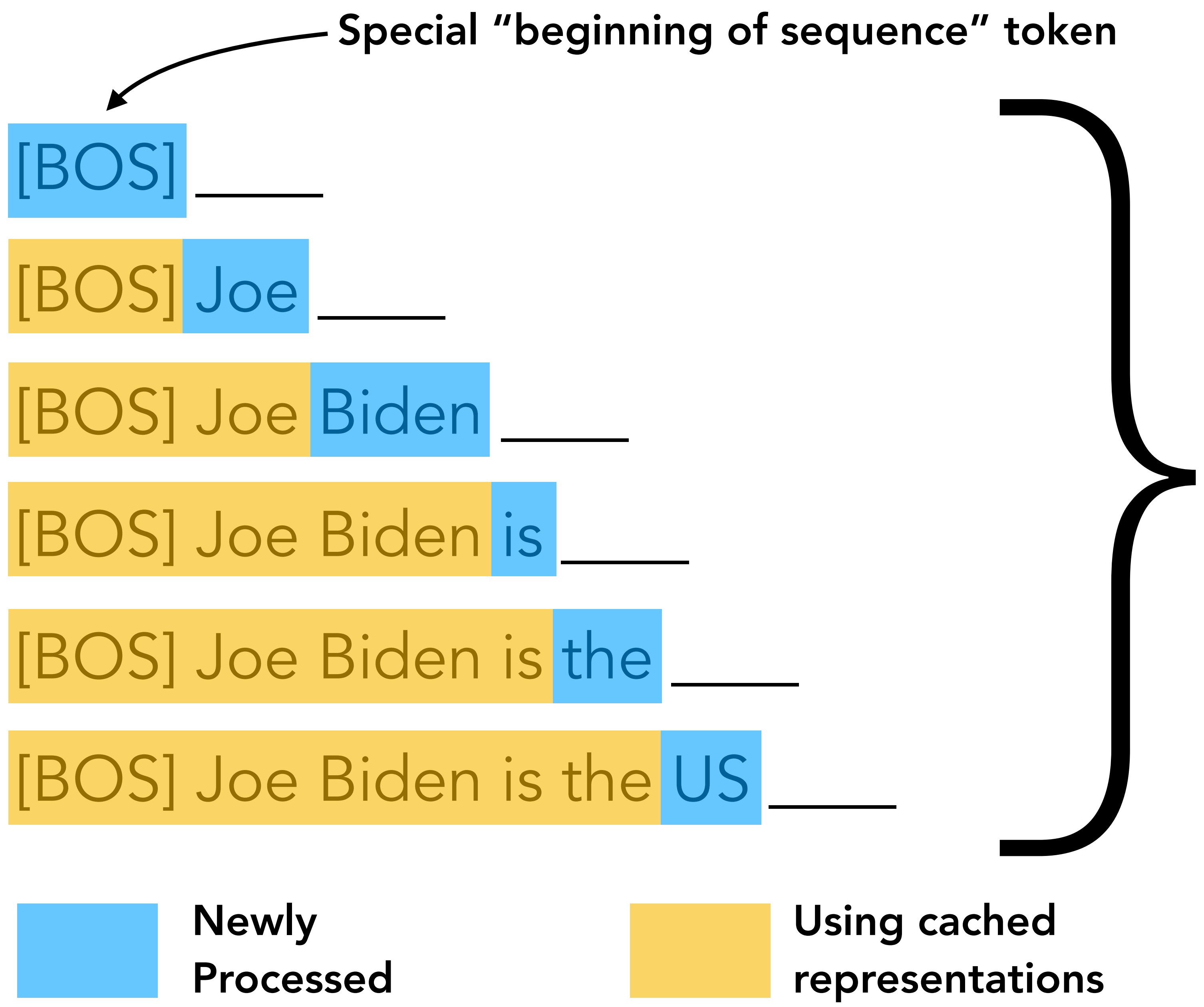
(recall GPT-3 from the black-box meta-learning lecture!)

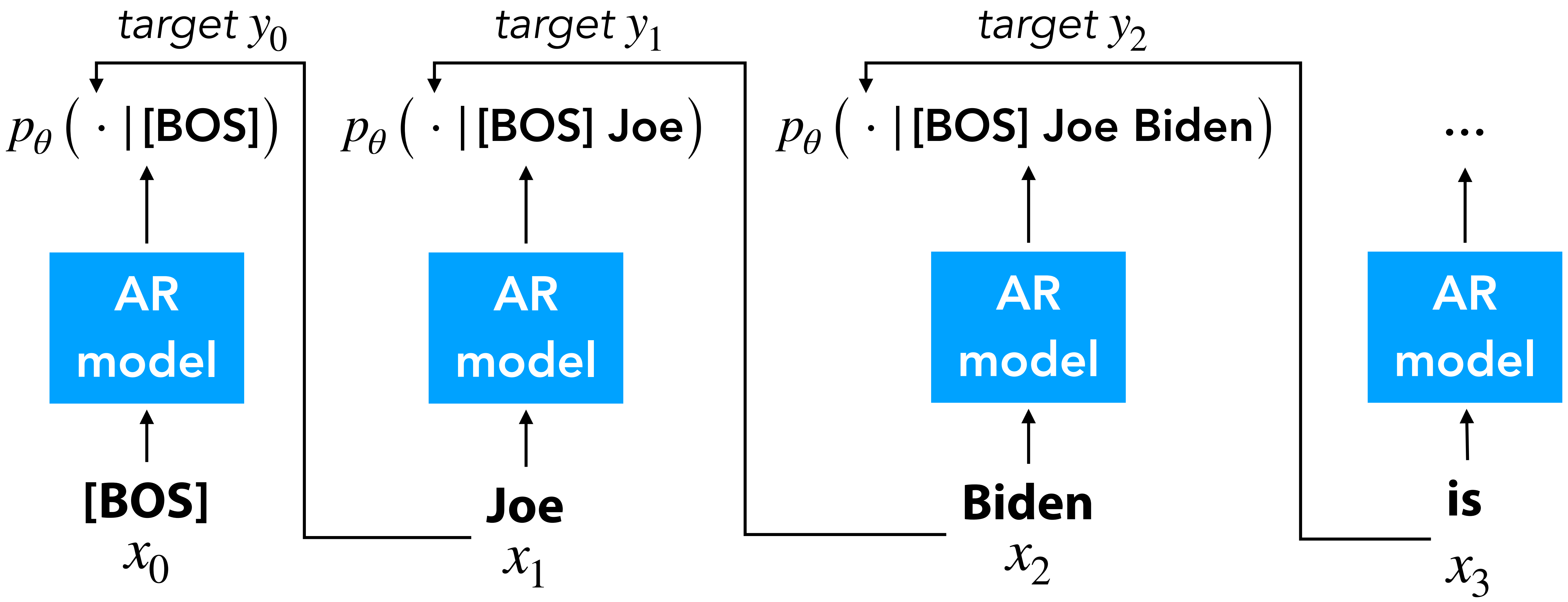
*What are some **downsides** of masked autoencoders?*

1. Need to pick `mask`
2. Only using ~15% of the example for training
3. Difficult to sample from

Instead of masking a **random subset,** what if we just *predict the next word/pixel/token?* → No need to pick a masking strategy; **mask every token!**

Simply learn $p_\theta(x_t | x_{<t})$, probability of the **next token** given the **previous tokens**





Autoregressive Transformers let us compute each $p_\theta(x_t | x_{<t})$ efficiently: we can **re-use** representations from the previous step

Autoregressive Transformers are *everywhere* these days

…for vision too!
…and RL/decision-making!
…and vision + language!

Improving Language Understanding by Generative Pre-Training

Language Models are Unsupervised Multitask Learners

Language Models are Few-Shot Learners

Megatron-LM: Training Multi-Billion Parameter Language Models Using Model Parallelism

OPT: Open Pre-trained Transformer Language Models

Announcing GPT-NeoX-20B

Announcing GPT-NeoX-20B, a 20 billion parameter model trained in collaboration with CoreWeave.

February 2, 2022 · Connor Leahy

As of February 9, 2022, GPT-NeoX-20B checkpoints are available for download from The Eye under Apache 2.0. More in-depth information on GPT-NeoX-20B can be found in the associated technical report on arXiv.

Looking for a demo? Try GPT-NeoX-20B via CoreWeave and Anlatan's inference service, GooseAI!

Generative Pretraining from Pixels

Decision Transformer: Reinforcement Learning via Sequence Modeling

RT-1: ROBOTICS TRANSFORMER FOR REAL-WORLD CONTROL AT SCALE

WebGPT: Browser-assisted question-answering with human feedback

DeepMind 28-04-2022

Flamingo: a Visual Language Model for Few-Shot Learning

Jean-Baptiste Alayrac[*,‡], Jeff Donahue[*], Pauline Luc[*], Antoine Miech[*], Iain Barr[†], Yana Hasson[†], Karel Lenc[†], Arthur Mensch[†], Katie Millican[†], Malcolm Reynolds[†], Roman Ring[†], Eliza Rutherford[†], Serkan Cabi, Tengda Han, Zhitao Gong, Sina Samangooei, Marianne Monteiro, Jacob Menick, Sebastian Borgeaud, Andrew Brock, Aida Nematzadeh, Sahand Sharifzadeh, Mikolaj Binkowski, Ricardo Barreira, Oriol Vinyals, Andrew Zisserman, Karen Simonyan[*,‡]
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Case study: **Flamingo**

How would you build a multimodal autoregressive model? From scratch? (NO)

[so far] Fine-tuning to **specialize:**

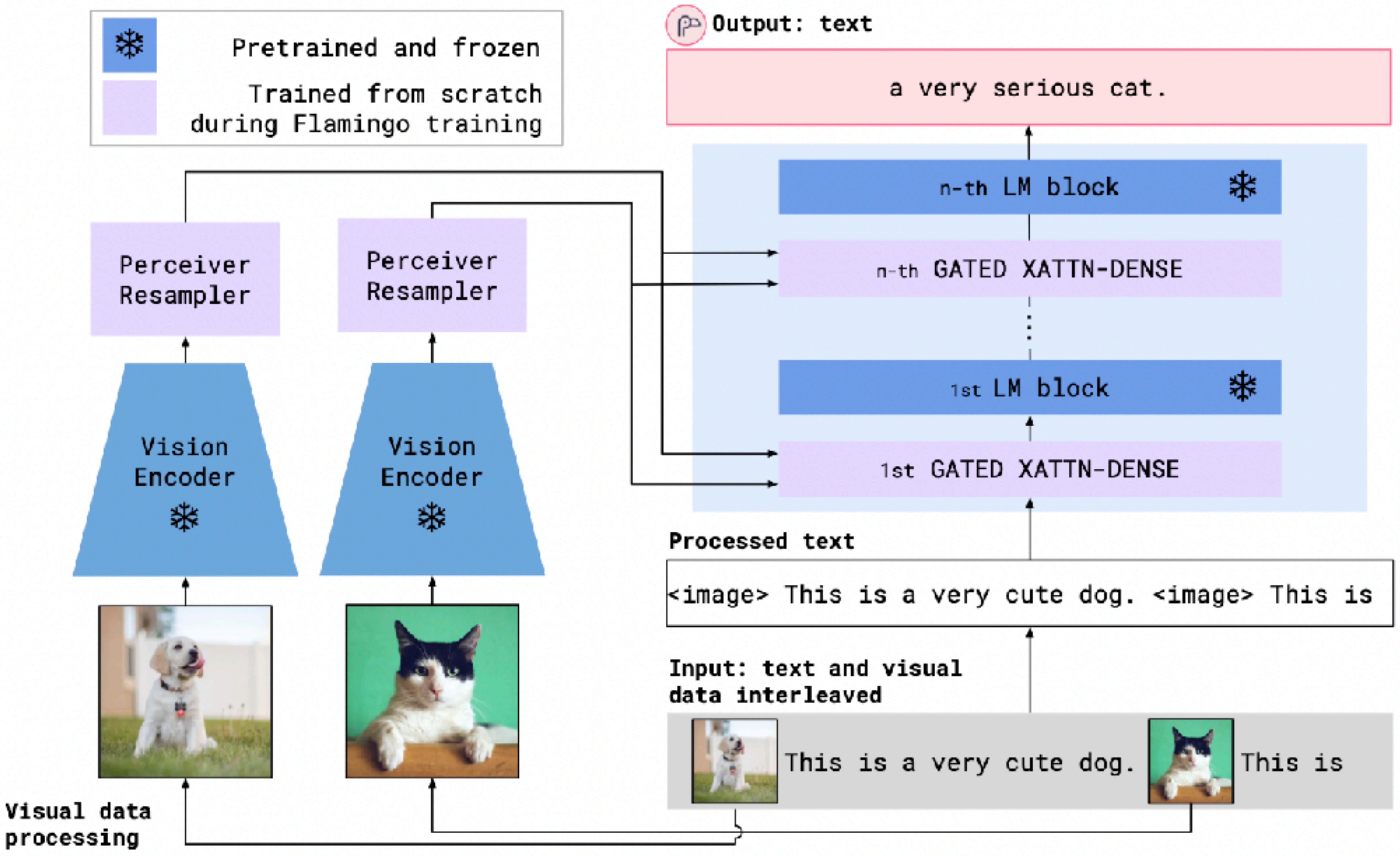
General-purpose LM + Few-shot data = Task-specific LM

Flamingo

Fine-tuning to **combine models:**

General-purpose LM + General-purpose Vision Model + Multimodal data

= General-purpose Vision-Language Model



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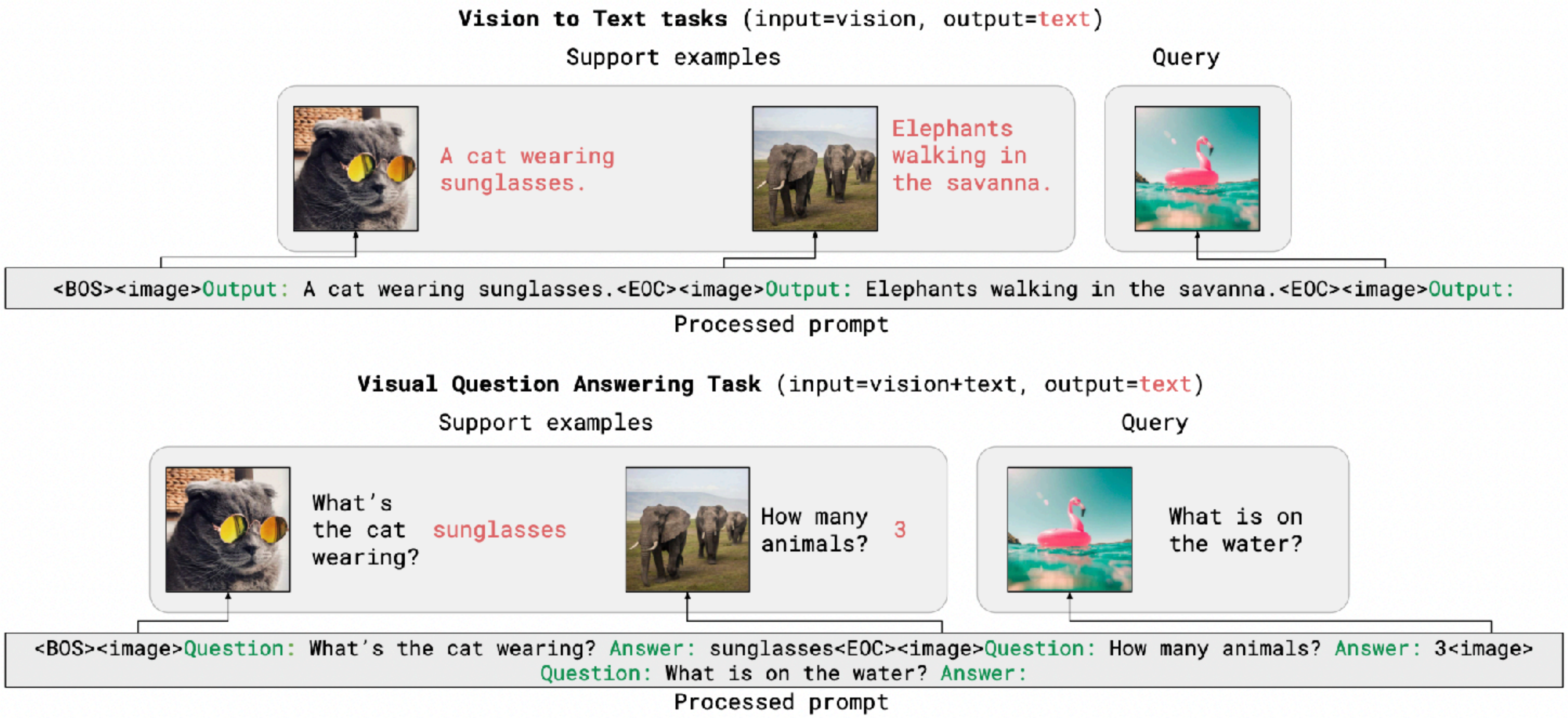

*In-context few-shot learning on sequences that freely mix **text** and **images!** Enables few-shot captioning, visual question-answering, etc.*

DeepMind 28-04-2022

Flamingo: a Visual Language Model for Few-Shot Learning

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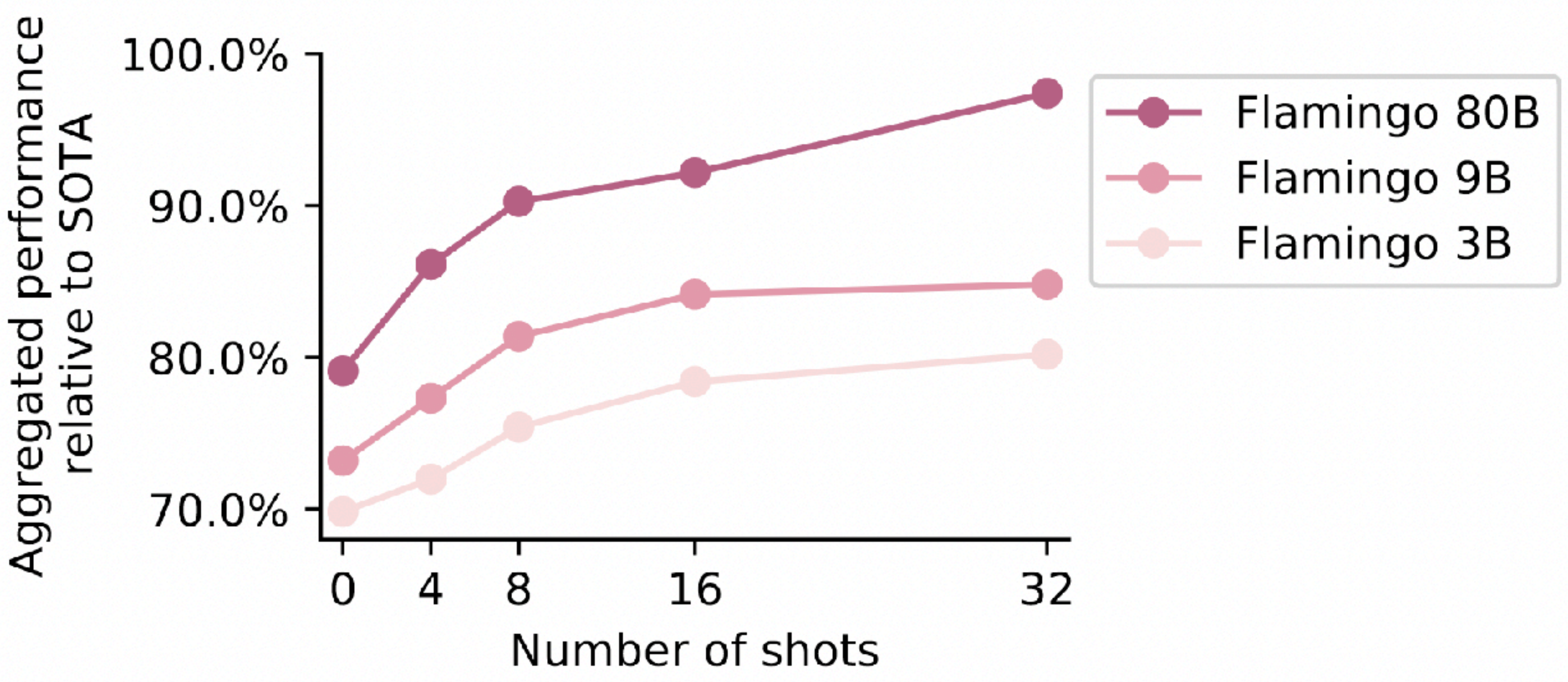
Case study: **Flamingo**



Few-shot Flamingo ≈ **Non-few-shot state of the art!**

Are AR models really **different** from masked autoencoders?

General recipe for training masked autoencoder f_θ:

1. Choose **distance function** $d(\cdot\,,\cdot) \to \mathbb{R}$
2. For **train batch** examples x_i :

   A. Sample $\tilde{x}_i, y_i \sim \texttt{mask}(x_i)$

   B. Make prediction $\hat{y}_i = f_\theta(\tilde{x}_i)$

   C. Compute loss $= d(y_i, \hat{y}_i)$

AR models are just masked AEs with a special choice of `mask`

Masked autoencoder:		*AR model:*	
$\tilde{x}$:	y :	$\tilde{x}$:	y :
Joe		**Joe**	
<mask>	**Biden**	**Biden**	
is		**is**	
the		**the**	
<mask>	**US**	**US**	
President		____	**President**

Summary of today

1. *Intuition for autoencoders (AEs): "A good* ***representation*** *lets us* ***reconstruct*** *the input"*
2. ***Masked*** *AEs learn to restore a* ***partially-deleted*** *input & help avoid degeneracies in unmasked AEs*
3. ***State of the art*** *in pre-training for few-shot learning in* ***language & vision***
4. ***Autoregressive*** *models (e.g., GPT-3) are* ***special case*** *of masked AEs; give a generative model for free at some cost to fine-tuning performance*

Contrastive Learning vs AEs vs Masked AEs

Contrastive learning:

+ Learns very high-quality representations
+ Don't need as large a model
- Need to select negatives carefully*
- Generally needs larger batch size*
- Cross-example dependencies can make implementation more difficult

** new methods are addressing these downsides but are more difficult to interpret/analyze*

(Bottlenecked) Autoencoders:

+ Simple to implement
+ No need to select pos/neg pairs; just $d(x, \hat{x})$
- Generally need a larger model
- Need to design a bottleneck
- (Comparatively) poor few-shot performance
- Not generally used in practice

Masked autoencoders:

+ **Few-shot** performance as good or better than contrastive
+ **AR special case** gives generative model for free
- **Raw representations** (without fine-tuning) still can be lower quality than contrastive

Reminders

Project proposal due **TODAY!**

Homework 2 due **Wednesday**

Make sure you have set-up Azure!

(well ***before*** the HW deadline)