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

CS 330

Logistics

Project proposal due TODAY!

Homework 2 due Monday, October 24

Kyle's office hours are hybrid going forward (see Ed for details)

Azure invites have been re-sent - **you have one week to accept!**

You will need Azure for HW3, so do this today!

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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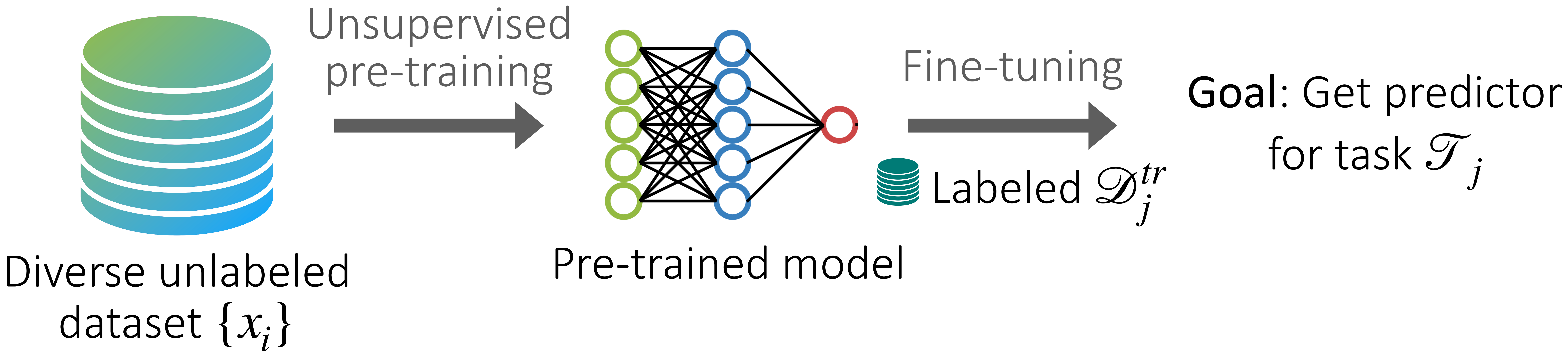
Unsupervised Pre-Training Set-Up



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Key Idea of Contrastive Learning

Similar examples should have **similar representations**

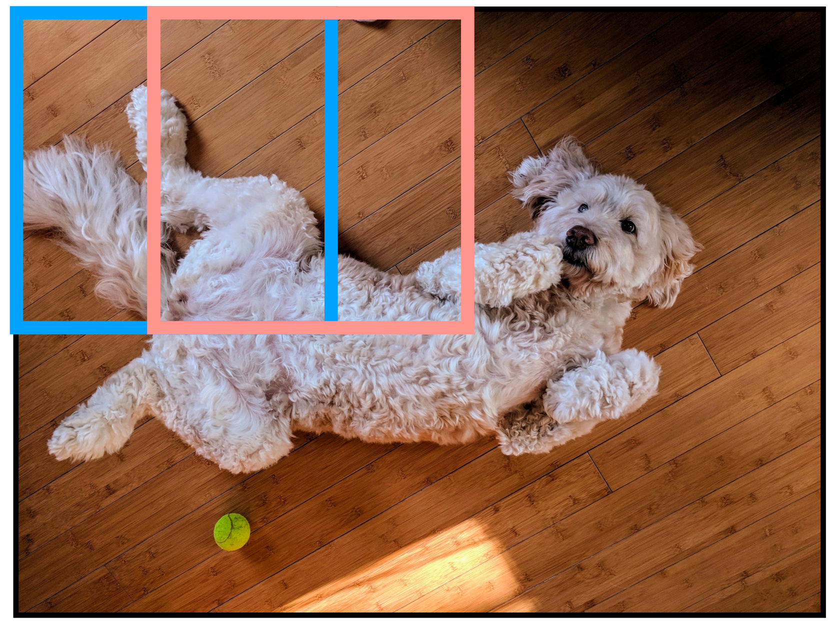
Examples with the same class label

(Requires labels, related to Siamese nets, ProtoNets)

Augmented versions of the example

(flip & crop)

Nearby image patches



Nearby video frames

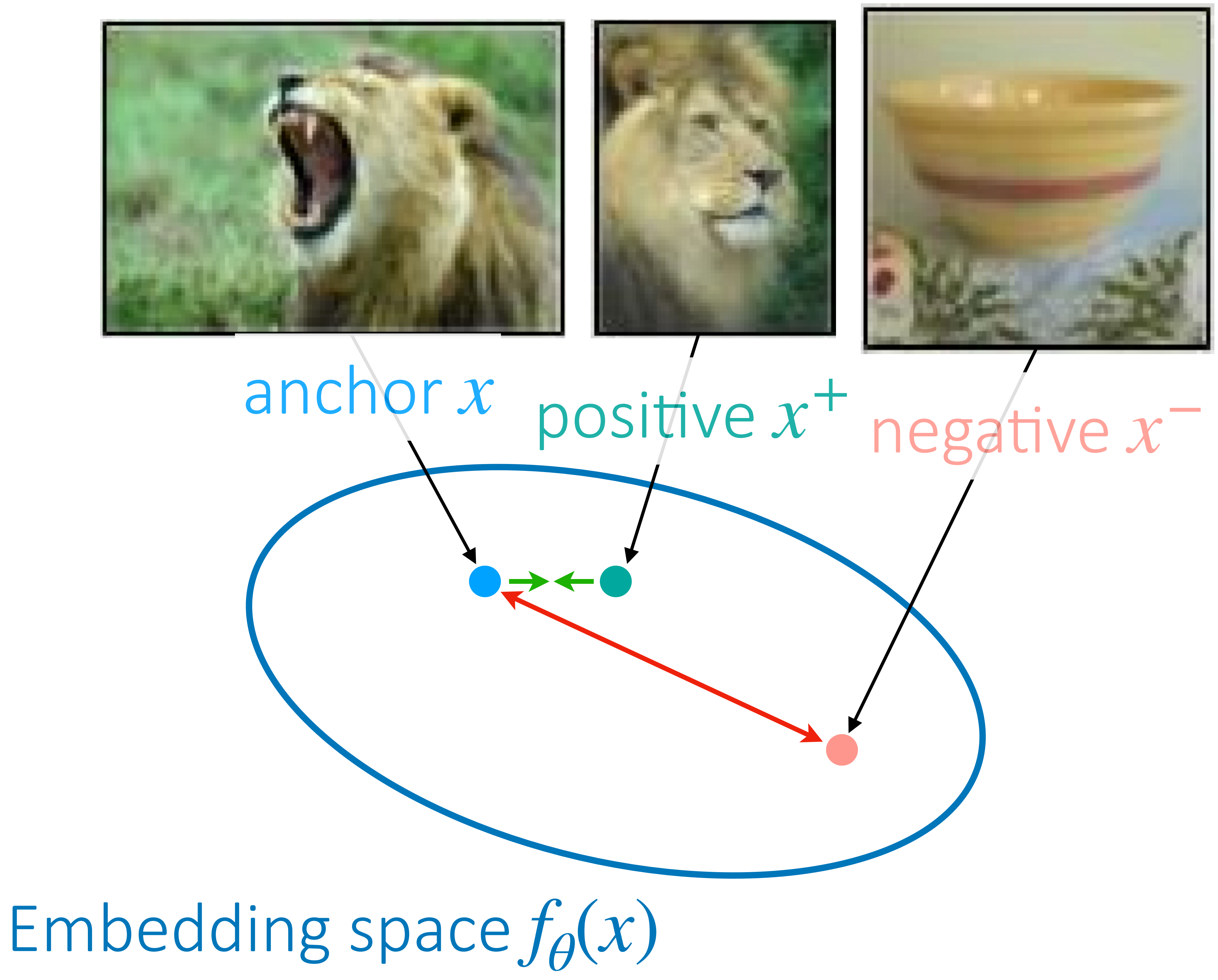
Dog credit to Maggie & Luke

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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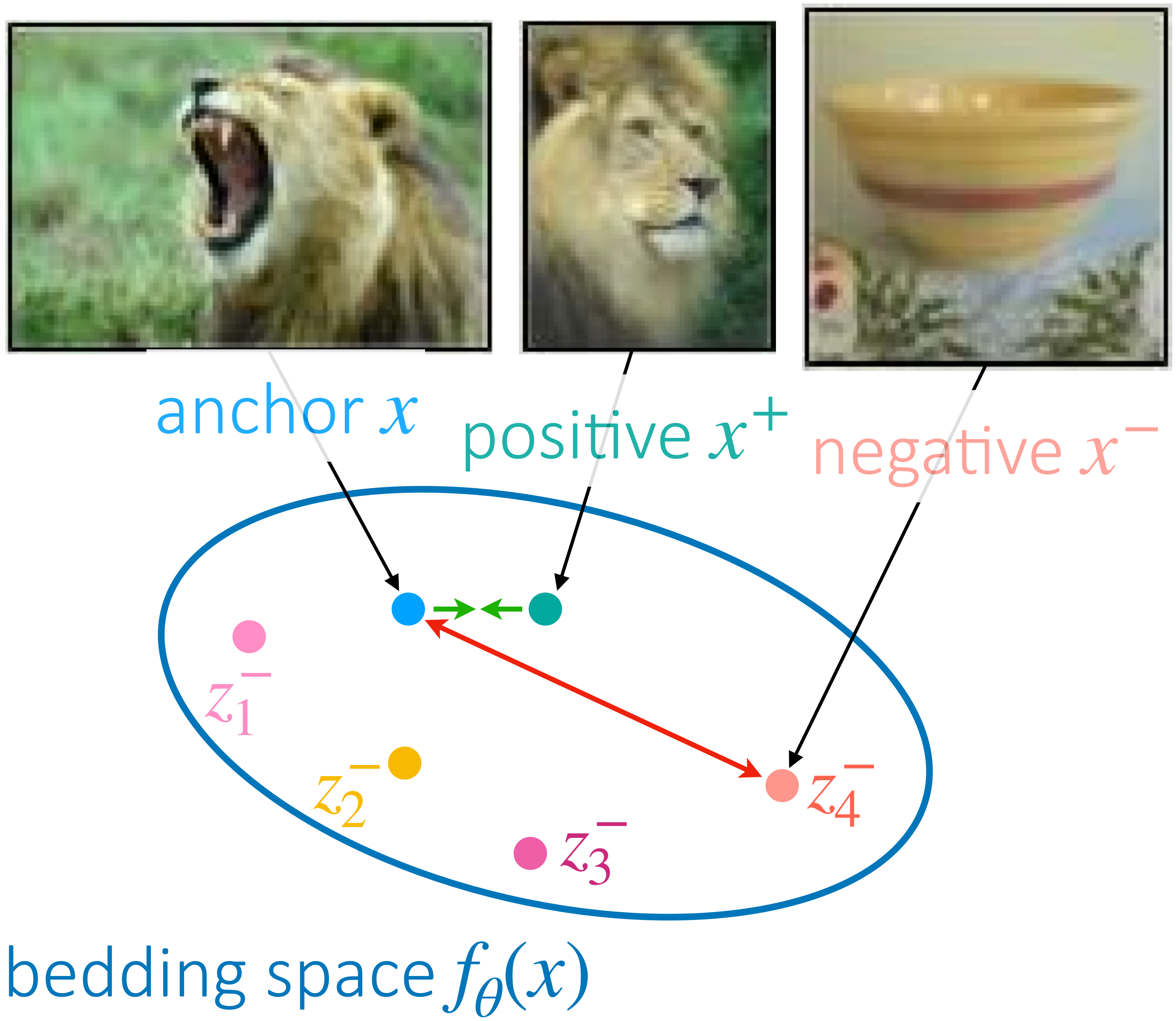

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V2. From binary to N-way classification (aka **simCLR***):

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

*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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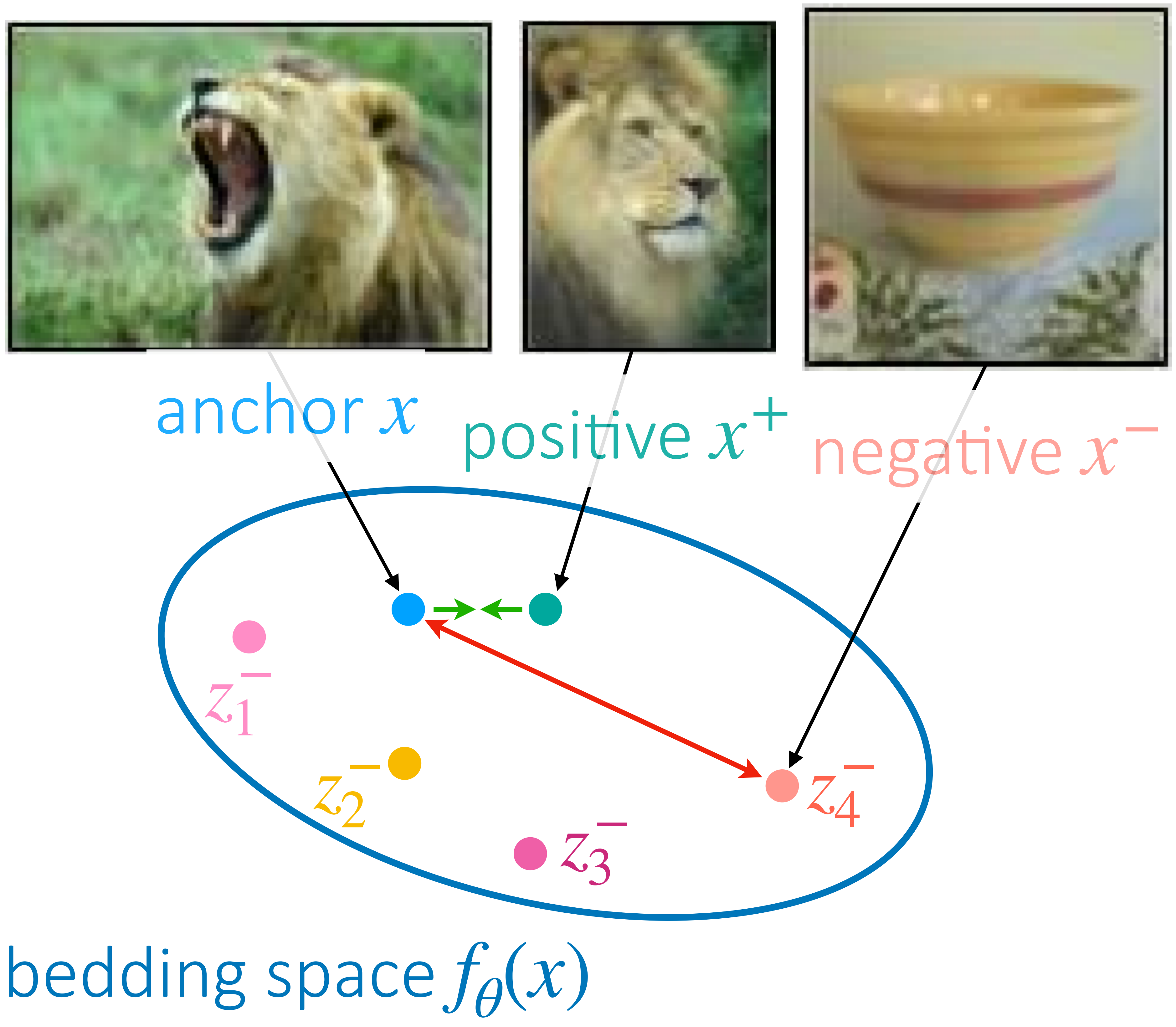

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V2. From binary to N-way classification (aka **simCLR***):

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

Positive score in denominator → 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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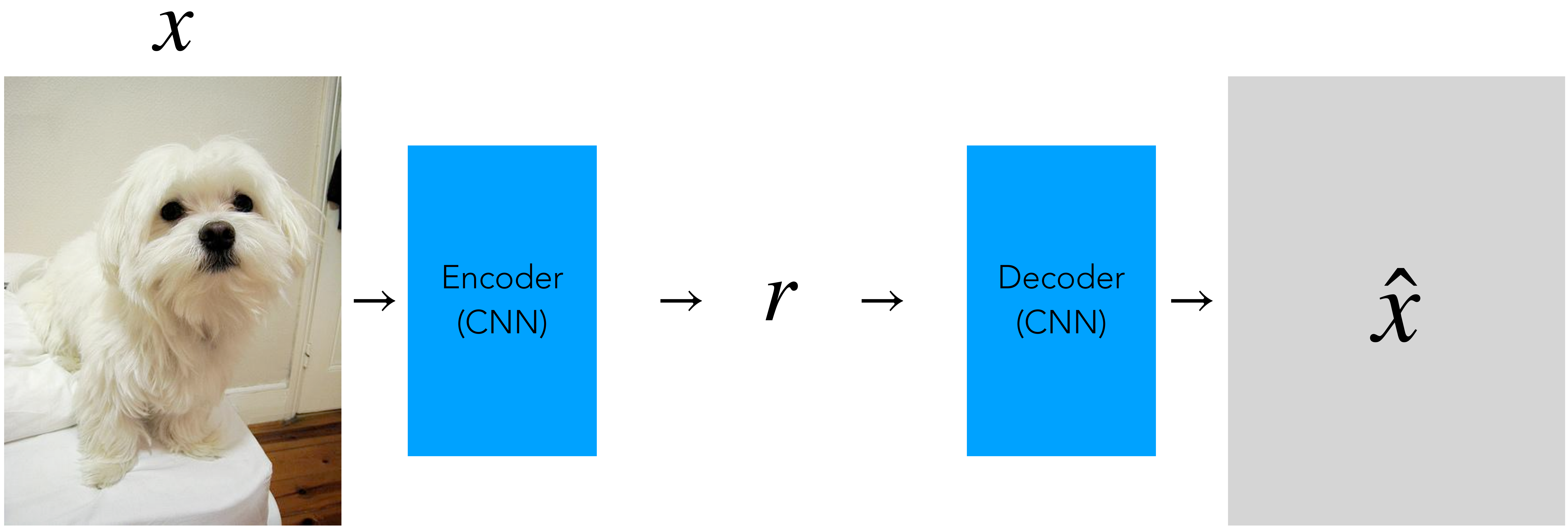
Reconstruction-based unsupervised pre-training

- **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

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

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

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

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

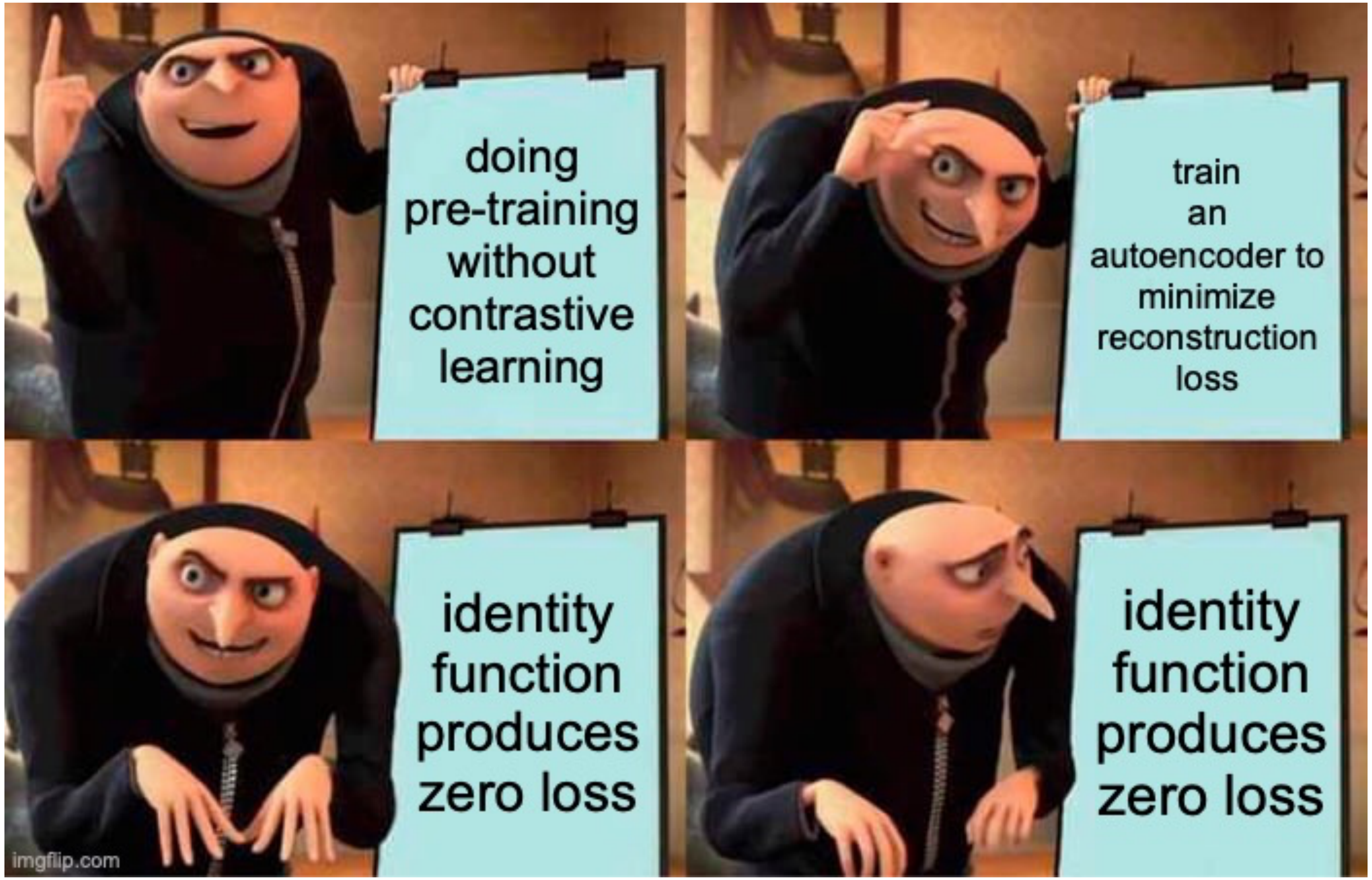
Input image, sentence, audio signal, etc.

Reconstruction of input image

What can go wrong here?

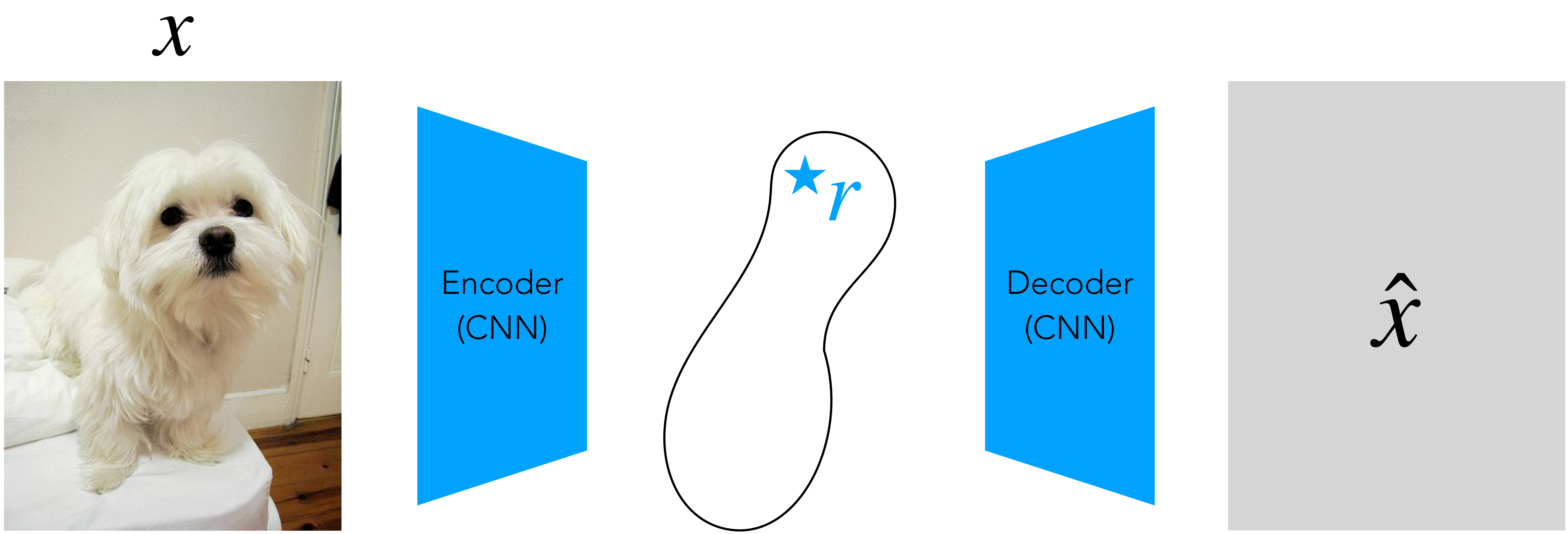
Is the **identity function** a good encoder/decoder?

Autoencoders: a first attempt



How to fix???

Autoencoders: adding a bottleneck



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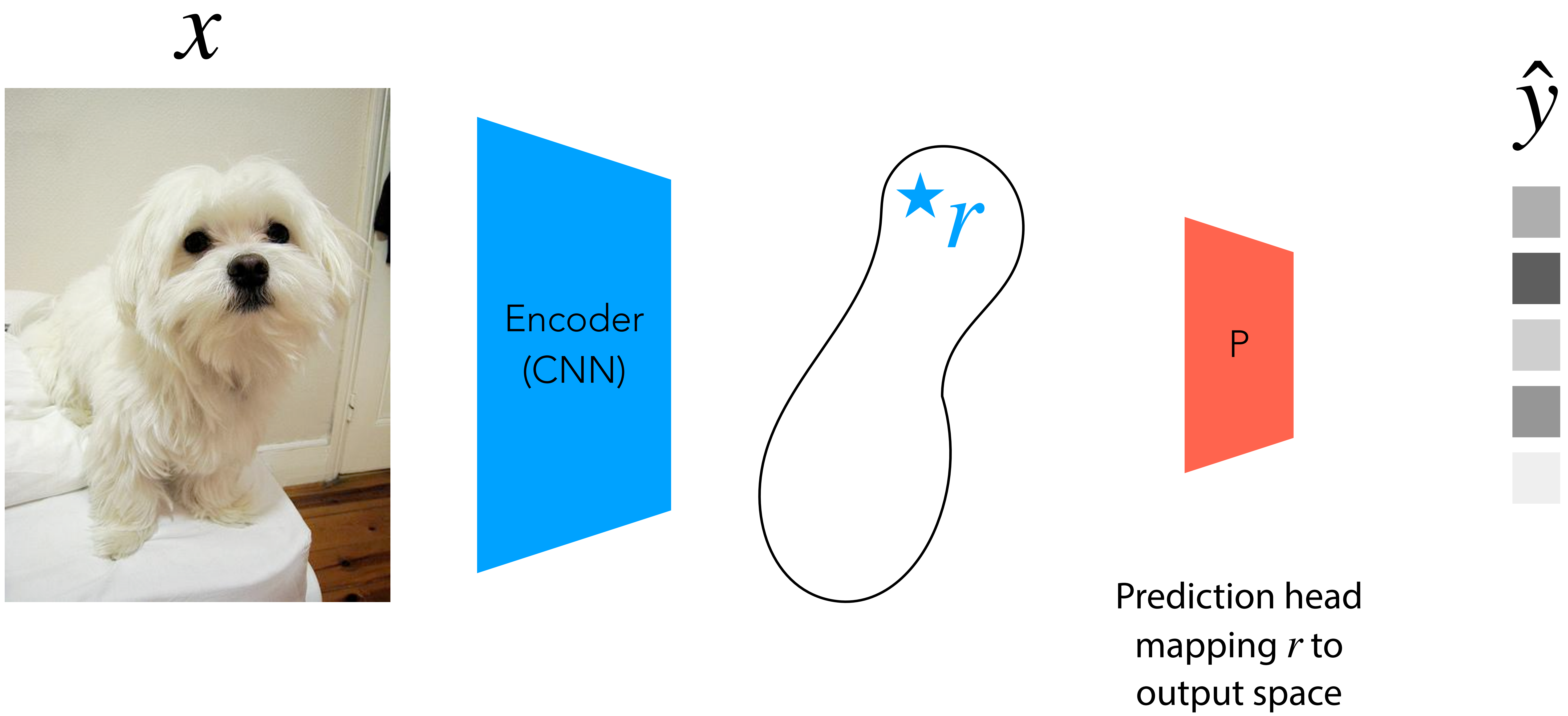
Input image, sentence, audio signal, etc.

Compact, latent representation of input image

Reconstruction of input image

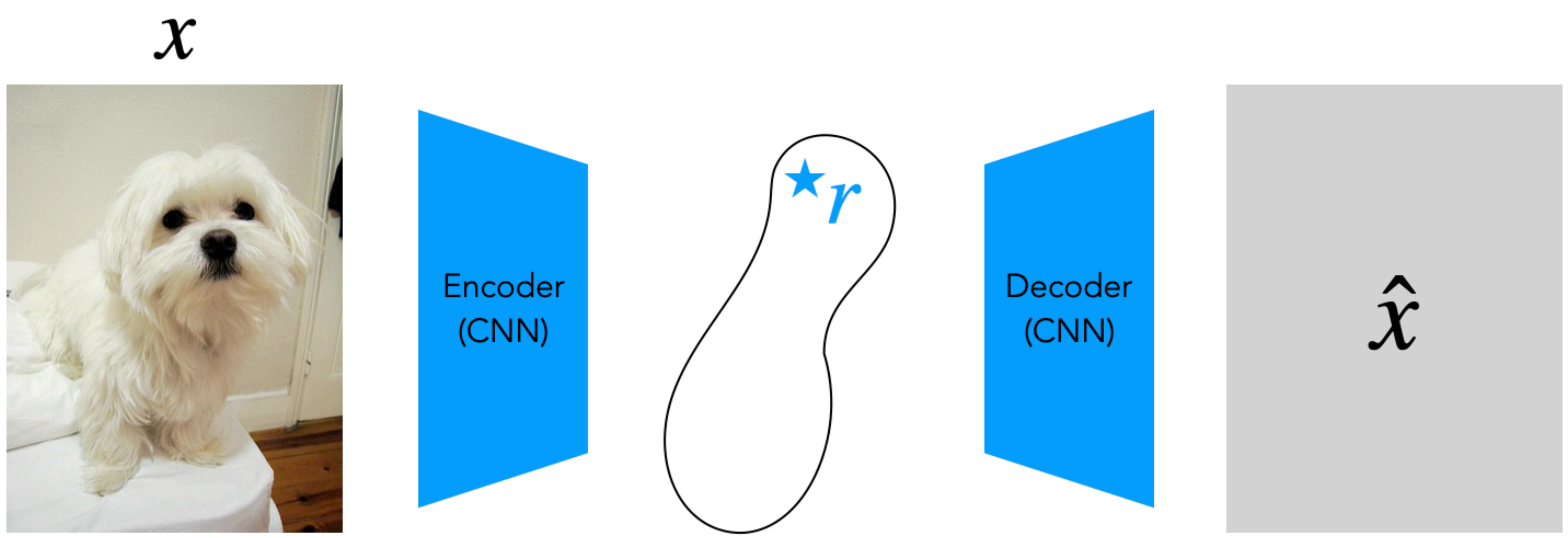
Key idea: latent representation is **bottlenecked**, e.g., **lower-dimensional** than the input → *Hope:* latent dimensions are forced to represent **high-level** concepts that **generalize** to other tasks

Autoencoders: few-shot learning



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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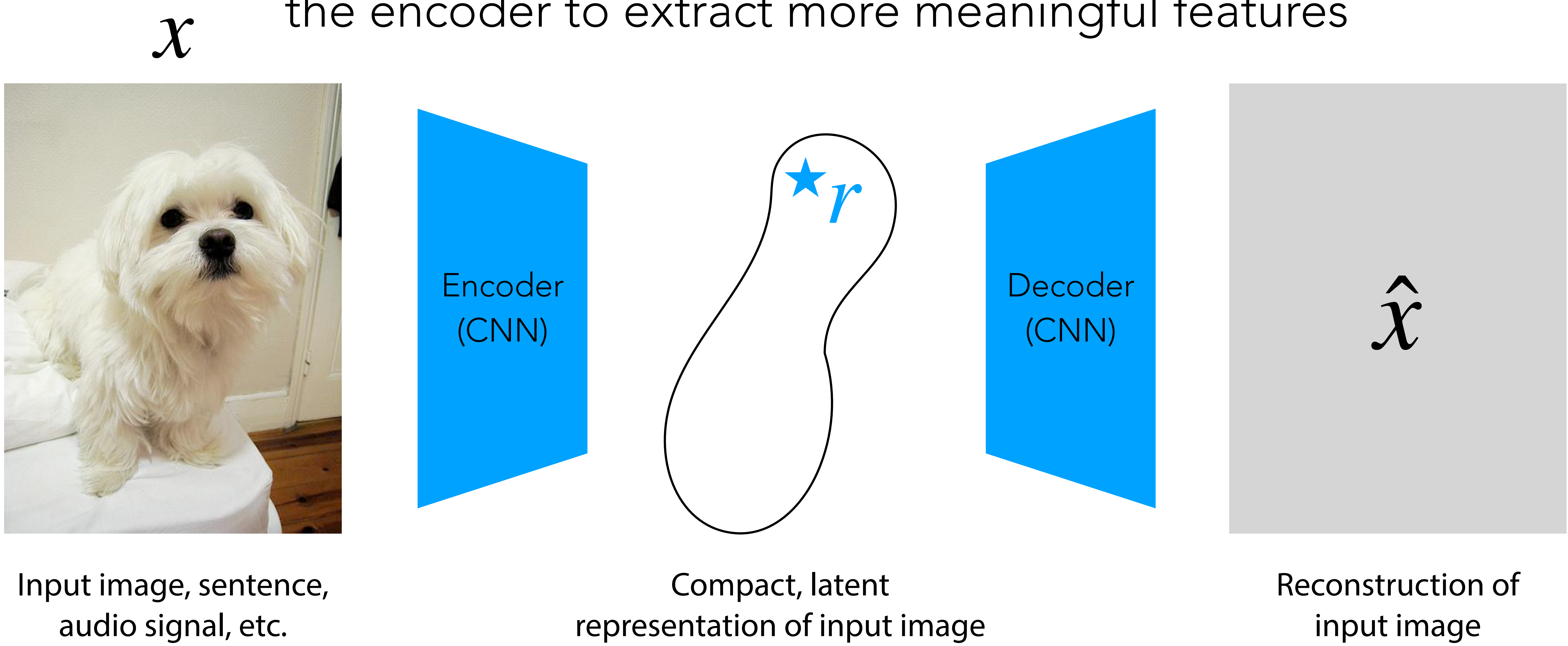
- ***Masked* autoencoders**: BERT, MAE
- Autoregressive models: GPT, Flamingo

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

Ultimately, **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



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

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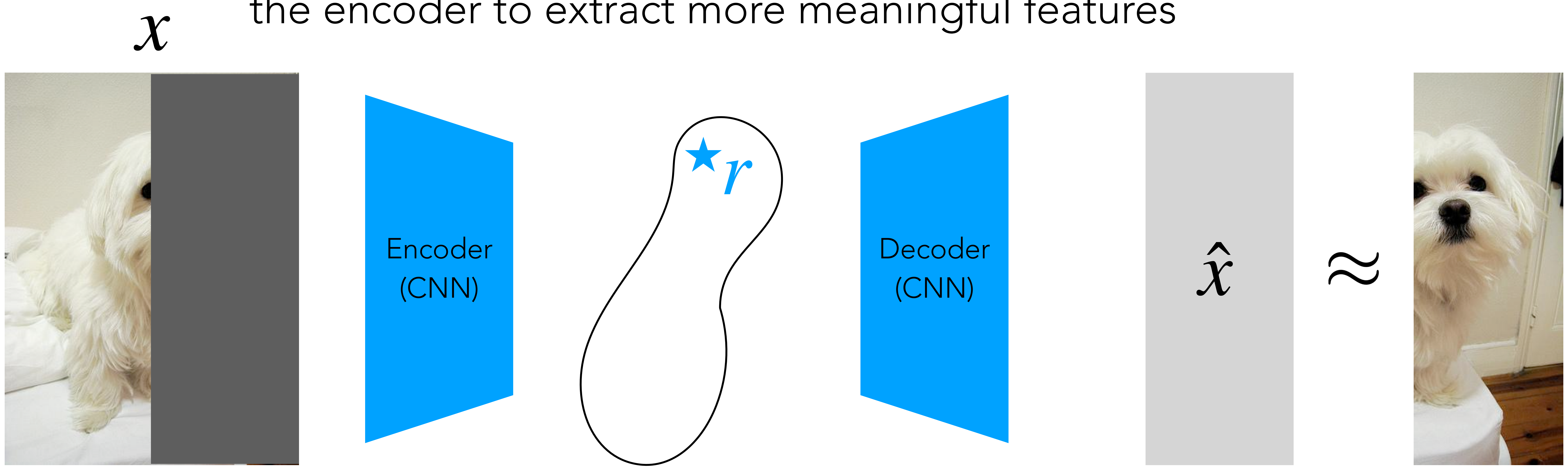


Masked input image

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 `)`

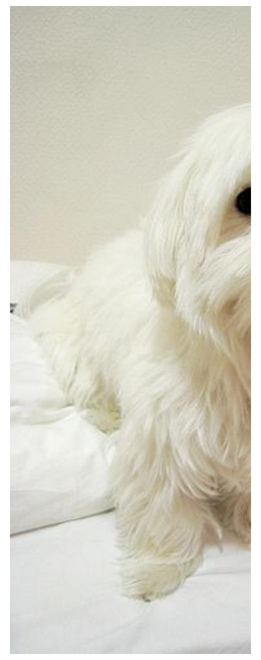
*$\tilde{x}_i, y_i$ are typically two **disjoint** sub-regions of x_i*

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 $\tilde{x}_i$ 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* `)` =

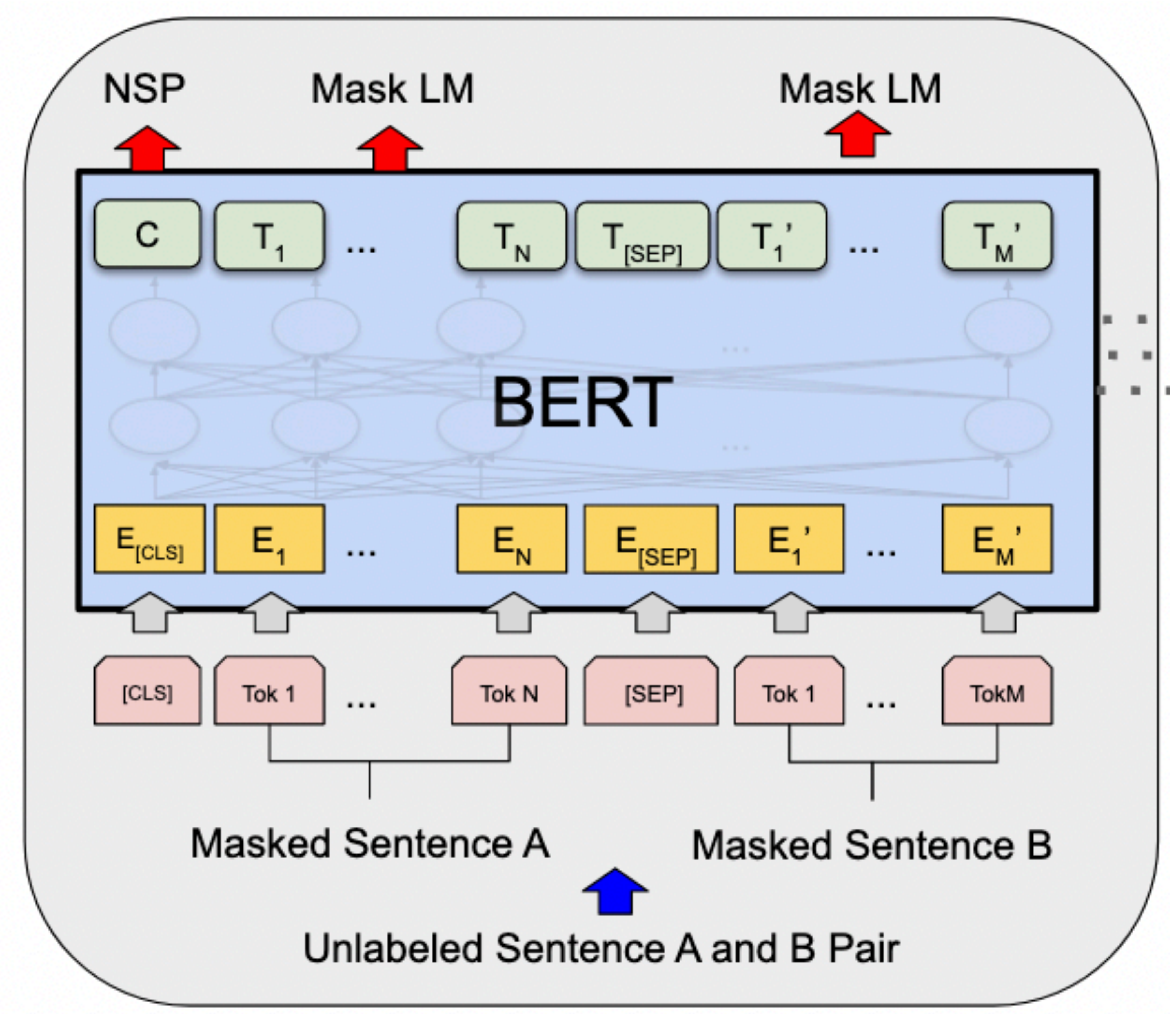
$\tilde{x}_i$ y_i

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

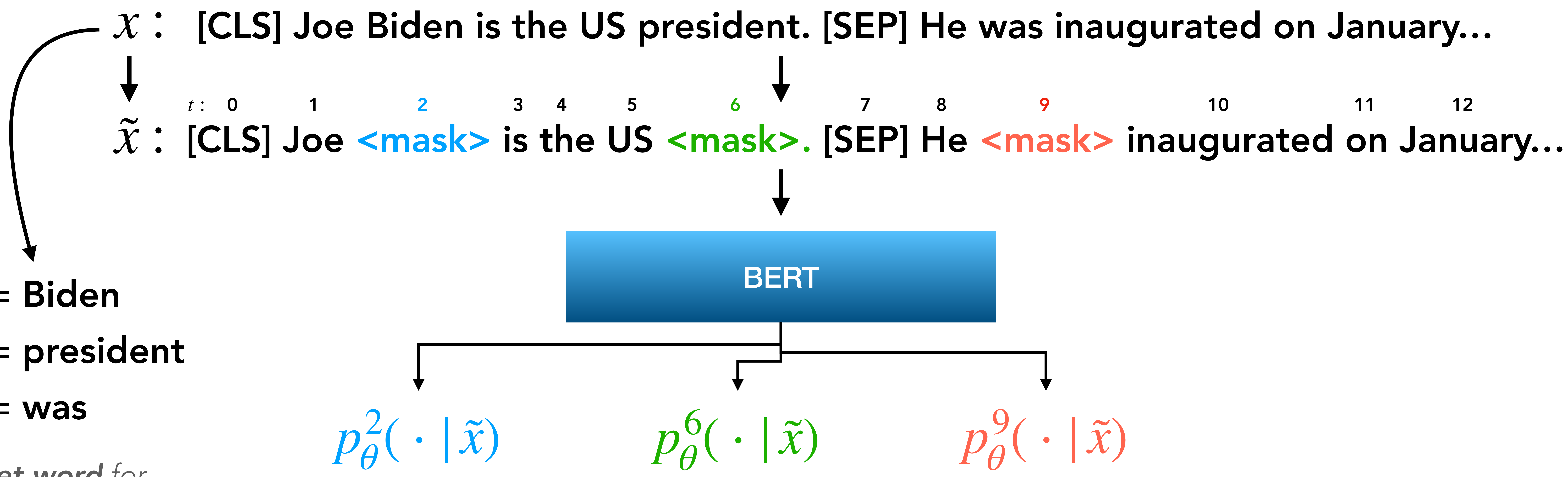
f_θ **: Transformer (**e.g., **BERT**; stay tuned**)**

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

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



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



***Target word** for each masked index*

***Probability distribution** over possible words at each masked index j*

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

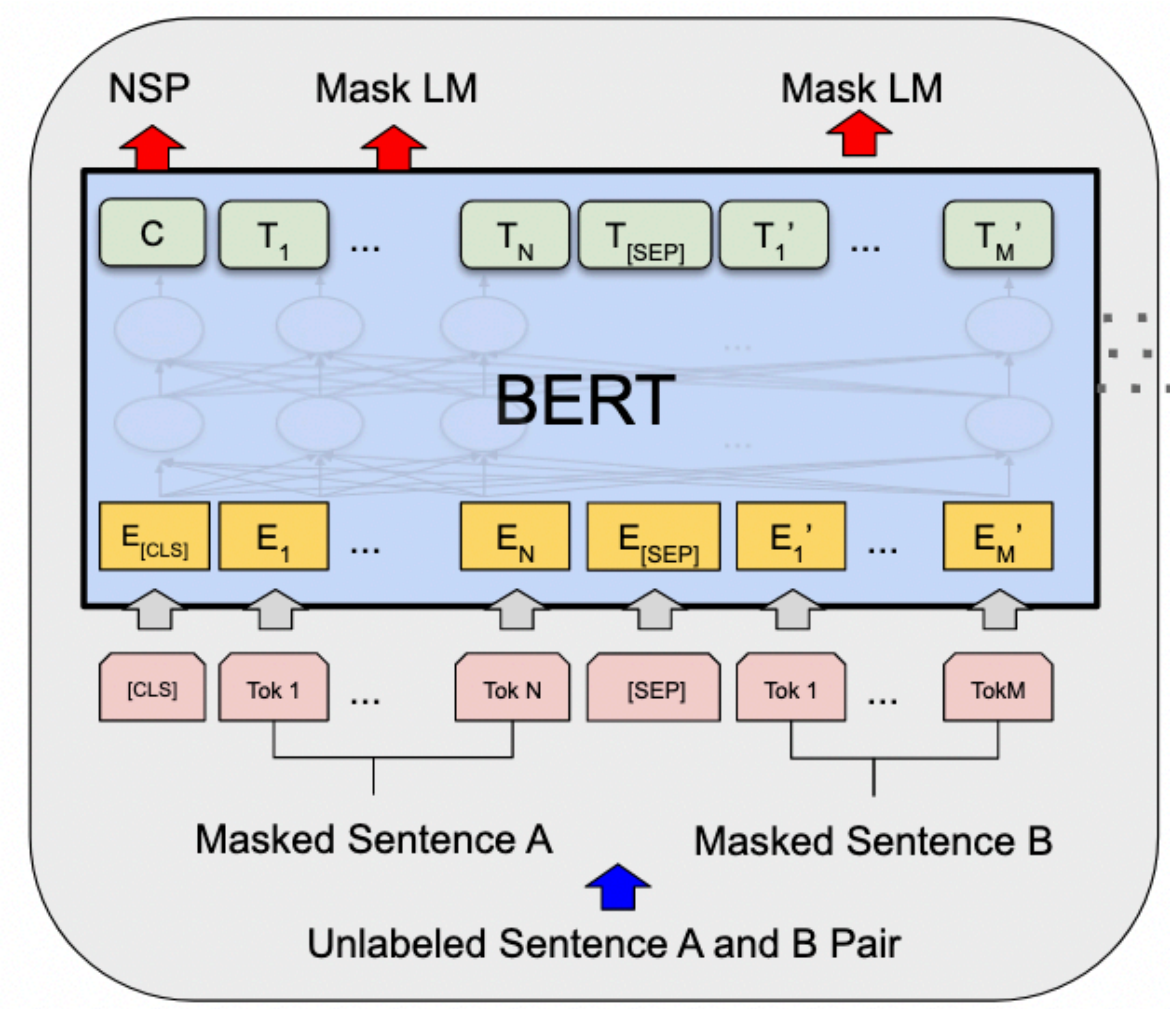
Details of BERT masking:

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

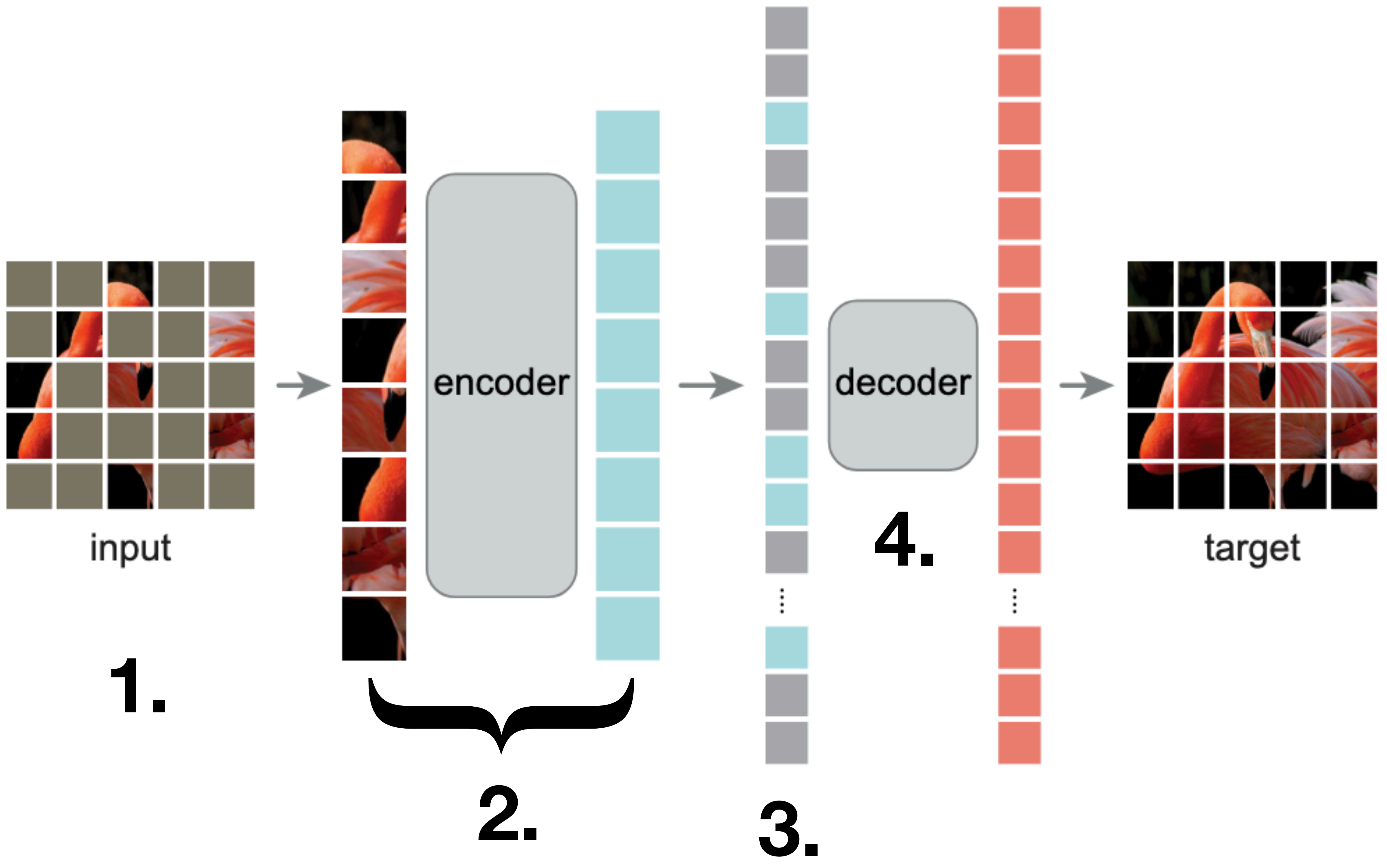
*It's possible we can do better than just picking **random** timesteps:

- 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***

More recently: Masked AEs give state-of-the-art **few-shot image classification** performance

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

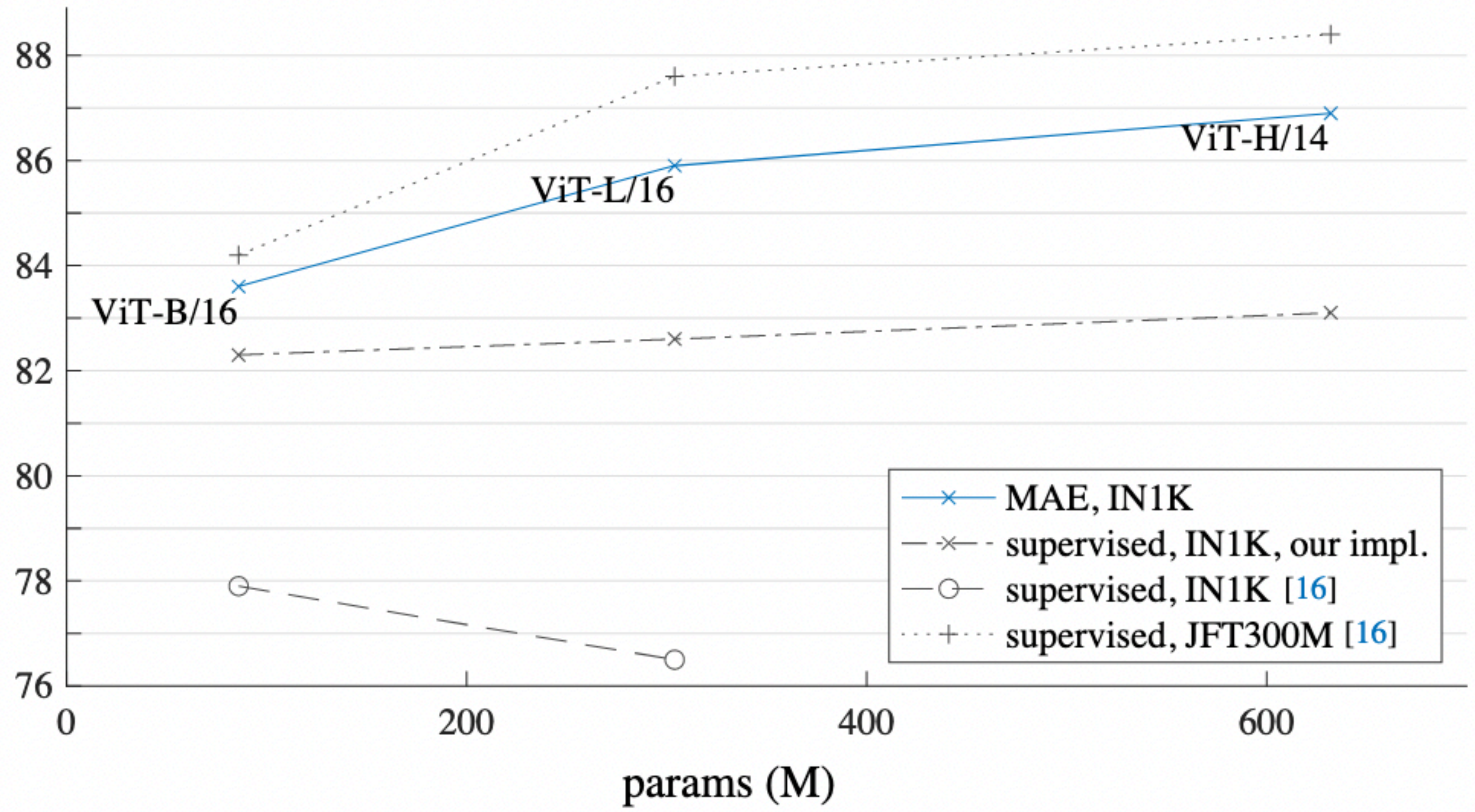


Figure 8. **MAE pre-training *vs.* supervised pre-training**, evaluated by fine-tuning in ImageNet-1K (224 size). We compare with the original ViT results [16] trained in IN1K or JFT300M.

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

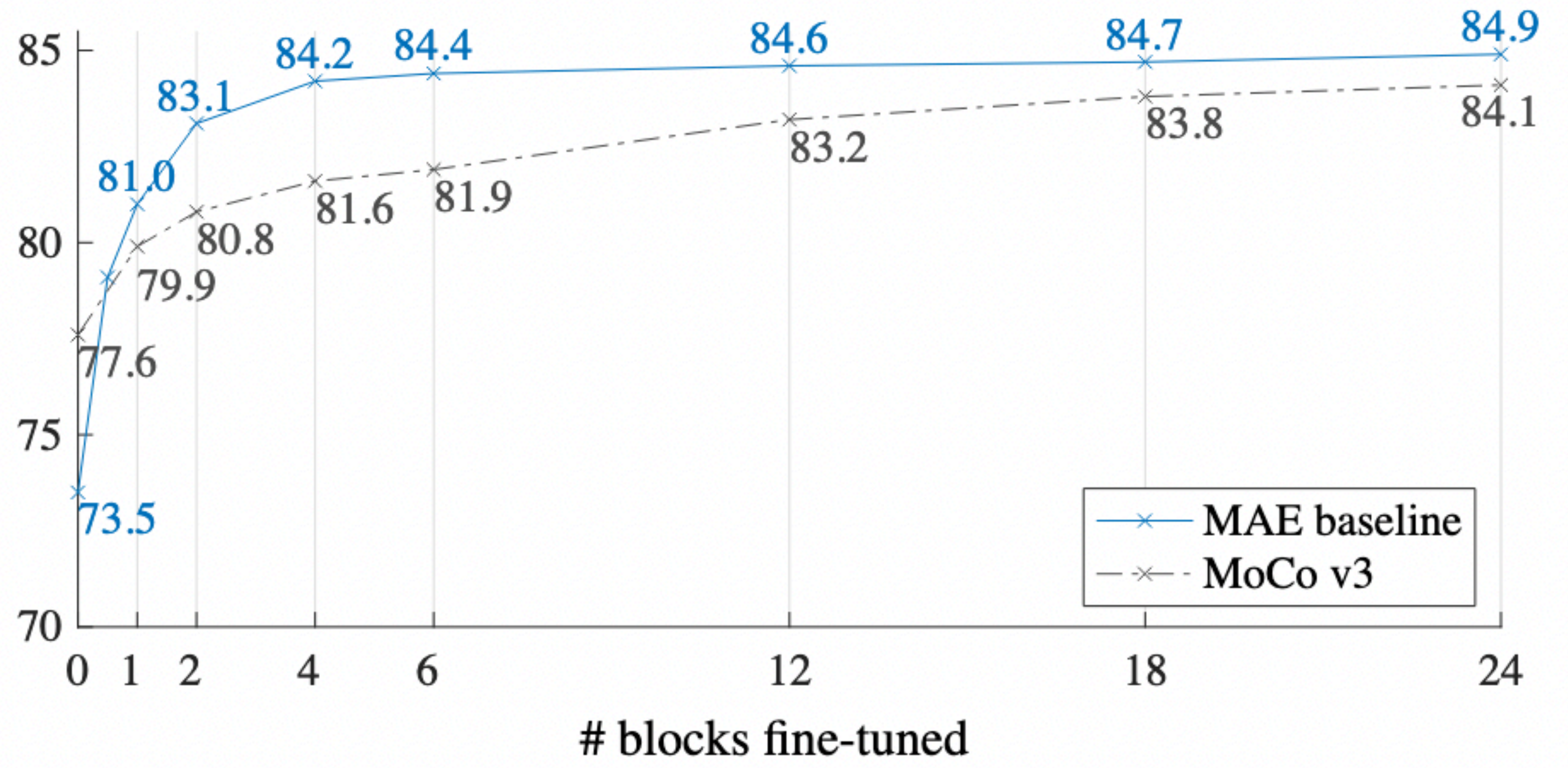


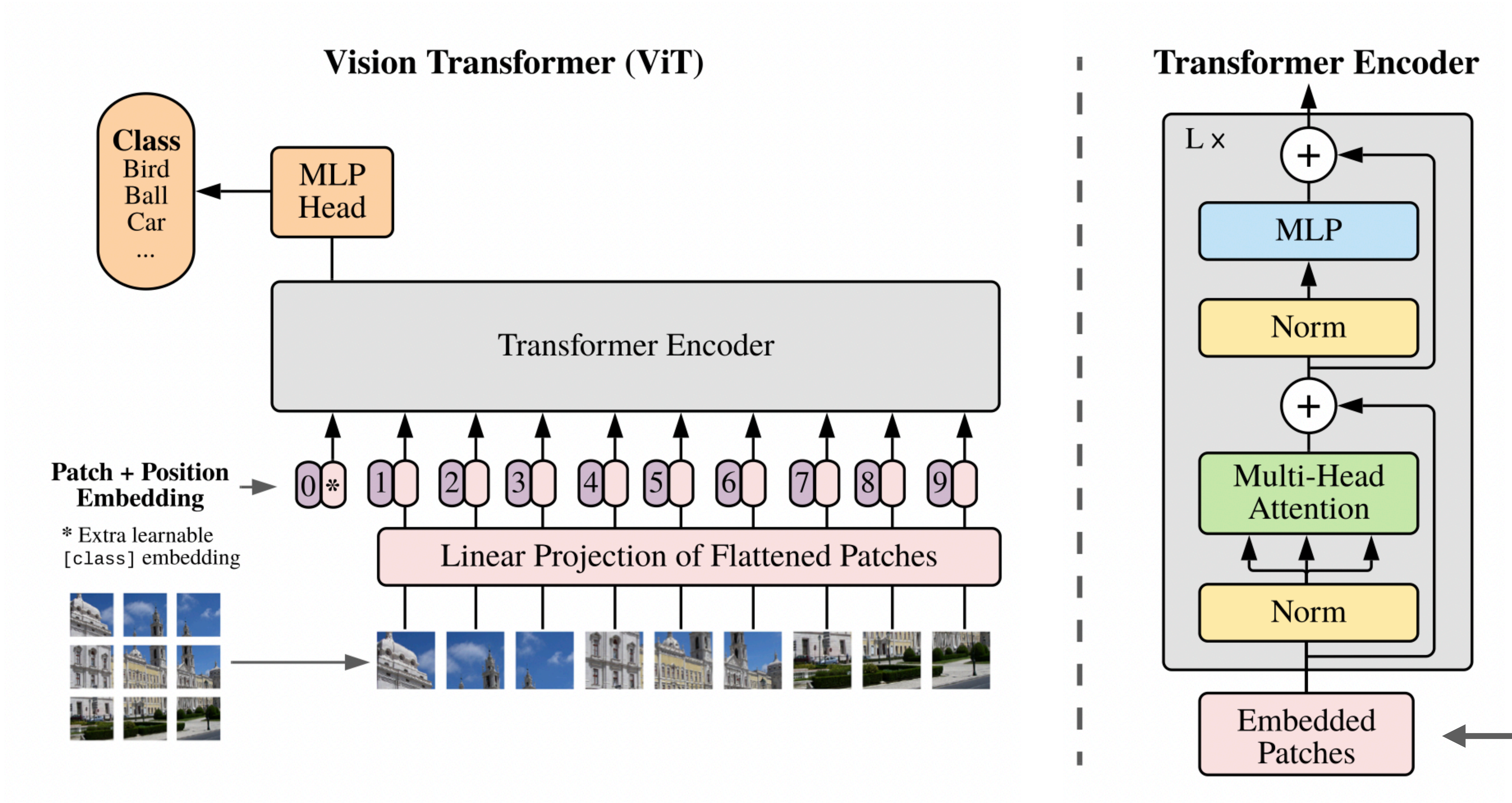
Figure 9. **Partial fine-tuning** results of ViT-L w.r.t. the number of fine-tuned Transformer blocks under the default settings from Table 1. Tuning 0 blocks is linear probing; 24 is full fine-tuning. Our MAE representations are less linearly separable, but are consistently better than MoCo v3 if one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

He et al, 2021

A (very quick) overview of Transformers

Image by Ray Shrewsberry from Pixabay

A (very quick) overview of Transformers



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)

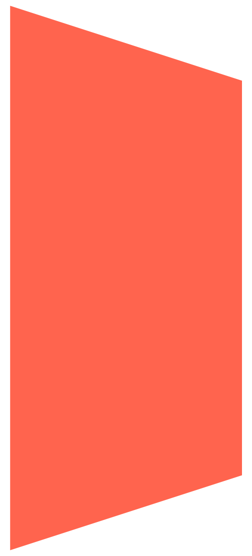
Transformers in a bit more detail

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?

Image by Cedric Yong from Pixabay

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)*

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

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

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

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

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)*

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

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*

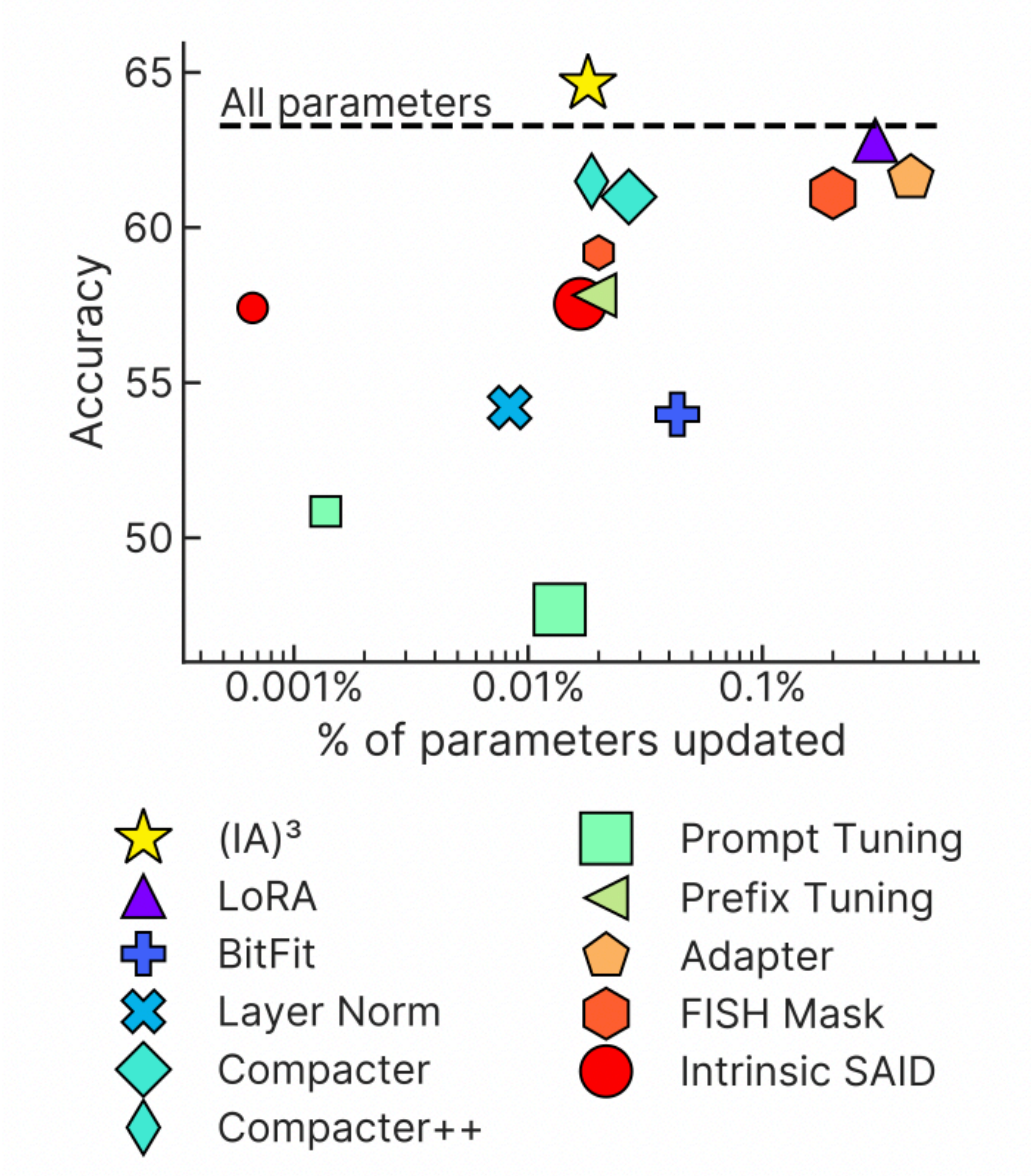
LoRA: $$W_{ft} = W_0 + AB^\top, \quad A, B \in \mathbb{R}^{d \times p}$$

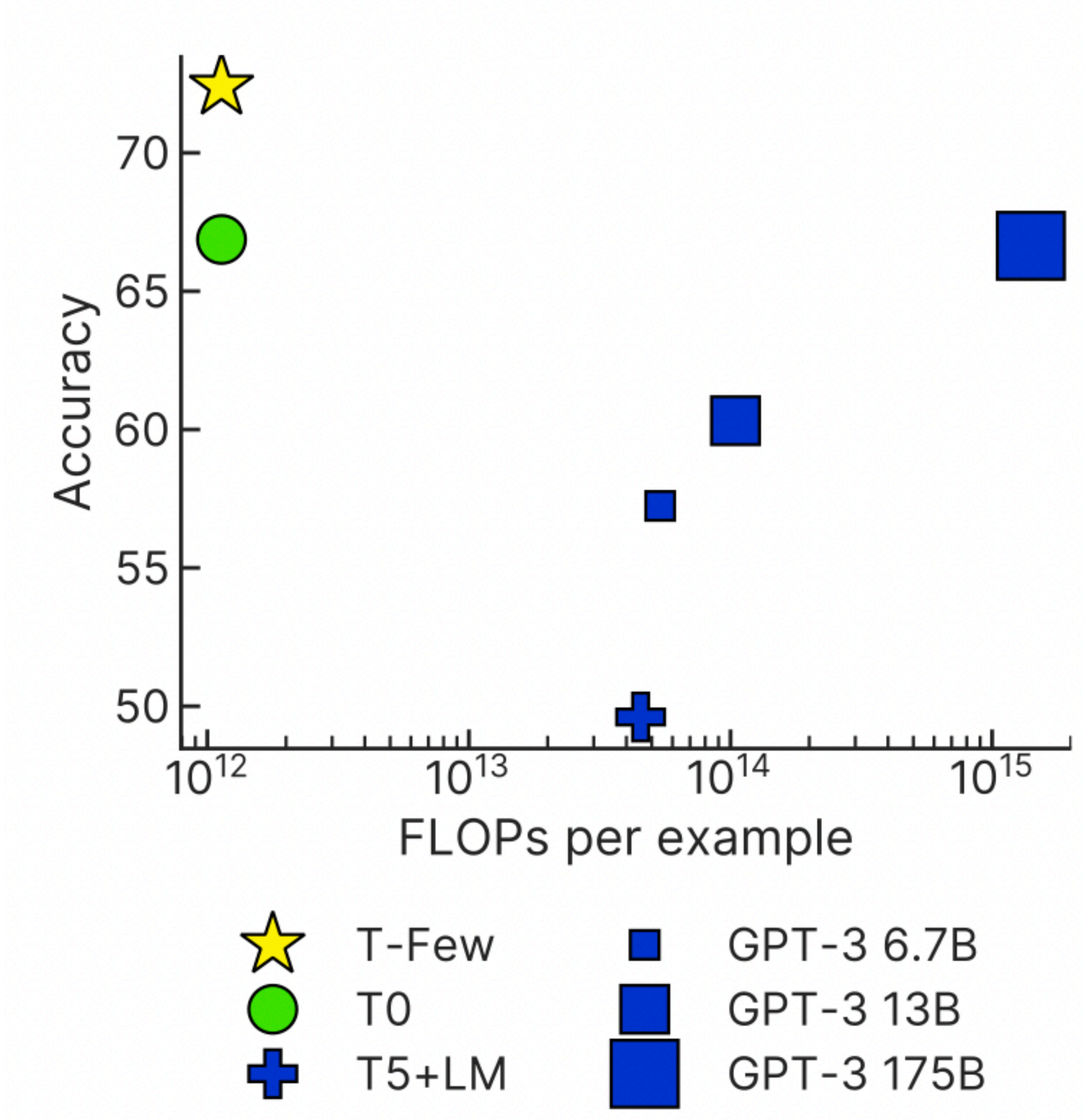
pre-trained weights **(frozen)**

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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- **Autoregressive models**: GPT, Flamingo

Striving for simplicity: **autoregressive models**

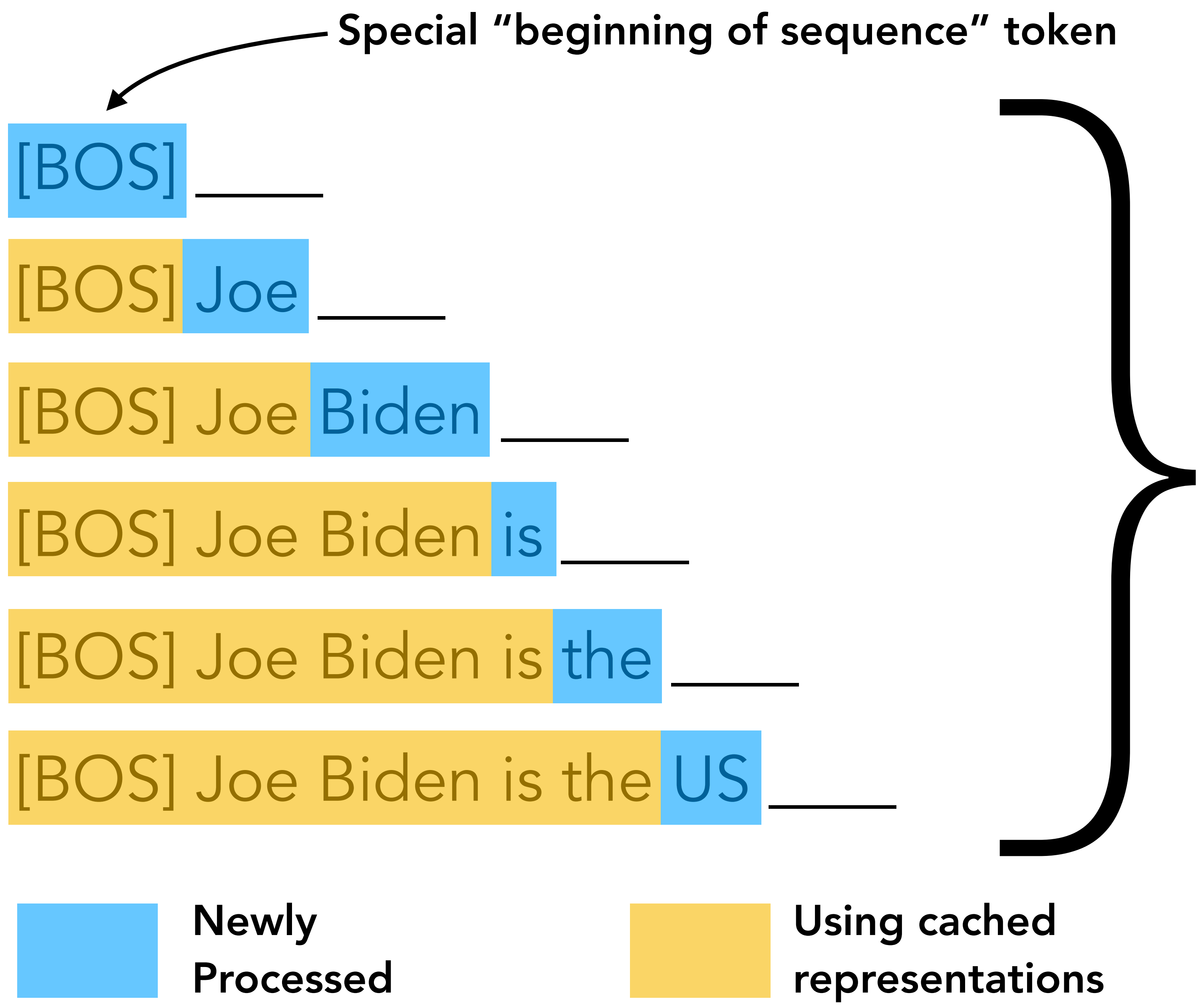
(recall from the black-box meta-learning lecture!)

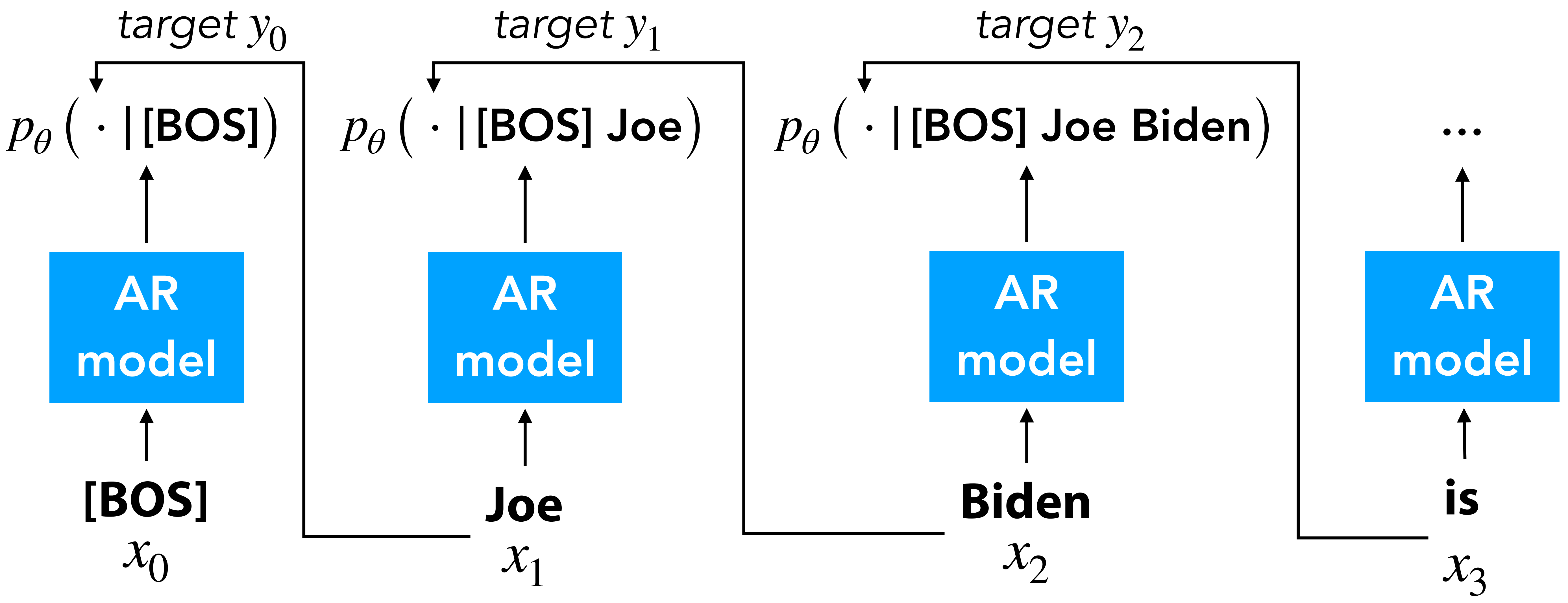
*What are some **downsides** of masked autoencoders?*

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

Generative Pretraining from Pixels

Mark Chen [1] Alec Radford [1] Rewon Child [1] Jeff Wu [1] Heewoo Jun [1] Prafulla Dhariwal [1] David Luan [1]

Decision Transformer: Reinforcement Learning via Sequence Modeling

WebGPT: Browser-assisted question-answering with human feedback

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 unde 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!

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[*,‡]

[*]Equal contributions, ordered alphabetically, [†]Equal contributions, ordered alphabetically, [‡]Equal senior contributions

Case study: **Flamingo**

DeepMind 28-04-2022

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[*]Equal contributions, ordered alphabetically, [†]Equal contributions, ordered alphabetically, [‡]Equal senior contributions

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

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

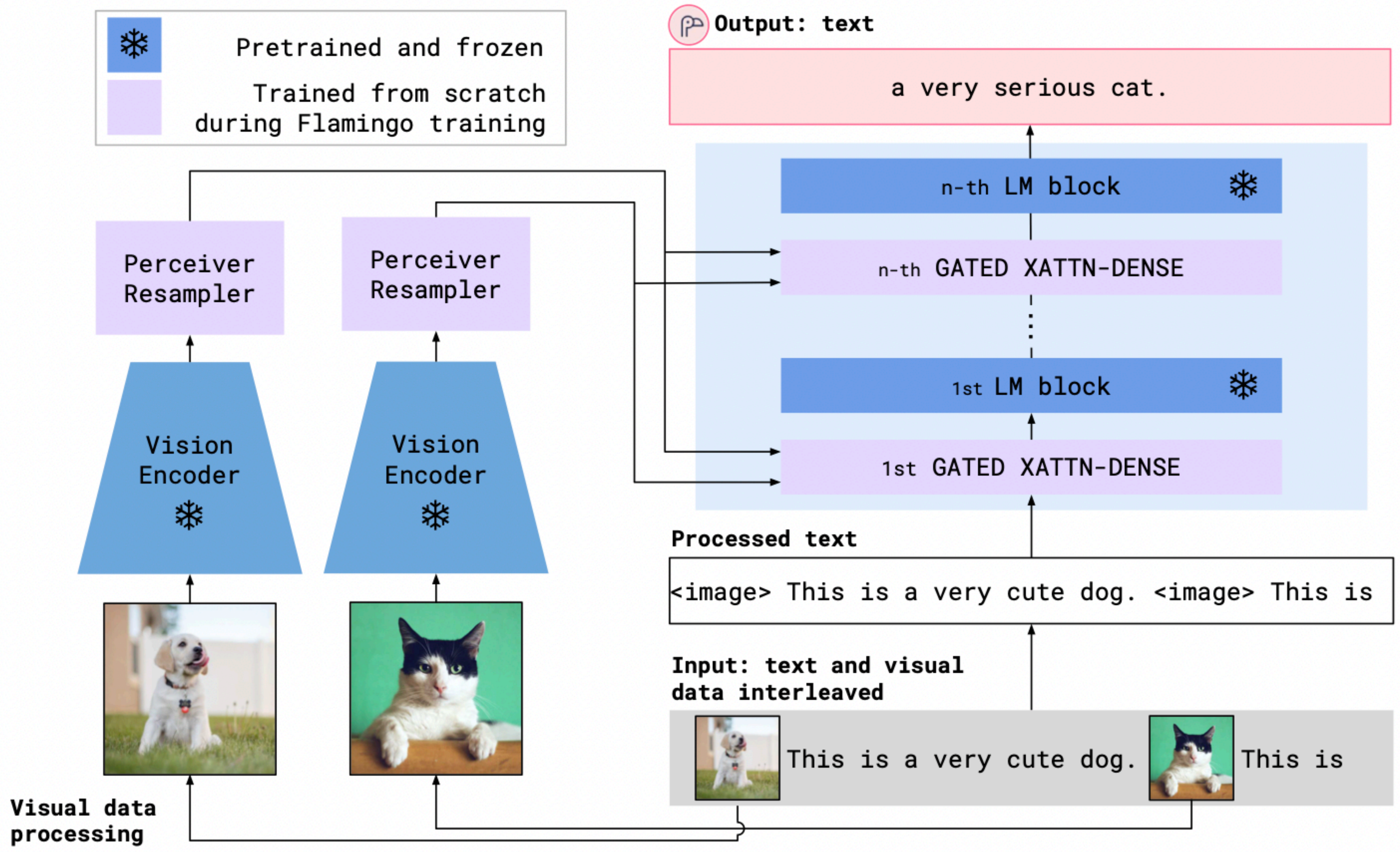
General-purpose LM + Few-shot data = Task-specific LM

Flamingo

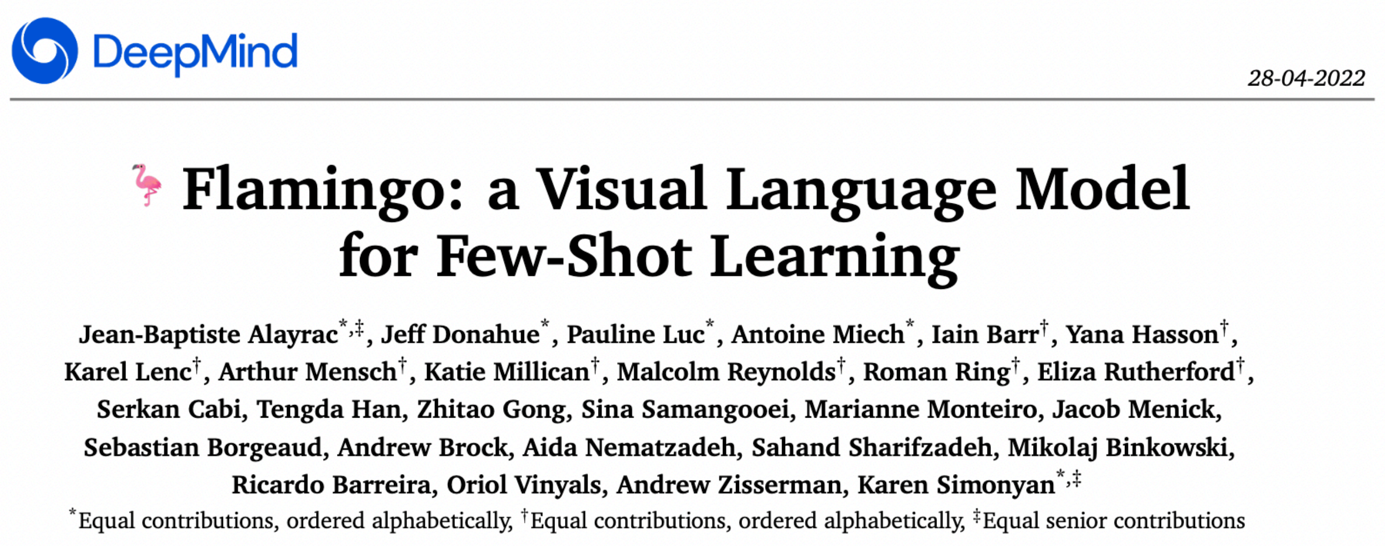
Fine-tuning to **combine models:**

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

= General-purpose Vision-Language Model



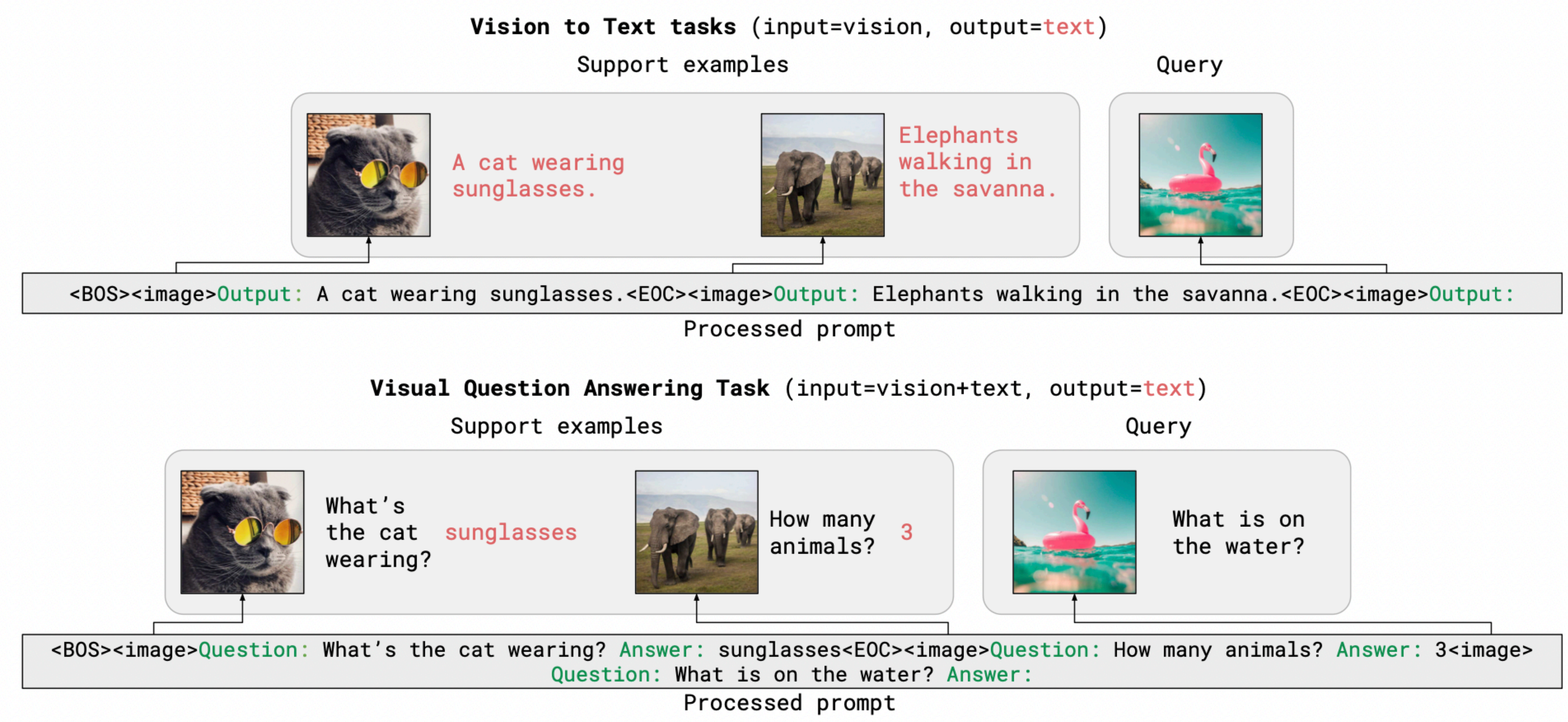
Case study: **Flamingo**


DeepMind 28-04-2022

Flamingo: a Visual Language Model for Few-Shot Learning

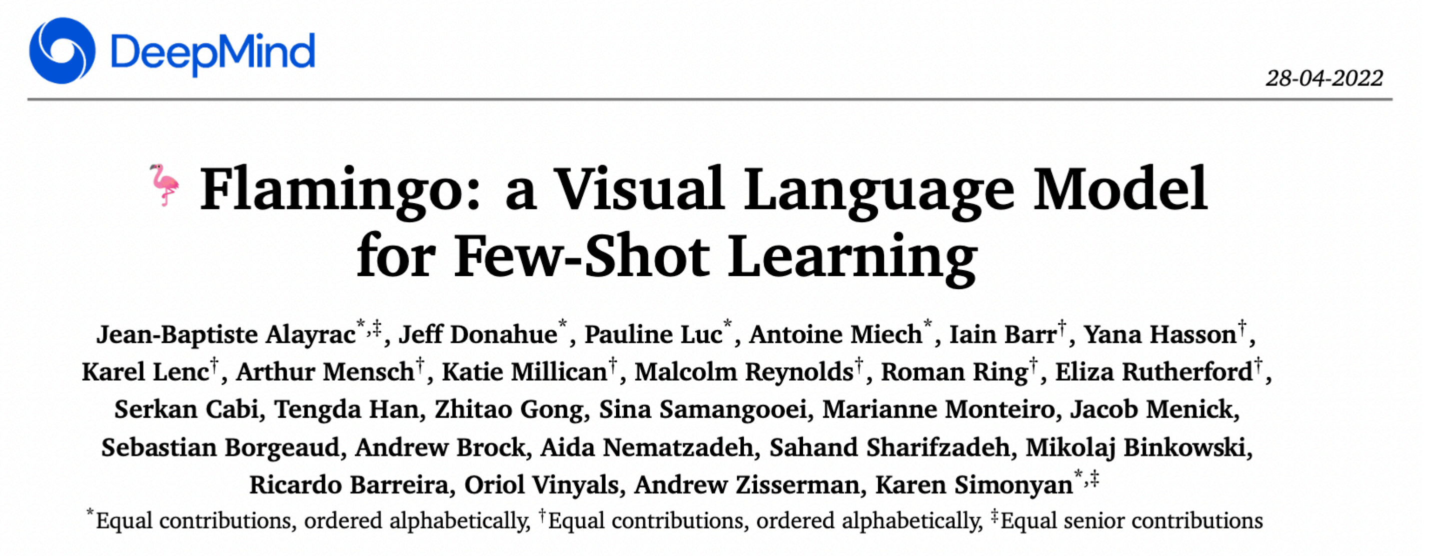
Jean-Baptiste Alayrac*,‡, Jeff Donahue*, Pauline Luc*, Antoine Miech*, Iain Barr†, Yana Hasson†, Karel Lenc†, Arthur Mensch†, Katie Millican†, Malcolm Reynolds†, Roman Ring†, Eliza Rutherford†, Serkan Cabi, Tengda Han, Zhitao Gong, Sina Samangooei, Marianne Monteiro, Jacob Menick, Sebastian Borgeaud,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

*Equal contributions, ordered alphabetically, †Equal contributions, ordered alphabetically, ‡Equal senior contributions



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

Case study: **Flamingo**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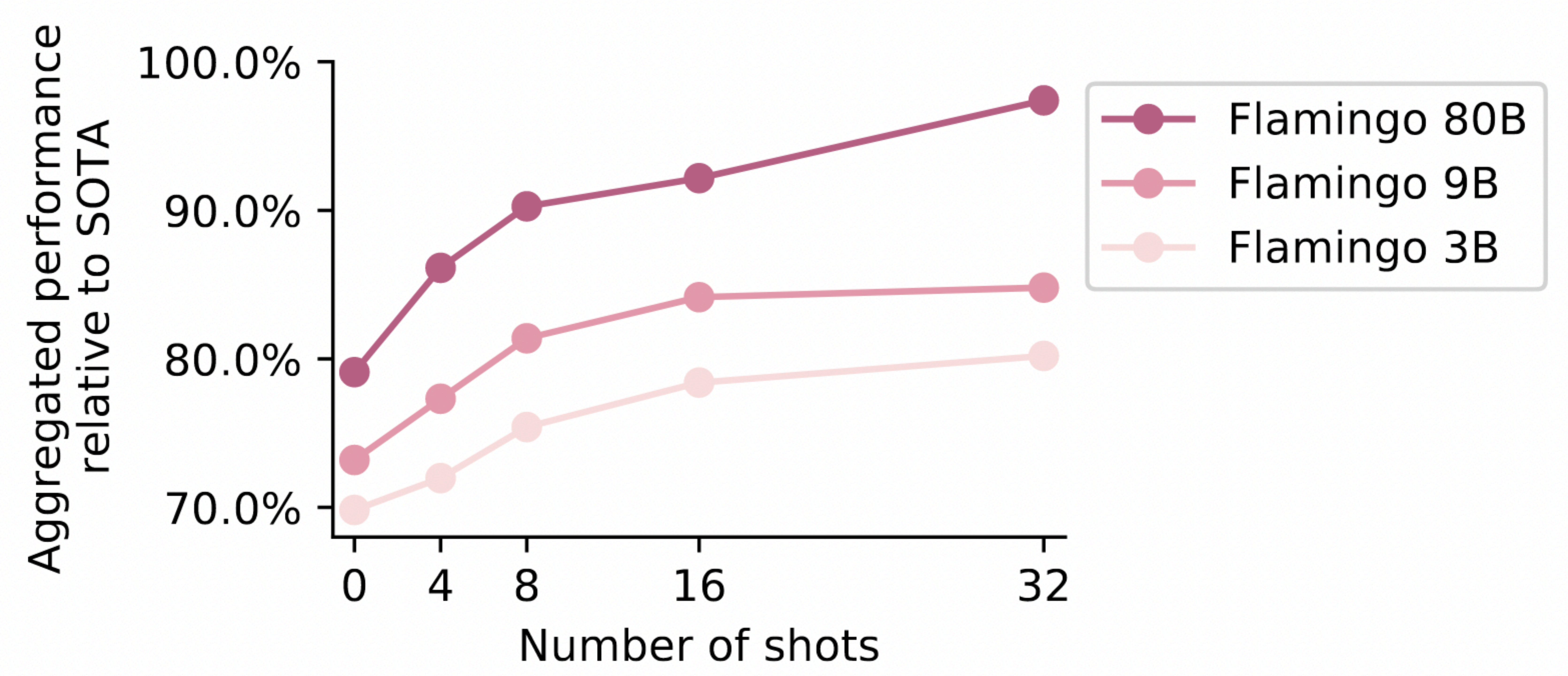

Few-shot Flamingo ≈ **Non-Few-shot state of the art!**

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:

$\tilde{x}$:	y :
Joe	
<mask>	**Biden**
is	
the	
<mask>	**US**
President	

AR model:

$\tilde{x}$:	y :
Joe	
Biden	
is	
the	
US	
____	**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: / *Masked autoencoders:*

+ *Simple to implement*
+ *No need to select pos/neg pairs; just $d(x, \hat{x})$*
- *Generally need a larger model*

(Bottlenecked) Autoencoders:

- *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 Monday, October 24

Kyle's office hours are hybrid going forward (see Ed for details)

Azure invites have been re-sent - **you have one week to accept!**

You will need Azure for HW3, so do this today!