

Self-supervised learning

CMPSCI 682: Neural Networks: A Modern Introduction

Subhransu Maji

December 7, 2023

College of
**INFORMATION AND
COMPUTER SCIENCES**



**UMASS
AMHERST**

Administrivia

Final report and video due **today** (Thursday, 12/7)

- Upload report to grade scope
- Upload video via the google form posted on piazza

Fill out SRTIs

- Different from course feedback from (should have received an email)
- Different questions
- Very important to us (and you...)

Today's Class

- Recap
 - Supervised vs Unsupervised Learning
 - Why not always label data?
- Semi-supervised Learning
 - Concepts
 - Example: pseudo-labels / self-training
- Self-supervised Learning
 - Concepts
 - Pretext tasks
 - Contrastive Learning
 - Beyond images

Today's Class

- **Recap**
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 - Beyond images

Recap: Supervised vs Unsupervised Learning

Supervised Learning

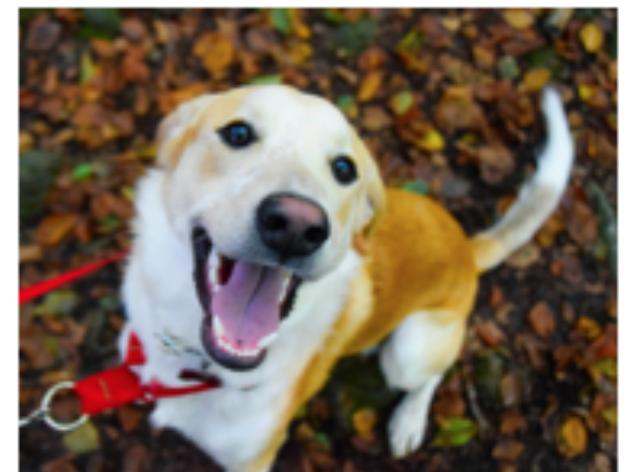
Data: (X, y)

X = input/feature/image/...

y = label/target



→ Cat



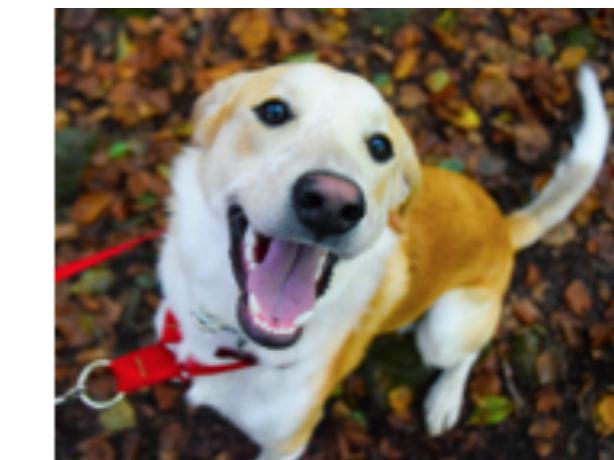
→ Dog

Unsupervised Learning

Data: X

Just X , no labels

Learn about the *structure* of the data,
i.e. $P(X)$



.....

So let's always use Supervised Learning?

Supervised Learning

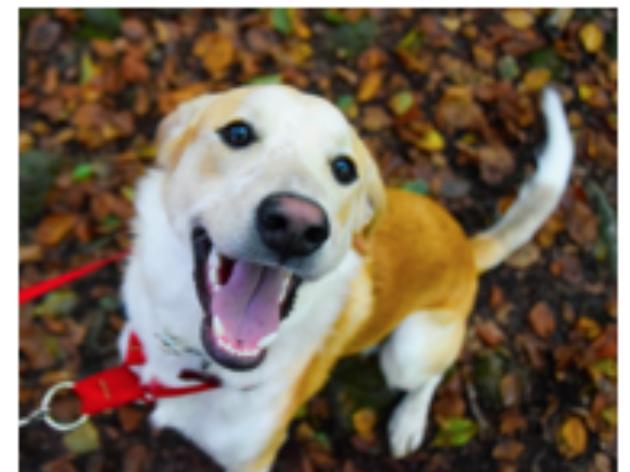
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→ Cat



→ Dog

“Standard” Supervised Learning:

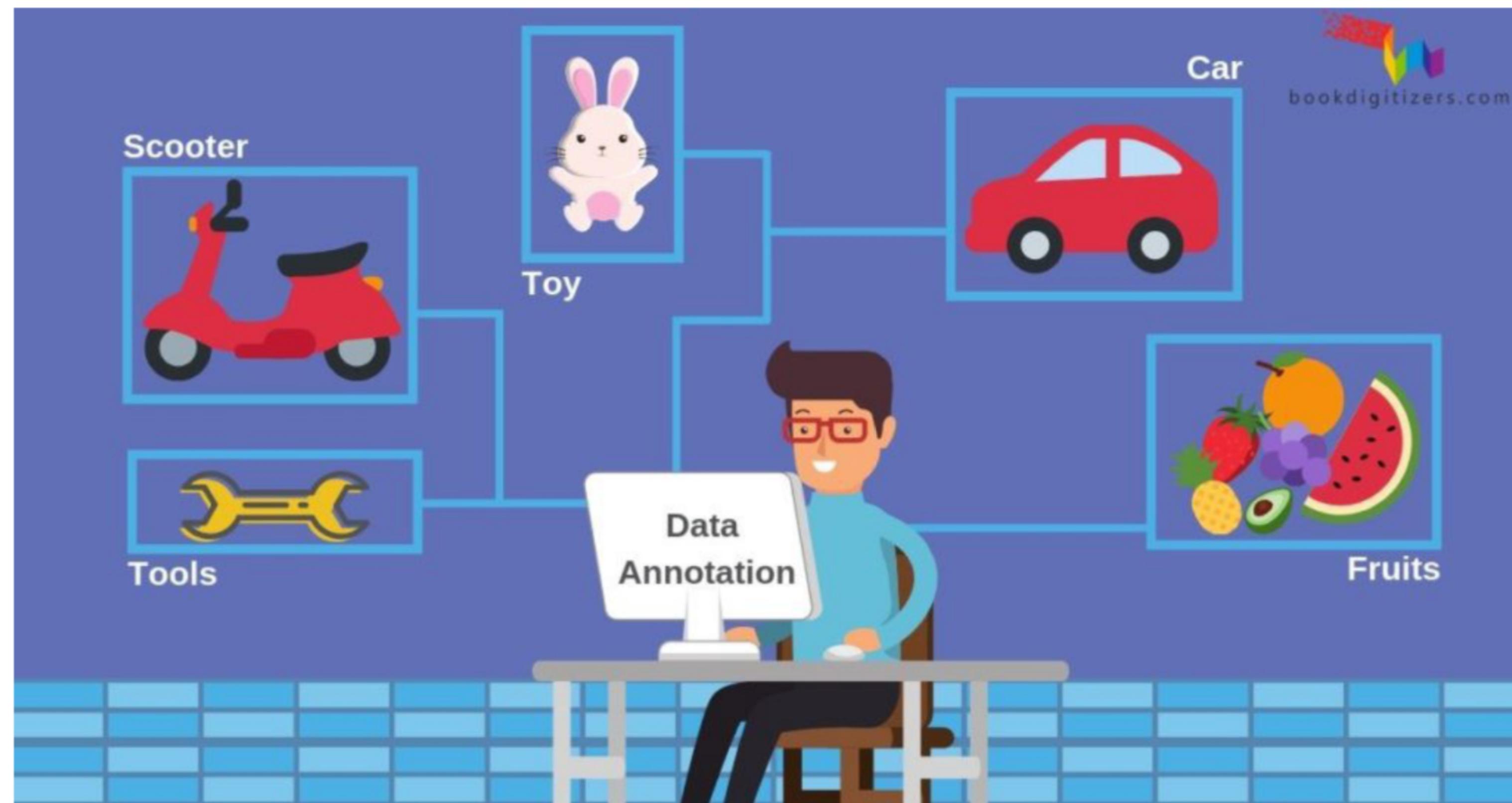
1. Collect a large set of data (images..) as the “training set”
2. Label each one as cat / dog / monkey / ...
3. Train a model mapping image to label

$$f : X \rightarrow y$$

4. Go forth and classify the world with f !

Data Annotation

Supervised Learning first requires labeling a very large amount of data

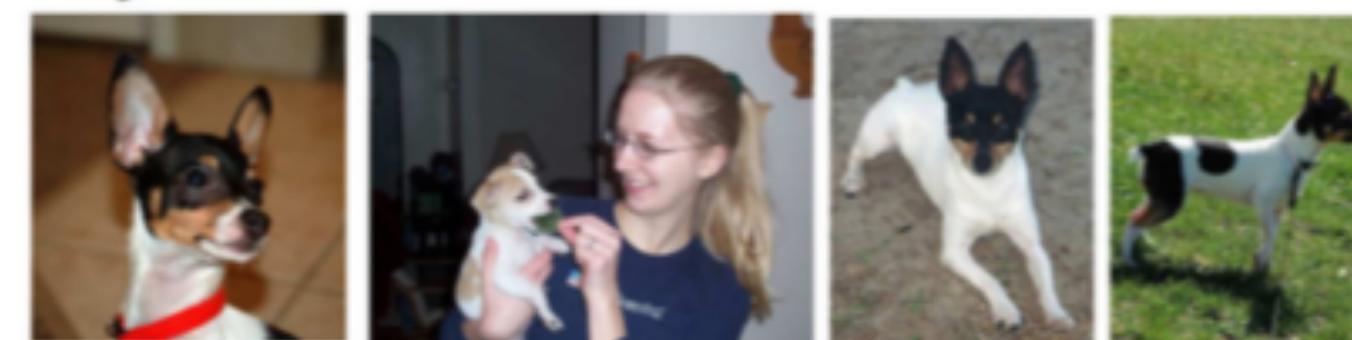


Labeling Image Categories - “Easy” Until

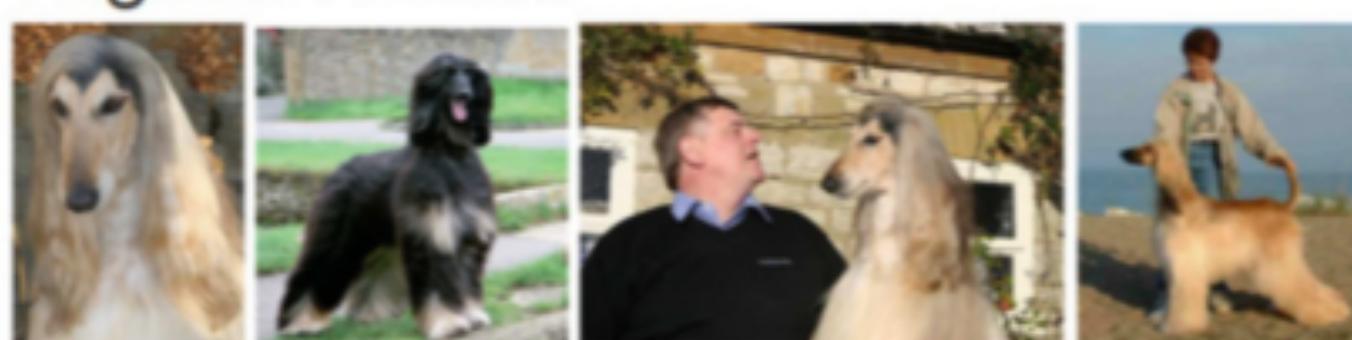
Blenheim Spaniel



Toy Terrier



Afghan Hound



Beagle



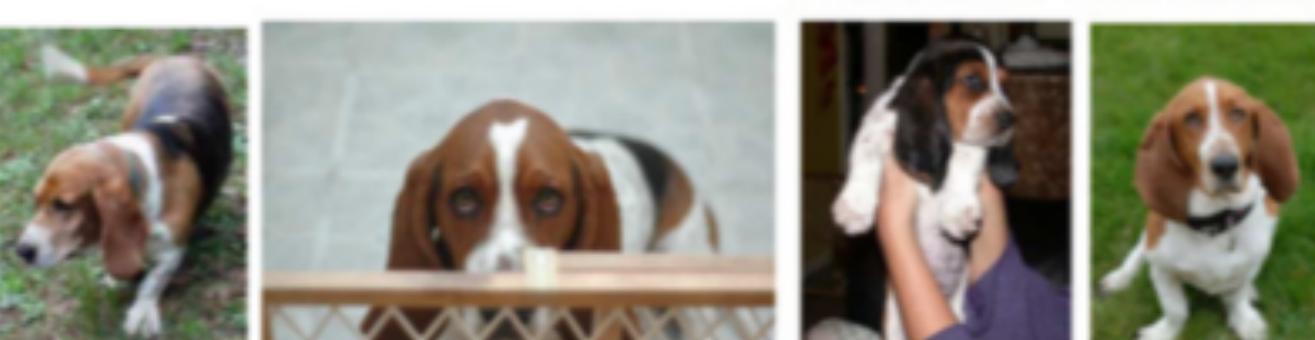
Papillon



Rhodesian Ridgeback



Basset Hound



Bloodhound



- Over 120 dog breeds in ImageNet dataset for image classification

- Non-expert labelers may not be aware of these **fine-grained** differences, leading to ***labeling errors***

- **E.g.,** the Caltech UCSD birds dataset has 4% labeling error (NABirds, Van horn et al. CVPR15)

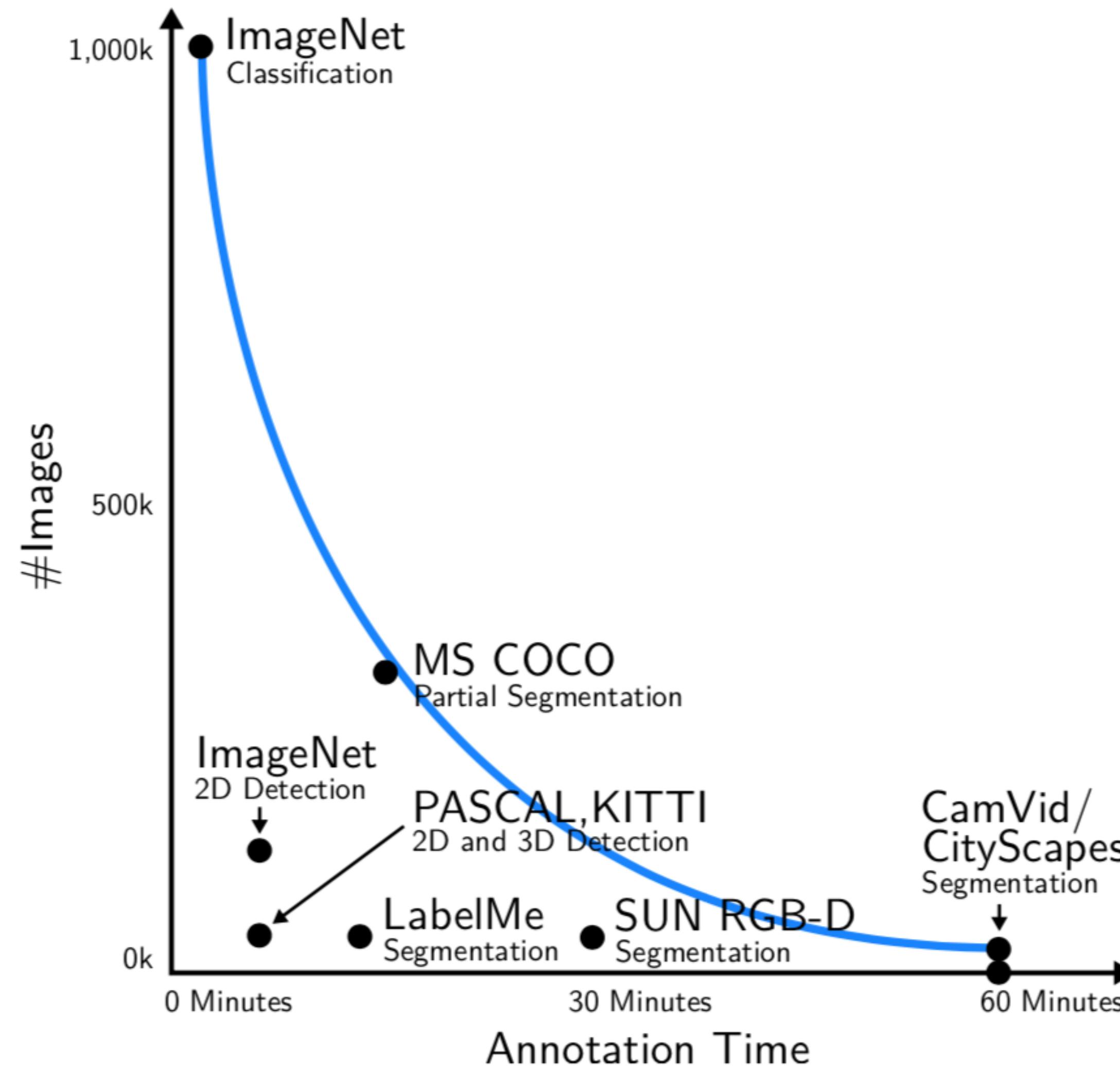
Dense Semantic and Instance Labels



“Cityscape” dataset: Labeling every pixel as person/road/sidewalk ...

Annotation time **60-90 minutes per image**

Annotate Everything — Expensive, doesn't Scale!



Motivation - Humans learn with little supervision

Provided with very few “labeled” examples (someone pointing something out to us explicitly), we can generalize quite well.

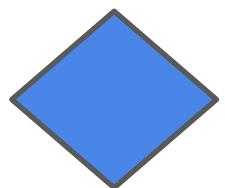
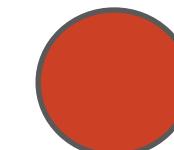


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 - Supervised vs Unsupervised Learning
 - Why not always label data?
- **Semi-supervised Learning**
 - Concepts
 - Example: pseudo-labels / self-training
 - Example: Distillation, Student/Teacher
- Self-supervised Learning
 - Concepts
 - Pretext tasks
 - Contrastive Learning

Semi-supervised Learning

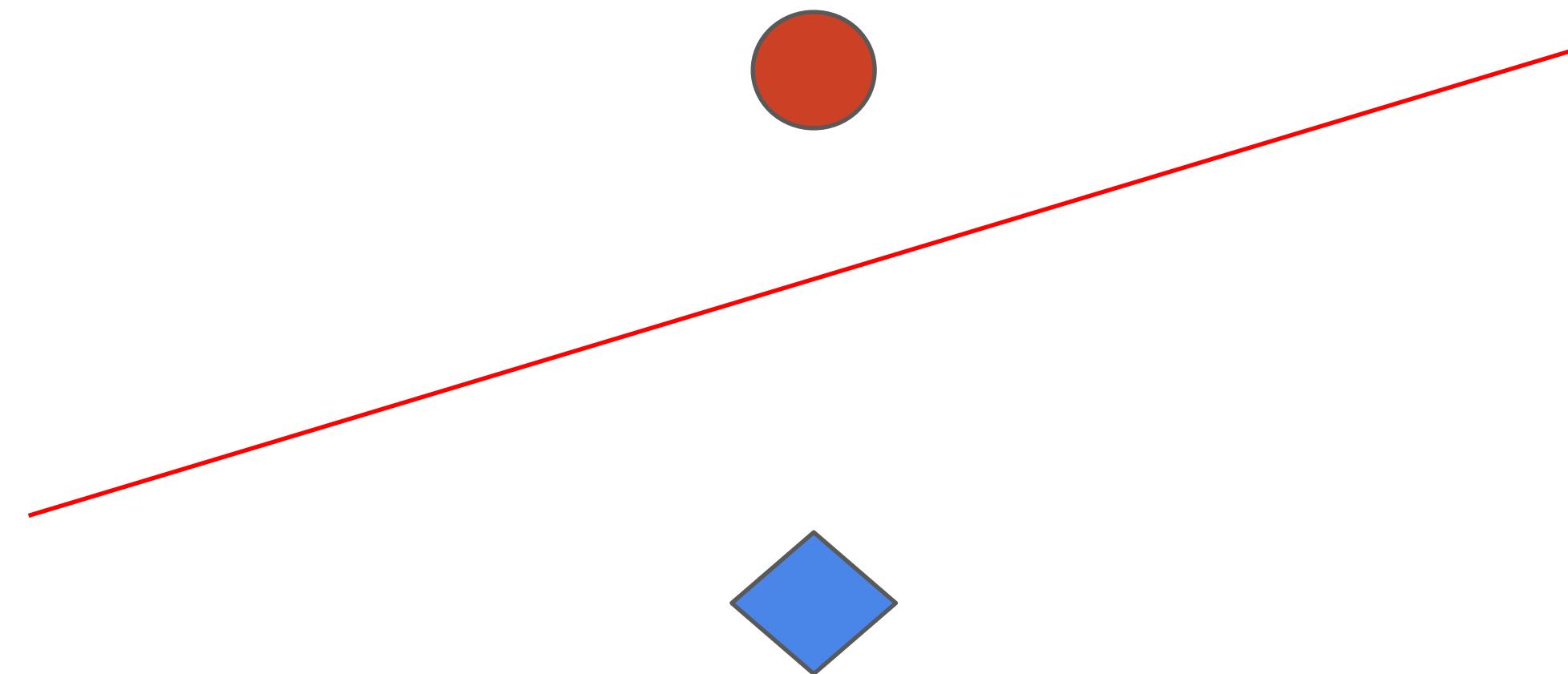
- Given a small amount of *labeled* data \mathcal{X}_L
- Given (usually) large amount of *unlabeled* data \mathcal{X}_U
- Can \mathcal{X}_U help us in getting a better model?



What is a good decision boundary for these points?

Semi-supervised Learning

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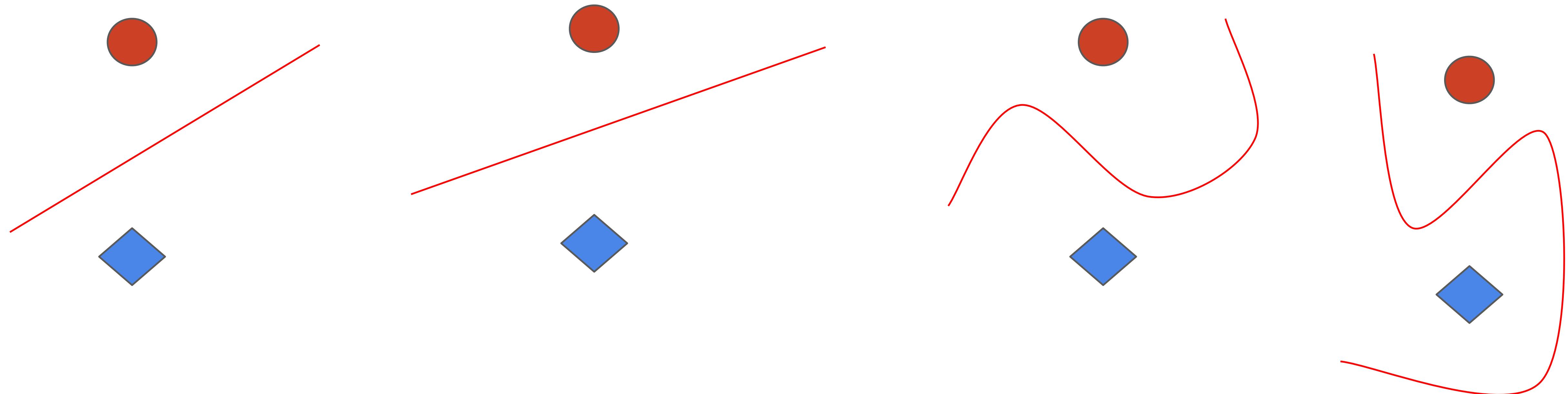


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Semi-supervised Learning

- Given a small amount of *labeled* data \mathcal{X}_L
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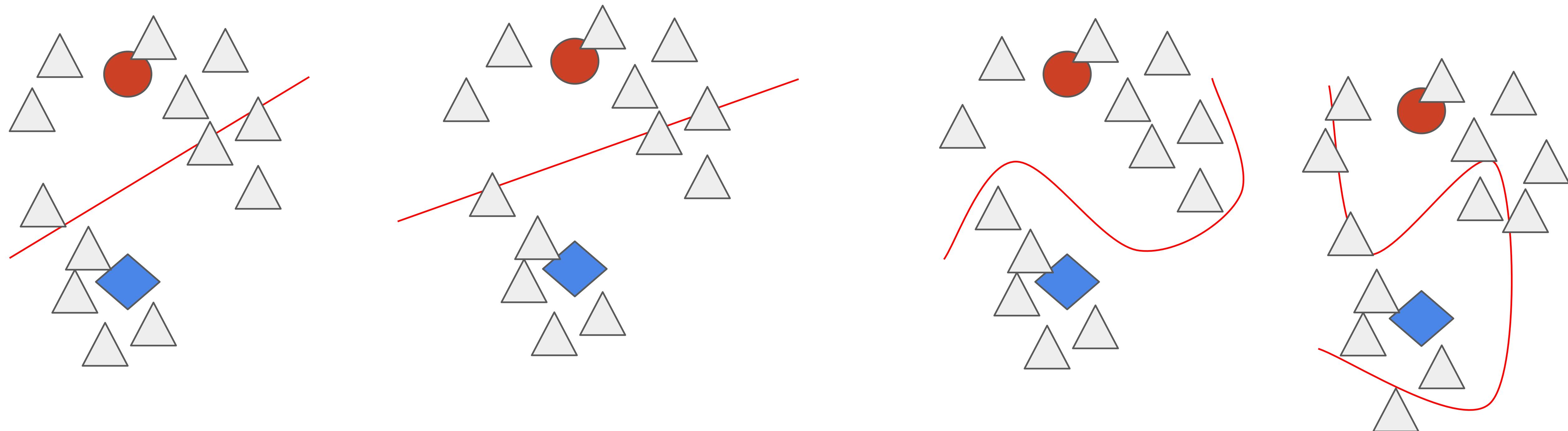
Which one is
your
favourite?



Semi-supervised Learning

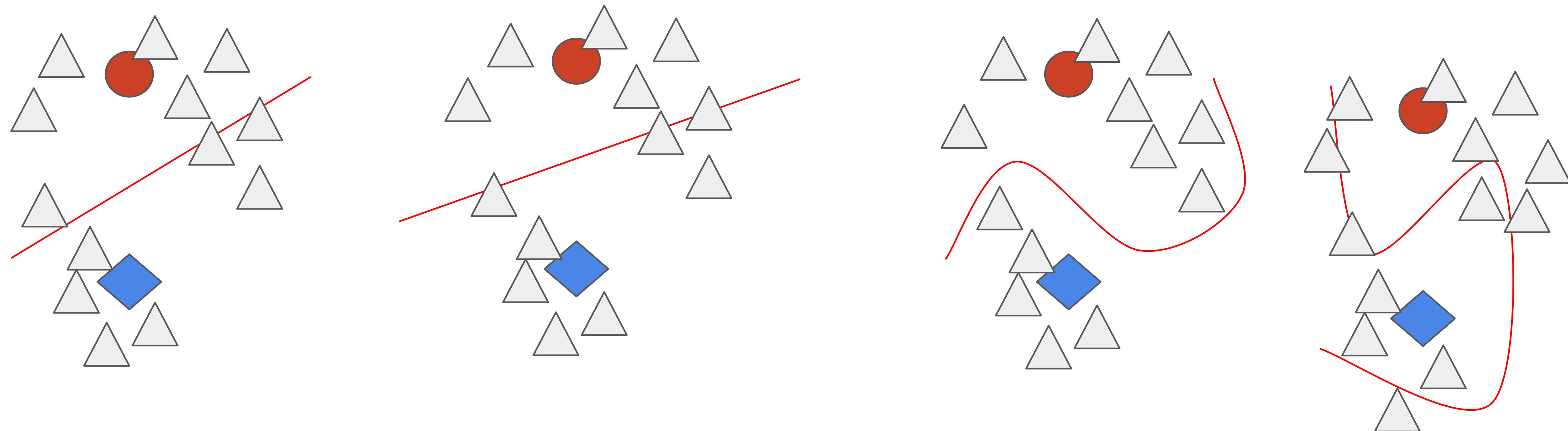
- Given a small amount of *labeled* data \mathcal{X}_L
- Given (usually) large amount of *unlabeled* data \mathcal{X}_U
- Can \mathcal{X}_U help us in getting a better model?

Now we see
some unlabeled
data points



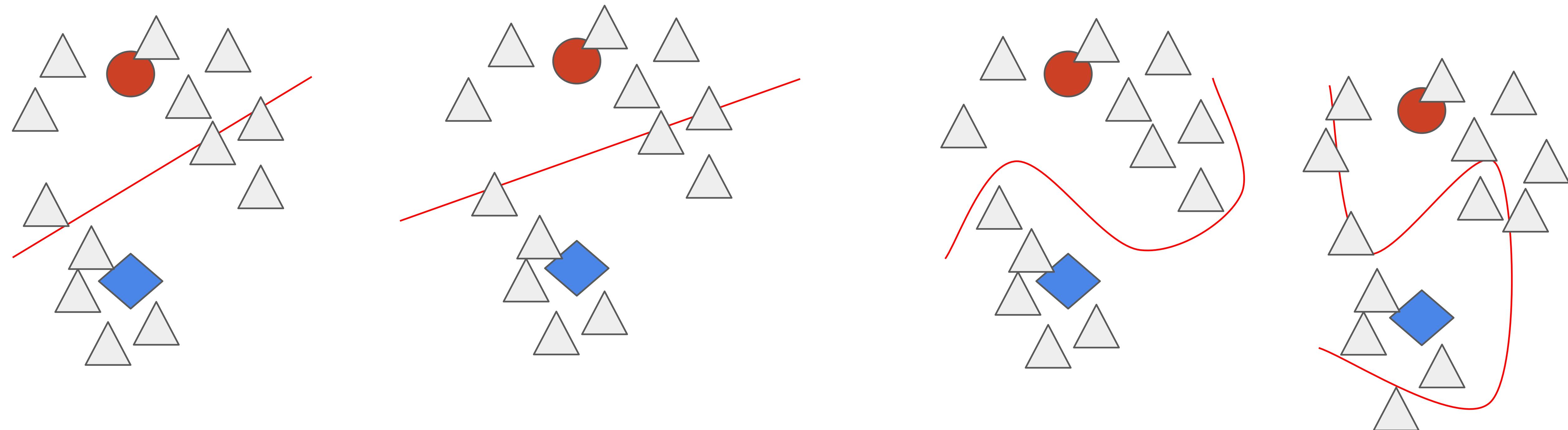
Semi-supervised Learning - intuitions

- Unlabeled samples tell us about $P(\mathbf{X})$, which is useful in the predictive posterior $P(y | \mathbf{X})$



Semi-supervised Learning - definitions

- **Smoothness assumption:** if x_1, x_2 are close, labels y_1, y_2 are also “close”
- **Low-density separation:** x_1, x_2 are separated by *low-density region* then labels are not “close”
- **Cluster assumption:** points in same cluster likely to have same label



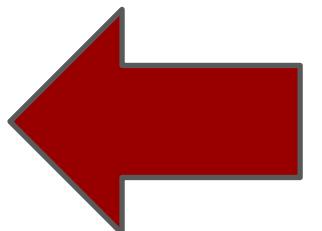
Semi-supervised Learning Approaches

- We will look at a *simple approach* to semi-supervised learning
- **Self-training or pseudo-labeling**
 - Age-old method
 - Surprisingly good with modern deep learning methods
 - But many variations ...

Self-training

- Assume: one's own high confidence predictions are correct!
- Train model f on $\mathcal{X}_L := \{x_L, y_L\}$
- Use f to predict “pseudo-labels” on $\mathcal{X}_U := \{x_u\}$
- Add $\{x_u, f(x_u)\}$ to labeled data
- Repeat

Self-training - variations

- Assume: one's own high confidence predictions are correct!
 - Train model f on $\mathcal{X}_L := \{x_L, y_L\}$
 - Use f to predict “pseudo-labels” on $\mathcal{X}_U := \{x_u\}$
 - Add $\{x_u, f(x_u)\}$ to labeled data
 - Repeat
- 1) Add only a few most confident predictions on X_U
2) Add all predictions on X_U
3) Add all predictions, weighted by the confidence of the prediction
....
- 

Self-training advantages

- The simplest semi-supervised method!
- It's a “wrapper” - the classifiers or models can be arbitrarily complex, we do not need to delve into those details to apply self-training
- Often quite good in practice, e.g. in natural language tasks
- Also some vision tasks ...

Data Distillation: Towards Omni-Supervised Learning

Ilija Radosavovic Piotr Dollár Ross Girshick Georgia Gkioxari Kaiming He
Facebook AI Research (FAIR)

Abstract

We investigate omni-supervised learning, a special regime of semi-supervised learning in which the learner exploits all available labeled data plus internet-scale sources of unlabeled data. Omni-supervised learning is lower-bounded by performance on existing labeled datasets, offering the potential to surpass state-of-the-art fully supervised methods. To exploit the omni-supervised setting, we propose data distillation, a method that ensembles predictions from multiple transformations of unlabeled data, using a single model, to automatically generate new training annotations. We argue that visual recognition models have recently become accurate enough that it is now possible to apply classic ideas about self-training to challenging real-world data. Our experimental results show that in the cases of human keypoint detection and general object detection, state-of-the-art models trained with data distillation surpass the performance of using labeled data from the COCO dataset alone.

1. Introduction

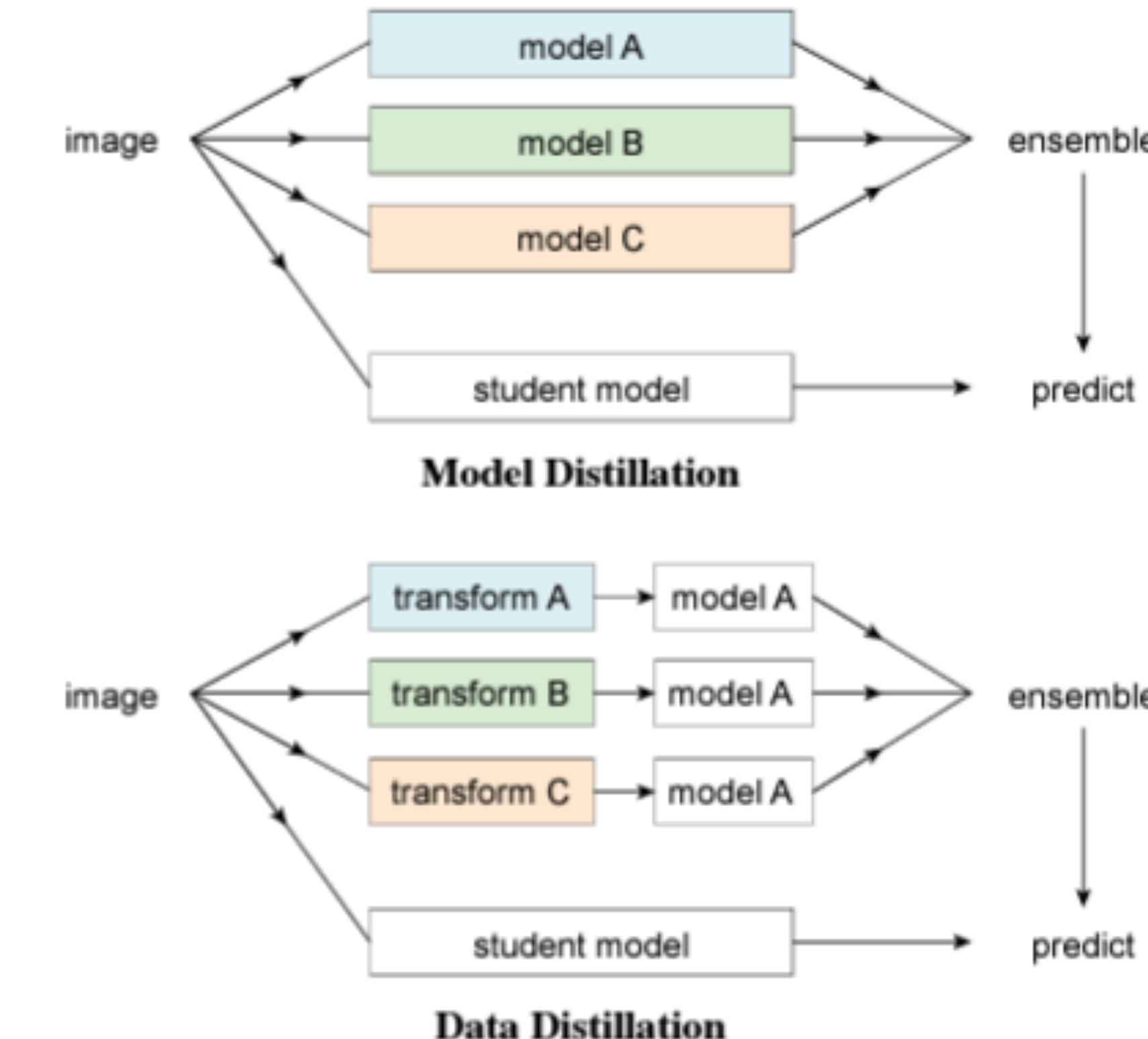


Figure 1. **Model Distillation [18] vs. Data Distillation.** In data distillation, ensembled predictions from a single model applied to multiple transformations of an unlabeled image are used as automatically annotated data for training a student model.

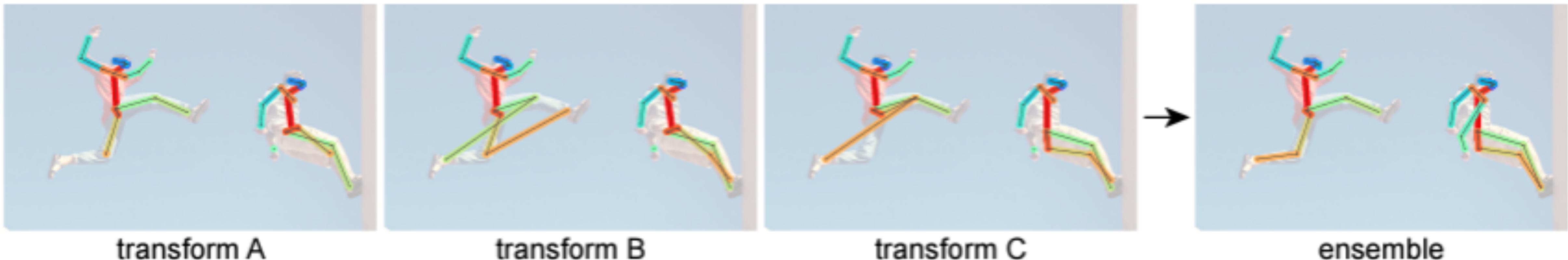


Figure 2. Ensembling keypoint predictions from multiple data transformations can yield a single superior (automatic) annotation.
For visualization purposes all images and keypoint predictions are transformed back to their original coordinate frame.

backbone	DD	AP	AP ₅₀	AP ₇₅	AP _M	AP _L
ResNet-50		65.1	86.6	70.9	59.9	73.6
ResNet-50	✓	66.6	87.3	72.6	61.6	75.0
ResNet-101		66.1	87.7	71.7	60.5	75.0
ResNet-101	✓	67.5	87.9	73.9	62.4	75.9
ResNeXt-101-32×4		66.8	87.5	73.0	61.6	75.2
ResNeXt-101-32×4	✓	68.0	88.1	74.2	63.1	76.2
ResNeXt-101-64×4		67.3	88.0	73.3	62.2	75.6
ResNeXt-101-64×4	✓	68.5	88.8	74.9	63.7	76.5

(c) **Large-scale, dissimilar-distribution data.** Data distillation (DD) is performed on `co-115` with labels and `s1m-180` without labels, comparing with the supervised counterparts trained on `co-115`.

Table 1. Data distillation for COCO keypoint detection. Keypoint AP is reported on COCO val2017.

Disadvantages of self-training?

Any guesses?

Disadvantages of self-training?

- Early mistakes can reinforce themselves
 - We have heuristic solutions, like discarding samples if the confidence of prediction falls below some threshold
- Convergence
 - Hard to say if these steps of self-train and repeat will converge

Domain shifts can have a large impact

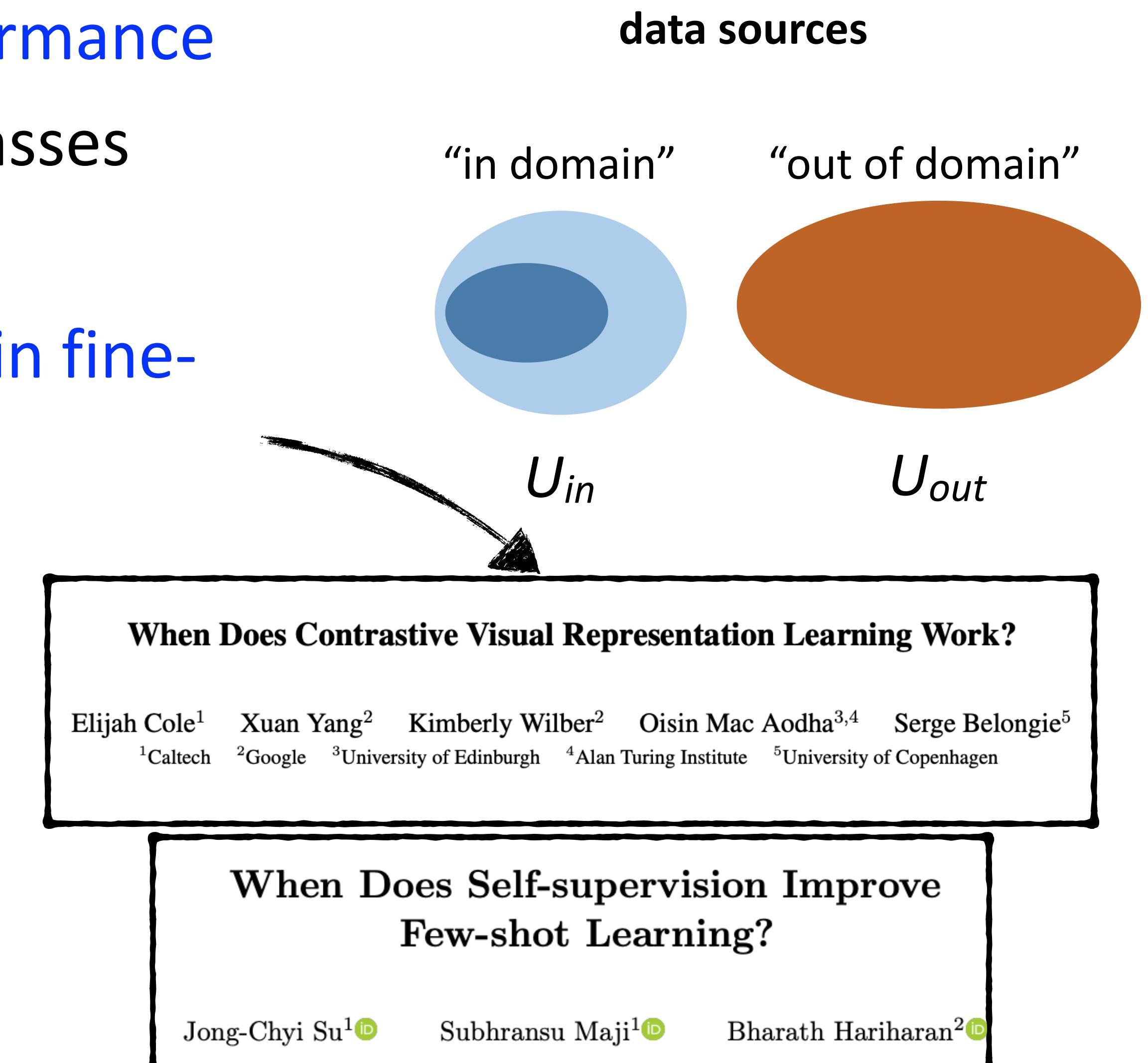
“Small” domain shifts can impact performance

- resolution, size/pose/class, novel classes

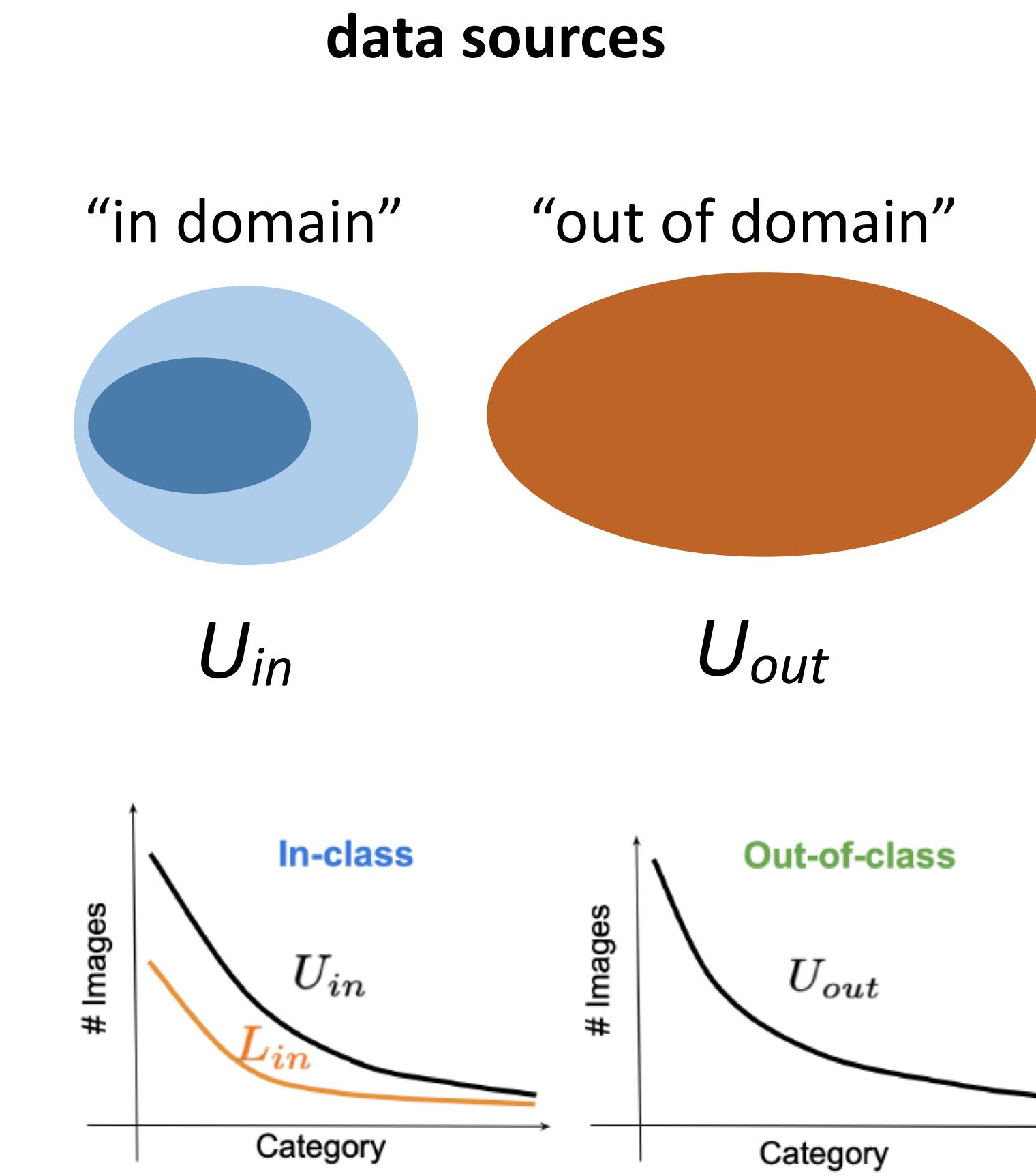
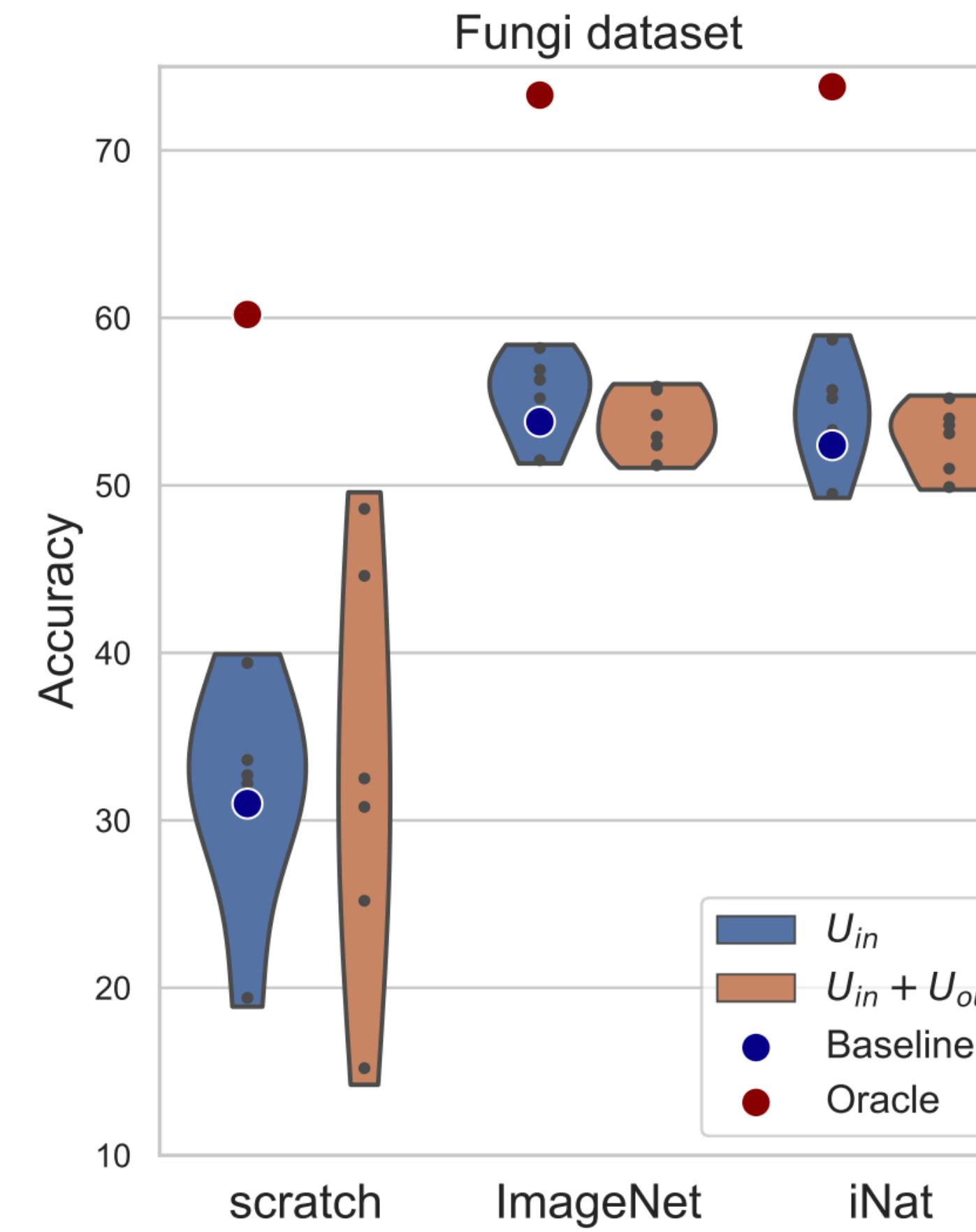
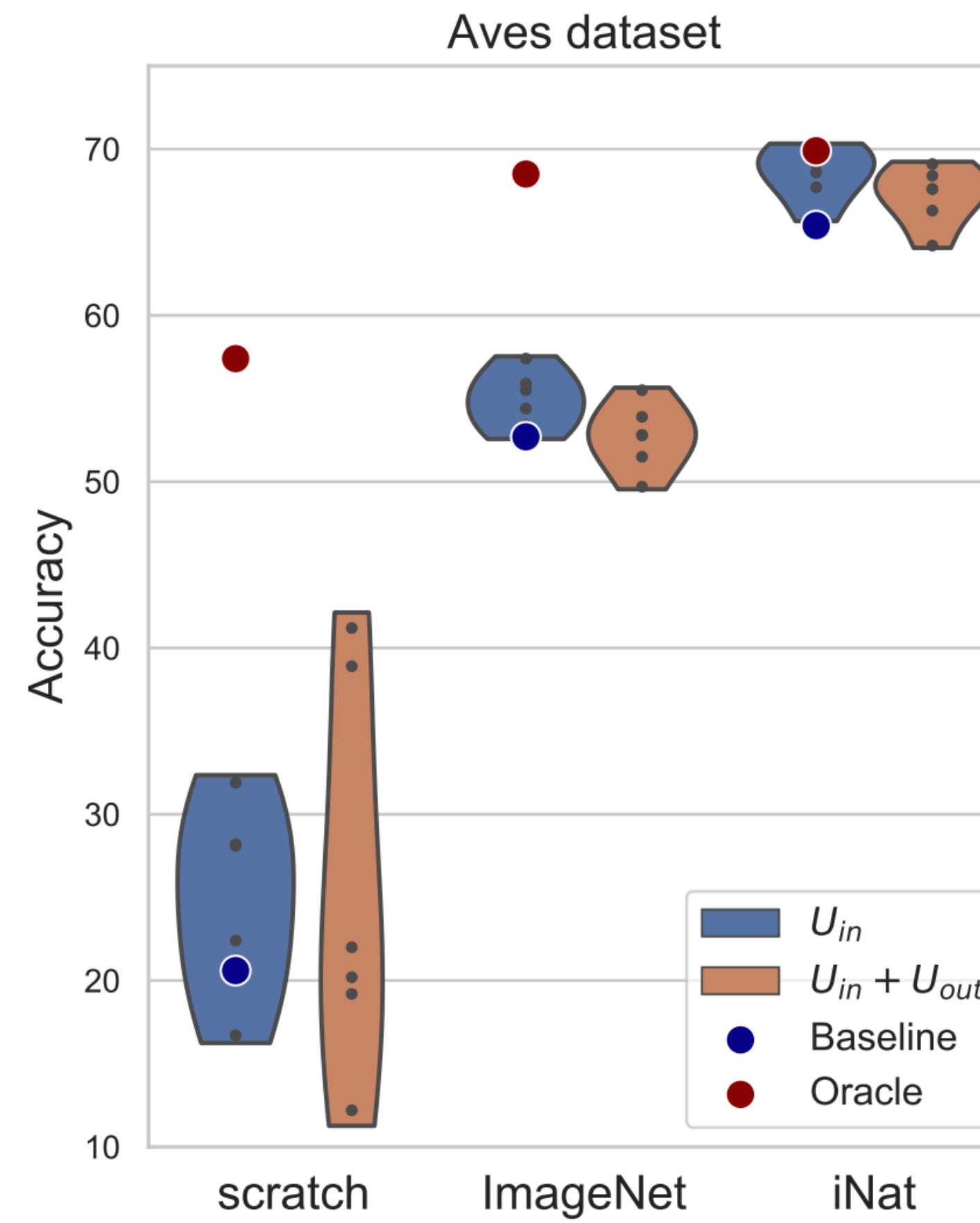
Self/semi-supervised learning is brittle in fine-grained domains

- difficult task, long-tailed data

Need “guardrails” against biased data



How robust is semi-supervised learning?



More pointers on semi-supervised learning

- Vast literature both in terms of theory and applications
- Other methods:
 - **Entropy minimization:** adds a loss that encourages the neural network model to make high confidence predictions (minimize “entropy”) on all unlabeled samples
 - [Mean Teacher](#), FixMatch, NoisyStudent, ...
 - Combine with methods to detect “out of domain” data

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Self-supervised learning: Outline

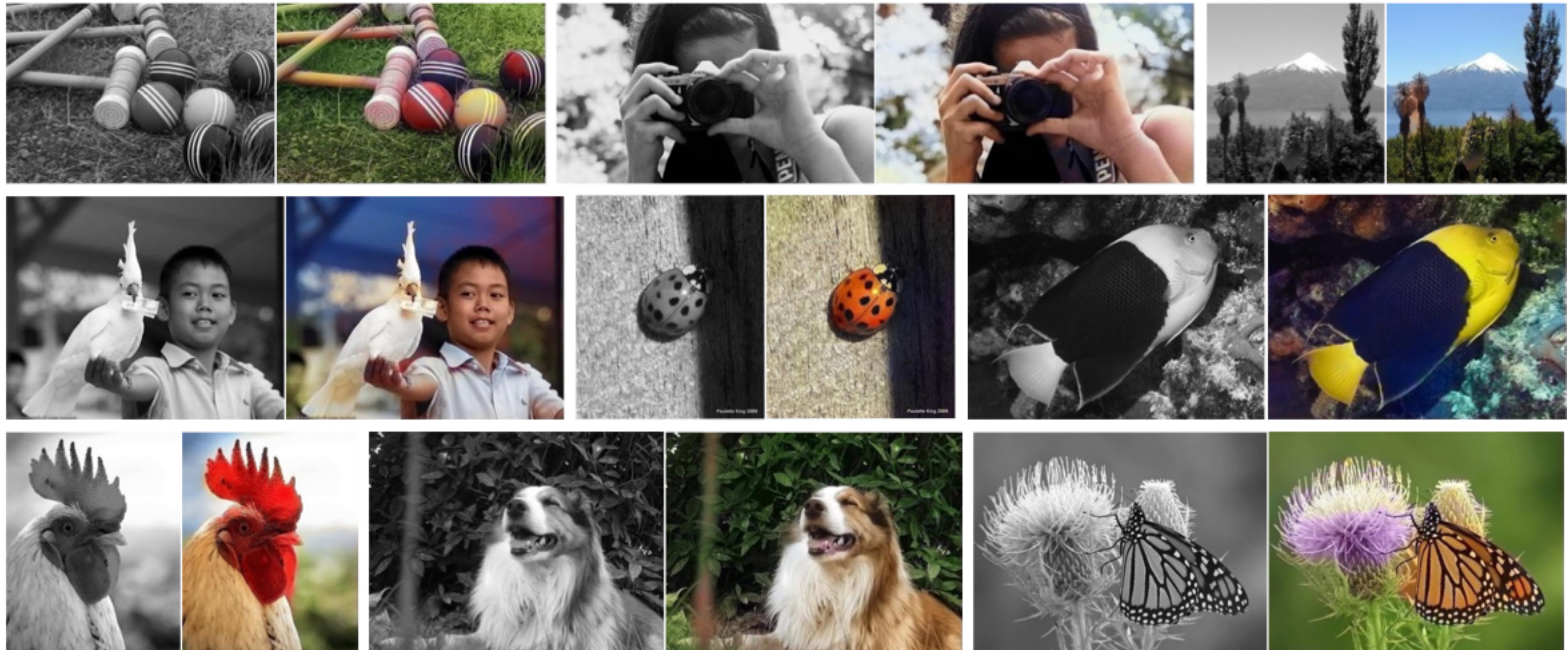
- Data prediction
 - Colorization
- Transformation prediction
 - Context prediction, jigsaw puzzle solving, rotation prediction
 - “Siamese” methods
 - Contrastive methods
 - Non-contrastive methods
- Self-supervision beyond still images
 - 3D, audio, video, language

Self-supervision as data prediction

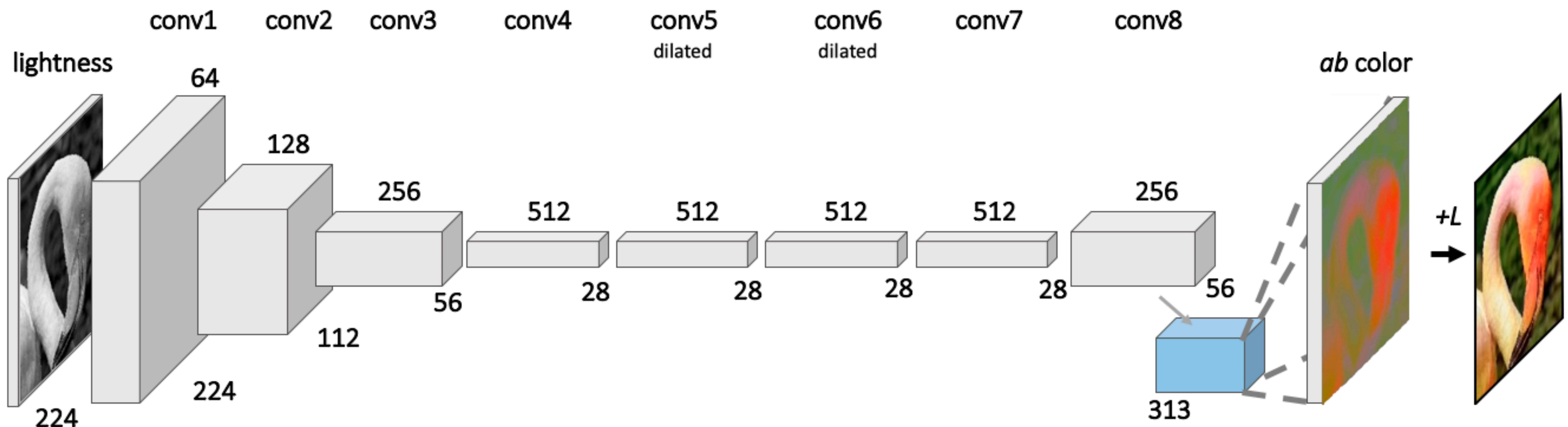


- Colorization
- Inpainting
- Future prediction
- ...

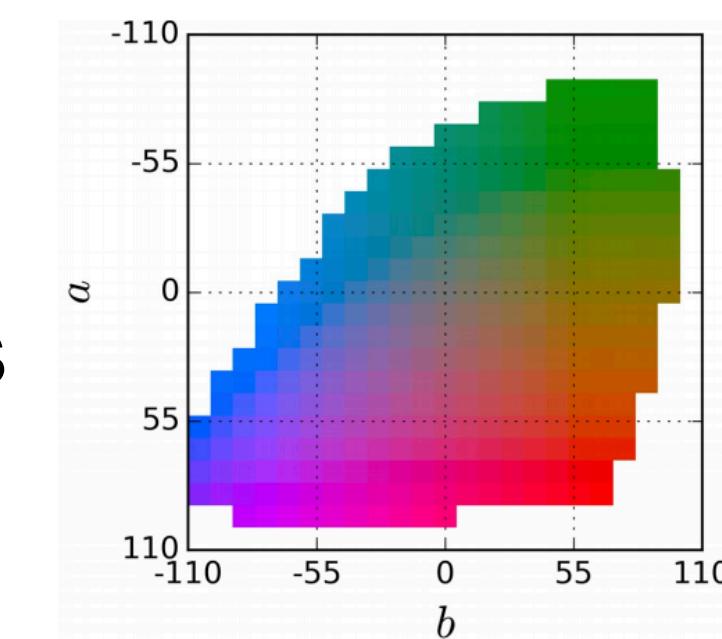
Colorization



Colorization: Architecture



At each spatial location, predict probability distribution over 313 quantized (a,b) values



Self-supervised learning: Outline

- Data prediction
 - Colorization
- Transformation prediction

Self-supervision by transformation prediction

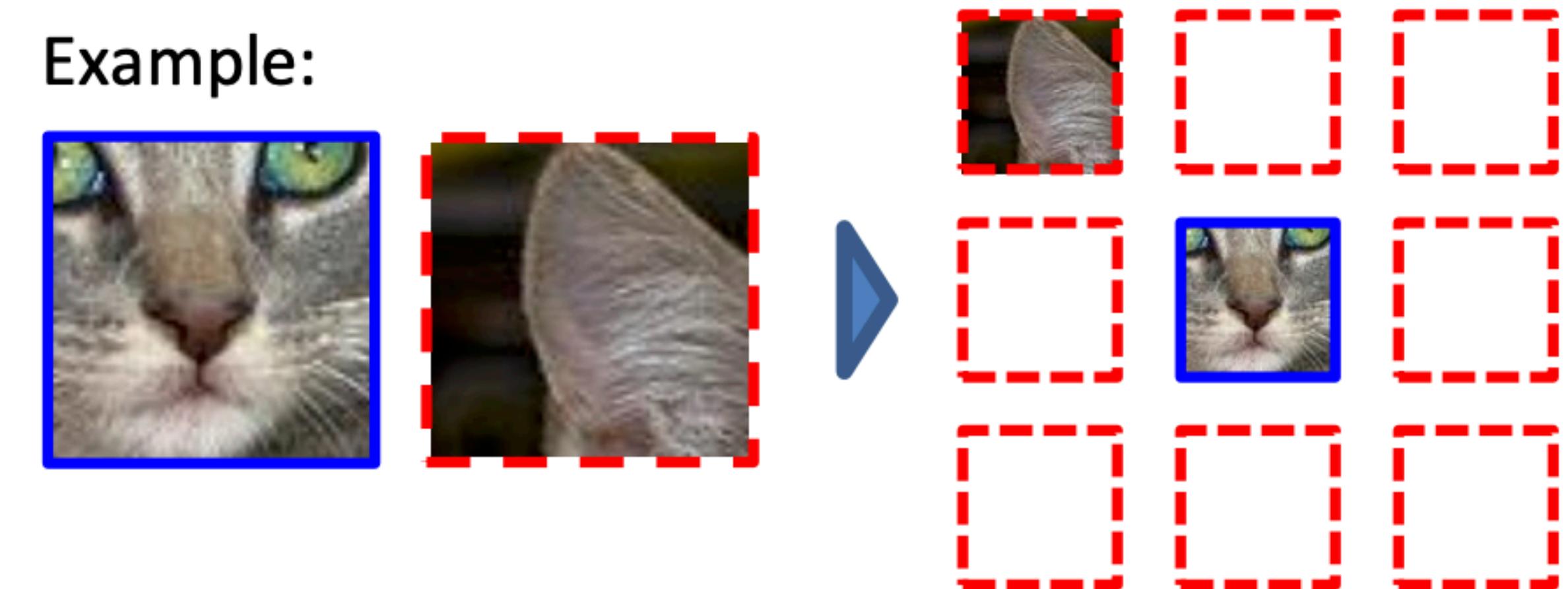


- Context prediction
- Jigsaw puzzle solving
- Rotation prediction

Context prediction

- *Pretext task:* randomly sample a patch and one of 8 neighbors
- Guess the spatial relationship between the patches

Example:



Question 1:



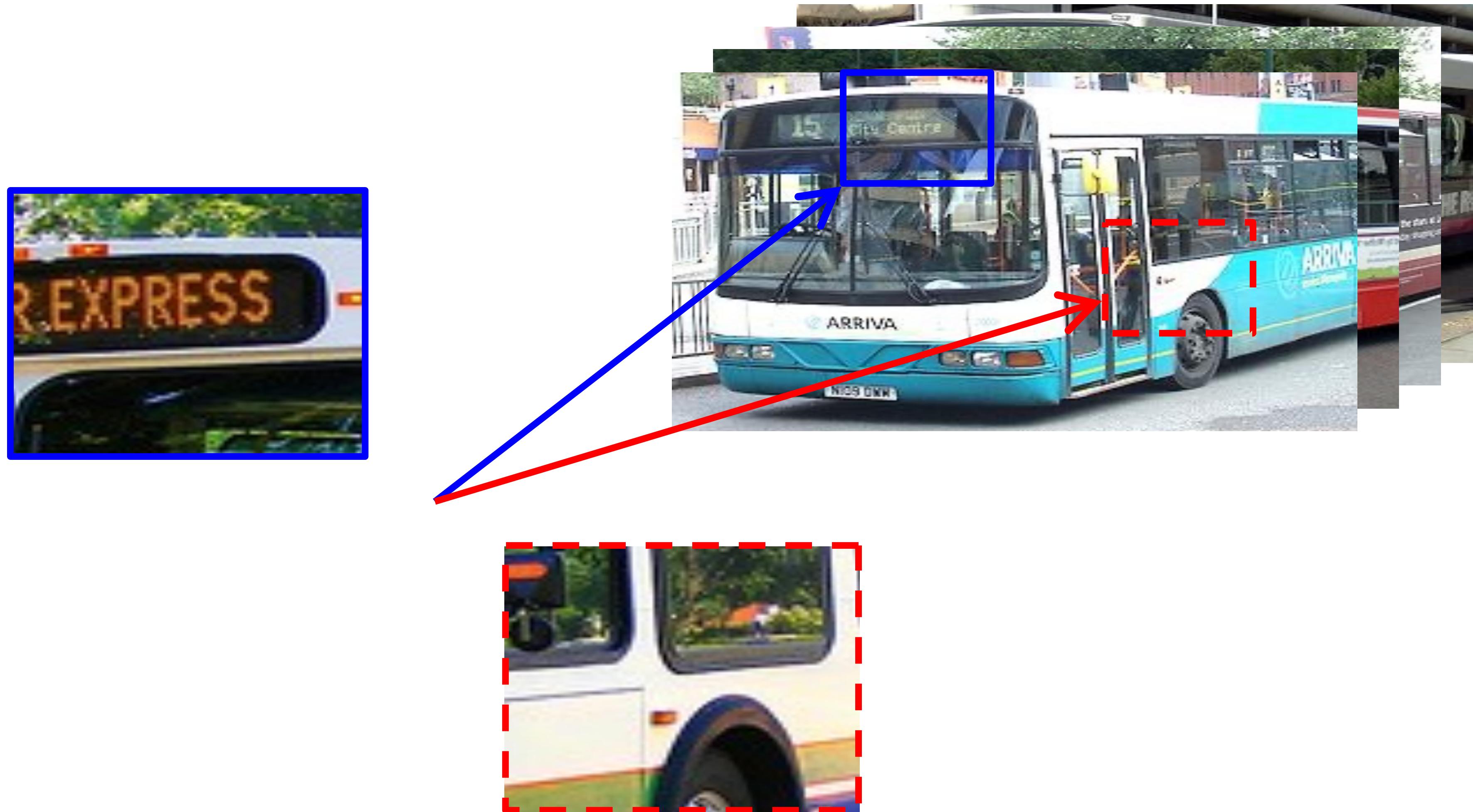
A: Bottom right

Question 2:



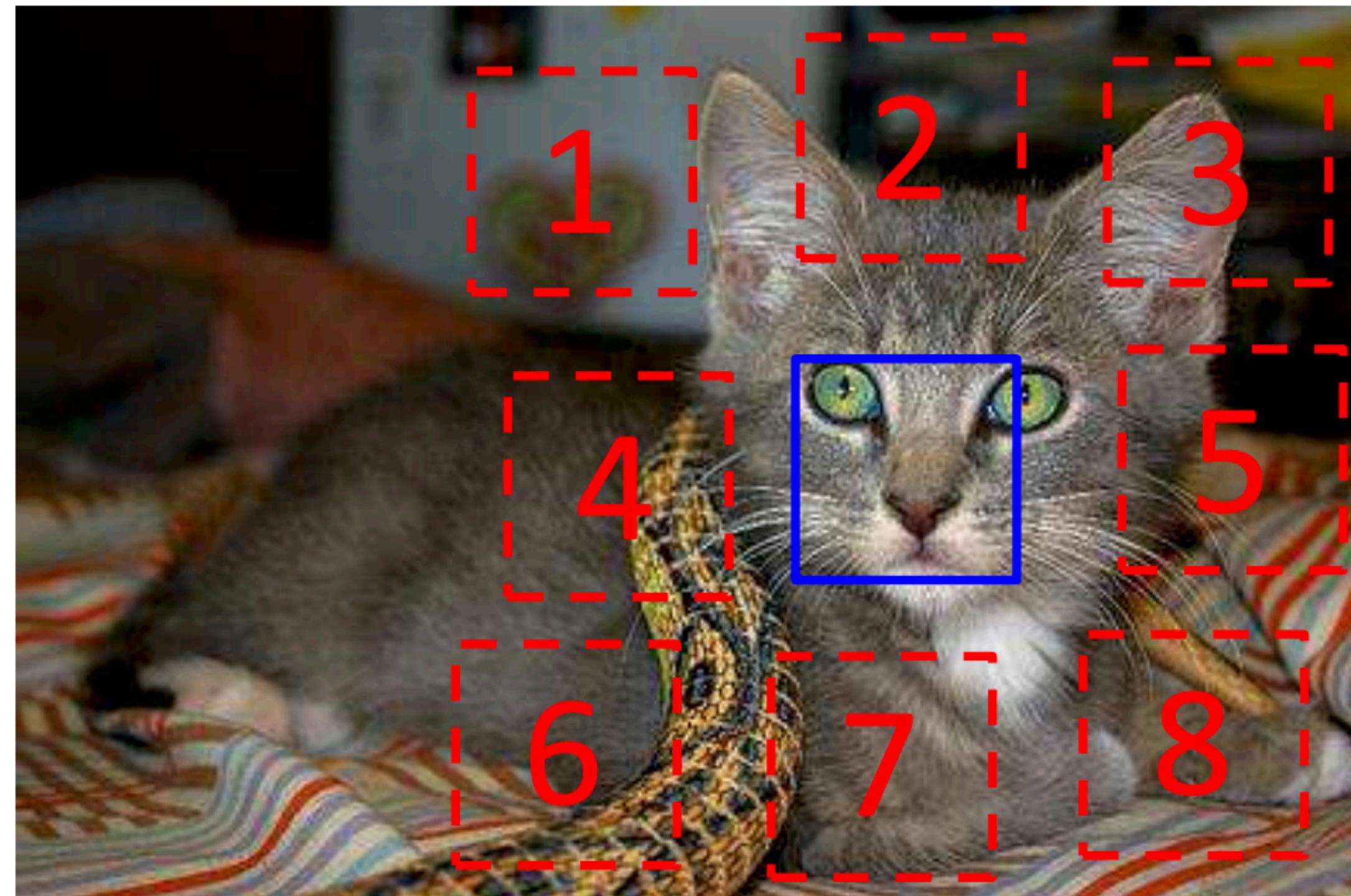
A: Top center

Context prediction: Semantics from a non-semantic task



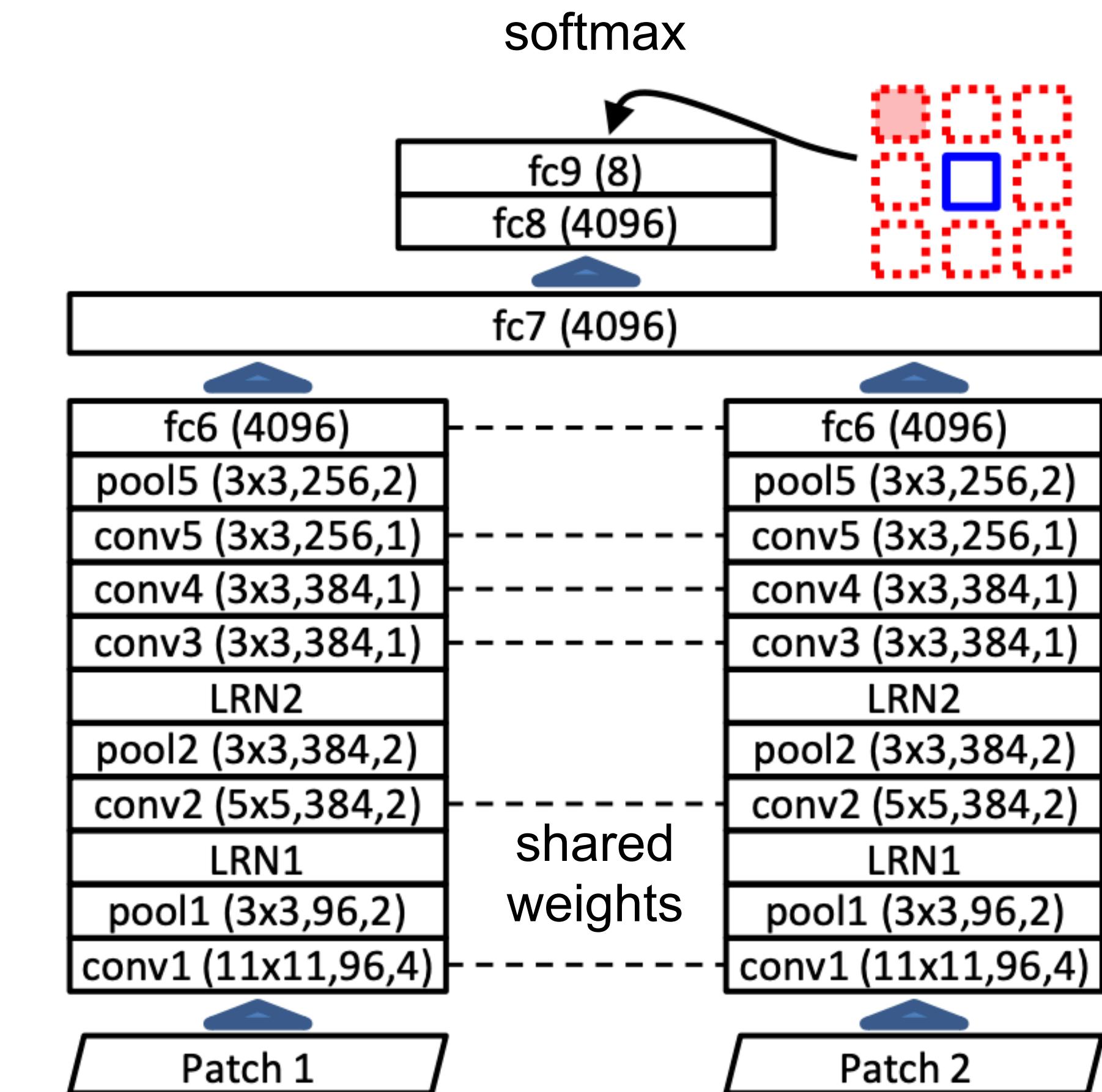
Source: A. Efros

Context prediction: Details



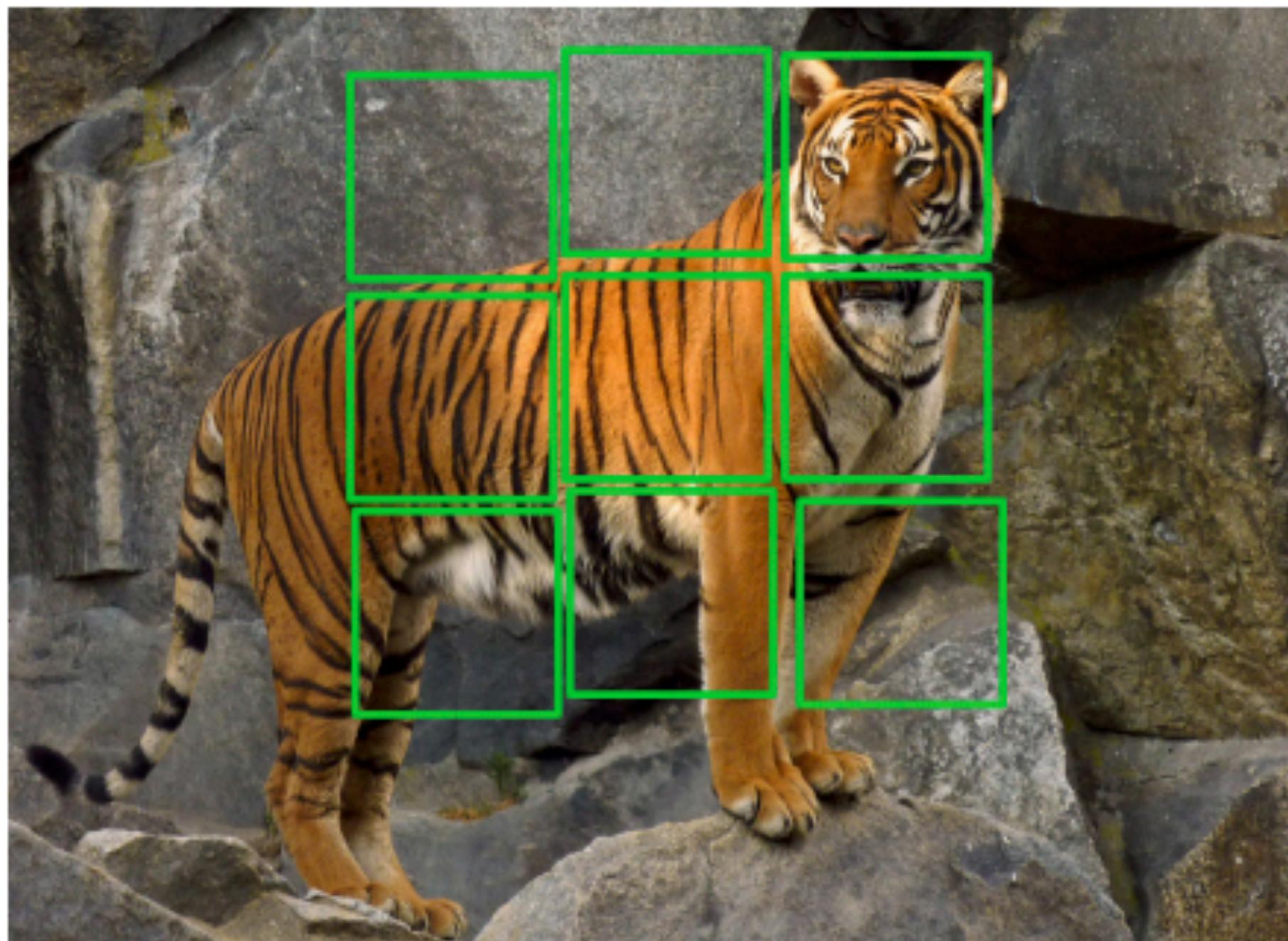
Prevent “cheating”: sample patches with gaps, pre-process to overcome chromatic aberration

AlexNet-like architecture

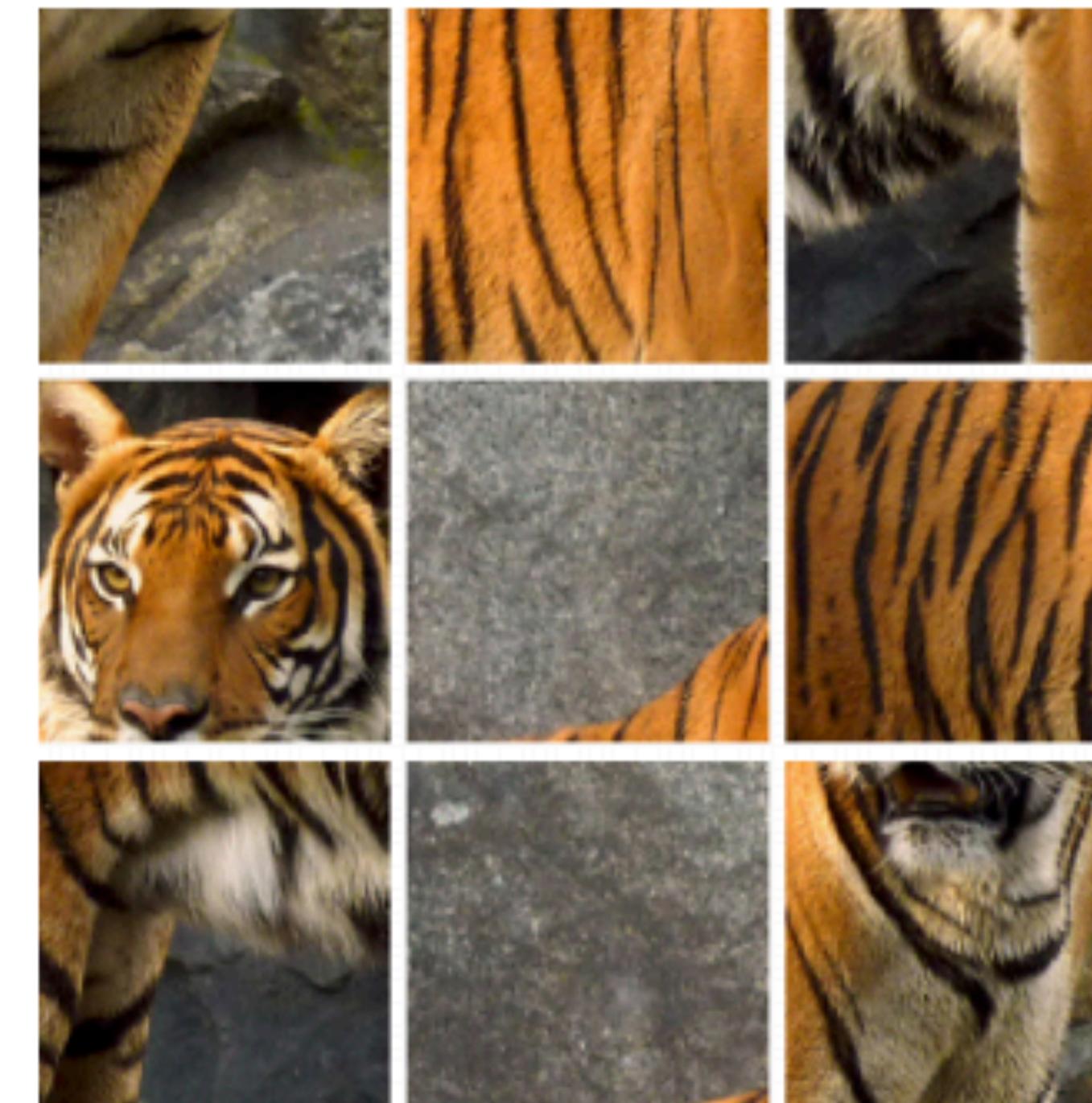


Jigsaw puzzle solving

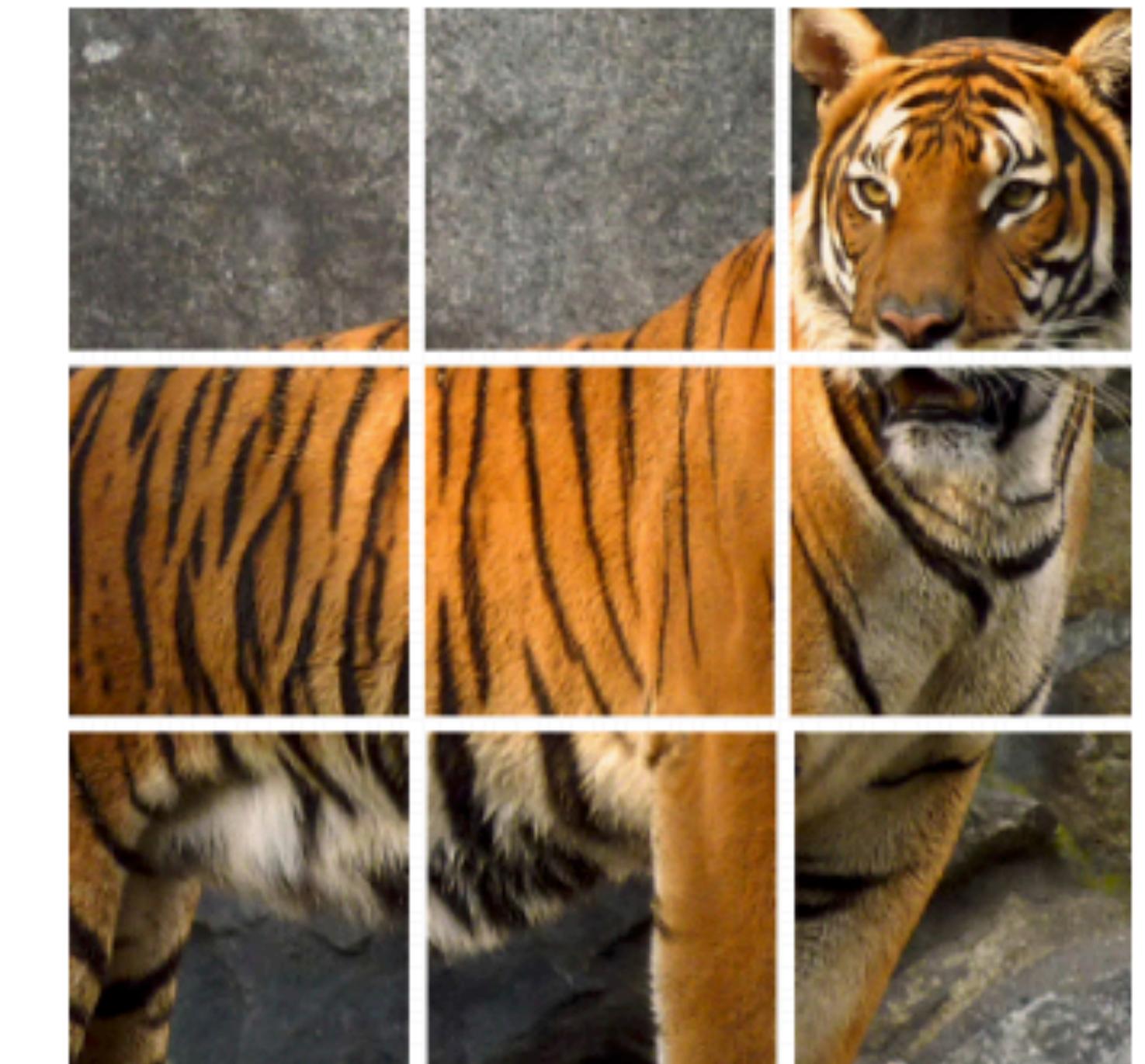
Crop out tiles



Shuffle



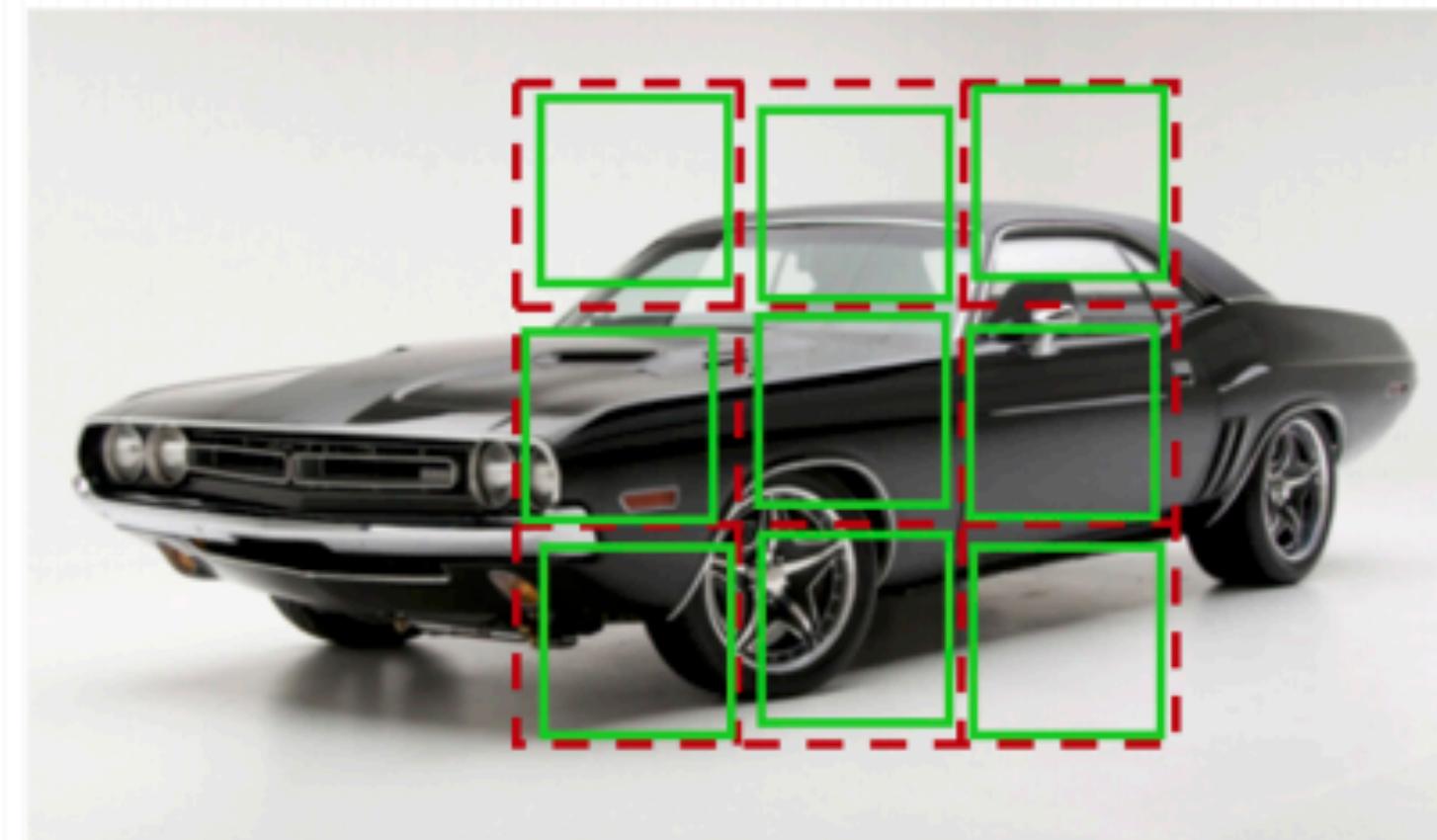
Pretext task: reassemble



Claim: jigsaw solving is easier than context prediction, trains faster, transfers better

Jigsaw puzzle solving: Details

Context free network (CFN)

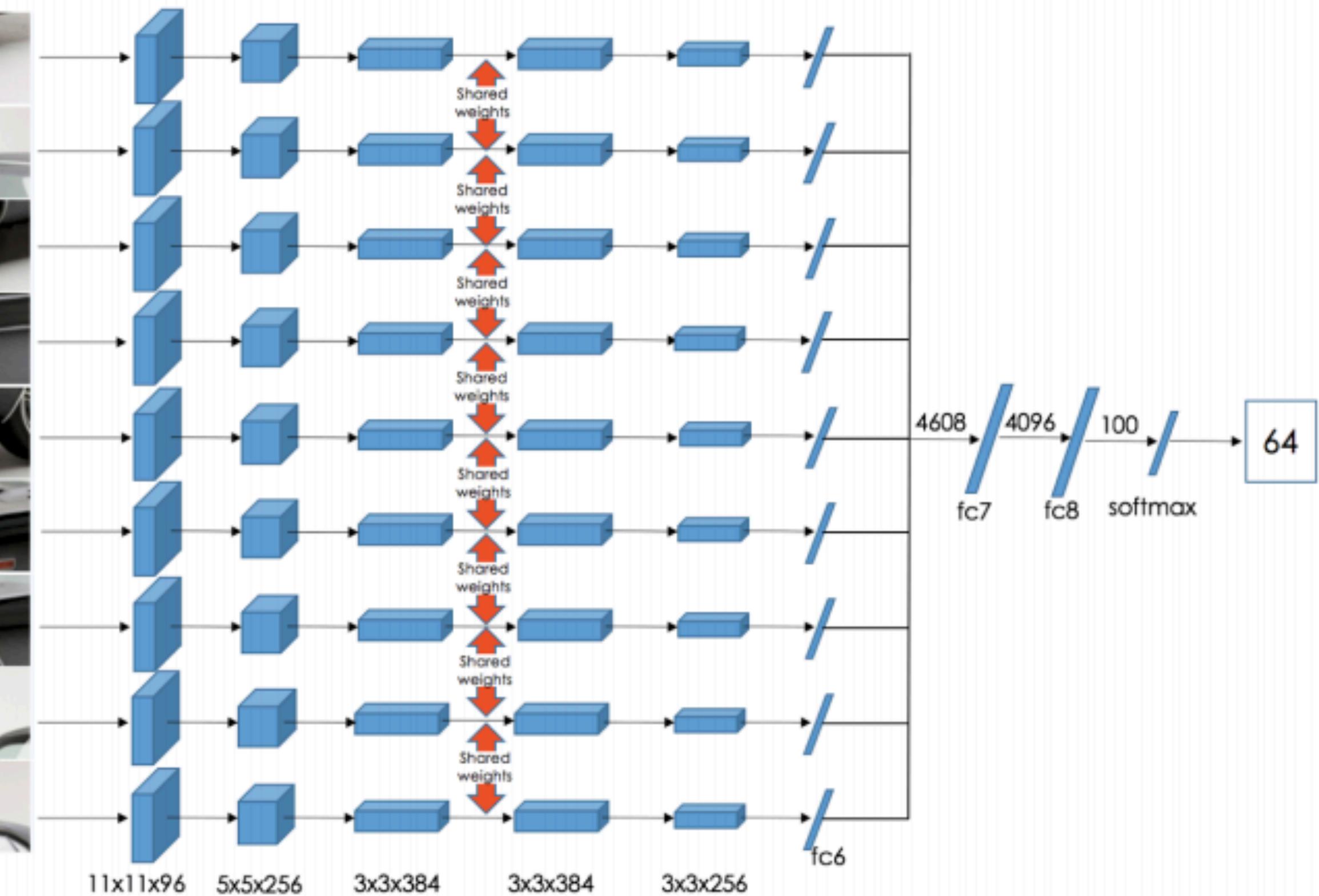
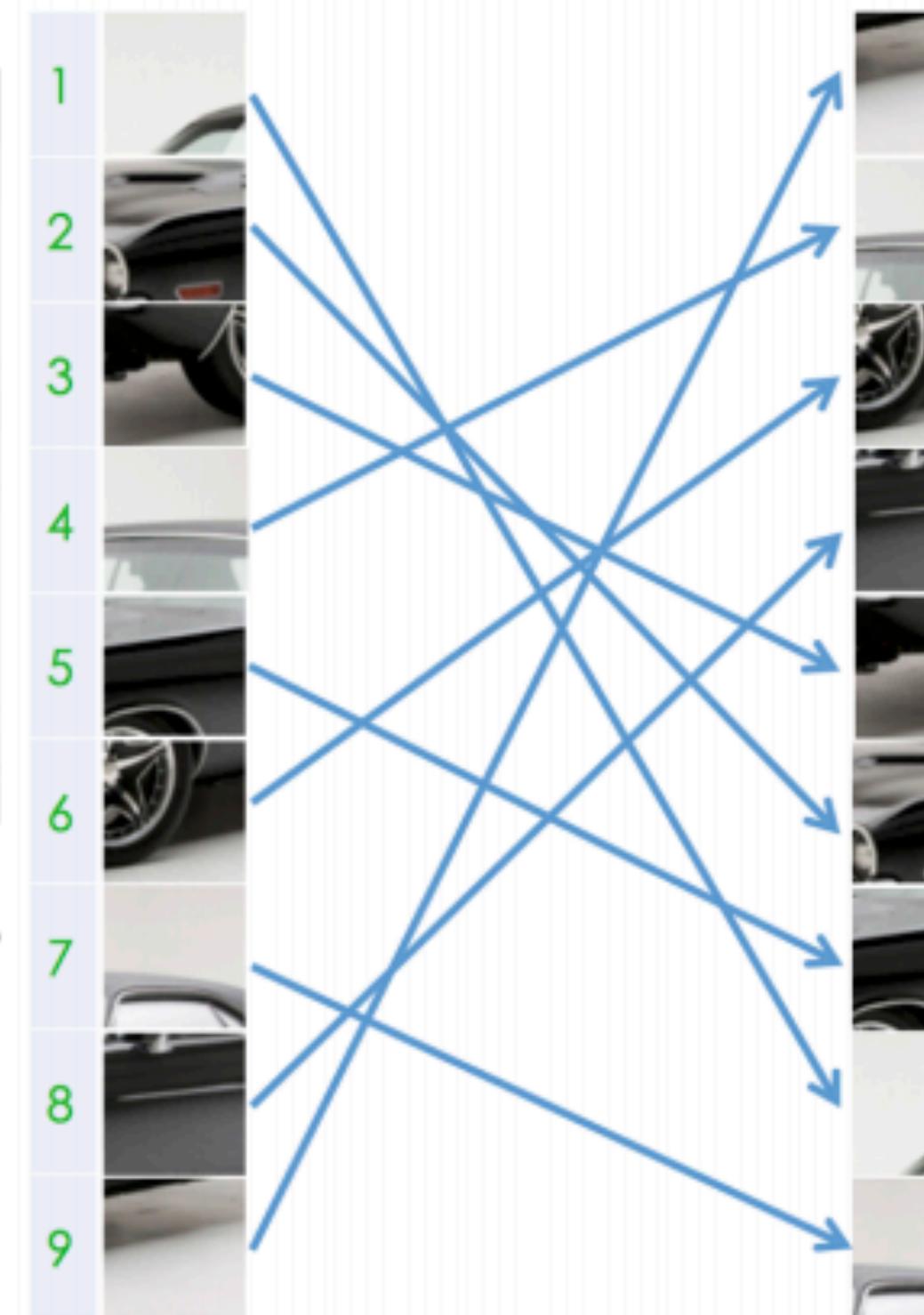


Permutation Set

index	permutation
64	9,4,6,8,3,2,5,1,7

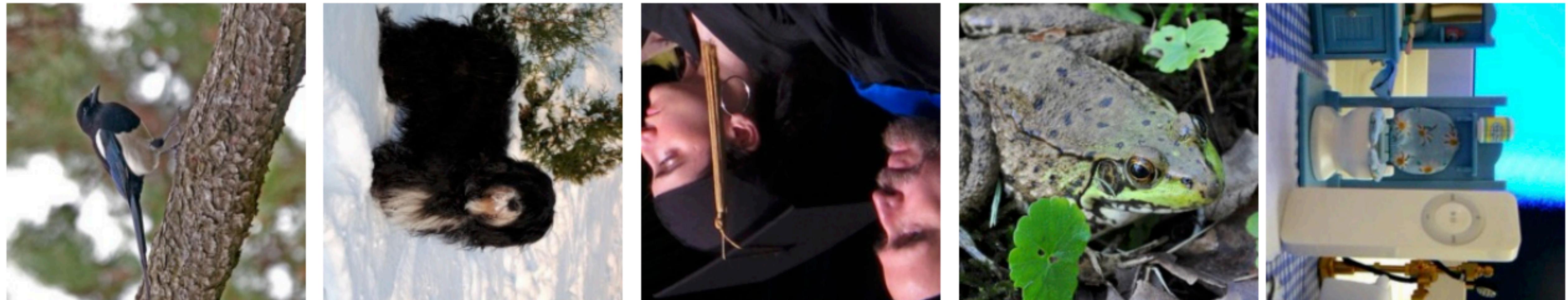
Reorder patches according to
the selected permutation

Predetermined set of
1000 permutations
(out of 362,880
possible)

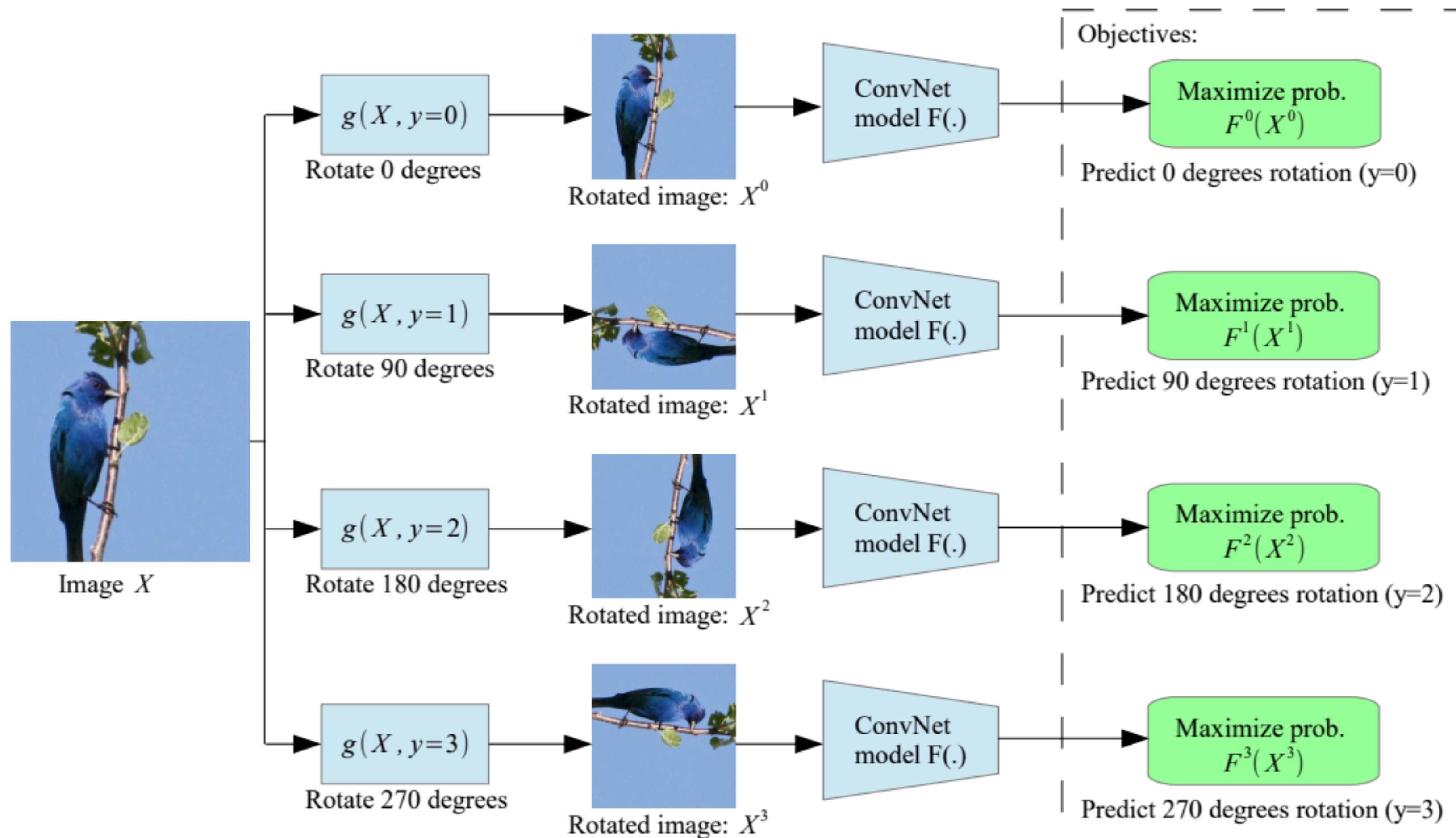


Rotation prediction

- Pretext task: recognize image rotation (0, 90, 180, 270 degrees)



Rotation prediction



During training, feed in all four rotated versions of an image in the same mini-batch

PASCAL VOC Transfer Results

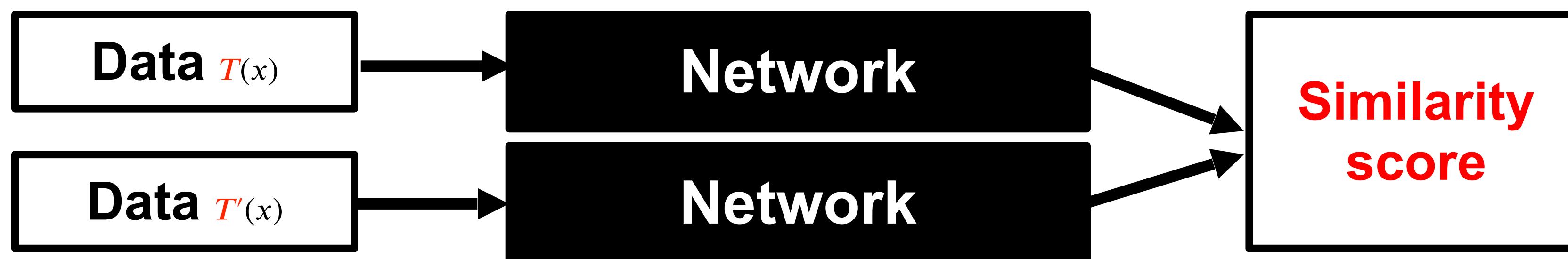
Method	Classification	Detection (mAP)	Segmentation (mIoU)
Supervised (ImageNet)	79.9	56.8	48.0
Colorization	65.6	46.9	35.6
Context	65.3	51.1	
Jigsaw	67.6	53.2	37.6
Rotation	73.0	54.4	39.1

Self-supervised learning: Outline

- Data prediction
 - Colorization
- Transformation prediction
 - Context prediction, jigsaw puzzle solving, rotation prediction
- “Siamese” methods

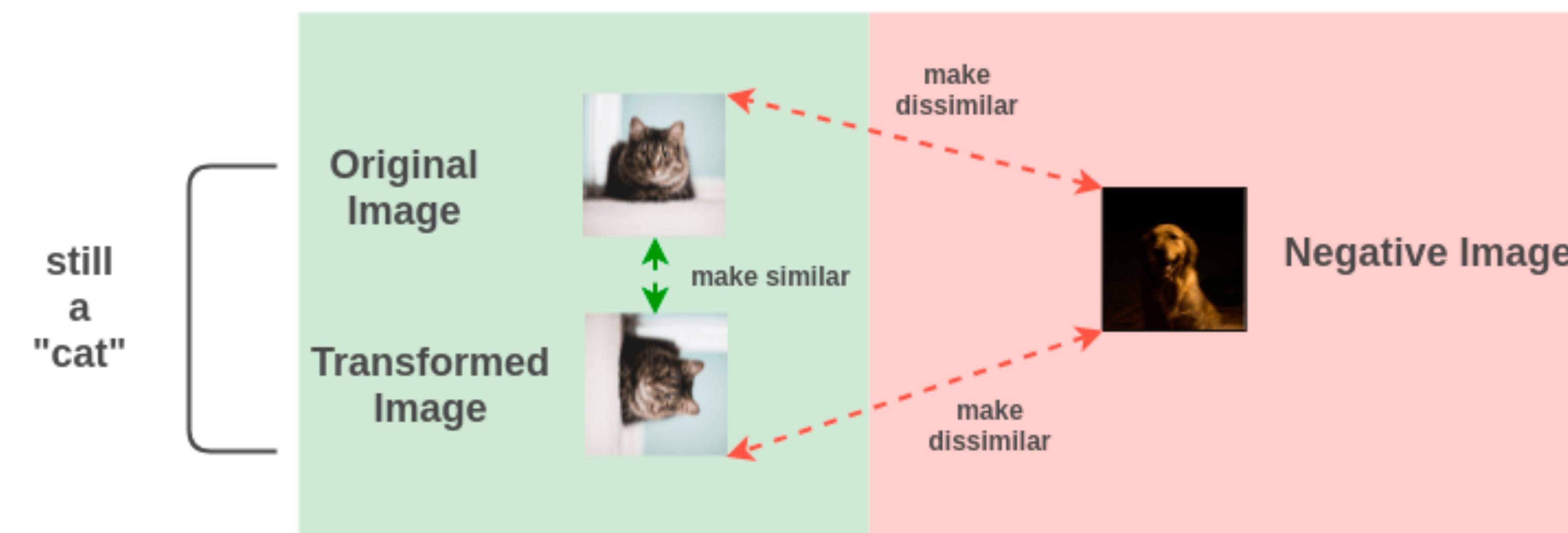
“Siamese” methods

- Extract representations from two transformed versions of a data point, encourage these representations to be similar (or to have other desirable properties)
 - **Contrastive methods:** train using both positive (similar) and negative (dissimilar) pairs
 - **Non-contrastive methods:** train with only positive examples



Contrastive methods

- Encourage representations of transformed versions of the same image to be the same and different images to be different



Contrastive loss formulation

- Given:
 - Query point x
 - Positive sample x^+ : version of x subjected to a random transformation or augmentation (cropping, rotation, color change, etc.)
 - Negative samples x^-

 x  x^+  x^- 

Contrastive loss formulation

- Given: query x , positive sample x^+ , negative samples x^-
- Measure similarity by dot product of L2-normalized feature representations:

$$\text{sim}(x, y) = \frac{f(x)}{\|f(x)\|_2} \cdot \frac{f(y)}{\|f(y)\|_2}$$

- Contrastive loss:** make x similar to x^+ , dissimilar from x^- :

$$l(x, x^+) = -\log \frac{\exp(\text{sim}(x, x^+)/\tau)}{\exp(\text{sim}(x, x^+)/\tau) + \sum_{j=1}^N \exp(\text{sim}(x, x_j^-)/\tau)}$$

- Intuitively, this is the loss of a softmax classifier that tries to classify x as x^+

Mechanisms for obtaining negative samples

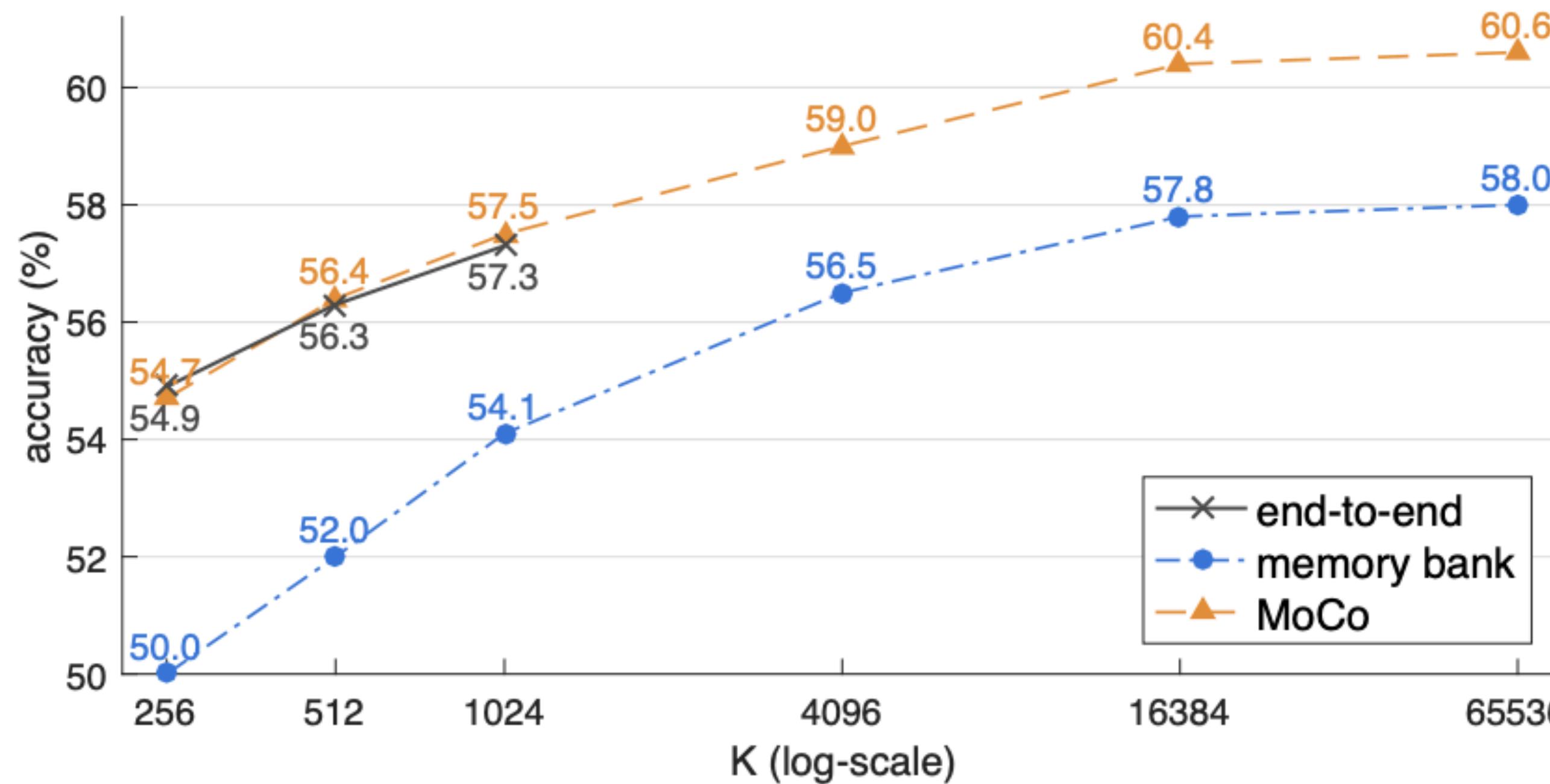
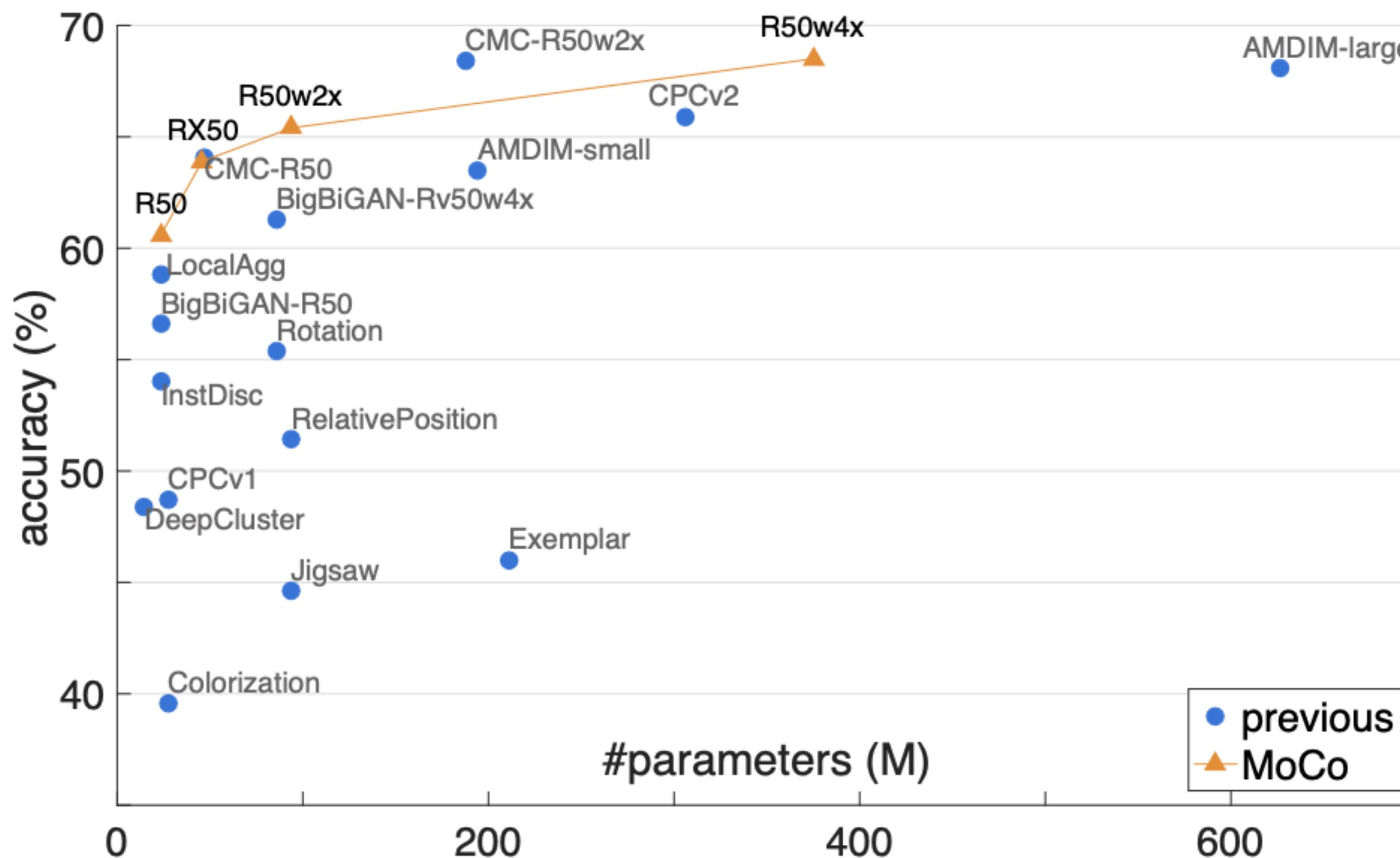


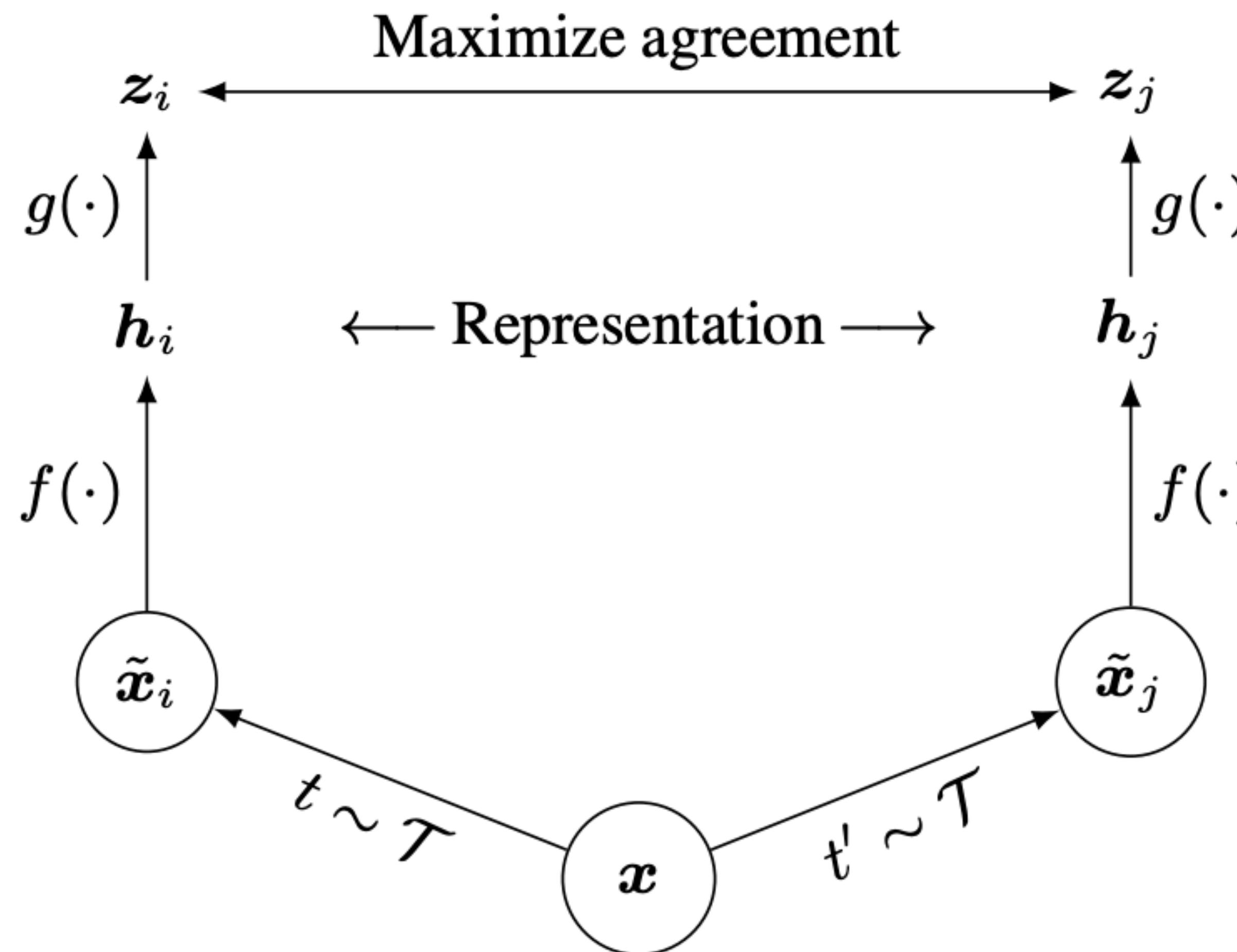
Figure 3. Comparison of three contrastive loss mechanisms under the ImageNet linear classification protocol. We adopt the same pretext task (Sec. 3.3) and only vary the contrastive loss mechanism (Figure 2). The number of negatives is K in memory bank and MoCo, and is $K - 1$ in end-to-end (offset by one because the positive key is in the same mini-batch). The network is ResNet-50.

MoCo results

Comparison on linear ImageNet classification
(supervised accuracy above 75%)



SimCLR



- Instead of memory bank or queue, use large mini-batch size (on cloud TPU)
- Introduce nonlinear *projection* (g) between representation (h) and feature used for computing contrastive loss (z)

SimCLR

- Performed extensive ablation study of data augmentations
- Found that composing multiple augmentations gives the best results

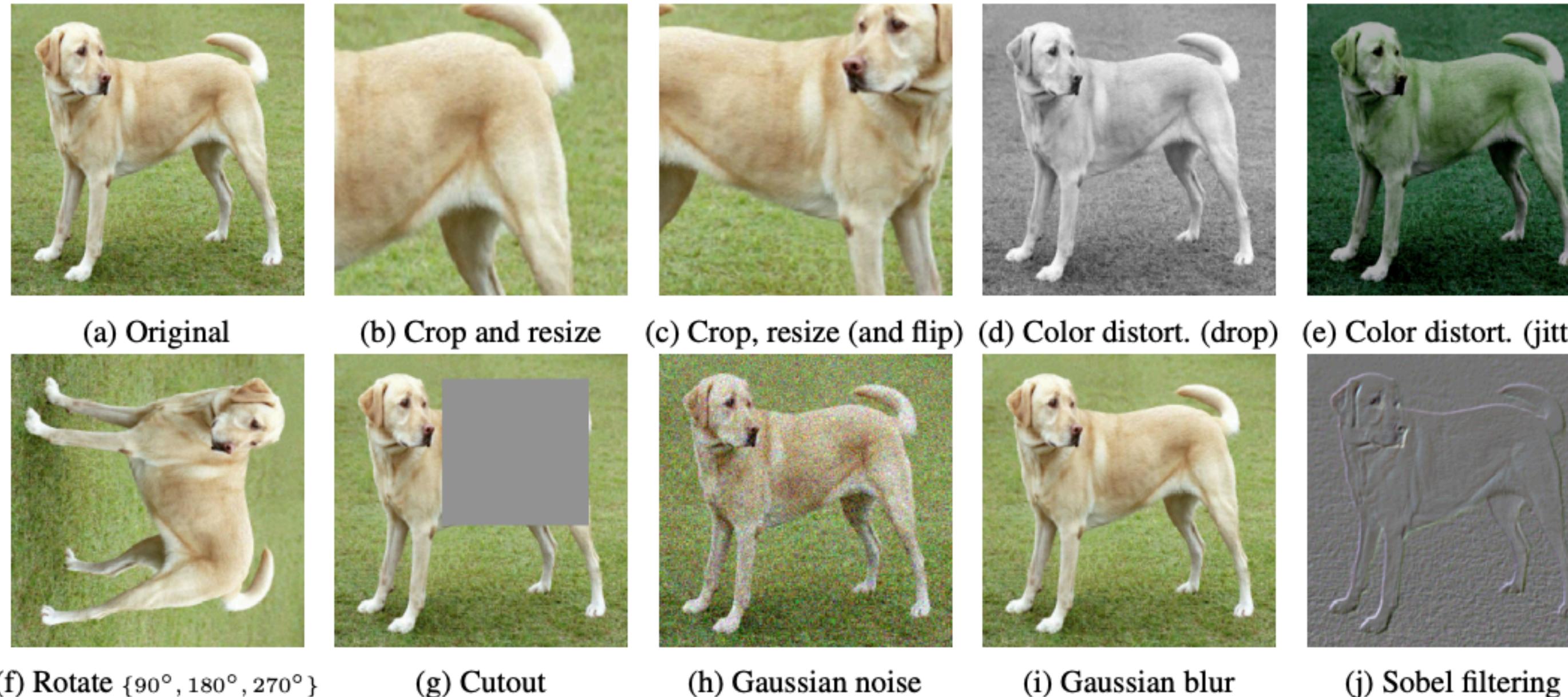


Figure 4. Illustrations of the studied data augmentation operators. Each augmentation can transform data stochastically with some internal parameters (e.g. rotation degree, noise level). Note that we *only* test these operators in ablation, the *augmentation policy used to train our models* only includes *random crop (with flip and resize), color distortion, and Gaussian blur*. (Original image cc-by: Von.grzanka)

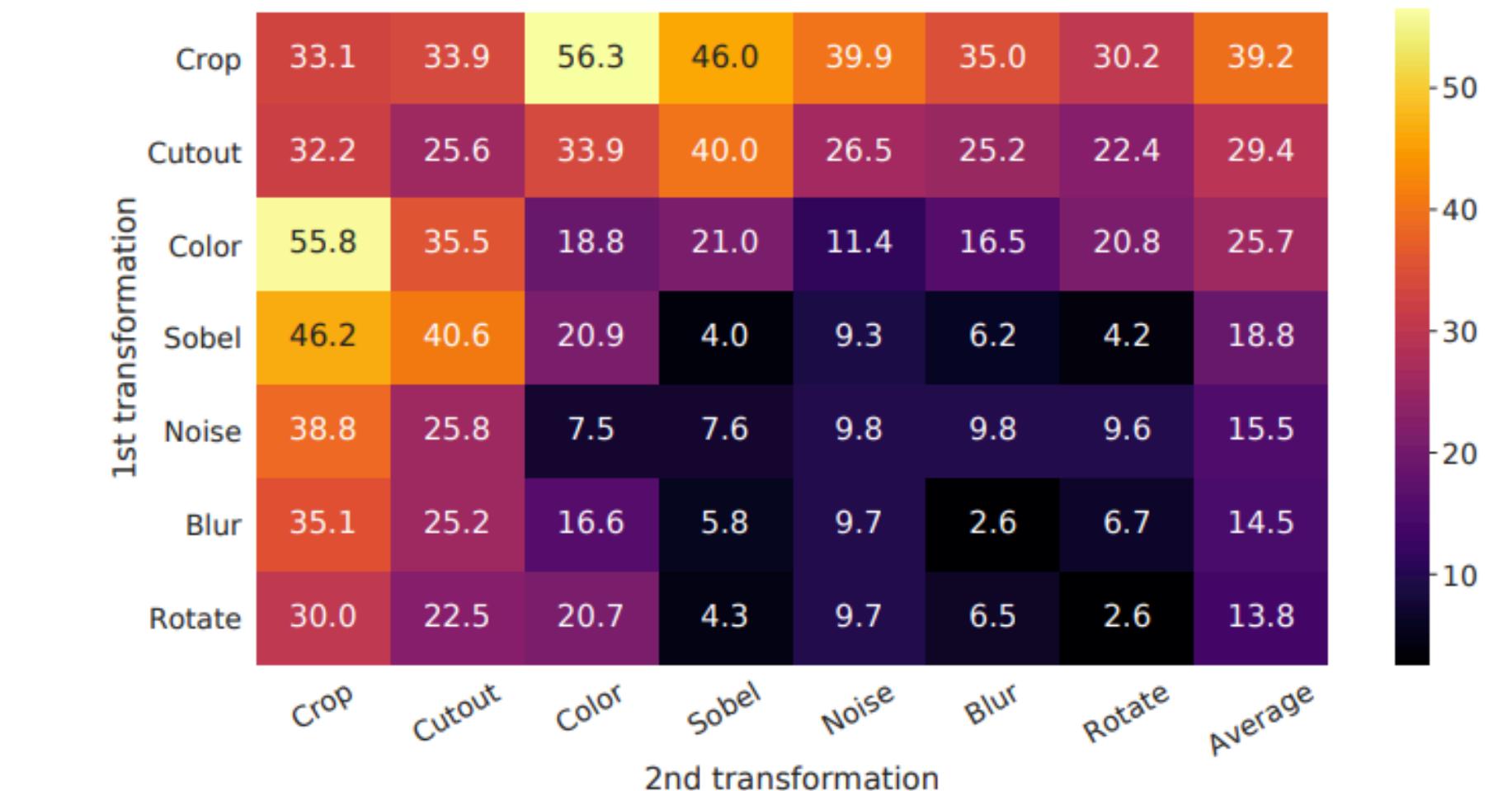
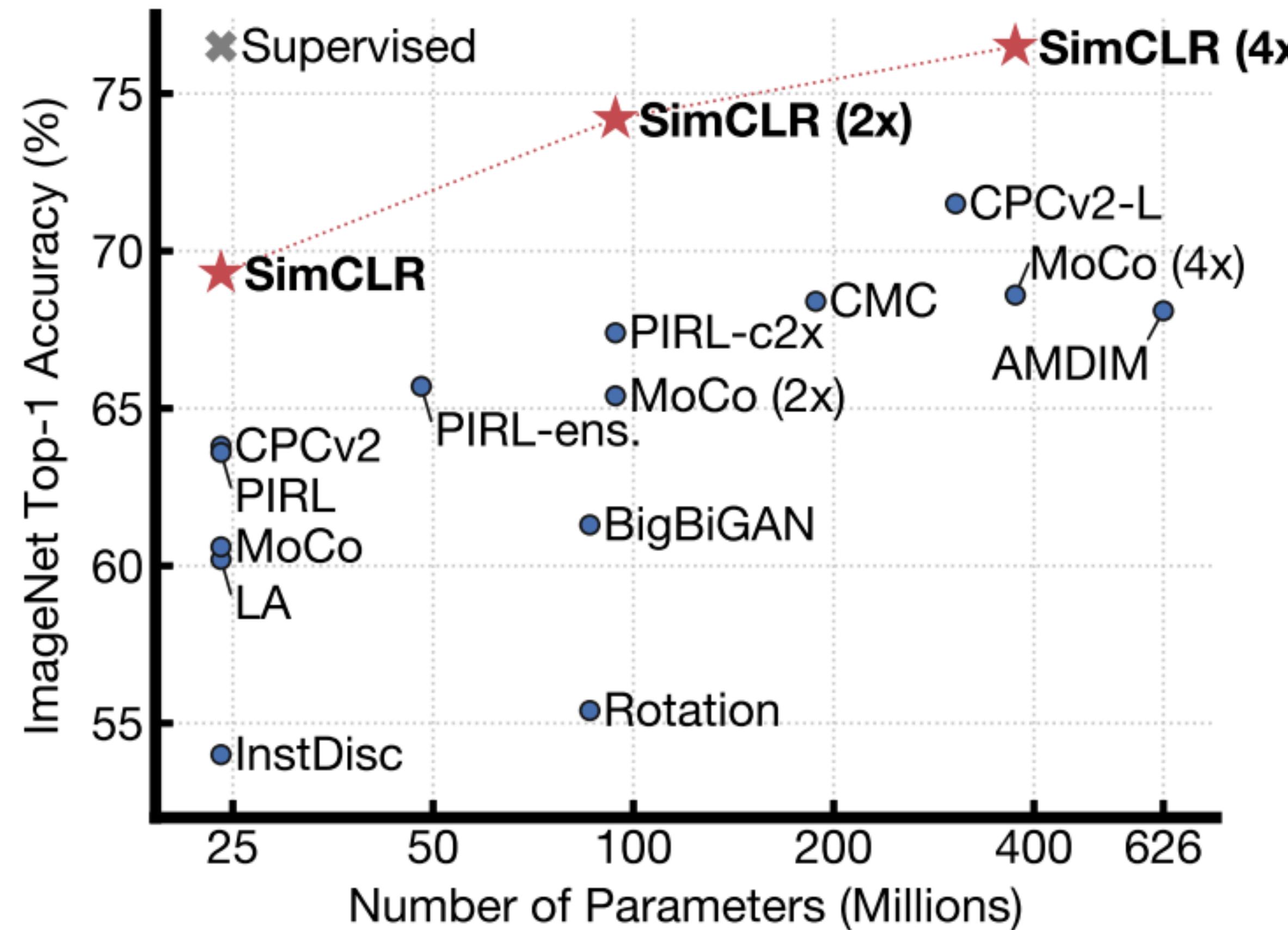


Figure 5. Linear evaluation (ImageNet top-1 accuracy) under individual or composition of data augmentations, applied only to one branch. For all columns but the last, diagonal entries correspond to single transformation, and off-diagonals correspond to composition of two transformations (applied sequentially). The last column reflects the average over the row.

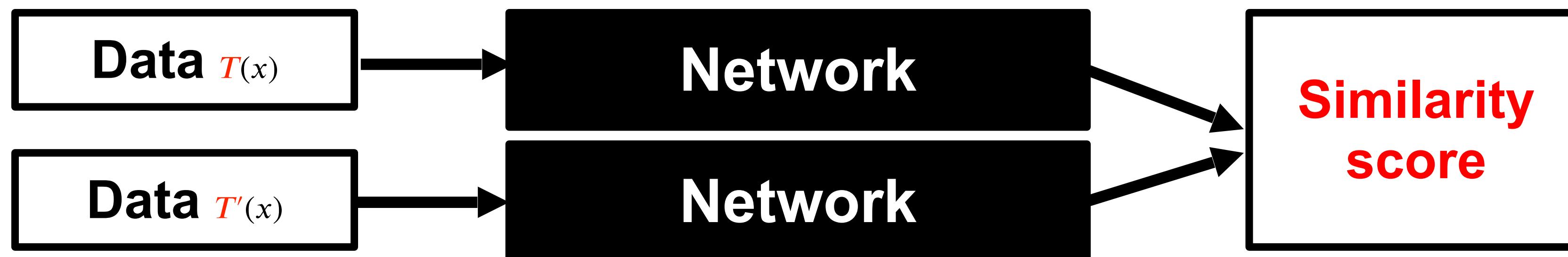
SimCLR: Evaluation



No detection evaluation

Non-contrastive methods

- Extract representations from two transformed versions of a data point, encourage these representations to be similar (or to have other desirable properties)
 - **Contrastive methods:** train using both positive (similar) and negative (dissimilar) pairs
 - Key challenge: sampling of negative pairs
 - **Non-contrastive methods:** train with only positive examples
 - Key challenge: avoiding degenerate solutions (all representations collapsing to constant output value)



BYOL

- Use momentum encoder, but without the queue of negative examples
- Use projection head like SimCLR, add prediction head to online network

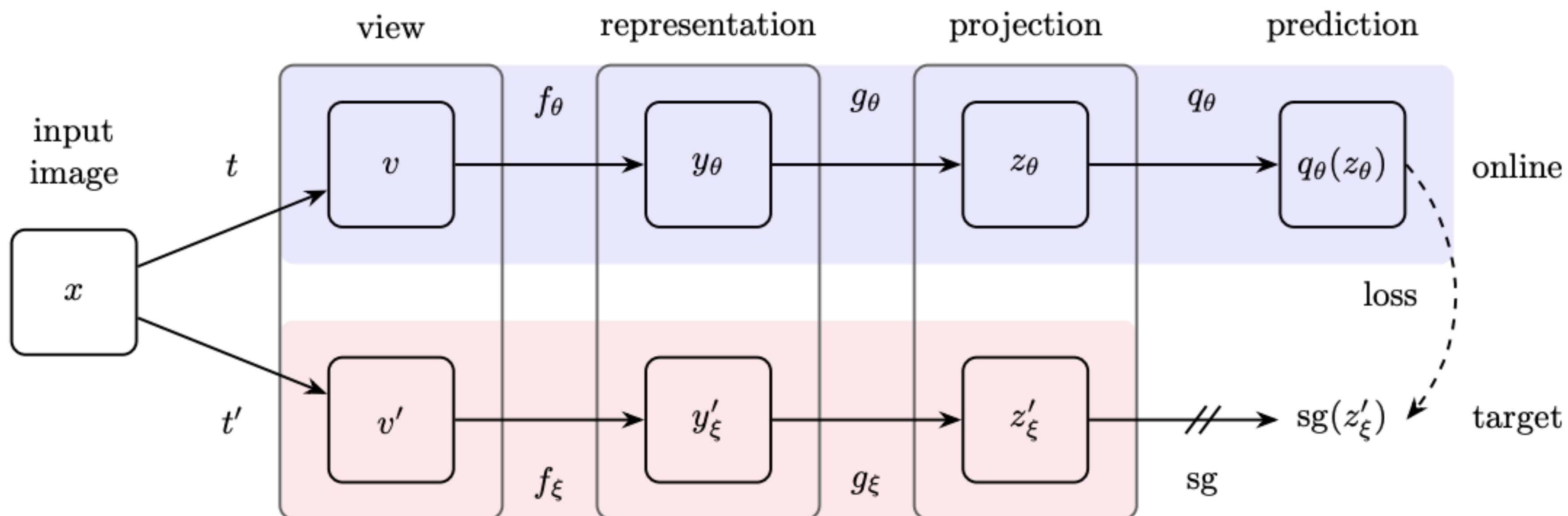


Figure 2: BYOL’s architecture. BYOL minimizes a similarity loss between $q_\theta(z_\theta)$ and $sg(z'_\xi)$, where θ are the trained weights, ξ are an exponential moving average of θ and sg means stop-gradient. At the end of training, everything but f_θ is discarded, and y_θ is used as the image representation.

BYOL: Evaluation

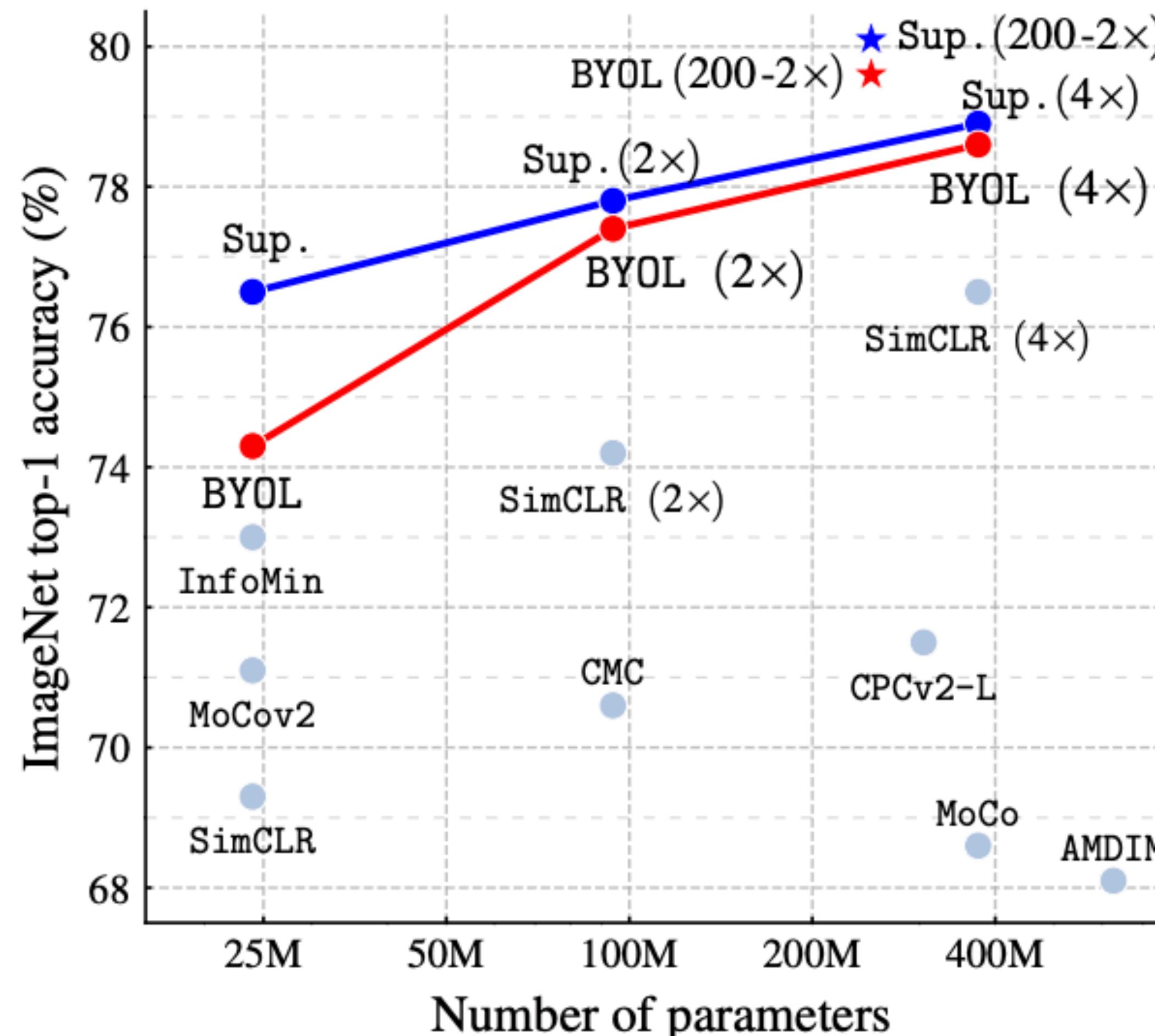


Figure 1: Performance of BYOL on ImageNet (linear evaluation) using ResNet-50 and our best architecture ResNet-200 ($2\times$), compared to other unsupervised and supervised (Sup.) baselines [8].

But remember ...

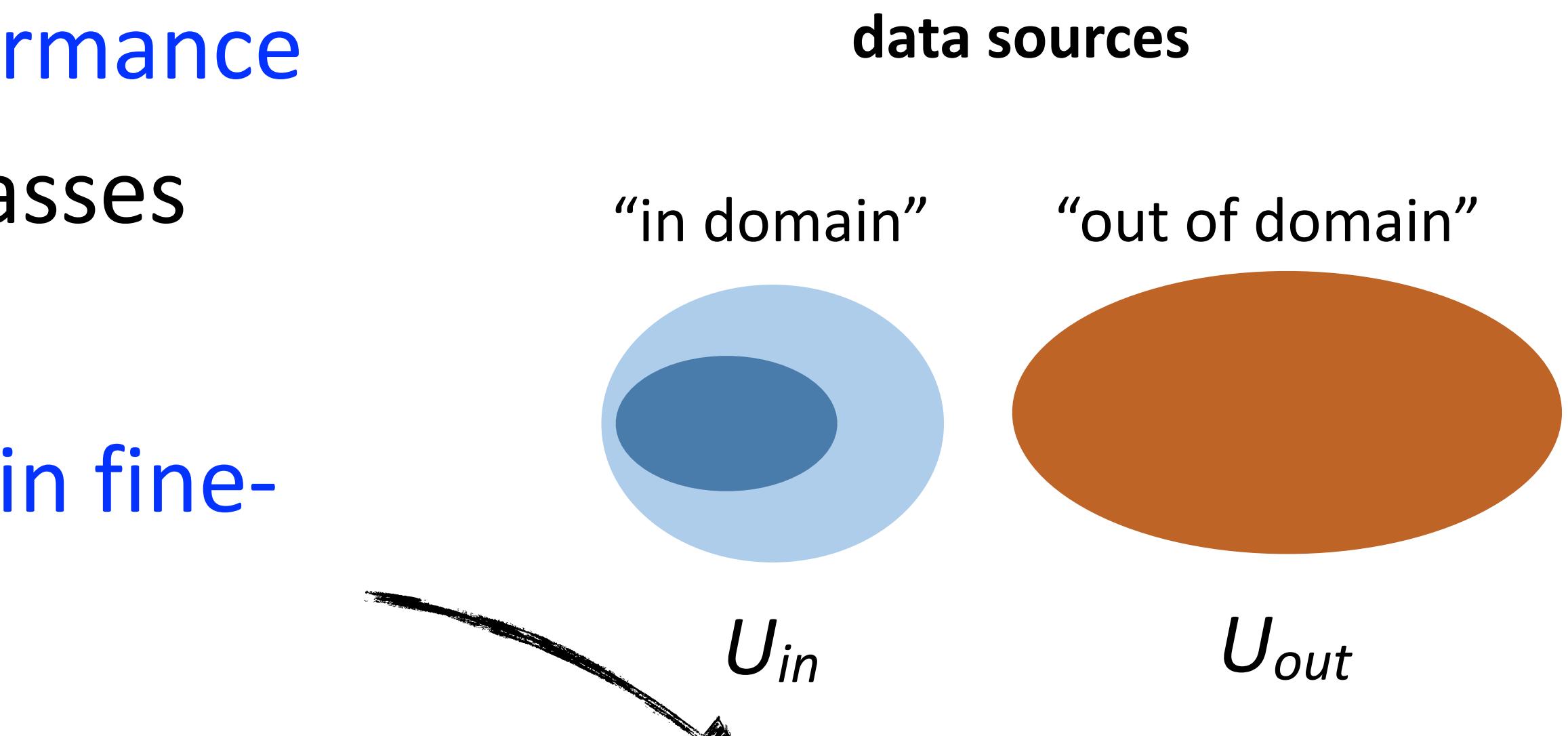
“Small” domain shifts can impact performance

- resolution, size/pose/class, novel classes

Self/semi-supervised learning is brittle in fine-grained domains

- difficult task, long-tailed data

Far from working on non-curated data!



When Does Contrastive Visual Representation Learning Work?

Elijah Cole¹ Xuan Yang² Kimberly Wilber² Oisin Mac Aodha^{3,4} Serge Belongie⁵
¹Caltech ²Google ³University of Edinburgh ⁴Alan Turing Institute ⁵University of Copenhagen

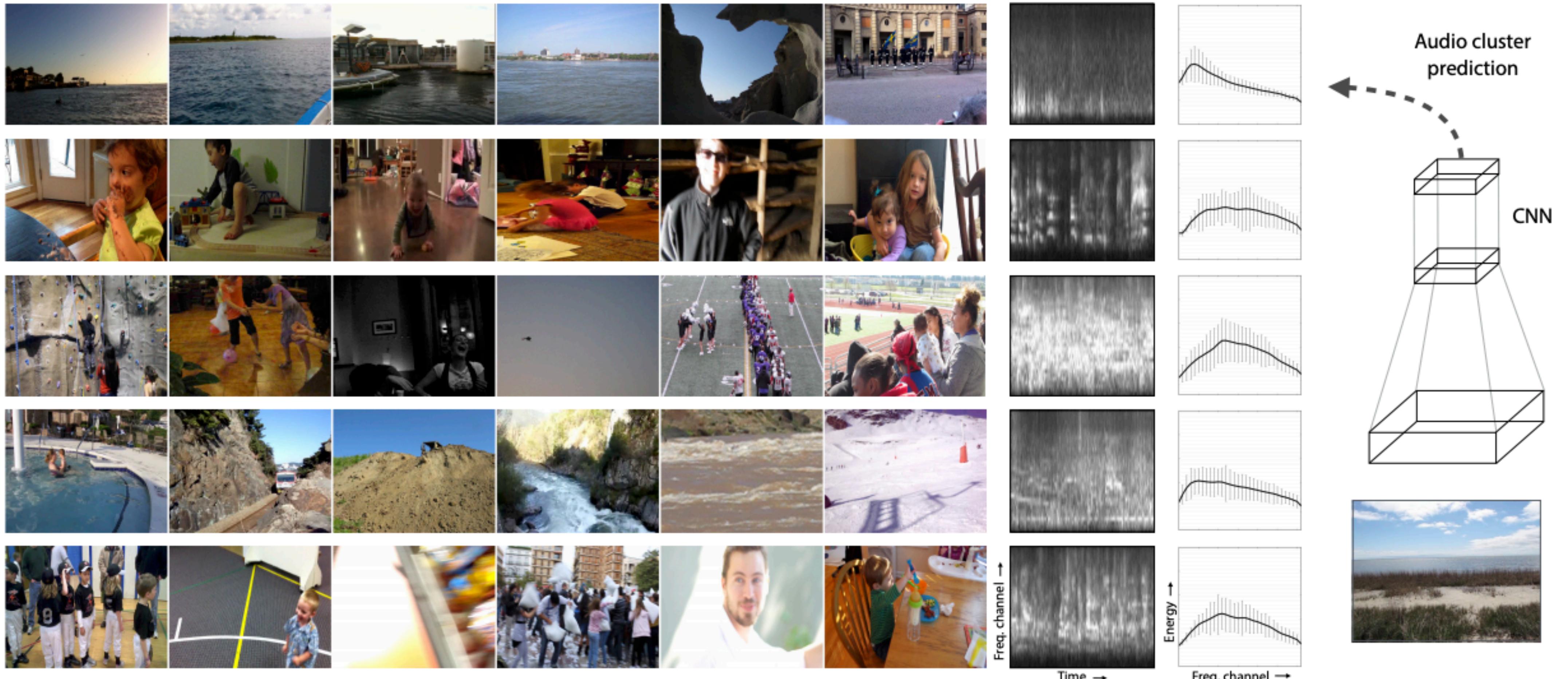
When Does Self-supervision Improve Few-shot Learning?

Jong-Chyi Su¹ Subhransu Maji¹ Bharath Hariharan²

Self-supervised learning: Outline

- Data prediction
 - Colorization
- Transformation prediction
 - Context prediction, jigsaw puzzle solving, rotation prediction
- “Siamese” methods
 - Contrastive methods
 - Non-contrastive methods
- **Self-supervision beyond still images**
 - Video, audio, language

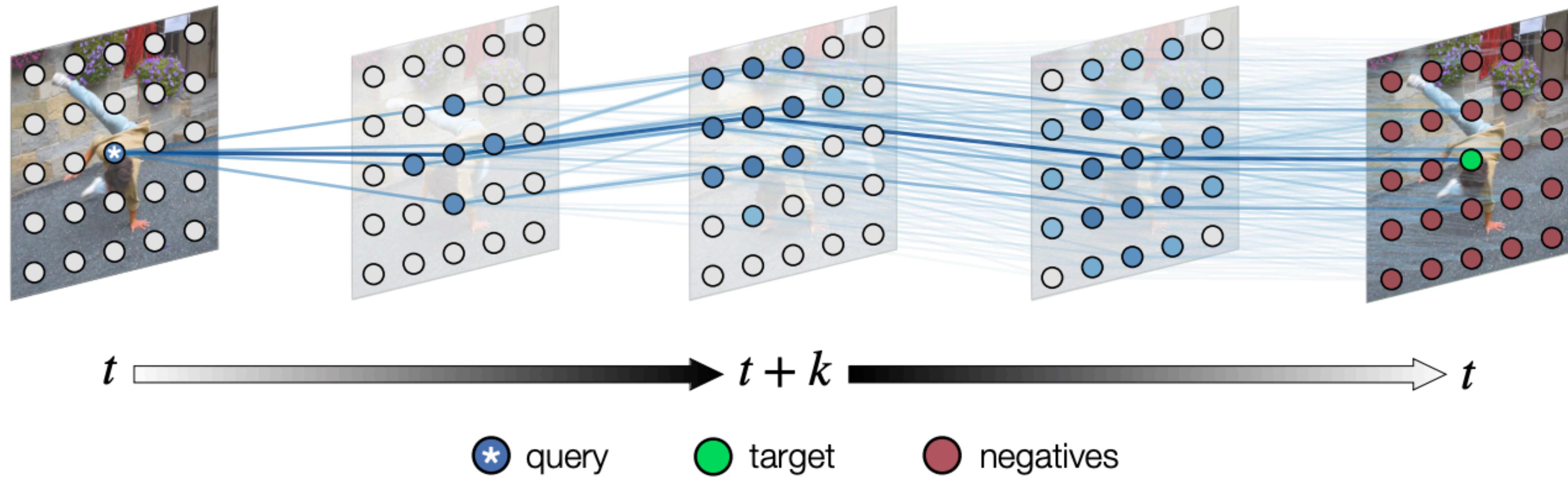
Learning from audio



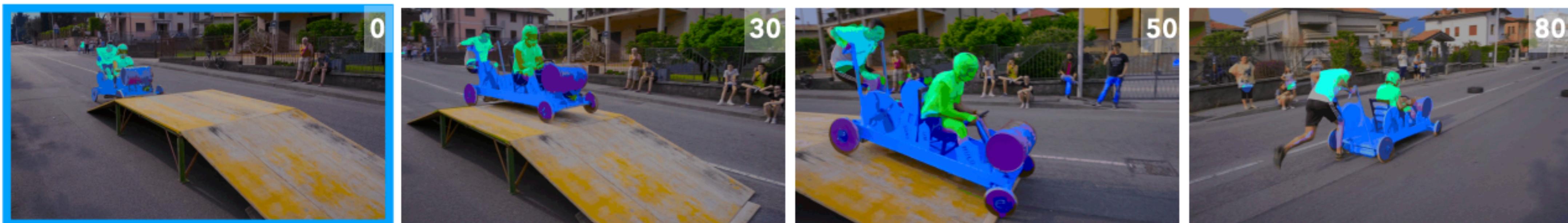
(a) Images grouped by audio cluster

(b) Clustered audio stats. (c) CNN model

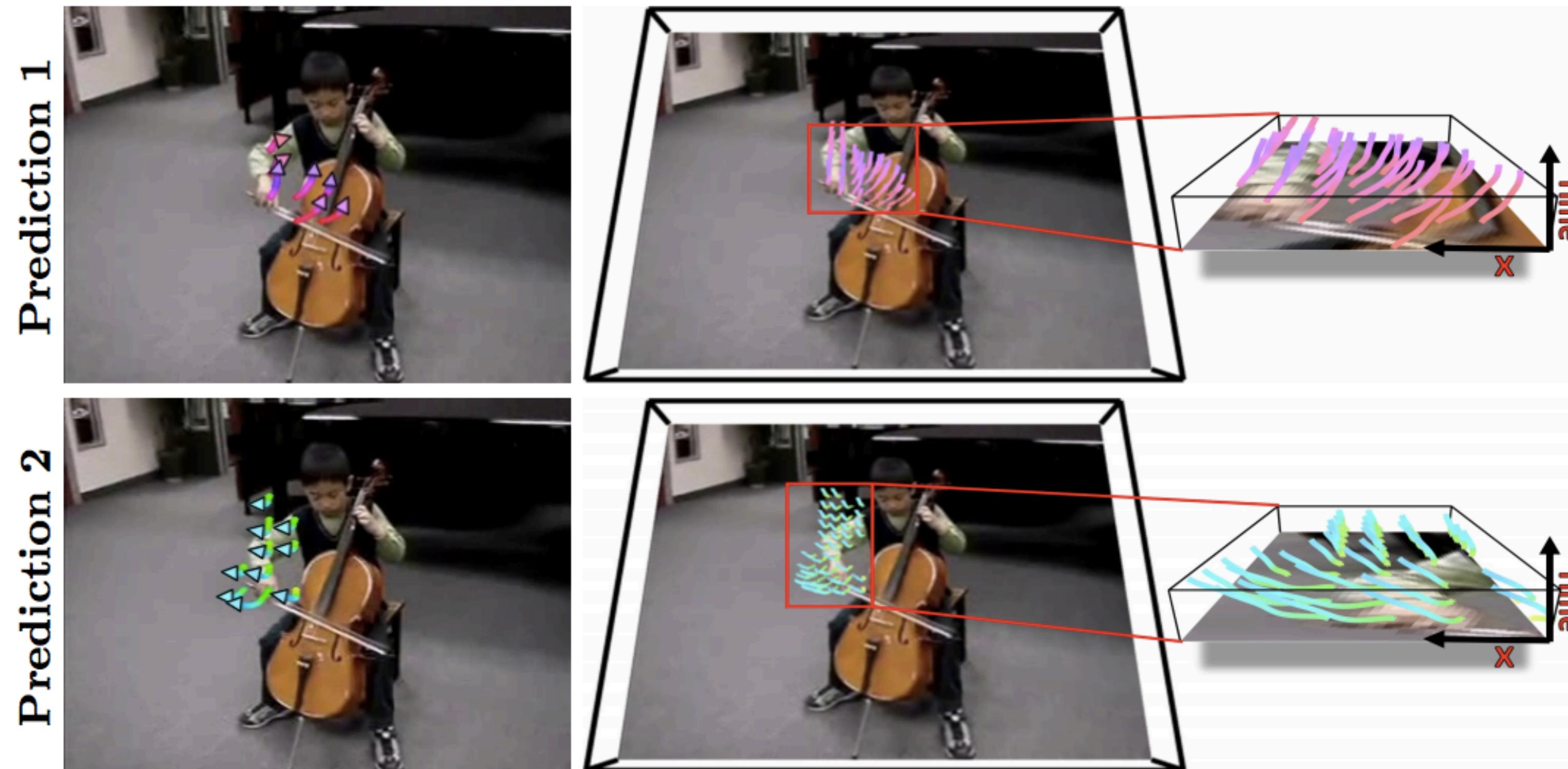
Video correspondence features



Object Propagation 1-4 Objects



Future prediction



3D shapes and convexity

- **Final Task:** separate 3D *objects* (chairs, tables..) into *parts* (legs, back, handles...)

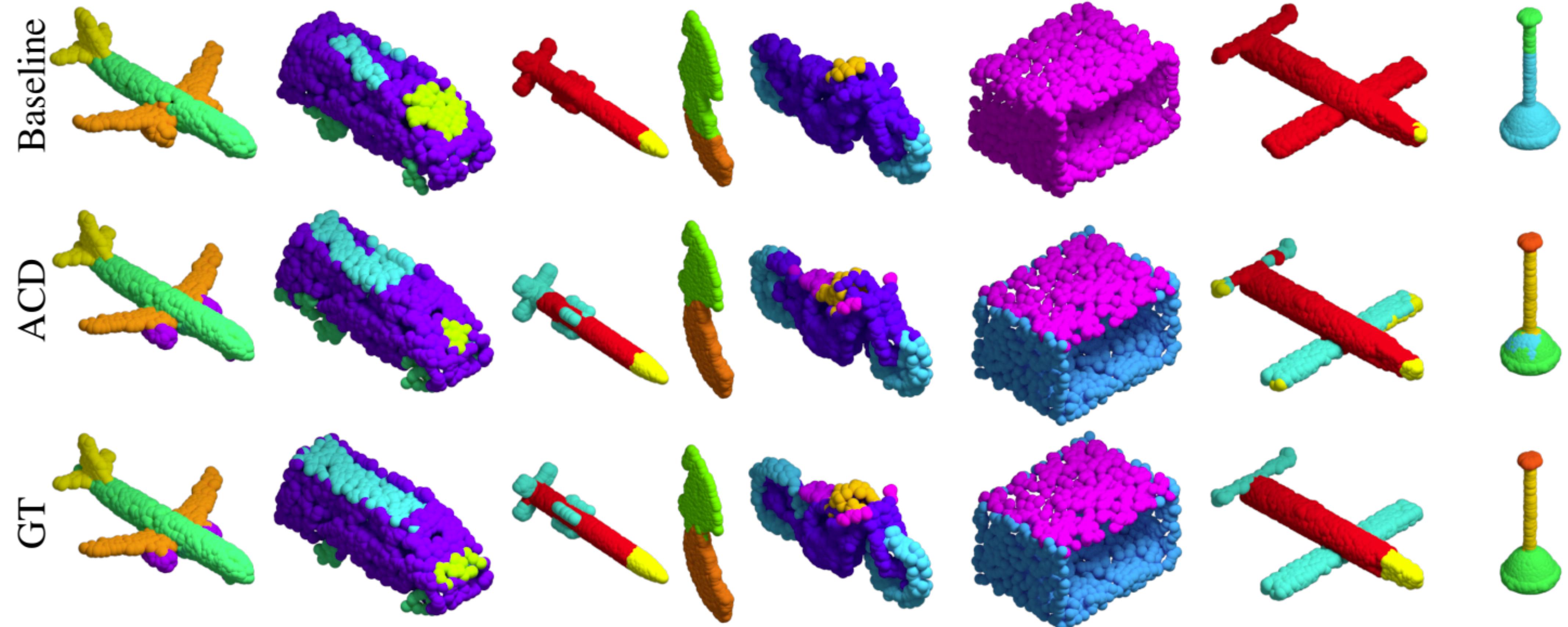


More on the pretext task - approx convexity

- **Pretext Task:** off-the-shelf package for “approximate convex decomposition”
 - Get a large number of unlabeled 3D shapes
 - Run **off-the-shelf “ACD” software** to get decompositions
 - Train your favorite 3D neural network on this, and then apply on final task



10-Shot Segmentation Results



Large Language Models

pre-train transformers on text

Next-token-prediction

The model is given a sequence of words with the goal of predicting the next word.

Example:
Hannah is a ___

Hannah is a *sister*
Hannah is a *friend*
Hannah is a *marketer*
Hannah is a *comedian*

Masked-language-modeling

The model is given a sequence of words with the goal of predicting a 'masked' word in the middle.

Example
Jacob [mask] reading

Jacob *fears* reading
Jacob *loves* reading
Jacob *enjoys* reading
Jacob *hates* reading

Human examples
Human preferences
RLHF



Finetuning



ChatGPT

Summary of self-supervision via pretext-tasks

Pretext Tasks:

- ▶ Pretext tasks focus on “visual common sense”, e.g., rearrangement, predicting rotations, inpainting, colorization, etc.
- ▶ The models are forced learn good features about natural images, e.g., semantic representation of an object category, in order to solve the pretext tasks
- ▶ We don’t care about pretext task performance, but rather about the utility of the learned features for downstream tasks (classification, detection, segmentation)

Problems:

- ▶ Designing good pretext tasks is tedious and some kind of “art”
- ▶ The learned representations may not be general