Augment with Care: Contrastive Learning for Combinatorial Problems

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Supervised learning for combinatorial problems

	Input	Label	ML model (e.g.,)
Boolean satisfiability (SAT)	$(x_1 \lor x_2 \lor \neg x_3)$ $\land (\neg x_1 \lor x_2 \lor x_3)$	SAT/UNSAT	NeuroSAT (Selsam et al, 2019)
Mixed Integer Programming	max $x_1 - 3x_2$ s.t. $x_1 > x_2$ $x_1, x_2 \in \mathbb{Z}$	Variable assignments	Neural Diving (Nair et al, 2020)
Travelling salesman		Shortest routes	Attention Model (Kool et al, 2018)

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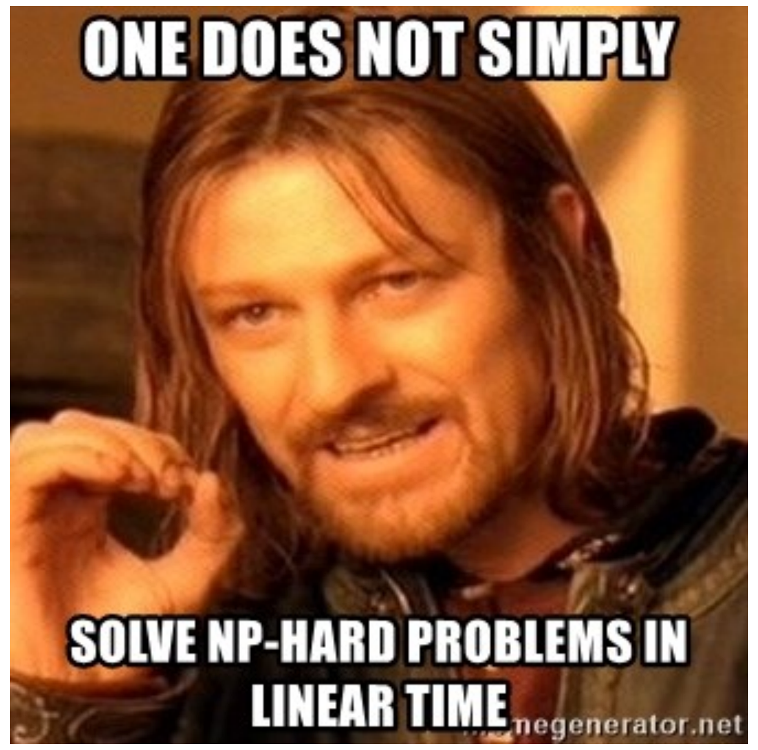
Limitation:

- Combinatorial optimization is NP-hard
- Worst-case exponential complexity
- Labelling = Not scaling



Self-supervised pre-training for image and vision

- Language: BERT (Kenton et al, 2019)

BERT's Performance - SWAG (Situations With Adversarial Generations)

System	Dev	Test
BERT$_{LARGE}$	**86.6**	**86.3**
Human (expert)	-	85.0
OpenAI GPT	-	78
ESIM+GloVe	51.9	52.7
ESIM+ELMo	59.1	59.2

✓ Better sample efficiency in downstream tasks
✓ Better multi-task performance
✓ Better transfer performance
✓ Better robustness
✓ ……

- Vision: CLIP (Radford et al, 2021)

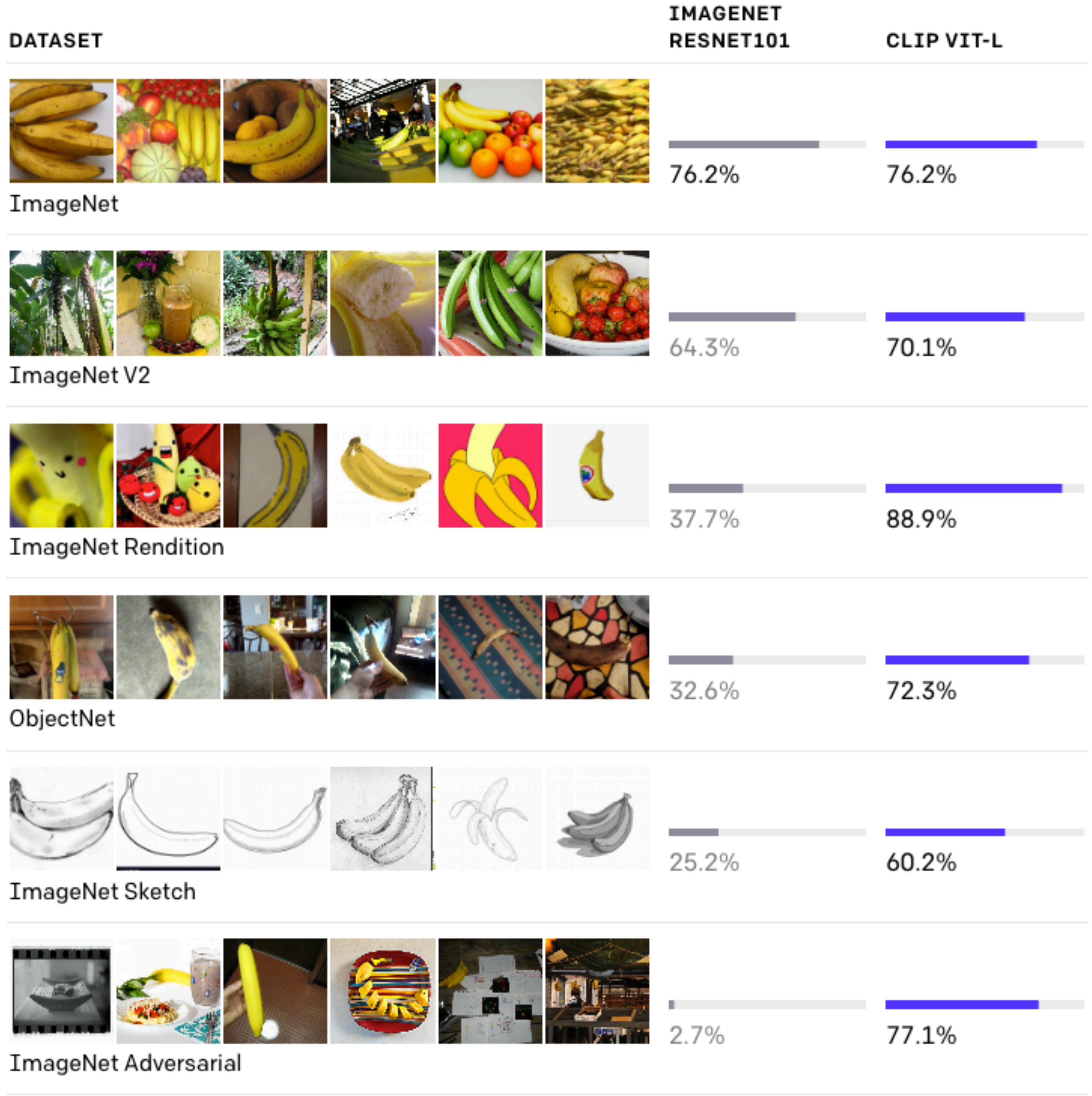
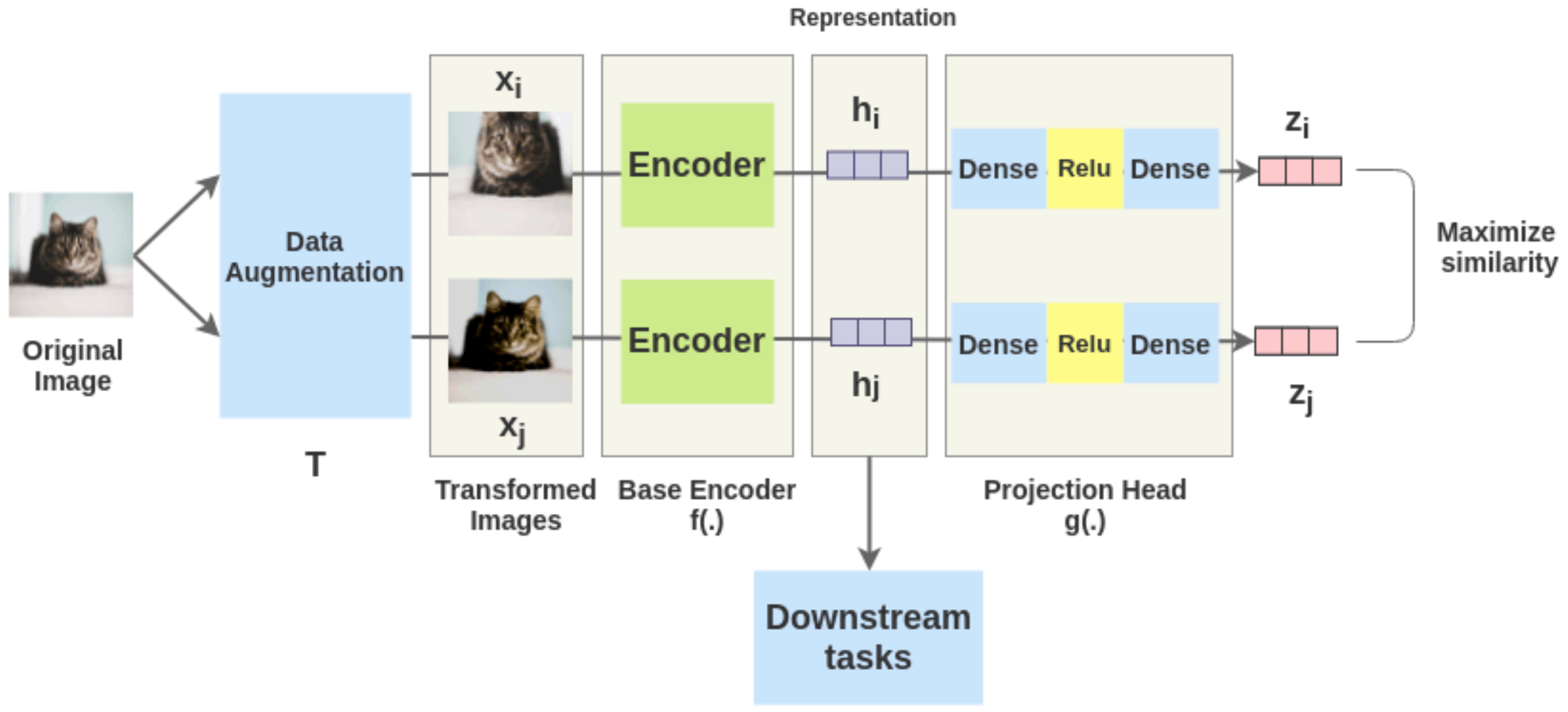


Image source: https://huggingface.co/blog/bert-101
https://openai.com/blog/clip/

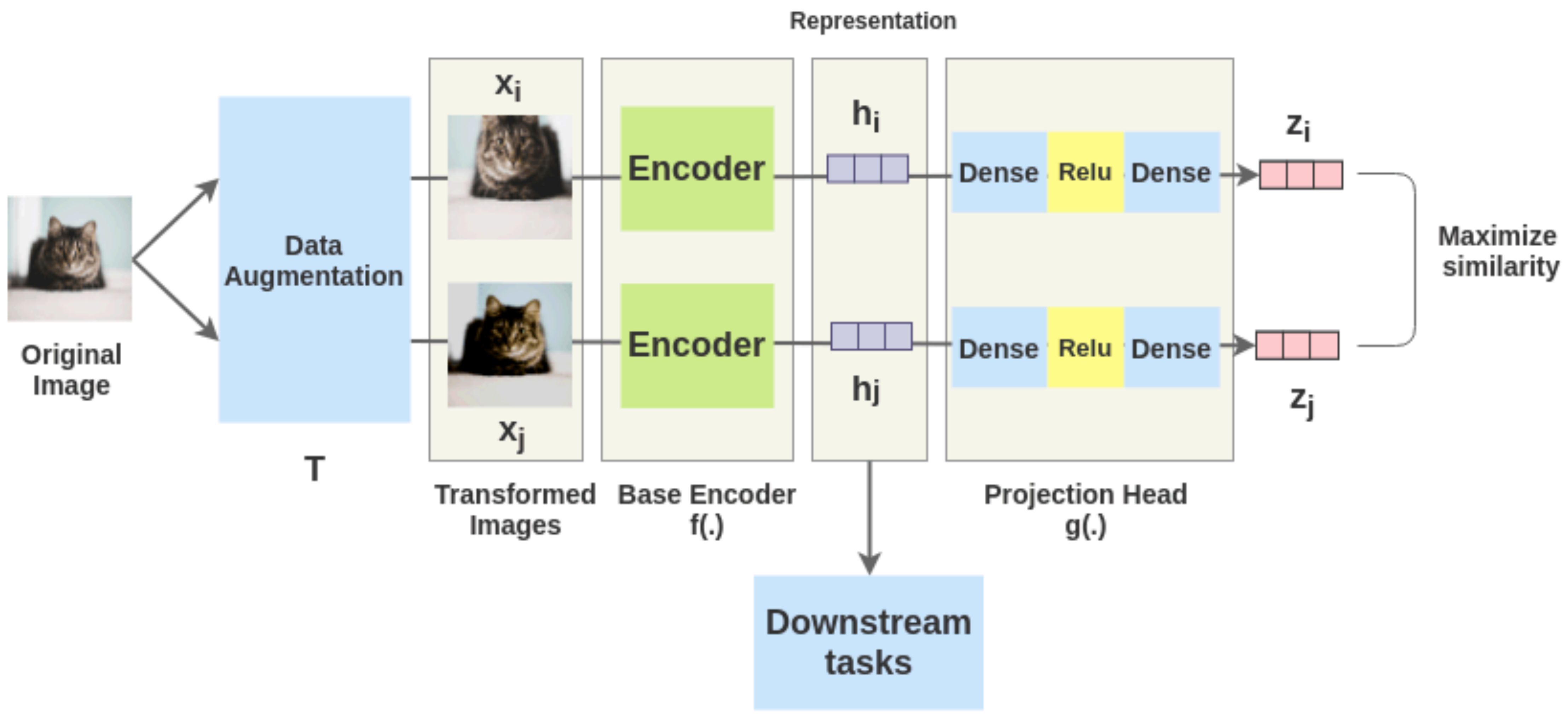
SimCLR: contrastive learning for image representations



Maximize the agreement between different augmented views of the same data

Image source: https://amitness.com/2020/03/illustrated-simclr/

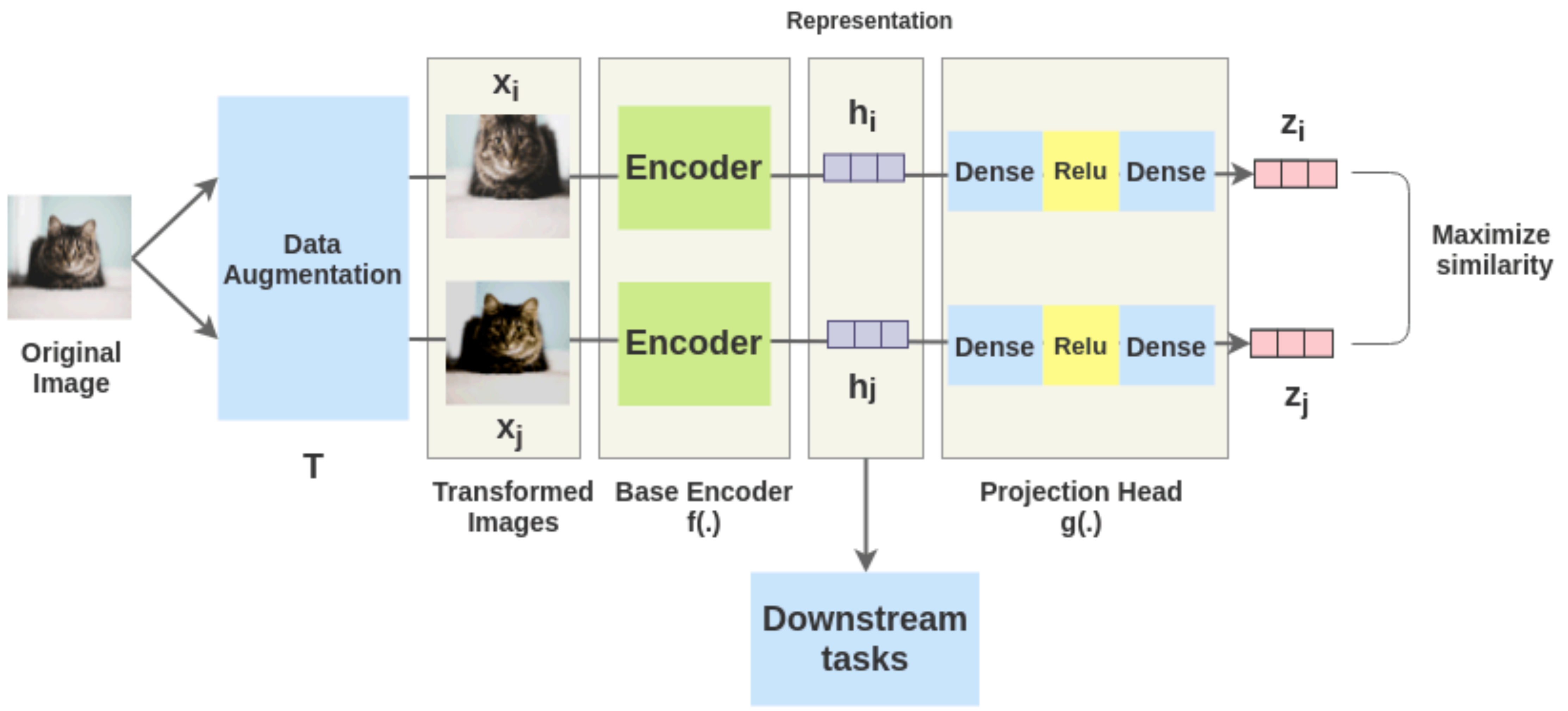
SimCLR: contrastive learning for image representations



Outperforming AlexNet on ImageNet using only 1% of the labels

Image source: https://amitness.com/2020/03/illustrated-simclr/

SimCLR: contrastive learning for image representations

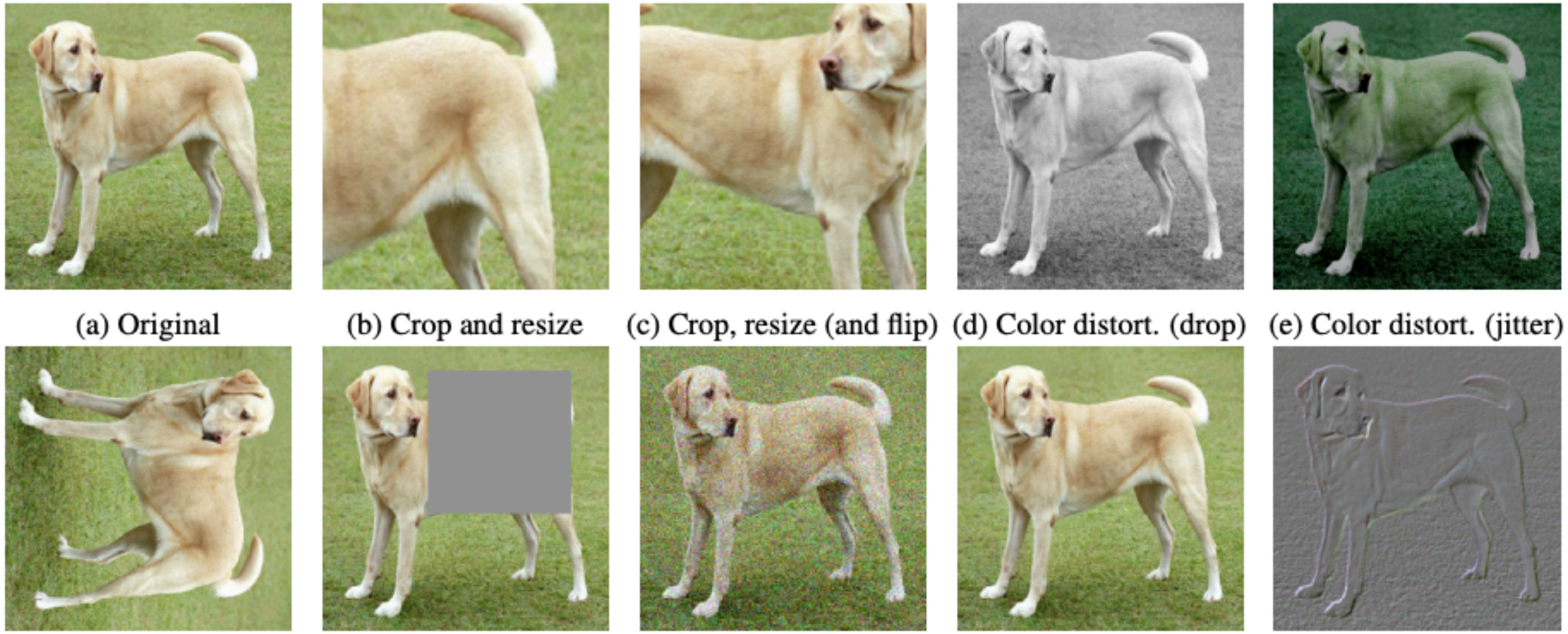


Outperforming AlexNet on ImageNet using only 1% of the labels

SimCLR for SAT representations?

Image source: https://amitness.com/2020/03/illustrated-simclr/

How to design augmentations? - Image



(a) Original (b) Crop and resize (c) Crop, resize (and flip) (d) Color distort. (drop) (e) Color distort. (jitter)

(f) Rotate {90°, 180°, 270°} (g) Cutout (h) Gaussian noise (i) Gaussian blur (j) Sobel filtering

Image source: https://arxiv.org/pdf/2002.05709.pdf

How to design augmentations? - SAT

- Requirements: the augmentations should
    - preserve labels (satisfiability): SAT => SAT, UNSAT => UNSAT
    - efficient to compute

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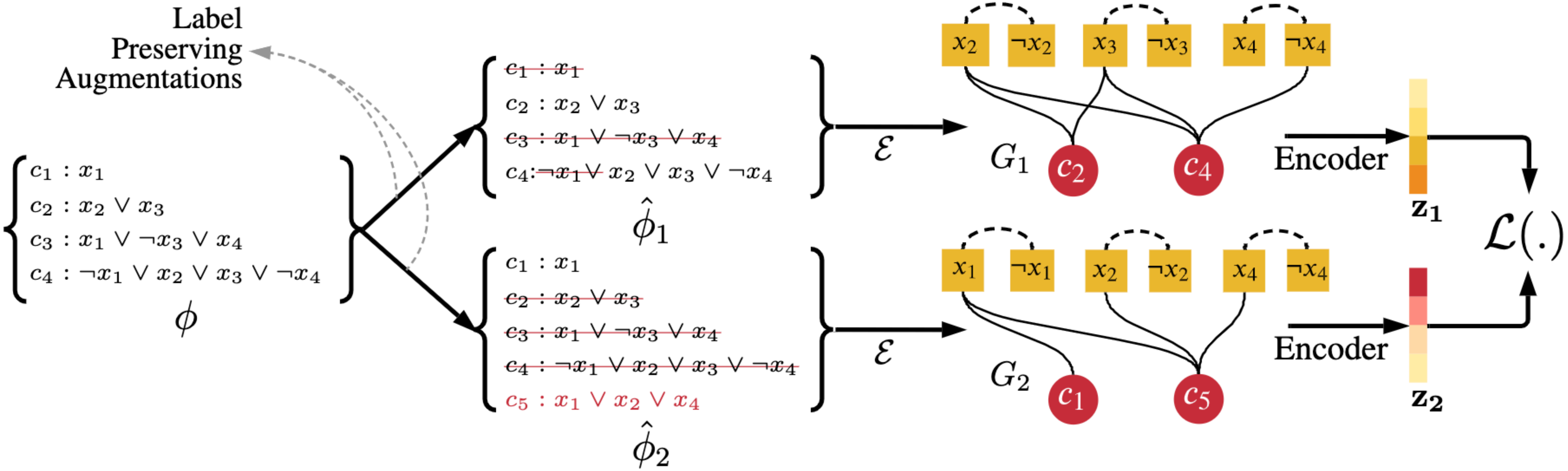
- The algorithms used in preprocessing components of SAT solvers are the perfect candidate.

Label-preserving augmentations (LPAs)

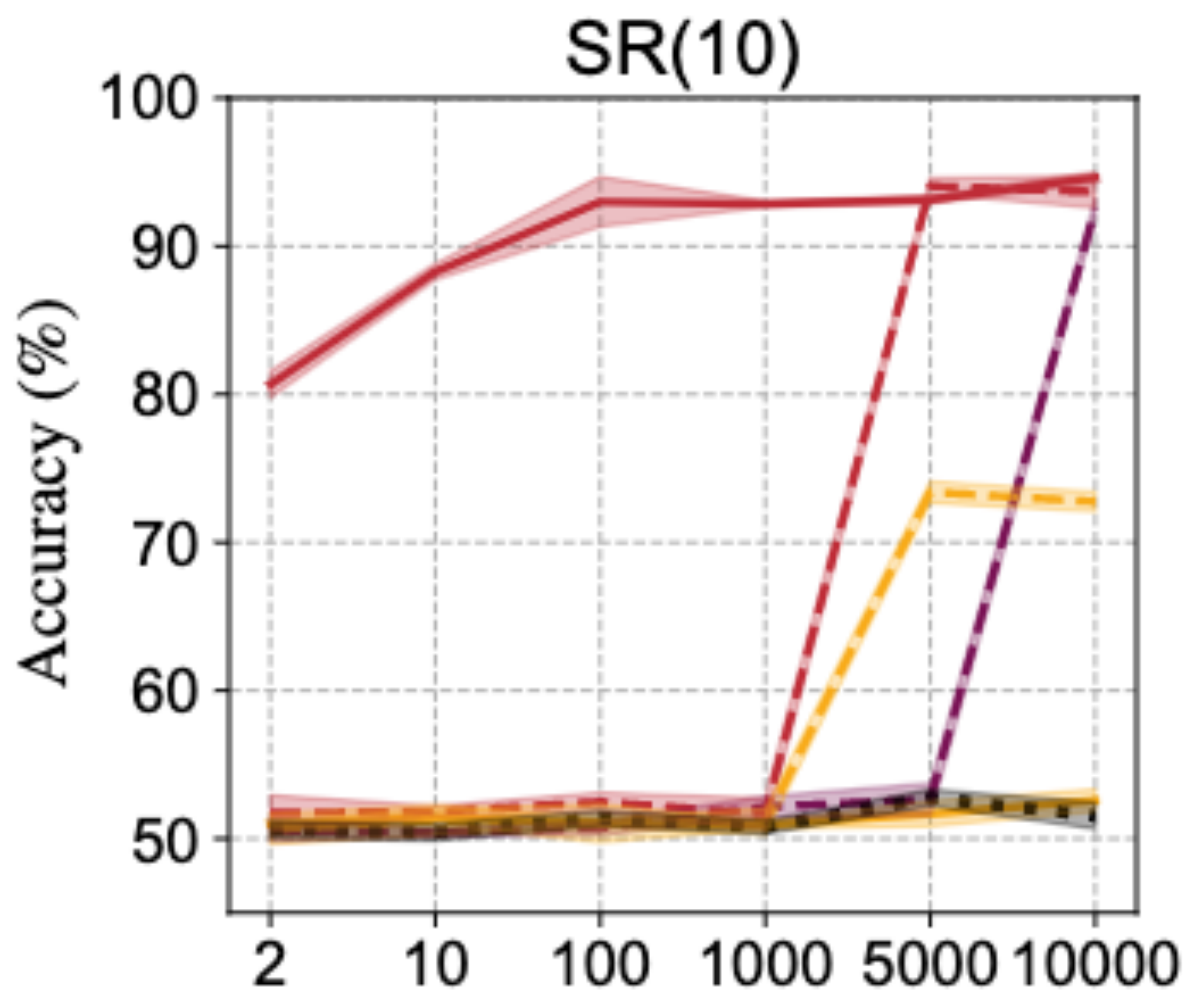
- Unit propagation (UP)
- Clause resolution (CR)
- Variable elimination (VE)
- Subsumed clause elimination (SC)
- ……

Original	UP
$c_1 : x_1$	$\cancel{x_1}$
$c_2 : x_2 \lor x_3$	$x_2 \lor x_3$
$c_3 : x_1 \lor \neg x_3 \lor x_4$	$\cancel{x_1 \lor \neg x_3 \lor x_4}$
$c_4 : \neg x_1 \lor x_2 \lor x_3 \lor \neg x_4$	$\cancel{\neg x_1 \lor} x_2 \lor x_3 \lor \neg x_4$
AU	**SC**
$\neg x_5$	
$x_5 \lor x_1$	x_1
$x_2 \lor x_3$	$x_2 \lor x_3$
$x_1 \lor \neg x_3 \lor x_4$	$x_1 \lor \neg x_3 \lor x_4$
$\neg x_1 \lor x_2 \lor x_3 \lor \neg x_4$	$\cancel{\neg x_1 \lor x_2 \lor x_3 \lor \neg x_4}$
$\neg x_5 \lor x_1 \lor \neg x_2 \lor x_3$	
CR	**VE**
x_1	x_1
$x_2 \lor x_3$	$\cancel{x_2 \lor x_3}$
$x_1 \lor \neg x_3 \lor x_4$	$\cancel{x_1 \lor \neg x_3 \lor x_4}$
$\neg x_1 \lor x_2 \lor x_3 \lor \neg x_4$	$\cancel{\neg x_1 \lor x_2 \lor x_3 \lor \neg x_4}$
$x_1 \lor x_2 \lor x_4$	$x_1 \lor x_2 \lor x_4$

Our framework



Results: pre-training improves sample efficiency by 100x



Number of training labels

- Red line: Our pre-training + linear evaluation
- Purple line: Fully-supervised NeuroSAT

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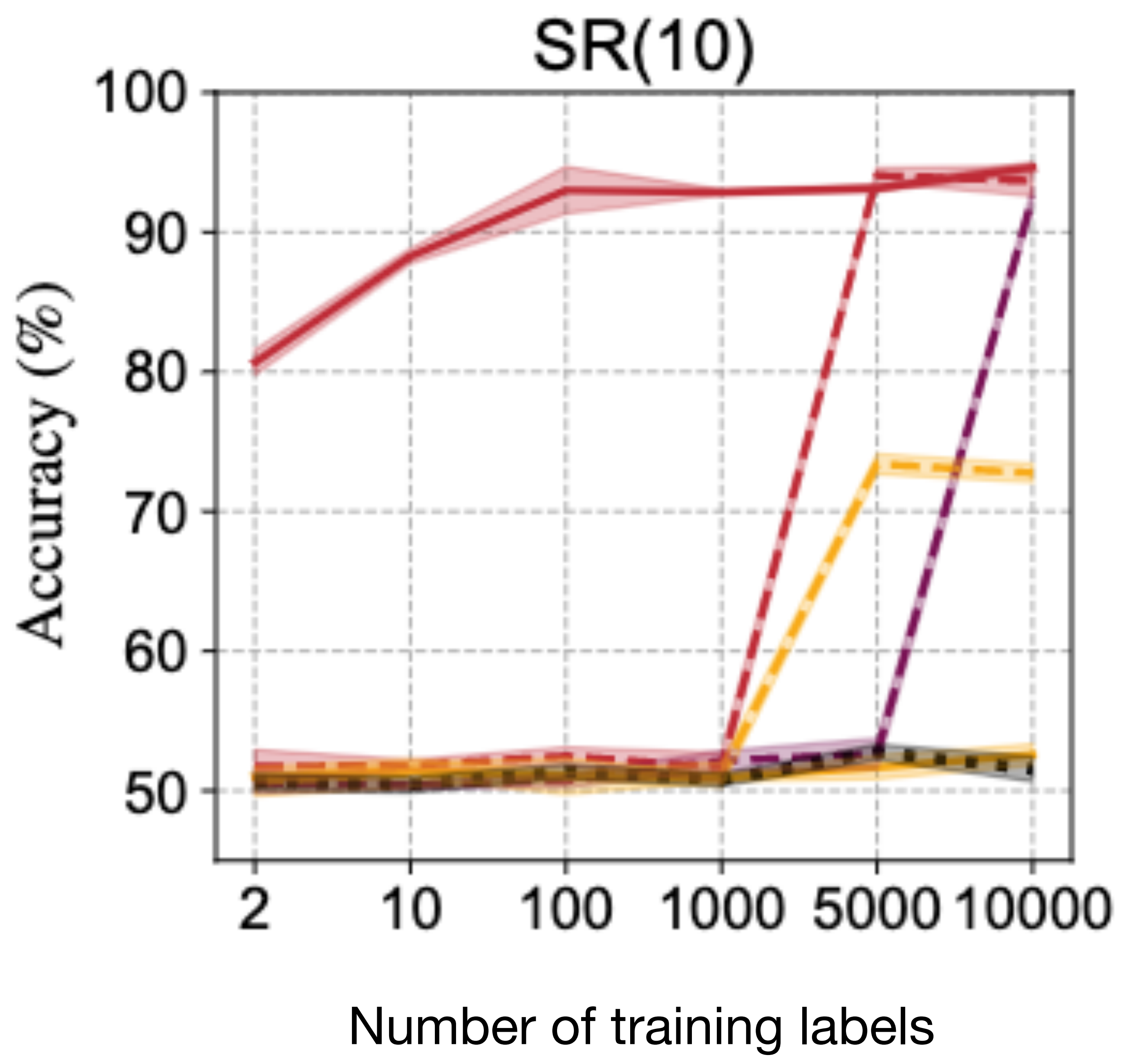
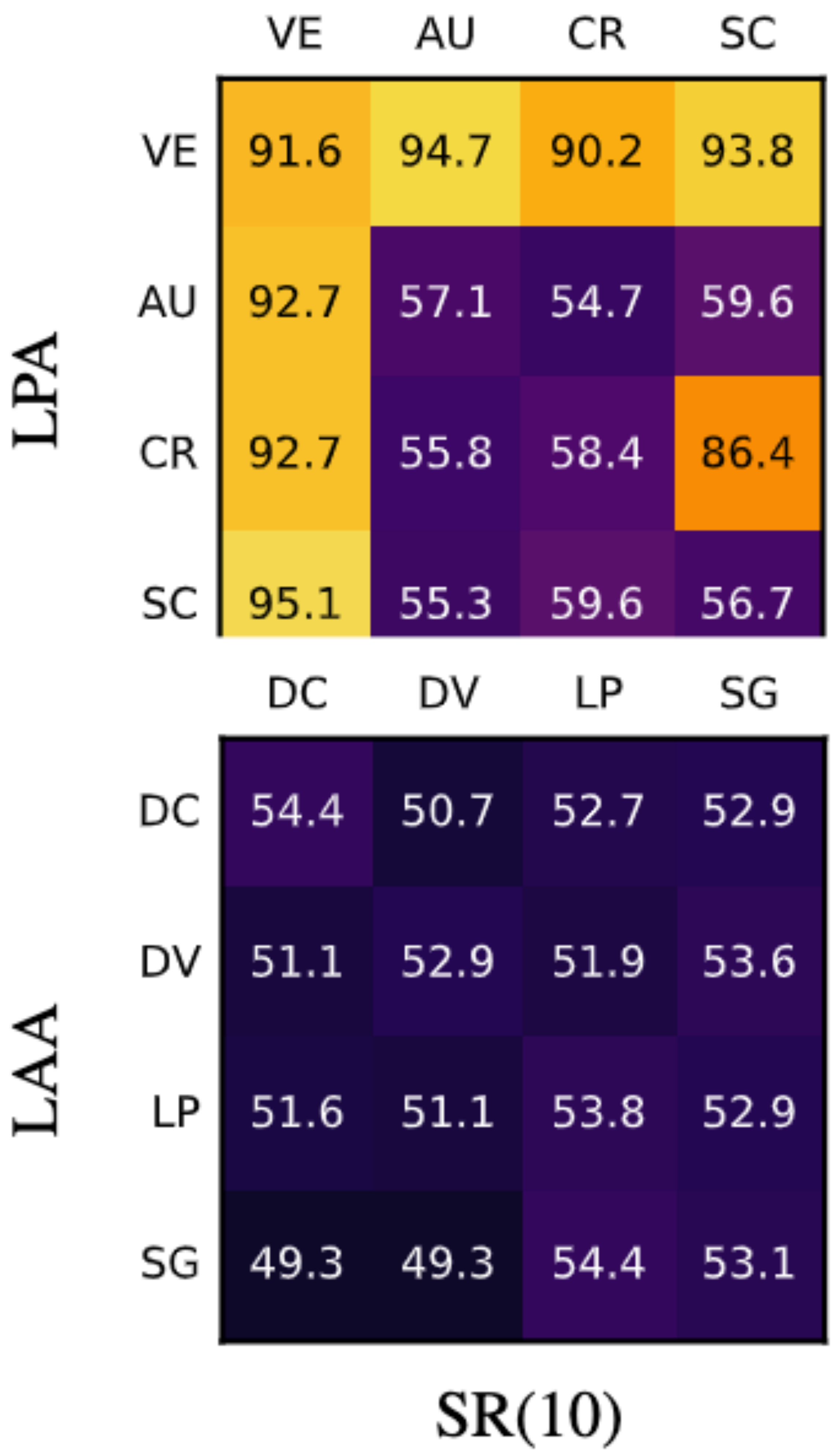


- Red line: Our pre-training + linear evaluation
- Purple line: Fully-supervised NeuroSAT
- Red with 100 labels > Purple with 10000 labels
- More datasets and settings? Check out our paper

Label-preserving augmentations are necessary



- Label-agnostic augmentations (LAAs):
  - Node dropping/adding
  - Edge perturbations
  - Subgraph

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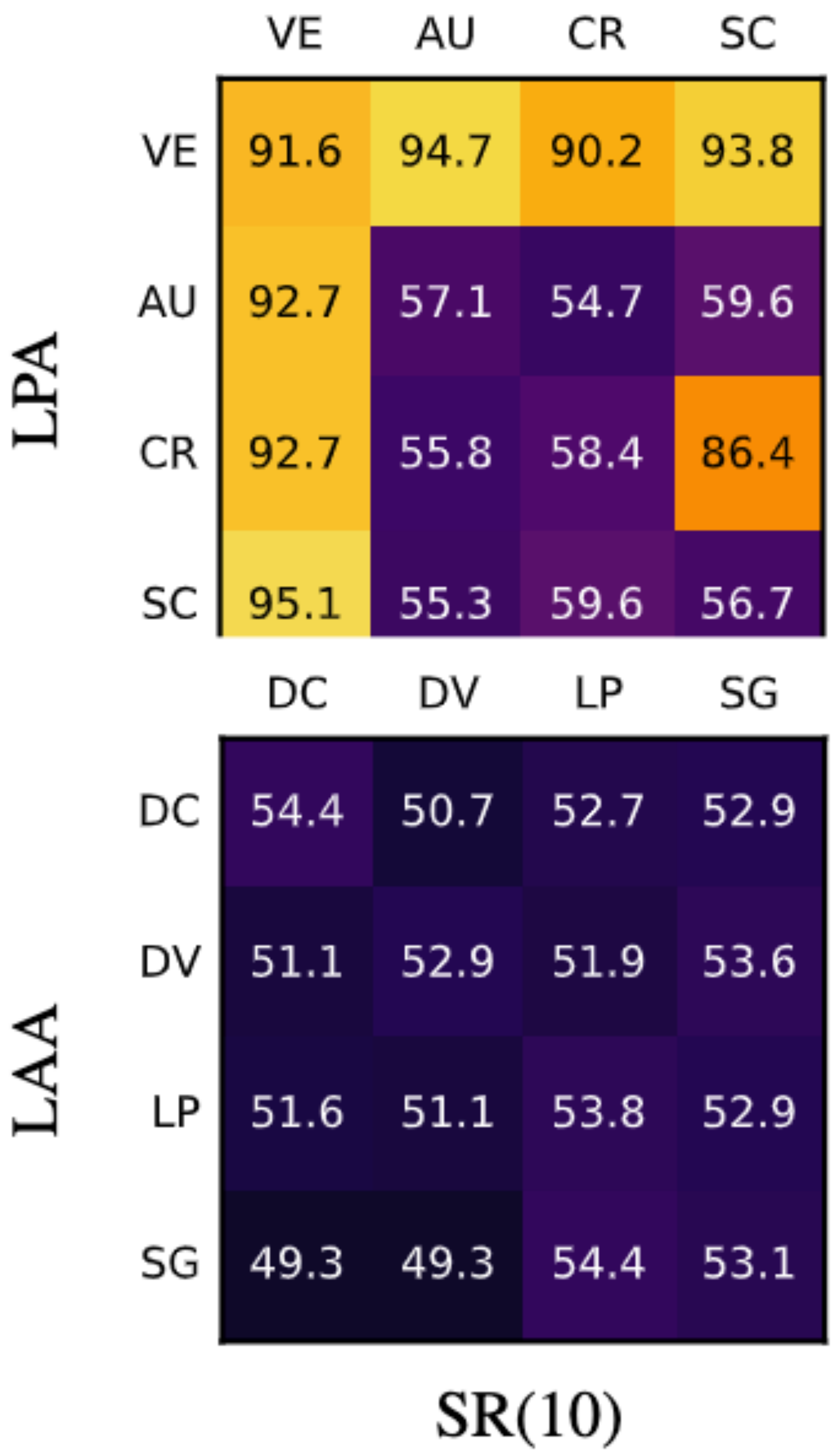

- Label-agnostic augmentations (LAAs):
  - Node dropping/adding
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- Best LPA (95.1) >> Best LAA (54.4)

Thanks!

Chat with us at our poster session: 6- 8pm, Hall E #403