



Augmentation and Generalization in Contrastive Self-Supervised Learning



Towards the Generalization of Contrastive Self-Supervised Learning

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Background

Contrastive Learning

- Alignment: Similar samples have similar features.
- Uniformity: Preserve maximal information.

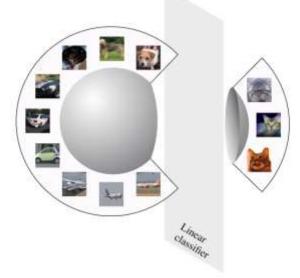
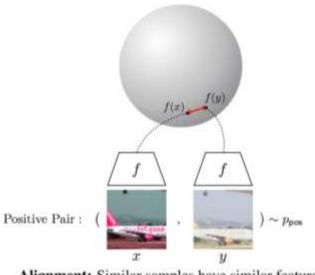


Figure 2: **Hypersphere:** When classes are well-clustered (forming spherical caps), they are linearly separable. The same does not hold for Euclidean spaces.





Alignment: Similar samples have similar features. (Figure inspired by Tian et al. (2019).)



Uniformity: Preserve maximal information.

The generalization of contrastive SSL is related to three key factors

- Alignment of positive samples
- **Divergence** of class centers

Background

• Concentration of augmented data

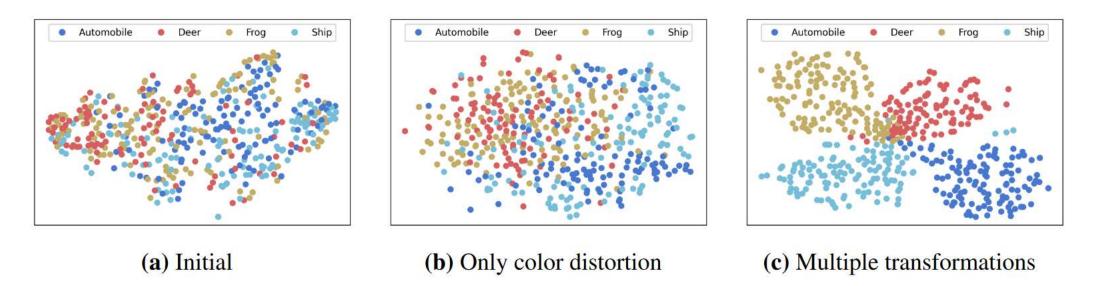


Figure 1: SimCLR's embedding space with different richnesses of data augmentations on CIFAR-10.

Background



The generalization of contrastive SSL is related to three key factors

- Alignment of positive samples
- **Divergence** of class centers
- Concentration of augmented data

The first two factors are properties of learned representations. The third one is determined by pre-defined data augmentation.

Experiments



Dataset CIFAR-10		Trans	sforma	ations		Accuracy					
	(a)	(b)	(c)	(d)	(e)	SimCLR	Barlow Twins	MoCo	SimSiam		
	1	~	1	1	~	89.76 ± 0.12	$\textbf{86.91} \pm \textbf{0.09}$	$\textbf{90.12} \pm \textbf{0.12}$	90.59 ± 0.11		
	1	1	\checkmark	~		88.48 ± 0.22	85.38 ± 0.37	89.69 ± 0.11	89.34 ± 0.09		
CIFAR-10	1	1	~			83.50 ± 0.14	82.00 ± 0.59	86.78 ± 0.07	85.38 ± 0.09		
	1	1				63.23 ± 0.05	67.83 ± 0.94	75.12 ± 0.28	63.27 ± 0.30		
	1					62.74 ± 0.18	67.77 ± 0.69	74.94 ± 0.22	61.47 ± 0.74		
	1	~	~	1	1	57.74 ± 0.12	$\textbf{57.99} \pm \textbf{0.29}$	$\textbf{64.19} \pm \textbf{0.14}$	$\textbf{63.48} \pm \textbf{0.16}$		
	1	1	~	~		55.43 ± 0.10	55.22 ± 0.25	62.50 ± 0.28	60.31 ± 0.41		
CIFAR-100	1	1	1			45.10 ± 0.25	50.40 ± 0.64	57.04 ± 0.21	51.42 ± 0.14		
	1	1				28.01 ± 0.18	34.11 ± 0.59	40.18 ± 0.04	26.26 ± 0.30		
	1					27.95 ± 0.09	34.05 ± 1.13	39.63 ± 0.31	25.90 ± 0.83		

Table 1: Downstream performance under different richness of augmentations.

(a) random cropping(b) random Gaussian blur

(c) color dropping

(d) color distortion

(e) random horizontal flipping

Table 2: Downstream performance under different strength of augmentations.

D	Color Distortion	1	Accu	iracy	
Dataset CIFAR-10	Strength	SimCLR	Barlow Twins	MoCo	SimSiam
	1	82.75 ± 0.24	$\textbf{82.58} \pm \textbf{0.25}$	$\textbf{86.68} \pm \textbf{0.05}$	$\textbf{82.50} \pm \textbf{1.05}$
CIFAR-10	1/2	78.76 ± 0.18	81.88 ± 0.25	84.30 ± 0.14	81.80 ± 0.15
	1/4	76.37 ± 0.11	79.64 ± 0.34	82.76 ± 0.09	78.80 ± 0.17
	1/8	74.23 ± 0.16	77.96 ± 0.16	81.20 ± 0.12	76.09 ± 0.50
	1	46.67 ± 0.42	$\textbf{50.39} \pm \textbf{1.09}$	$\textbf{58.50} \pm \textbf{0.51}$	$\textbf{49.94} \pm \textbf{2.01}$
CIFAR-100	1/2	40.21 ± 0.05	48.76 ± 0.25	55.08 ± 0.09	46.27 ± 0.46
CIFAR-100	1/4	36.67 ± 0.08	46.22 ± 0.71	52.09 ± 0.18	42.02 ± 0.34
	1/8	34.75 ± 0.20	44.72 ± 0.26	49.43 ± 0.16	36.26 ± 0.34



ARCL: ENHANCING CONTRASTIVE LEARNING WITH AUGMENTATION-ROBUST REPRESENTATIONS

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Augmentation Set \mathcal{A} Transformation-induced domain D_A Training domain set $\{D_A\}_{A \in \mathcal{A}}$

The goal of contrastive learning is equivalent to align different D_A

We naturally expect that the features it learn are domain invariant **The learned representation is not domain-invariant**

Formulation



The population loss of InfoNCE (Chen et al., 2020a; He et al., 2020) is well known as:

$$\mathcal{L}_{\text{InfoNCE}} = - \mathop{\mathbb{E}}_{\boldsymbol{x}, \boldsymbol{x}'} \mathop{\mathbb{E}}_{\boldsymbol{x}_1, \boldsymbol{x}_2 \in A(\boldsymbol{x})} \log \frac{e^{f(\boldsymbol{x}_1)^\top f(\boldsymbol{x}_2)}}{e^{f(\boldsymbol{x}_1)^\top f(\boldsymbol{x}_2)} + e^{f(\boldsymbol{x}_1)^\top f(\boldsymbol{x}^{-})}},$$

where encoder f is normalized by ||f|| = 1. It can be divided into two parts:

$$\mathcal{L}_{\text{InfoNCE}} = \underset{\substack{\boldsymbol{x}, \boldsymbol{x}' \ \boldsymbol{x}_{1}, \boldsymbol{x}_{2} \in A(\boldsymbol{x}) \\ \boldsymbol{x}^{-} \in A(\boldsymbol{x}')}}{\mathbb{E}} \left[-f(\boldsymbol{x}_{1})^{\top} f(\boldsymbol{x}_{2}) + \log \left(e^{f(\boldsymbol{x}_{1})^{\top} f(\boldsymbol{x}_{2})} + e^{f(\boldsymbol{x}_{1})^{\top} f(\boldsymbol{x}^{-})} \right) \right]$$

$$= \underbrace{\frac{1}{2} \underset{\substack{\boldsymbol{x}_{1}, \boldsymbol{x}_{2} \in A(\boldsymbol{x}')}}{\mathbb{E}} \underset{=:\mathcal{L}_{1}^{\text{InfoNCE}}(f)}{\mathbb{E}} \left[\| f(\boldsymbol{x}_{1}) - f(\boldsymbol{x}_{2}) \|^{2} \right] - 1}_{=:\mathcal{L}_{2}^{\text{InfoNCE}}(f)} \underbrace{\underset{\substack{\boldsymbol{x}_{2} \in A(\boldsymbol{x}')}}{\mathbb{E}} \left[\log \left(e^{f(\boldsymbol{x}_{1})^{\top} f(\boldsymbol{x}_{2})} + e^{f(\boldsymbol{x}_{1})^{\top} f(\boldsymbol{x}^{-})} \right) \right]}_{=:\mathcal{L}_{2}^{\text{InfoNCE}}(f)}$$

$$(5)$$

Methods



The original align loss:

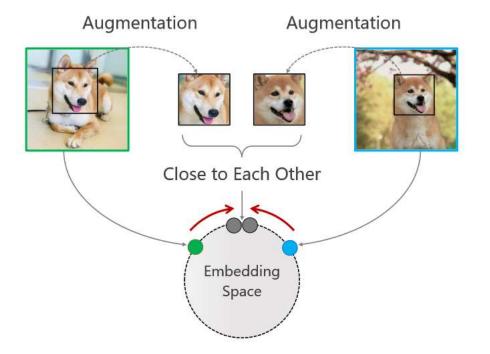
 $\mathcal{L}_{\text{align}}(f; \mathcal{D}, \pi) := \mathbb{E}_{X \sim \mathcal{D}} \mathbb{E}_{(A_1, A_2) \sim \pi^2} \| f(A_1(X)) - f(A_2(X)) \|^2$

Define the augmentation-robust loss as

$$\mathcal{L}_{AR}(f;\mathcal{D}) := \mathop{\mathbb{E}}_{X \in \mathcal{D}} \sup_{A,A' \in \mathcal{A}} \|f(A(X)) - f(A'(X))\|^2$$

An approximation:

$$\widehat{\mathcal{L}}_{AR}(f) := \frac{1}{n} \sum_{i=1}^{n} \sup_{A_1, A_2 \in \widehat{\mathcal{A}}_m(X_i)} \| f(A_1(X_i)) - f(A_2(X_i)) \|_2^2.$$



Methods



Algo	orithm 1: SimCLR + ArCL
in	put : Batch size N, temperature τ , augmentation π , number of views m, epoch T, encoder f, projector g.
1 fo	$\mathbf{r} \ t = 1, \dots, T \ \mathbf{do}$
2	sample minibatch $\{X_i\}_{i=1}^N$;
3	for $i = 1, \ldots, N$ do
4	draw <i>m</i> augmentations $\widehat{\mathcal{A}} = \{A_1, \ldots, A_m\} \sim \pi;$
5	$z_{i,j} = g(f(A_j X_i))$ for $j \in [m]$;
6	# select the worst positive samples;
7	$s_i^+ = \min_{j,k \in [m]} \{ z_{i,j}^\top z_{i,k} / (\ z_{i,j} \ \ z_{i,k} \) \};$
8	# select the negative samples;
9	for $j = 1, \ldots, N$ do
10	$ s_{i,j}^- = z_{i,1}^\top z_{j,1} / (z_{i,1} z_{j,1});$
11	$ \sum_{i,j+N} = z_{i,1}^{\top} z_{j,2} / (z_{i,1} z_{j,2}); $
12	compute $L = -\frac{1}{N} \sum_{i=1}^{N} \log \frac{\exp(s_i^+/\tau)}{\sum_{j=1, j \neq i}^{2N} \exp(s_{i,j}^-/\tau)};$
13	update f and g to minimize L;
14 re	turn f

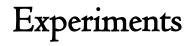




Table 1: 5 different augmentations.

	Grayscale	RandomCrop	HorizontalFlip	ColorJitter
Aug 1	 ✓ 	-	-	
Aug 2	<u></u>	~		2
Aug 3	-	877	1	-
Aug 4	-	-		~
Aug 5	~	8 <u>-</u>		1

Table 2: Linear evaluation results (%) of pretrained CIFAR10 models on CIFAR10, CIFAR100 and their modified versions.

	Method	Batch Size	Aug 1	Aug 2	Aug 3	Aug 4	Aug 5	Origina
	SimCLR	256	86.36	83.21	86.93	86.42	86.13	86.76
\sim	SimCLR + ArCL (views=4)	256	88.68	86.77	89.01	88.70	88.31	88.95
R1(SimCLR + ArCL (views=6)	256	88.95	87.18	89.54	88.92	88.61	89.11
CIFARI	SimCLR	512	88.62	86.27	88.96	88.56	88.37	88.81
U	SimCLR + ArCL (views=4)	512	89.97	88.06	90.48	89.91	89.59	90.20
	SimCLR + ArCL (views=6)	512	90.24	89.54	90.69	90.43	90.07	90.69
	SimCLR + ArCL (views=8)	512	90.44	88.96	90.98	90.63	90.31	90.84
	SimCLR	256	51.65	47.55	53.17	52.05	51.36	52.75
0	SimCLR+ArCL(views=4)	256	53.76	49.80	55.68	54.19	52.96	54.83
210	SimCLR+ArCL(views=6)	256	54.13	50.74	55.74	54.75	53.46	55.29
CIFAR100	SimCLR	512	52.28	48.09	53.45	52.58	51.53	53.12
5	SimCLR+ArCL(views=4)	512	53.40	50.16	54.92	53.77	52.61	54.20
	SimCLR+ArCL(views=6)	512	54.00	50.57	56.24	55.04	53.77	55.60
	SimCLR+ArCL(views=8)	512	54.59	50.85	55.74	54.62	53.21	55.96



		Epochs	ImageNet	Aircraft	Caltech101	Cars	CIFAR10	CIFAR100	DTD	Flowers	Food	Pets	Avg
	MoCo	800	70.68	41.79	87.92	39.31	92.28	74.90	73.88	90.07	68.95	83.30	72.49
	MoCo	800+50	70.64	41.00	87.63	39.01	92.27	75.14	74.31	88.31	68.57	83.69	72.21
	MoCo + ArCL(views=2)	800+50	69.70	44.29	89.79	42.15	93.07	76.70	74.20	90.40	70.94	83.68	73.91
	MoCo + ArCL(views=3)	800+50	69.80	44.57	89.48	42.11	93.29	77.33	74.63	91.13	71.16	84.23	74.21
	MoCo + ArCL(views=4)	800+50	69.80	44.62	89.66	42.88	93.22	76.83	75.00	91.59	71.35	83.99	74.35
Linear	МоСо	800+100	70.64	41.65	87.64	39.31	92.12	75.03	73.94	89.53	68.31	83.55	72.34
in	MoCo + ArCL(views=2)	800+100	70.26	41.86	89.52	40.21	92.64	75.73	74.04	88.97	70.06	84.31	73.04
-	MoCo + ArCL(views=3)	800+100	70.92	43.87	89.36	42.37	93.30	76.93	72.93	90.50	71.14	84.03	73.83
	MoCo + ArCL(views=4)	800+100	69.42	45.55	89.61	41.91	93.55	77.05	74.04	91.17	70.93	85.48	74.37
	MoCo	200	67.72	40.02	86.59	37.41	90.90	72.43	73.88	87.97	66.97	80.00	70.69
	MoCo + ArCL(views=2)	200	68.04	42.34	87.92	36.45	92.29	71.71	74.68	89.00	67.87	81.42	71.85
	MoCo + ArCL(views=3)	200	68.74	43.21	88.26	38.27	92.49	75.02	74.68	89.61	68.31	81.64	72.39
	MoCo + ArCL(views=4)	200	68.92	41.65	88.42	38.77	92.70	75.73	75.43	88.95	68.63	81.60	72.43
	Supervised*		77.20	43.59	90.18	44.92	91.42	73.90	72.23	89.93	69.49	91.45	74.12
	МоСо	800		83.56	82.54	85.09	95.89	71.81	69.95	95.26	76.81	88.83	83.30
	МоСо	800+50		83.15	84.50	85.90	96.13	72.58	70.16	94.44	79.34	86.12	83.59
	MoCo + ArCL(views=2)	800+50		86.05	87.38	87.28	96.33	79.39	72.18	95.89	81.36	89.03	86.10
	MoCo + ArCL(views=3)	800+50		84.03	87.64	86.34	96.88	80.98	72.87	96.14	81.90	89.20	86.22
	MoCo + ArCL(views=4)	800+50		84.19	88.42	86.67	96.68	81.17	73.09	95.90	81.70	89.52	86.37
Finetune	MoCo	800+100		83.18	84.50	84.27	96.01	72.14	70.27	95.53	78.23	88.73	83.65
ne	MoCo + ArCL(views=2)	800+100		84.45	86.84	87.20	96.40	78.40	71.91	95.93	80.54	88.56	85.58
ΪĒ	MoCo + ArCL(views=3)	800+100		85.94	86.85	87.34	96.36	79.75	71.44	96.00	81.48	88.26	85.94
	MoCo + ArCL(views=4)	800+100		85.65	88.50	86.39	96.91	81.29	73.35	96.17	81.82	89.30	86.60
	MoCo	200		83.18	82.66	84.47	95.51	72.54	70.43	94.99	77.39	86.12	83.03
	MoCo + ArCL(views=2)	200		81.09	83.93	86.54	95.88	76.18	70.69	94.44	76.78	86.98	83.61
	MoCo + ArCL(views=3)	200		84.79	85.61	85.39	96.56	78.81	70.59	95.84	80.71	87.91	85.13
	MoCo + ArCL(views=4)	200		84.88	86.19	85.90	96.35	78.62	70.69	95.77	80.46	88.00	85.21
	Supervised*			83.50	91.01	82.61	96.39	82.91	73.30	95.50	84.60	92.42	86.92

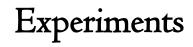




Table 7: Linear evaluation results of pretrained models using SimCLR with two different alignment losses on MNIST-CIFAR dataset. The average results under three diffrent random seeds are given.

Methods	Accuracy(%)	Methods	Accuracy(%)
SimCLR	85.6		
SimCLR + ArCL(views=3)	86.0	SimCLR+AAL(views=3)	85.4
SimCLR + ArCL(views=4)	87.2	SimCLR+AAL(views=4)	86.1
SimCLR + ArCL(views=5)	87.3	SimCLR+AAL(views=5)	86.3
SimCLR + ArCL(views=6)	88.4	SimCLR+AAL(views=6)	85.8



WHAT SHOULD NOT BE CONTRASTIVE IN CONTRASTIVE LEARNING

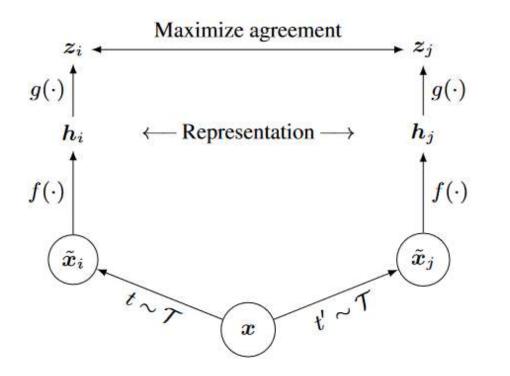
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Background



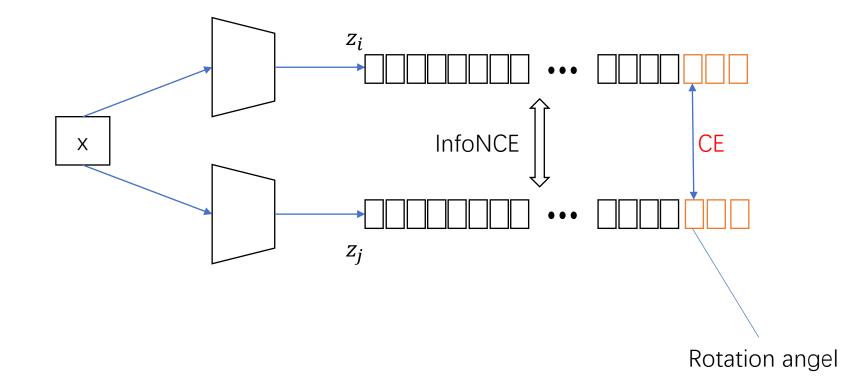
Is the classical contrastive learning framework capable of achieving optimal in generalization?



Consider the extreme situation:

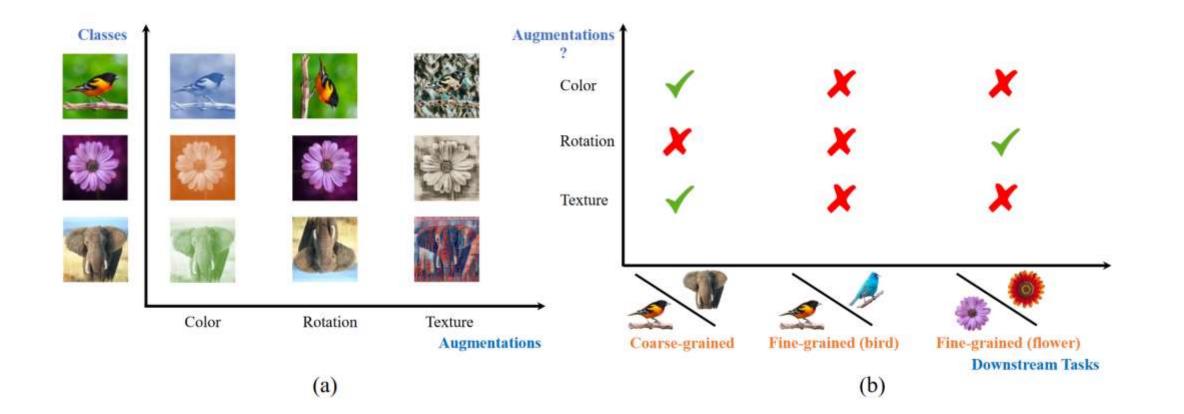
 $z_i = z_j, \forall x \in D_x$ If *T* contains Rotation, then the features contains non information to justify the rotation angel in some rotation-sensitive tasks. Background





Motivation





Method



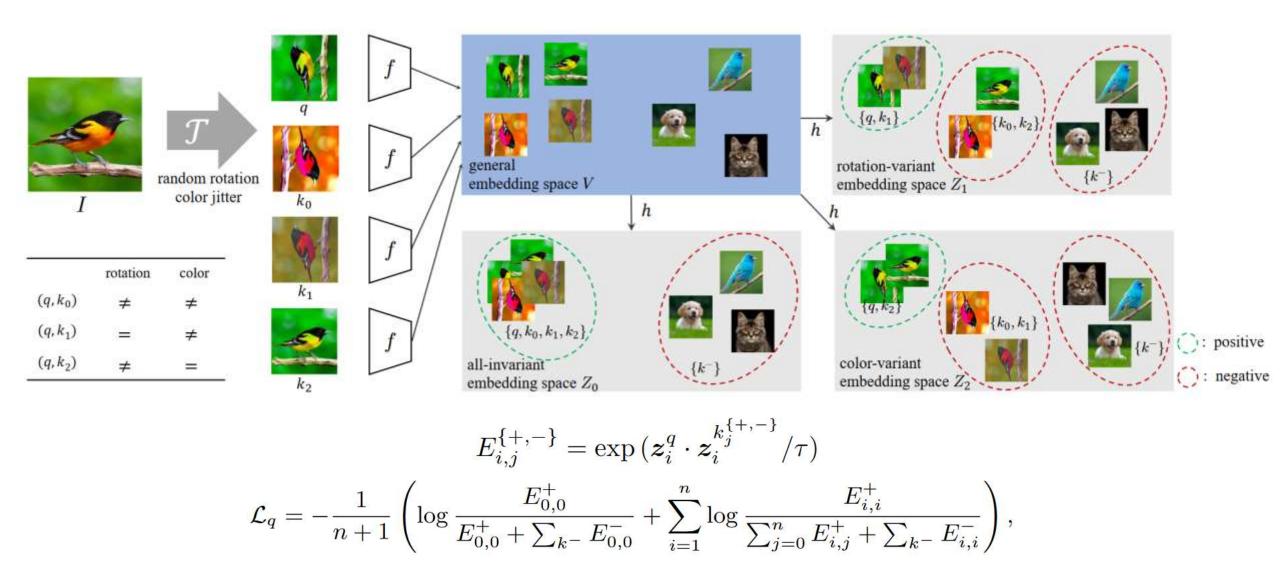




Table 1: Classification accuracy on 4-class rotation and IN-100 under linear evaluation protocol. Adding rotation augmentation into baseline MoCo significantly reduces its capacity to classify rotation angles while downgrades its performance on IN-100. In contrast, our method better leverages the information gain of the new augmentation.

Experiments

modal	Rotation	IN-100		
model	Acc.	top-1	top-5	
Supervised	72.3	83.7	95.7	
MoCo	61.1	81.0	95.2	
MoCo + Rotation	43.3	79.4	94.1	
MoCo + Rotation (same for q and k)	45.5	78.1	94.3	
LooC + Rotation [ours]	65.2	80.2	95.5	

Table 2: Evaluation on multiple downstream tasks. Our method demonstrates superior generalizability and transferability with increasing number of augmentations.

model			iNat-1k					IN-100		
model	Color	Rotation	top-1	top-5	top-1	top-5	5-shot	10-shot	top-1	top-5
MoCo	~		36.2	62.0	36.7	64.7	67.9 (± 0.5)	77.3 (± 0.1)	81.0	95.2
LooC	1		41.2	67.0	40.1	69.7	68.2 (± 0.6)	77.6 (± 0.1)	81.1	95.3
		\checkmark	40.0	65.4	38.8	67.0	$70.1 (\pm 0.4)$	79.3 (± 0.1)	80.2	95.5
	\checkmark	\checkmark	44.0	69.3	39.6	69.2	$70.9 (\pm 0.3)$	80.8 (± 0.2)	79.2	94.7
LooC++	~	~	46.1	71.5	39.3	69.3	68.1 (± 0.4)	78.8 (± 0.2)	81.2	95.2

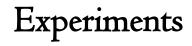




Table 5: **Comparisons of concatenating features from different embedding spaces in LooC++** jointly trained on color, rotation and texture augmentations. Different downstream tasks show non-identical preferences for augmentation-dependent or invariant representations.

Model	Vari	ance H	Iead	IN-	100	iNat-1k		Flowe	IN-C-100	
Widder	Col.	Rot.	Tex.	top-1	top-5	top-1	top-5	5-shot	10-shot	all-top-1
LooC++				78.5	94.3	38.5	64.7	$68.6 (\pm 0.6)$	$77.6 (\pm 0.1)$	48.0
	\checkmark			79.7	94.4	42.9	68.7	$69.1 (\pm 0.7)$	$79.5 (\pm 0.2)$	47.1
		\checkmark		81.5	94.9	41.4	67.4	$70.5 (\pm 0.6)$	$80.0 (\pm 0.2)$	52.6
			\checkmark	80.3	94.9	43.0	68.6	$70.4 (\pm 0.5)$	$80.5 (\pm 0.2)$	44.1
	\checkmark	\checkmark	\checkmark	82.2	95.3	45.9	71.4	$71.0 (\pm 0.7)$	81.9 (± 0.3)	48.0

Experiments



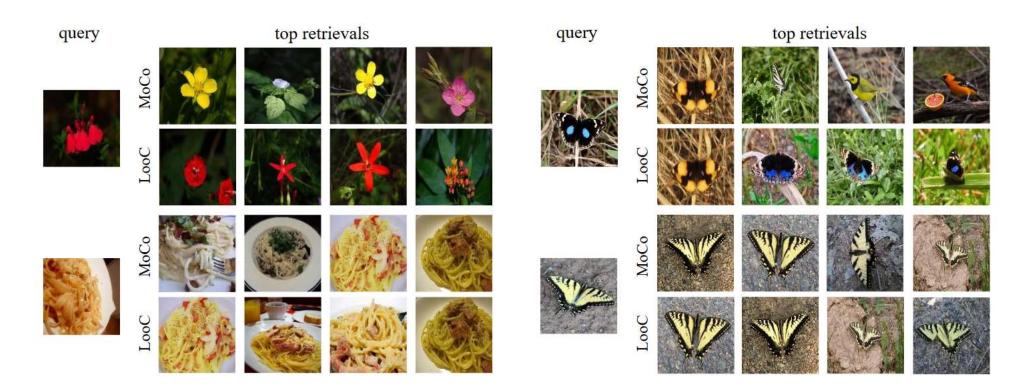


Figure 3: **Top nearest-neighbor retrieval results** of LooC vs. corresponding invariant MoCo baseline with color (left) and rotation (right) augmentations on IN-100 and iNat-1k. The results show that our model can better preserve information dependent on color and rotation despite being trained with those augmentations.



Thanks





Augmented Distance

$$d_A(x_1, x_2) = \min_{x_1' \in A(x_1), x_2' \in A(x_2)} \|x_1' - x_2'\|.$$

Definition 1 ((σ, δ) -Augmentation). The augmentation set A is called a (σ, δ) -augmentation, if for each class C_k , there exists a subset $C_k^0 \subseteq C_k$ (called a main part of C_k), such that both $\mathbb{P}[\boldsymbol{x} \in C_k^0] \geq \sigma \mathbb{P}[\boldsymbol{x} \in C_k]$ where $\sigma \in (0, 1]$ and $\sup_{\boldsymbol{x}_1, \boldsymbol{x}_2 \in C_k^0} d_A(\boldsymbol{x}_1, \boldsymbol{x}_2) \leq \delta$ hold.

Larger σ and smaller δ indicate the sharper concentration of augmented data.

For any $A' \supseteq A$, $d_{A'}(x_1, x_2) \le d_A(x_1, x_2)$

Theories



Theorem 1. Given a (σ, δ) -augmentation used in contrastive SSL, if

$$\mu_{\ell}^{\top}\mu_{k} < r^{2}\left(1 - \rho_{max}(\sigma, \delta, \varepsilon) - \sqrt{2\rho_{max}(\sigma, \delta, \varepsilon)} - \frac{\Delta_{\mu}}{2}\right)$$
(2)

holds for any pair of (ℓ, k) with $\ell \neq k$, then the downstream error rate of NN classifier G_f $\operatorname{Err}(G_f) \leq (1 - \sigma) + R_{\varepsilon},$ (3)
where $\rho_{max}(\sigma, \delta, \varepsilon) = 2(1 - \sigma) + \frac{R_{\varepsilon}}{\min_{\ell} p_{\ell}} + \sigma \left(\frac{L\delta}{r} + \frac{2\varepsilon}{r}\right)$ and $\Delta_{\mu} = 1 - \min_{k \in [K]} \|\mu_k\|^2 / r^2.$



Proof of Proposition 4.1. For any $\varepsilon > 0$, let $t = \sqrt{\varepsilon}/2$ and $f(x_1, x_2) = x_1 + tx_2$. Then, the alignment loss of f satisfies

$$\mathcal{L}_{\text{align}}(f; \mathcal{D}, \pi) = t^2 \mathbb{E} X_2^2 \underset{(\theta_1, \theta_2) \sim \mathcal{N}(0, 1)^2}{\mathbb{E}} (\theta_1 - \theta_2)^2 = 2t^2 < \varepsilon.$$

Let c = 0 and c' = 1/t. Then obviously

$$\mathcal{R}(f;\mathcal{D}_c)=0,$$

but

$$\mathcal{R}(f;\mathcal{D}_{c'}) = P(X_1 < 0, X_1 + X_2 \ge 0) + P(X_1 \ge 0, X_1 + X_2 \le 0) = \frac{1}{4}.$$

Formulation



$$\mathcal{R}(f; \mathcal{D}^{\text{tar}}) := \min_{h \in \mathbb{R}^{K \times m}} \mathbb{E}_{X \sim \mathcal{D}^{\text{tar}}} \ell(h \circ f(X), Y),$$

$$\mathcal{L}_{\text{align}}(f; \mathcal{D}, \pi) := \mathbb{E}_{X \sim \mathcal{D}} \mathbb{E}_{(A_1, A_2) \sim \pi^2} \| f(A_1(X)) - f(A_2(X)) \|^2$$

$$(2)$$

Proposition 4.1. Consider a two-dimensional classification problem with data $(X_1, X_2) \sim \mathcal{N}(0, I_2)$. The label Y satisfies $Y = 1(X_1 \ge 0)$, and the data augmentation is to multiply X_2 by standard normal noise, i.e.,

$$A_{\theta}(X) = (X_1, \theta \cdot X_2),$$

$$\theta \sim \mathcal{N}(0, 1).$$

The corresponding transformation-induced domain set is $\mathcal{P} = \{\mathcal{D}_c : \mathcal{D}_c = (X_1, c \cdot X_2) \text{ for } c \in \mathbb{R}\}$. We consider the 0-1 loss in equation 2. Then for every $\varepsilon > 0$, there exists representation f and two domains \mathcal{D}_c and $\mathcal{D}_{c'}$ such that

$$\mathcal{L}_{\text{align}}(f; \mathcal{D}, \pi) < \varepsilon,$$

but

$$|\mathcal{R}(f; \mathcal{D}_c) - \mathcal{R}(f; \mathcal{D}_{c'})| \ge \frac{1}{4}$$