LOTOS: Layer-wise Orthogonalization for Training robust ensembles

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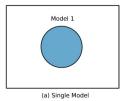
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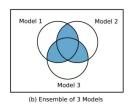


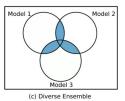
Why ensembles?



- Ensembles of models is known to be more robust to adversarial attacks.
 - It is harder to fool multiple models!







- The adversarial examples are transferable!
 - this reduces the effectiveness of using multiple models
 - introducing diversity among the models helps to counteract this effect
 - this is the basis of methods for training robust ensembles

¹ Kariyappa, S., & Qureshi, M. K. (2019). Improving adversarial robustness of ensembles with diversity training. arXiv preprint arXiv:1901.09981.



• For model $\mathcal{F}: \mathcal{X} \to \mathcal{Y}$, untargeted attack $\mathcal{A}(x) = x + \delta_x$, and a sample (x,y), \mathcal{A} maximizes $\ell_{\mathcal{F}}(x+\delta_x,y)$, s.t. $\|\delta_x\|_2 \le \epsilon$.



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- Given an untargetted attack A(x) on a surrogate model \mathcal{F} , transferability between \mathcal{F} and the target model \mathcal{G} is defined as:
 - Consider the samples for which:
 - \bigcirc \mathcal{F} makes correct prediction,
 - \bigcirc \mathcal{G} makes correct prediction,
 - \mathfrak{I} makes wrong prediction on $\mathcal{A}(x)$
 - And compute the ratio of them on which $\mathcal G$ makes wrong prediction on $\mathcal A(x)$ as well.



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- More specifically:

$$T_{rate}(\mathcal{A}_{\mathcal{F}}, \mathcal{F}, \mathcal{G}) = \mathbb{P}_{(x,y)\in\mathcal{X}\times\mathcal{Y}}[\mathcal{G}(\mathcal{A}_{\mathcal{F}}(x)) \neq y \mid \mathcal{F}(x) = \mathcal{G}(x) = y$$
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Controling the Lipschitz constant



• Function *f* is *L*-Lipschitz if:

$$||f(x_1) - f(x_2)||_2 \le L||x_1 - x_2||_2.$$

Consider a model

$$f(x,\theta) = W^{L+1}\sigma_L(W^L(\sigma_{L-1}(W^{L-1}(\dots\sigma_1(W^1x)\dots)))),$$

▶ Then:

$$||f||_{\text{Lip}} \le ||(W^{L+1})||_{\text{Lip}} \cdot ||\sigma_L||_{\text{Lip}} \cdot ||(W^L)||_{\text{Lip}} \cdots ||\sigma_1||_{\text{Lip}} \cdot ||(W^1)||_{\text{Lip}}$$

Effect of Lipschitz continuity



Controlling the Lipschitz factor of a model makes it more robust. [2]

We investigated how it affects the transferability rate among models!

² Ebrahimpour Boroojeny, A., Telgarsky, M., & Sundaram, H. (2024, April). Spectrum extraction and clipping for implicitly linear layers. In International Conference on Artificial Intelligence and Statistics (pp. 2971-2979). PMLR.

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Proposition

If $\ell_{\mathcal{F}}$ and $\ell_{\mathcal{G}}$ are L-Lipschitz w.r.t the inputs, and $\|\delta\|_2 \leqslant r$, for attack \mathcal{A} :

$$|R_{\mathcal{F}}(A(x),y) - R_{\mathcal{G}}(A(x),y)| \leq 2Lr + |R_{\mathcal{F}}(x,y) - R_{\mathcal{G}}(x,y)|.$$

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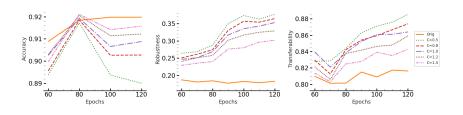
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What can we do?

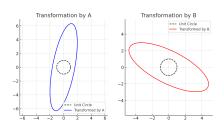


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What can we do?



- How to preserve the robustness of individual models and increase the diversity?
- We consider the layers-wise transformations of linear layers!
 - Consider two corresponding layers from the two models in the ensemble:
 - The direction along the largest singular vector of each one should cause small changes in the other!



New component in the loss function



 We define a new notion of similarity between the jth layers of models f and g, based on their top-k sub-spaces:

$$\begin{split} S_k^{(j)}(f^{(j)},g^{(j)},\text{mal}) \coloneqq & \sum_{i=1}^k w_i (\text{ReLU}(\|f^{(j)}(v_i')\|_2 - \text{mal})) \\ & + \text{ReLU}(\|g^{(j)}(v_i)\|_2 - \text{mal})), \end{split}$$

where mal is a threshold hyperparameter

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- where mal is a threshold hyperparameter
- LOTOS uses a new component in the loss that penalizes the similarity for all pairs of corresponding layers for the models of the ensemble:

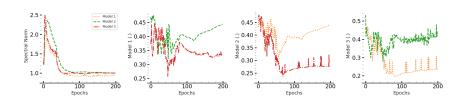
$$\begin{split} \mathcal{L}_{\text{train}} &= \frac{1}{N} \sum_{i=1}^{N} \mathcal{L}_{\text{CE}}(\mathcal{F}_{i}(x), y) + \\ &\frac{\lambda}{M \, N \, (N-1)} \sum_{z=1}^{N-1} \sum_{j=z+1}^{N} \sum_{l=1}^{M} S_{k}^{(l)}(f_{z}^{(l)}, f_{j}^{(l)}, \text{mal}) \end{split}$$

Does the new loss function work?



The effect of orthogonalization with different values of mal:

• When mal = 0.5:

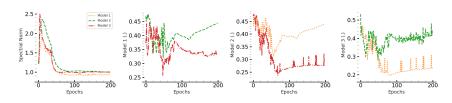


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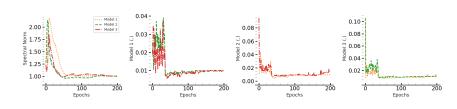


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• When mal = 0.01:

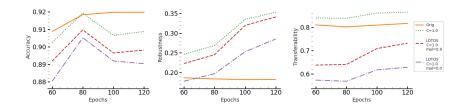


Does this help?



Experimental setup: ensembles of three ResNet-18 models

- LOTOS effectively decreases the transferability rate among pairs of models
- LOTOS still benefits from robustness of individual models
- By decreasing the value of mal transferability rate decreases, but individual accuracy and robust accuracy decreases, and therefore, introduces a trade-off



More robust ensembles!



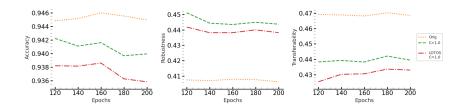
- Comparing the effectiveness in overall robustness of the ensembles:
 - Two different architectures (ResNet-18 and DLA)
 - ► Two different datasets (CIFAR-10 and CIFAR-100)

	CIFAR-10			CIFAR-100				
	ORIG	C = 1.0	LOTOS	ORIG	C = 1.0	LOTOS		
	Ensembles of ResNet-18 models							
Test Acc	95.3 ± 0.06	94.7 ± 0.24	94.6 ± 0.19	77.2 ± 0.17	76.6 ± 0.01	76.6 ± 0.10		
Robust Acc	30.3 ± 1.63	35.2 ± 0.72	36.3 ± 0.88	15.2 ± 0.45	18.9 ± 0.40	20.2 ± 0.47		
	Ensembles of DLA models							
Test Acc	95.4 ± 0.12	95.2 ± 0.05	95.05 ± 0.09	77.1 ± 0.09	78.8 ± 0.31	78.3 ± 0.38		
ROBUST ACC	26.7 ± 0.58	32.8 ± 1.28	34.5 ± 0.63	16.5 ± 0.78	19.4 ± 0.32	21.0 ± 0.39		

What about heterogeneous ensembles?



- The singular vectors of the first affine layer have the same dimension, which is equal to the input dimension!
 - They can be made orthogonal using LOTOS
- Ensembles of ResNet-18, ResNet-34, and DLA trained on CIFAR-10:
 - ▶ LOTOS still effective, but not as much as homogeneous ensembles



Works with other methods!



- Comparing the effectiveness of LOTOS when used along with TRS^[3], which is one of the prior SOTA in ensemble robust training
 - Two different architectures (ResNet-18 and DLA)
 - ► Two different datasets (CIFAR-10 and CIFAR-100)

		CIFAR-10		CIFAR-100				
	TRS	$\mathrm{TRS}+C=1$	${ m TRS} + { m LOTOS}$	TRS	$\mathrm{TRS}+C=1$	TRS + LOTOS		
	Ensembles of ResNet-18 models							
Test Acc	94.4 ± 0.05	94.1 ± 0.17	92.7 ± 0.09	73.28 ± 0.46	72.94 ± 0.29	67.23 ± 1.22		
ROBUST ACC	30.8 ± 0.65	35.9 ± 1.35	41.5 ± 1.04	12.3 ± 0.53	16.3 ± 0.57	20.7 ± 0.99		
			Ensembles of	DLA MODELS				
Test Acc	94.72 ± 0.06	92.79 ± 0.13	93.18 ± 0.14	72.6 ± 0.54	63.3 ± 1.20	66.8 ± 1.26		
ROBUST ACC	31.2 ± 0.80	32.9 ± 0.77	35.3 ± 0.39	23.2 ± 0.41	23.7 ± 2.36	24.3 ± 1.67		

• Similar results with DVERGE^[4], another prior SOTA

³ Yang, Z., Li, L., Xu, X., Zuo, S., Chen, Q., Zhou, P., ... Li, B. (2021). Trs: Transferability reduced ensemble via promoting gradient diversity and model smoothness. Advances in Neural Information Processing Systems, 34, 17642-17655.

⁴ Yang, H., Zhang, J., Dong, H., Inkawhich, N., Gardner, A., Touchet, A., ... Li, H. (2020). Dverge: diversifying vulnerabilities for enhanced robust generation of ensembles. Advances in Neural Information Processing Systems, 33, 5505-5515.

Is it efficient?



- ullet LOTOS promotes orthogonality among the top-k sub-spaces.
- The (k+1)st singular vectors can still be highly correlated!
- The (k+1)st singular value can be as large as the 1st one!

Theorem

Given two convolutional layers, M_1 and M_2 with a single input and output channel and circular padding for which \mathbf{f} is the vectorized form of the filter with a length of T, and considering n to be the length of the vectorized input, if $\|Av_1'\|_2 \leqslant \epsilon$, then:

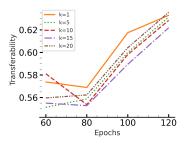
$$||Av_p'||_2 \le \sqrt{\epsilon^2 + \pi ||\mathbf{f}||_2^2 T^2 \frac{p}{n}},$$

where A is the corresponding linear transformation of M_1 and v_p' is singular vector of M_2 corresponding to its p-th largest singular value.

Is it efficient?



• Observing the effect of k in transferability rate:



- Increasing k slightly decreases the transferability rate, but up to k = 15
- $oldsymbol{k}$ larger than 15 does not show further improvements due to further optimization constraints and restrictions of convolutional layer's spectrum

Thank You!





• Observing the effect of k in transferability rate:

	Orig	Orig+ C = 1	ORIG + LOTOS
TRS	10.3 ± 0.33	13.2 ± 1.12	14.5 ± 0.81
DVERGE	19.7 ± 2.34	26.8 ± 0.75	29.2 ± 0.56

• Comparing the running times:

	Orig	C = 1	LOTOS	TRS	TRS + C = 1	TRS + LOTOS	Adv	$\mathrm{Adv}+C=1$	ADV + LOTOS
ResNet-18	33.2	74.9 ×2.3	79.3 ×2.4	158.2	224.4 ×1.4	227.3 ×1.4	312.6	479.2 ×1.5	485.2 ×1.5
DLA	63.1	$155.4_{\times 2.5}$	$165.4_{~\times 2.6}$	326.2	$466.1{\scriptstyle~\times 1.4}$	$477.4_{\times1.5}$	758.6.2	$942.5_{~\times1.2}$	$949.2{\scriptstyle~\times 1.2}$



- For model $\mathcal{F}: \mathcal{X} \to \mathcal{Y}$ and, attack $\mathcal{A}(x) = x + \delta_x$, and a sample (x,y):
 - for untargetted attack: \mathcal{A} maximizes $\ell_{\mathcal{F}}(x + \delta_x, y)$, s.t. $\|\delta_x\|_2 \le \epsilon$.
 - and targeted attack for y_t : $A_t(x) = \min_{\delta x} [\ell_{\mathcal{F}}(x + \delta_x.y_t)]$
- Given an untargetted attack $\mathcal{A}(x)$ on a surrogate model \mathcal{F} , transferability between \mathcal{F} and the target model \mathcal{G} is defined as:

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• And for targeted attack $A_t(x)$, it is defined as:

$$T_{rate}(\mathcal{A}_{\mathcal{F}}^{(t)}, \mathcal{F}, \mathcal{G}) = \mathbb{P}_{(x,y)\in\mathcal{X}\times\mathcal{Y}}[\mathcal{G}(\mathcal{A}_{\mathcal{F}}^{(t)}(x)) = y_t \mid \mathcal{F}(x) = \mathcal{G}(x) = y$$
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