How to Improve Model Robustness? A Distributional-Discrepancy Perspective

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Outline

- Background
- **ICML 2025:** Sample-specific Noise Injection for Diffusion-based Adversarial Purification
- **ICML 2025:** One Stone, Two Birds: Enhancing Adversarial Defense Through the Lens of Distributional Discrepancy

What is an adversarial example (attack)?

88% Tabby Cat

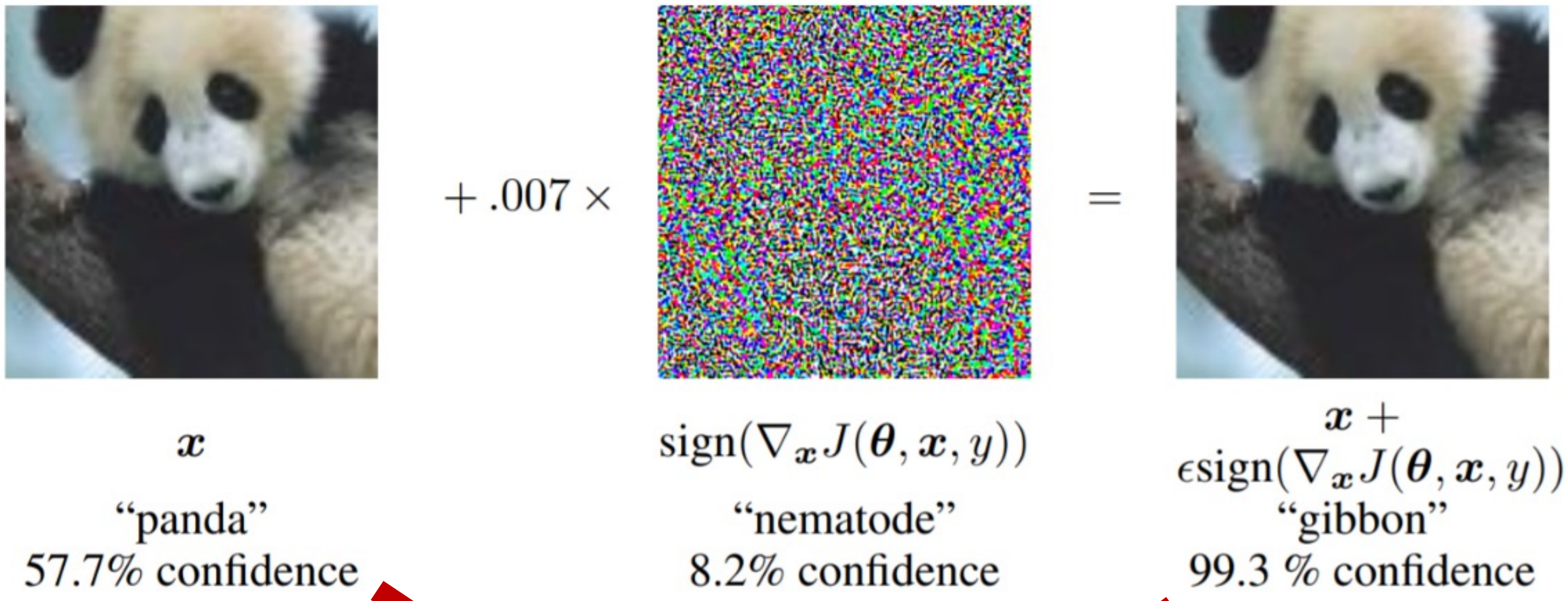
Adversarial

Perturbations

99% Guacamole

Why it works?

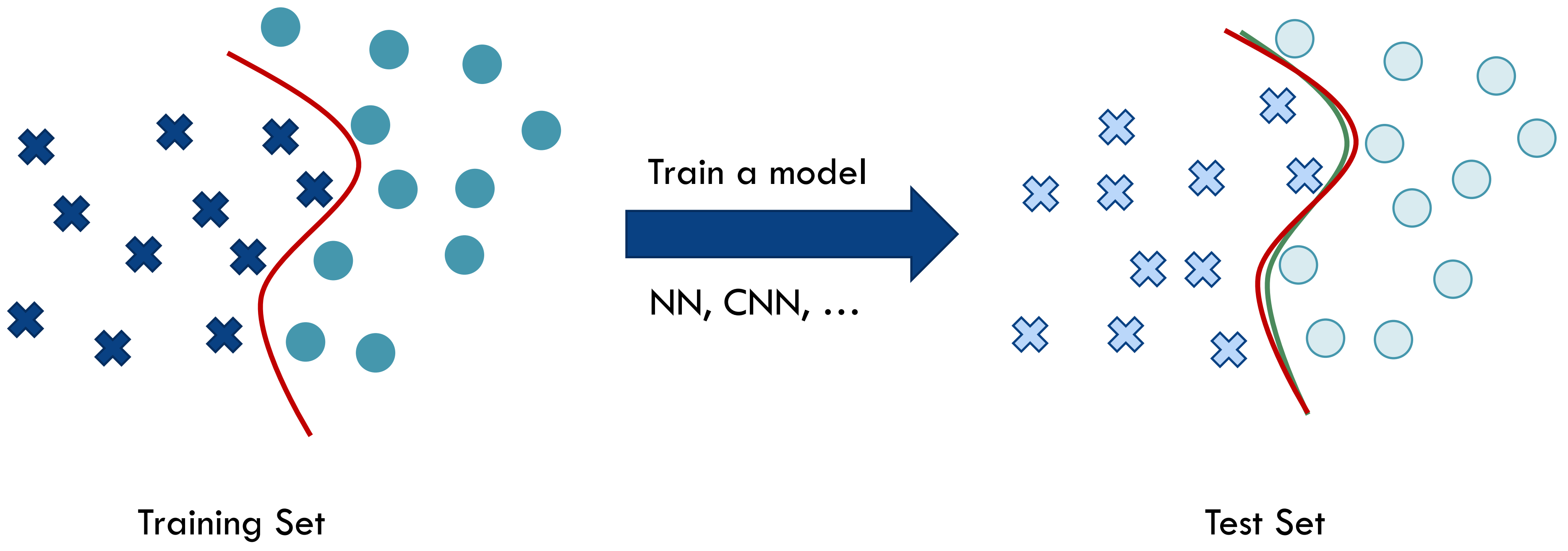
Why adversarial attack can be successful?



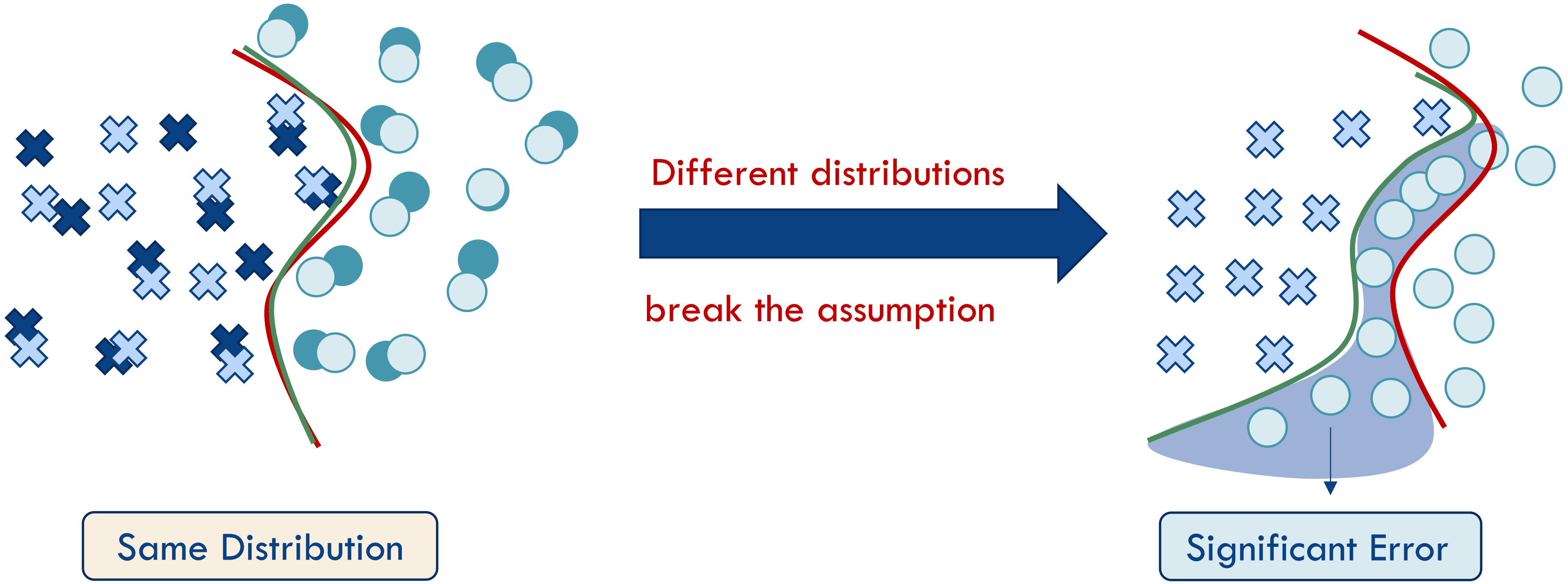
Different Distributions → Significant Error

Maximum Mean Discrepancy Test is Aware of Adversarial Attacks. In *ICML*, 2021.

Basic assumption in machine learning



Basic assumption in machine learning



Basic assumption in machine learning

Break the assumption!!!

How to defend against it?

Defend against adversarial attacks

Trustworthy Machine Learning Under Adversarial Data

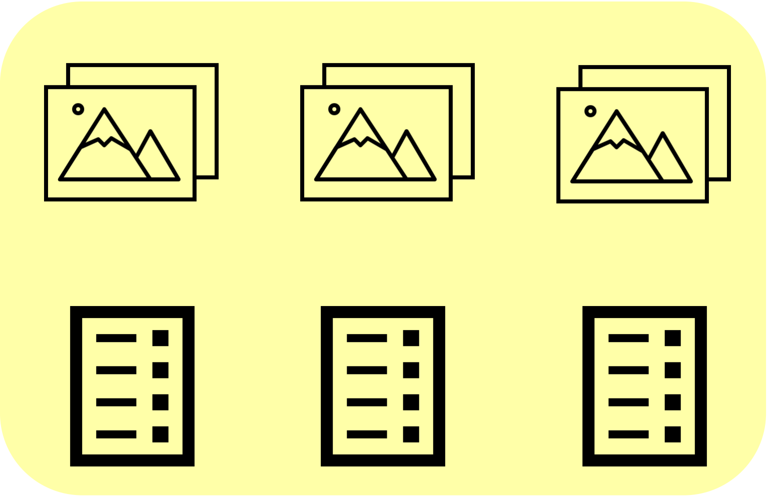
- Actively Handle Adversarial Data
  - Model Perspective — **Adversarial Training, Fine-tuning**
  - Data Perspective — **Adversarial Purification**
- Passively Handle Adversarial Data — **Adversarial Detection**

Today's Focus

Adversarial detection

- ❑ *Adversarial Detection* (AD): aims to detect and discard AEs.

Discard the adversarial data

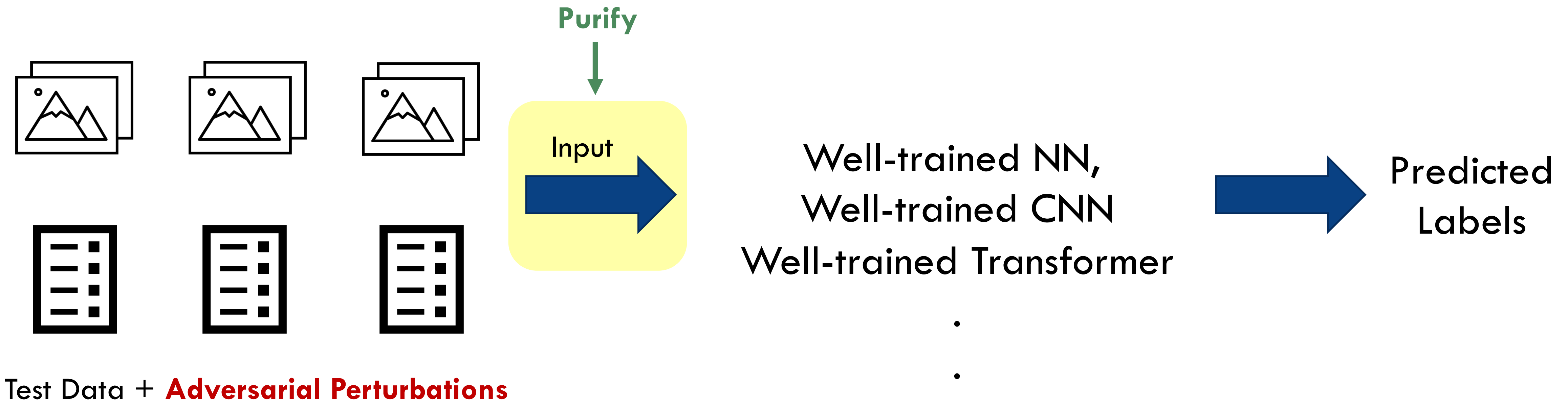


Test Data + **Adversarial Perturbations**

Input → Well-trained NN, Well-trained CNN Well-trained Transformer . . → Predicted Labels

Adversarial purification

- ❑ *Adversarial Purification* (AP): aims to shift AEs back towards their natural counterparts.



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Sample-specific Noise Injection for Diffusion-based Adversarial Purification

Yuhao Sun^, Jiacheng Zhang^, Zesheng Ye^, Chaowei Xiao, Feng Liu*

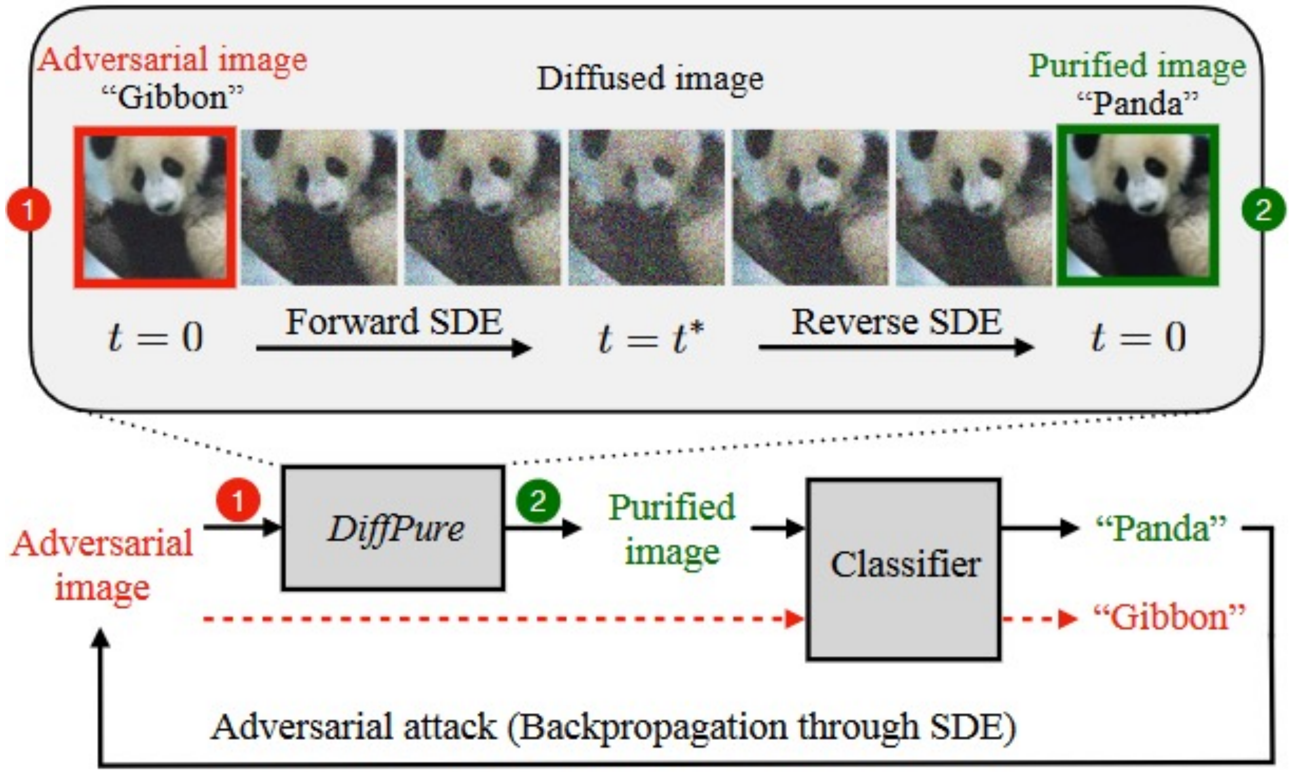
(^ Co-first authors, * Corresponding authors)

In *ICML*, 2025.

Paper

Code

Preliminary: diffusion-based adversarial purification

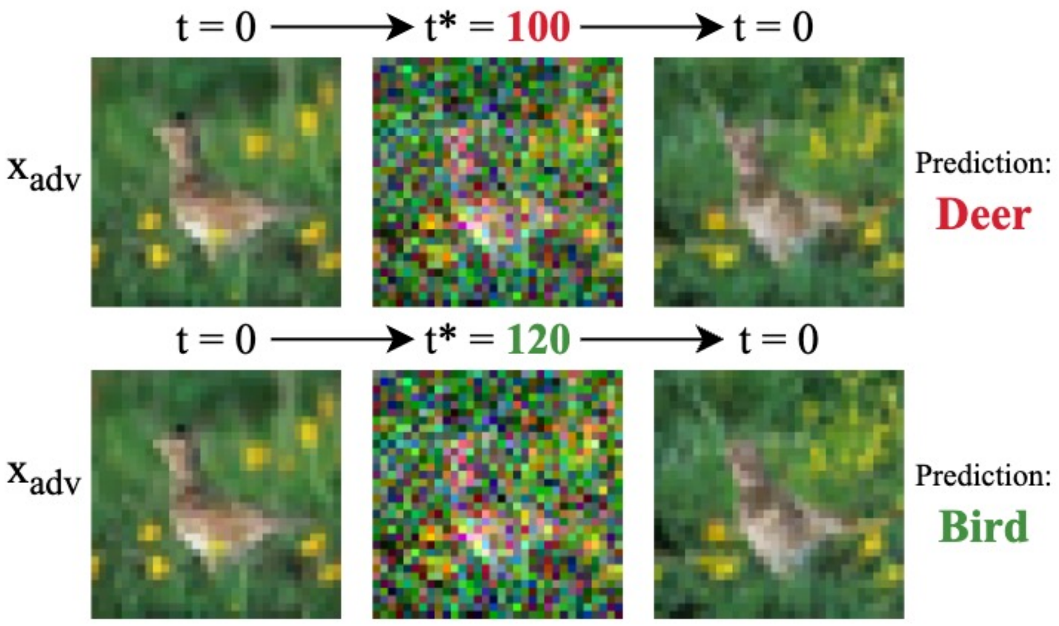


A Key Challenge: The Choice of t

- ❑ **If t is too small,** then adversarial noise cannot be fully removed.
- ❑ **If t is too large,** then the purified image may have a different semantic meaning.
- ❑ **Research gap:** current methods empirically select a *fixed* timestep t for all images, which is counterintuitive.

Diffusion Models for Adversarial Purification. In *ICML*, 2022.

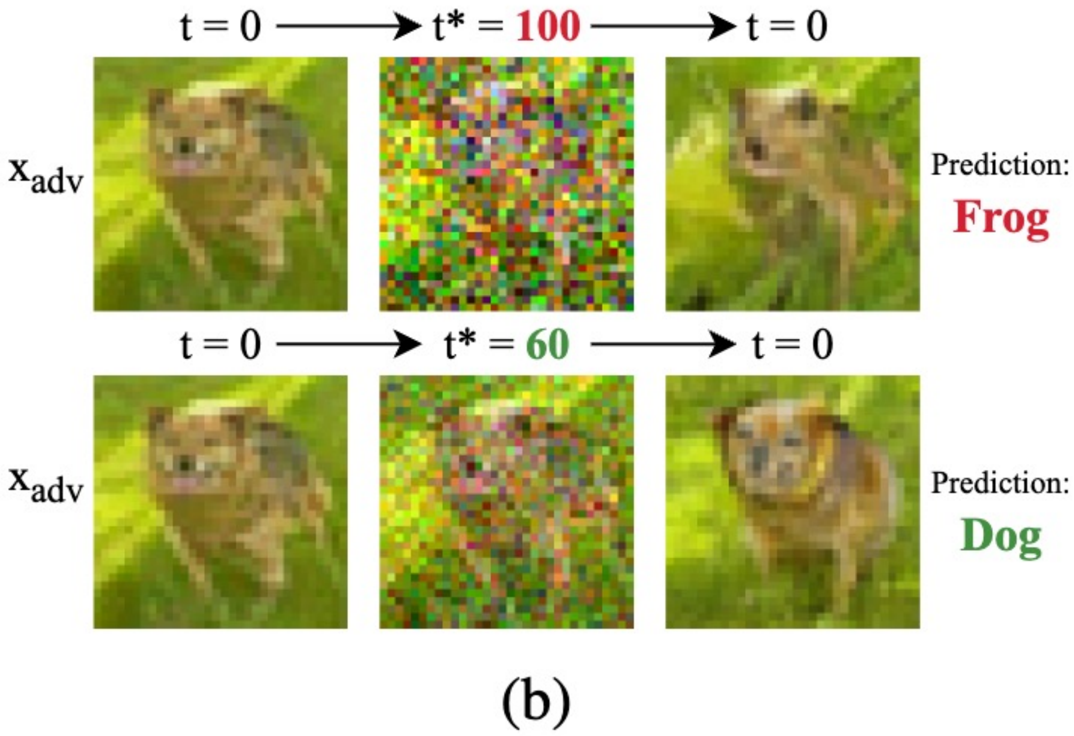
Motivation



(a)

- Sample-shared noise level is sometimes insufficient to remove adversarial perturbations.

Motivation



- Sample-shared noise level is sometimes too large, which causes excessive disruption of the sample's semantic information, making it difficult to recover the original semantics.

Sample-specific Noise Injection for Diffusion-based Adversarial Purification. In *ICML*, 2025.

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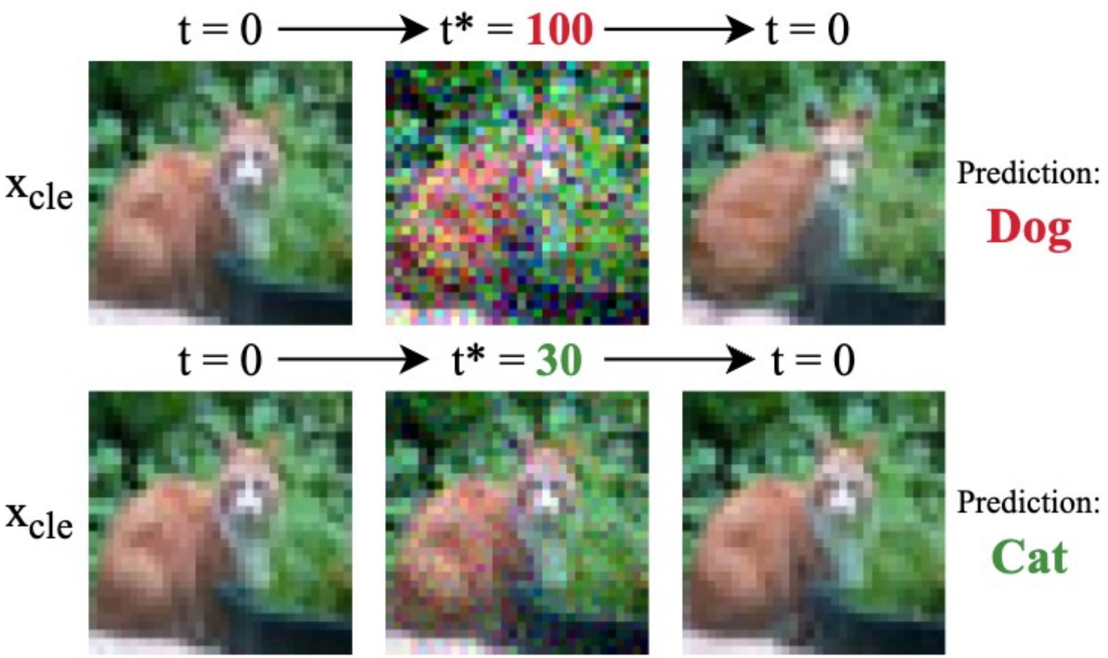
Motivation

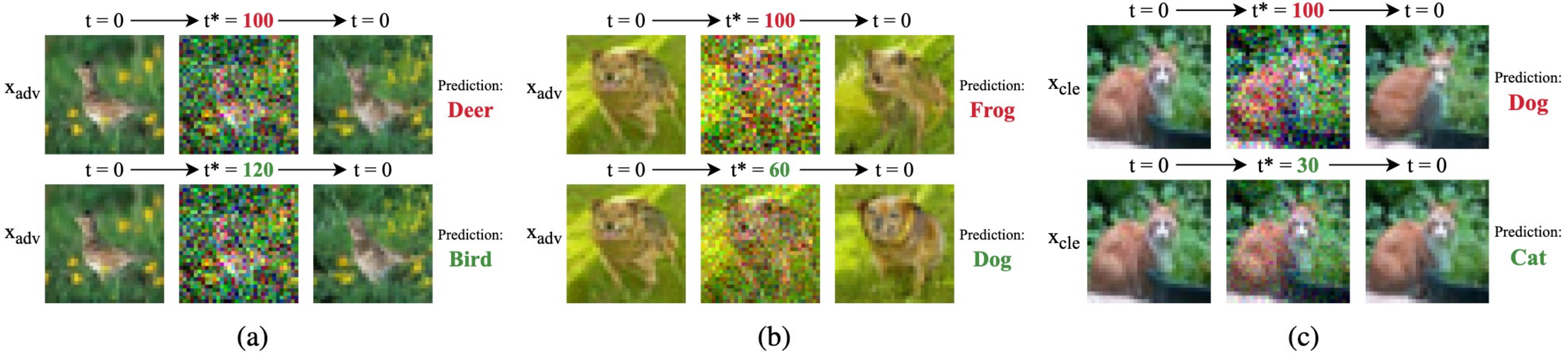


(c)

- ❑ Sample-shared noise level is often too large for clean examples, as they do not need to be purified.

Sample-specific Noise Injection for Diffusion-based Adversarial Purification. In *ICML*, 2025.

Proof-of-concept Experiment



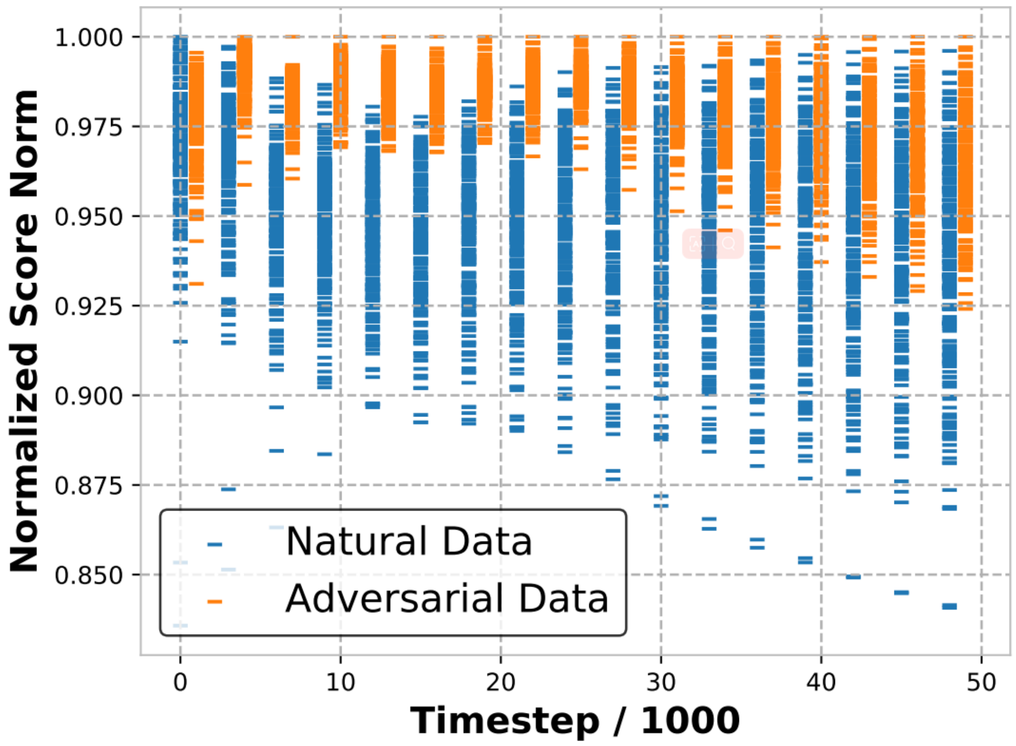
- ❑ Sample-shared noise level *fail* to address diverse adversarial perturbations.
- ❑ These findings *highlight* the need for sample-specific noise injection levels.

Sample-specific Noise Injection for Diffusion-based Adversarial Purification. In *ICML*, 2025.

What is the metric?

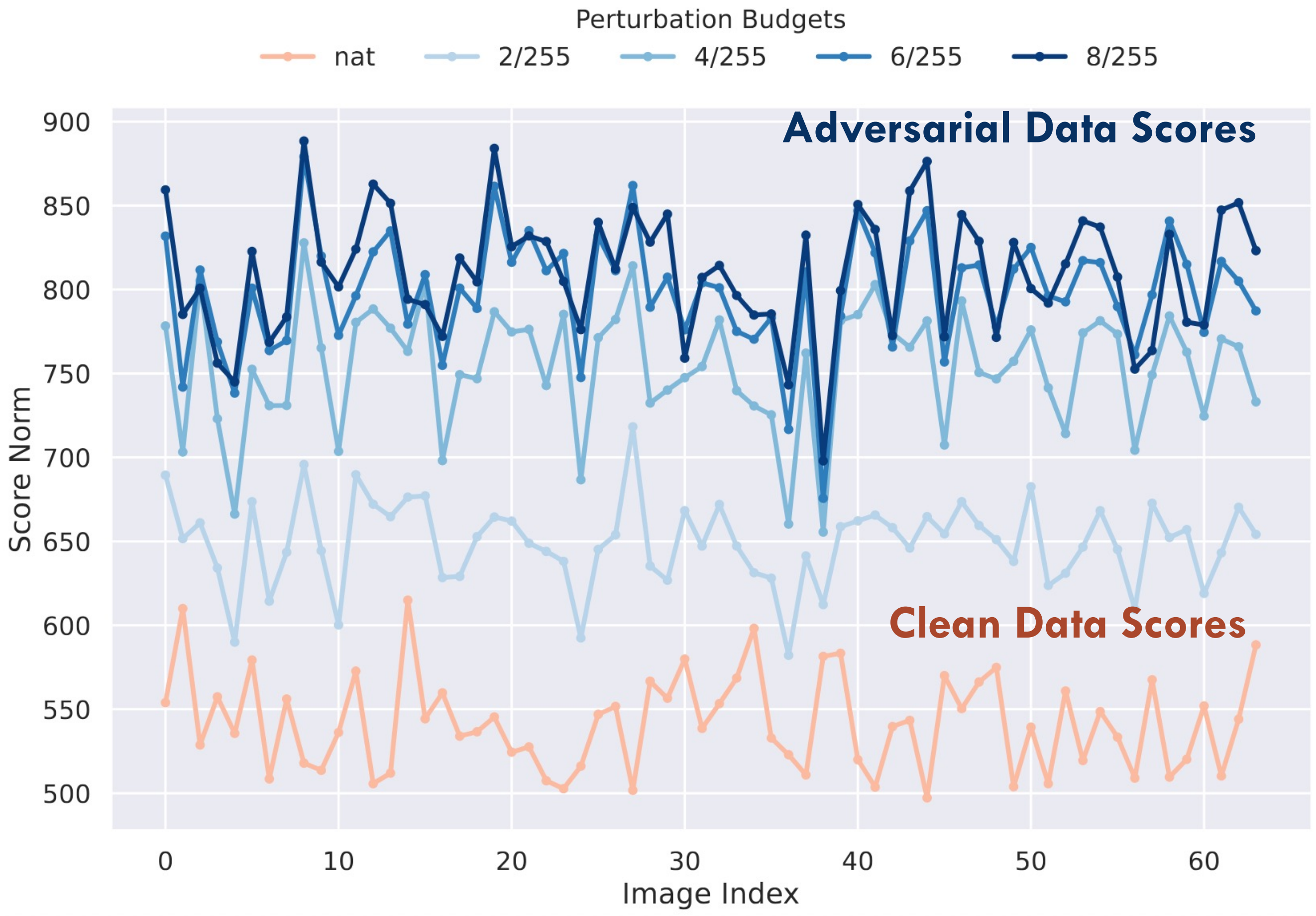
Intuition from score function

- Intuition from score function $\nabla_{\mathbf{x}} \log p(\mathbf{x})$
  - Score $\nabla_{\mathbf{x}} \log p(\mathbf{x})$ represents the momentum of the sample towards high density areas of natural data distribution (Song et al., 2019)
  - A lower score norm $||\nabla_{\mathbf{x}} \log p(\mathbf{x})||$ indicates the sample is closer to the high-density areas of natural data distribution



Detecting Adversarial Data by Probing Multiple Perturbations Using Expected Perturbation Score. In *ICML*, 2023.

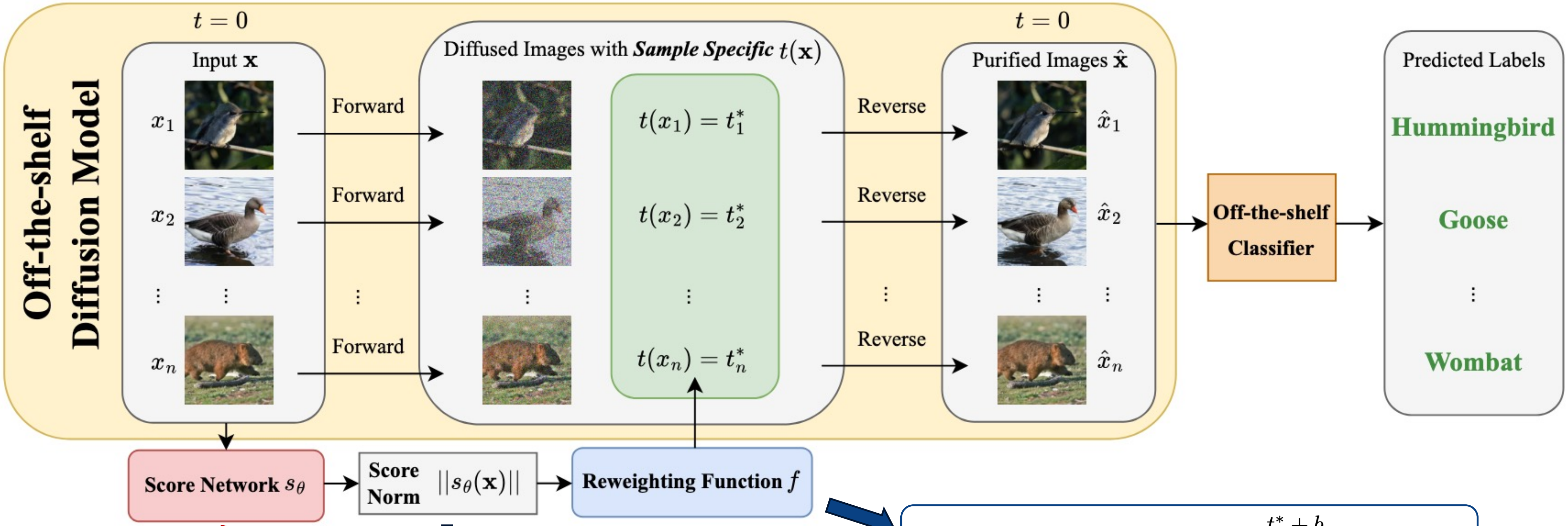
Score norms vs perturbation budgets



- ❑ We further find that score norms *scale directly* with perturbation budgets.
- ❑ Score norms can act as *proxies* for estimating the sample-specific noise level.

Sample-specific Noise Injection for Diffusion-based Adversarial Purification. In *ICML*, 2025.

Sample-specific Score-aware Noise Injection (SSNI)



estimate

$$||\mathrm{EPS}(\mathbf{x})|| = ||\mathbb{E}_{t \sim U(0,t^S)} \nabla_{\mathbf{x}} \log p_t(\mathbf{x})||$$

$$f_\sigma(\|\mathrm{EPS}(\mathbf{x})\|\,,\ t^*) = \frac{t^* + b}{1 + \exp\{-(\|\mathrm{EPS}(\mathbf{x})\| - \mu)/\tau\}}$$

Sample-specific Noise Injection for Diffusion-based Adversarial Purification. In *ICML*, 2025.

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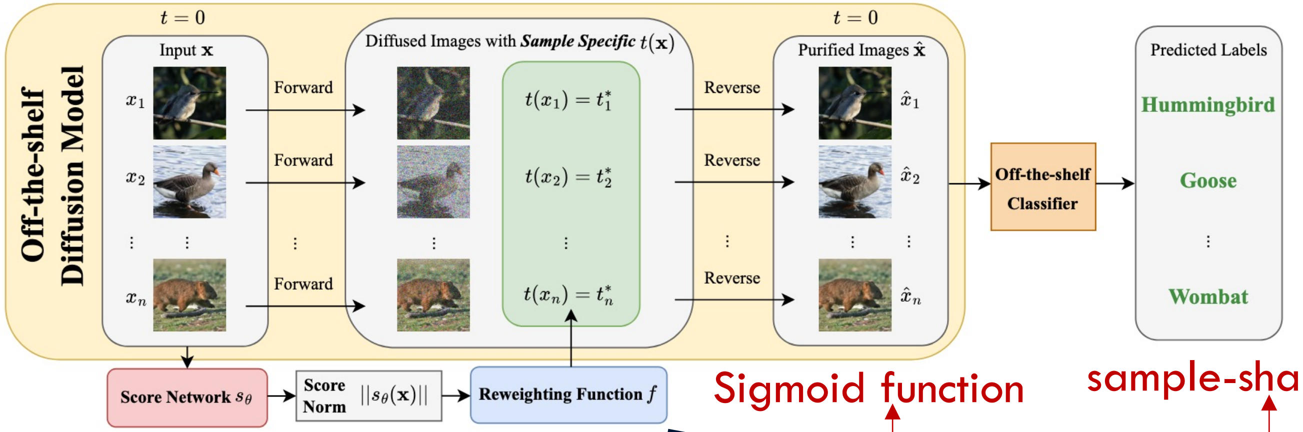
Sample-specific Score-aware Noise Injection (SSNI)



bias term

Sigmoid function

sample-shared noise level

temperature coefficient

$$f_\sigma(\|\mathrm{EPS}(\mathbf{x})\|, t^*) = \frac{t^* + b}{1 + \exp\{-(\|\mathrm{EPS}(\mathbf{x})\| - \mu)/\tau\}}$$

mean EPS norm values of clean examples

$$\|\mathrm{EPS}(\mathbf{x})\| = \|\mathbb{E}_{t\sim U(0,t^{S})} \nabla_{\mathbf{x}} \log p_t(\mathbf{x})\|$$

the expectation of the scores of perturbed images across different noise levels $t \sim U(0, t^S)$

Sample-specific Noise Injection for Diffusion-based Adversarial Purification. In *ICML*, 2025.

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Main results: CIFAR10

	PGD+EOT ℓ_∞ ($\epsilon = 8/255$)		
	DBP Method	Standard	Robust
WRN-28-10	Nie et al. (2022)	89.71±0.72	47.98±0.64
	+ *SSNI-N*	**93.29±0.37** (+3.58)	**48.63±0.56** (+0.65)
	Wang et al. (2022)	92.45±0.64	36.72±1.05
	+ *SSNI-N*	**94.08±0.33** (+1.63)	**40.95±0.65** (+4.23)
	Lee & Kim (2023)	90.10±0.18	56.05±1.11
	+ *SSNI-N*	**93.55±0.55** (+2.66)	**56.45±0.28** (+0.40)
WRN-70-16	Nie et al. (2022)	90.89±1.13	52.15±0.30
	+ *SSNI-N*	**94.47±0.51** (+3.58)	**52.47±0.66** (+0.32)
	Wang et al. (2022)	93.10±0.51	43.55±0.58
	+ *SSNI-N*	**95.57±0.24** (+2.47)	**46.03±1.33** (+2.48)
	Lee & Kim (2023)	89.39±1.12	56.97±0.33
	+ *SSNI-N*	**93.82±0.24** (+4.44)	**57.03±0.28** (+0.06)

	PGD+EOT ℓ_2 ($\epsilon = 0.5$)		
	DBP Method	Standard	Robust
WRN-28-10	Nie et al. (2022)	91.80±0.84	**82.81±0.97**
	+ *SSNI-N*	**93.95±0.70** (+2.15)	82.75±1.01 (-0.06)
	Wang et al. (2022)	92.45±0.64	82.29±0.82
	+ *SSNI-N*	**94.08±0.33** (+1.63)	**82.49±0.75** (+0.20)
	Lee & Kim (2023)	90.10±0.18	83.66±0.46
	+ *SSNI-N*	**93.55±0.55** (+3.45)	**84.05±0.33** (+0.39)
WRN-70-16	Nie et al. (2022)	92.90±0.40	82.94±1.13
	+ *SSNI-N*	**95.12±0.58** (+2.22)	**84.38±0.58** (+1.44)
	Wang et al. (2022)	93.10±0.51	**85.03±0.49**
	+ *SSNI-N*	**95.57±0.24** (+2.47)	84.64±0.51 (-0.39)
	Lee & Kim (2023)	89.39±1.12	84.51±0.37
	+ *SSNI-N*	**93.82±0.24** (+4.43)	**84.83±0.33** (+0.32)

Sample-specific Noise Injection for Diffusion-based Adversarial Purification. In *ICML*, 2025.

Main results: ImageNet-1K

	PGD+EOT ℓ_∞ $(\epsilon = 4/255)$		
	DBP Method	Standard	Robust
RN-50	Nie et al. (2022)	68.23±0.92	30.34±0.72
	+ *SSNI-N*	**70.25±0.56** (+2.02)	**33.66±1.04** (+3.32)
	Wang et al. (2022)	74.22±0.12	0.39±0.03
	+ *SSNI-N*	**75.07±0.18** (+0.85)	**5.21±0.24** (+4.82)
	Lee & Kim (2023)	70.18±0.60	42.45±0.92
	+ *SSNI-N*	**72.69±0.80** (+2.51)	**43.48±0.25** (+1.03)

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AutoAttack, DiffAttack and Diff-PGD

	ℓ_∞ $(\epsilon = 8/255)$				
	DBP Method	Standard	AutoAttack	DiffAttack	Diff-PGD
WRN-28-10	Nie et al. (2022)	89.71±0.72	66.73±0.21	47.16±0.48	54.95±0.77
	+ *SSNI-N*	**93.29±0.37** (+3.58)	**66.94±0.44** (+0.21)	**48.15±0.22** (+0.99)	**56.10±0.35** (+1.15)
	Wang et al. (2022)	92.45±0.64	64.48±0.62	54.27±0.72	41.45±0.60
	+ *SSNI-N*	**94.08±0.33** (+1.63)	**66.53±0.46** (+2.05)	**55.81±0.33** (+1.54)	**42.91±0.56** (+1.46)
	Lee & Kim (2023)	90.10±0.18	69.92±0.30	56.04±0.58	59.02±0.28
	+ *SSNI-N*	**93.55±0.55** (+3.45)	**72.27±0.19** (+2.35)	**56.80±0.41** (+0.76)	**61.43±0.58** (+2.41)

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Inference Time

DBP Method	Noise Injection Method	Time (s)
Nie et al. (2022)	-	3.934
	SSNI-L	4.473
	SSNI-N	4.474
Wang et al. (2022)	-	5.174
	SSNI-L	5.793
	SSNI-N	5.829
Lee & Kim (2023)	-	14.902
	SSNI-L	15.624
	SSNI-N	15.534

DBP Method	Noise Injection Method	Time (s)
Nie et al. (2022)	-	8.980
	SSNI-L	14.515
	SSNI-N	14.437
Wang et al. (2022)	-	11.271
	SSNI-L	16.657
	SSNI-N	16.747
Lee & Kim (2023)	-	35.091
	SSNI-L	40.526
	SSNI-N	40.633

Sample-specific Noise Injection for Diffusion-based Adversarial Purification. In *ICML*, 2025.

Limitations of DBP framework & SSNI

- **Limitation 1:** Having a pre-trained diffusion model is not always feasible, training a diffusion model is resource-consuming.
- **Limitation 2:** The inference speed of DBP-based methods is slow.
- **Limitation 3:** SSNI still injects noise to clean samples, which cannot fully preserve the utility (i.e., clean accuracy) of the model.

Sample-specific Noise Injection for Diffusion-based Adversarial Purification. In *ICML*, 2025.

One Stone, Two Birds: Enhancing Adversarial Defense Through the Lens of Distributional Discrepancy

Jiacheng Zhang, Benjamin I. P. Rubinstein, Jingfeng Zhang, Feng Liu*

(* Corresponding authors)

In *ICML*, 2025.

Paper

Code

Distributional discrepancy minimization improves robustness

Theorem 1. *For a hypothesis* $h \in \mathcal{H}$ *and a distribution* $\mathcal{D}_{\mathcal{A}} \in \mathbb{D}$*:*

$$R(h, f_{\mathcal{A}}, \mathcal{D}_{\mathcal{A}}) \leq R(h, f_{\mathcal{C}}, \mathcal{D}_{\mathcal{C}}) + d_1(\mathcal{D}_{\mathcal{C}}, \mathcal{D}_{\mathcal{A}}).$$

risk on adversarial data **risk on clean data** **distributional discrepancy**

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Distributional discrepancy minimization improves robustness

- Previous Studies: loose bound due to **an extra constant**

$$R(h, f_{\mathcal{A}}, \mathcal{D}_{\mathcal{A}}) \leq R(h, f_{\mathcal{C}}, \mathcal{D}_{\mathcal{C}}) + d_1(\mathcal{D}_{\mathcal{C}}, \mathcal{D}_{\mathcal{A}}) + \mathbf{C}$$

- Ours: **tight bound** without extra constants

$$R(h, f_{\mathcal{A}}, \mathcal{D}_{\mathcal{A}}) \leq R(h, f_{\mathcal{C}}, \mathcal{D}_{\mathcal{C}}) + d_1(\mathcal{D}_{\mathcal{C}}, \mathcal{D}_{\mathcal{A}})$$

very low if h is a well-trained classifier

risk on adversarial data $\leq$ distributional discrepancy

One Stone, Two Birds: Enhancing Adversarial Defense Through the Lens of Distributional Discrepancy. In *ICML*, 2025.

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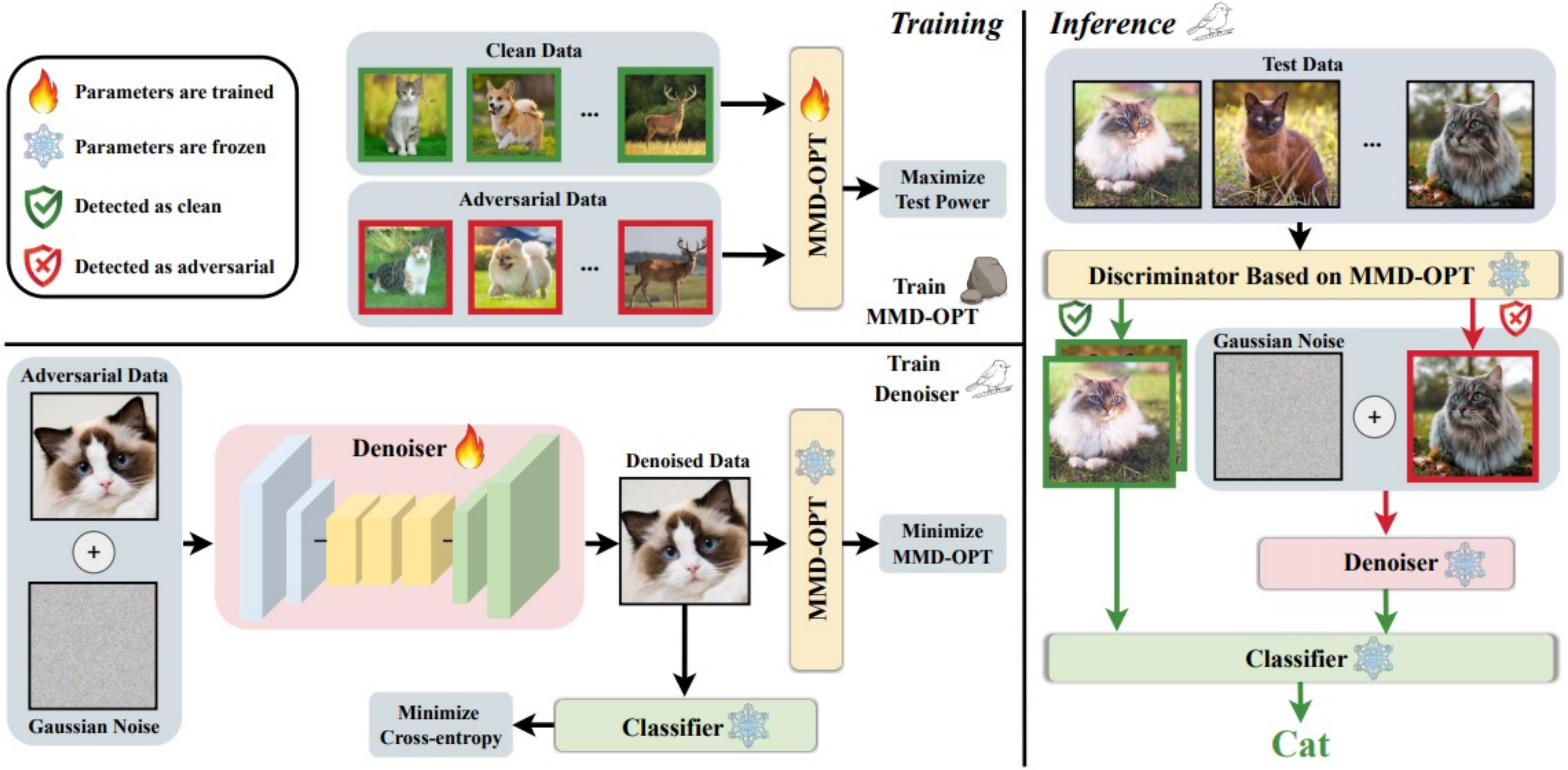
Distributional-discrepancy-based Adversarial Defense (DAD)



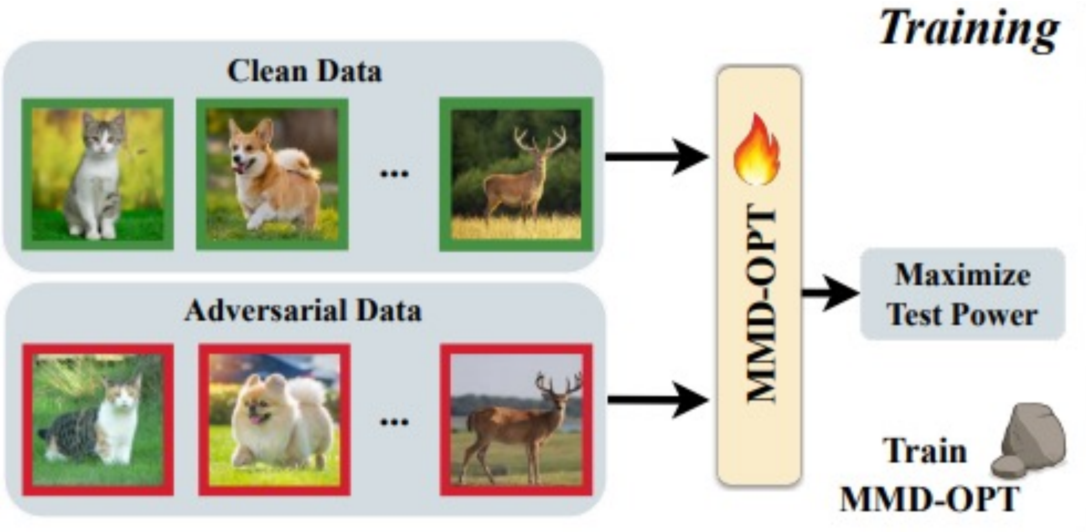
One Stone, Two Birds: Enhancing Adversarial Defense Through the Lens of Distributional Discrepancy. In *ICML*, 2025.

One stone: optimized MMD

$$\text{MMD-OPT}(S'_X, S'_Z) = \widehat{\text{MMD}}_u^2(S'_X, S'_Z; k^*_\omega)$$

MMD values

0 if same distribution
1 if different



Algorithm 1 Optimizing MMD (Liu et al., 2020).

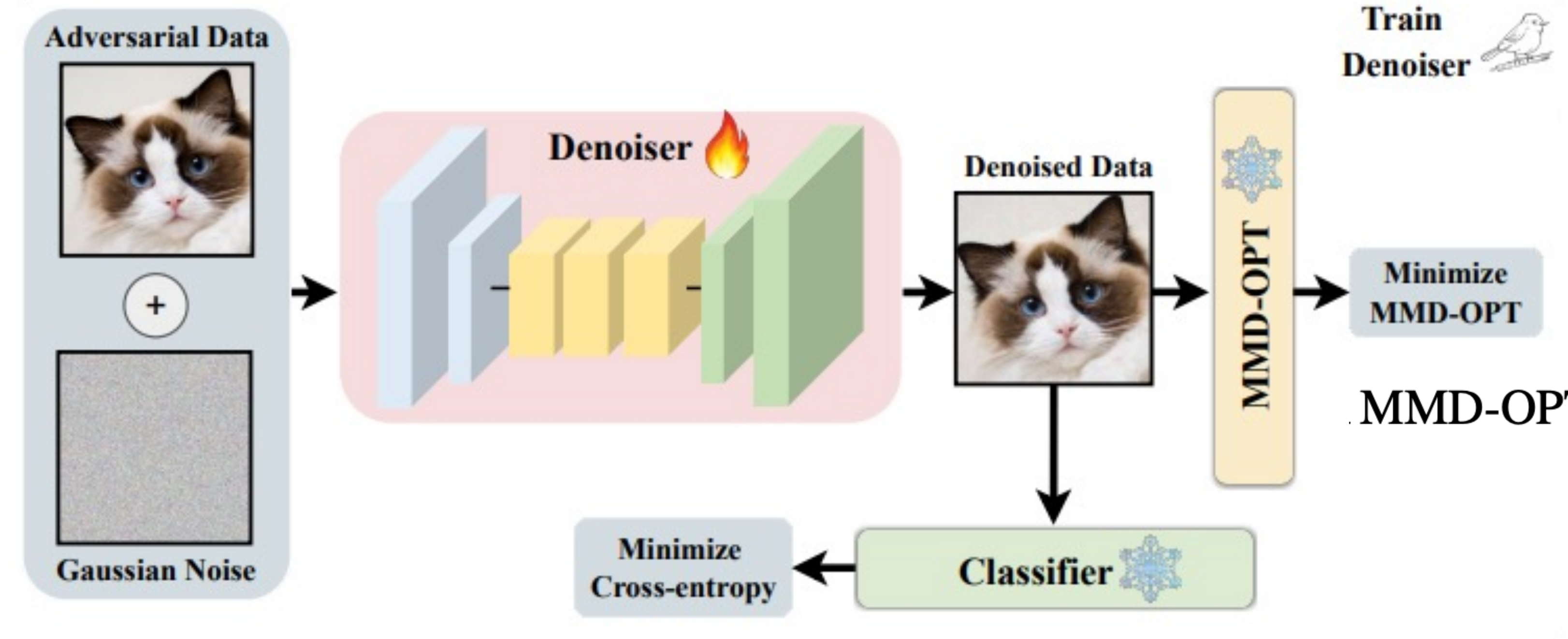
Input: clean data $S_{\mathcal{C}}^{\text{train}}$, adversarial data $S_{\mathcal{A}}^{\text{train}}$, learning rate η, epoch T;
Initialize $\omega \leftarrow \omega_0$; $\lambda \leftarrow 10^{-8}$;
for epoch $= 1, \ldots, T$ **do**
  $S'_{\mathcal{C}} \leftarrow$ minibatch from $S_{\mathcal{C}}^{\text{train}}$;
  $S'_{\mathcal{A}} \leftarrow$ minibatch from $S_{\mathcal{A}}^{\text{train}}$;
  $k_\omega \leftarrow$ kernel function with parameters ω using Eq. (3);
  $M(\omega) \leftarrow \widehat{\text{MMD}}_u^2(S'_{\mathcal{C}}, S'_{\mathcal{A}}; k_\omega)$ using Eq. (2);
  $V_\lambda(\omega) \leftarrow \hat{\sigma}_\lambda(S'_{\mathcal{C}}, S'_{\mathcal{A}}; k_\omega)$ using Eq. (5);
  $\hat{J}_\lambda(\omega) \leftarrow M(\omega)/\sqrt{V_\lambda(\omega)}$ using Eq. (4);
  $\omega \leftarrow \omega + \eta \nabla_{\text{Adam}} \hat{J}_\lambda(\omega)$;
end for
Output: k^*_ω

MMD-OPT serves as:

1. Guiding signal to to train a denoiser.
2. Discriminator to differentiate clean data and adversarial data during inference

One Stone, Two Birds: Enhancing Adversarial Defense Through the Lens of Distributional Discrepancy. In *ICML*, 2025.

First bird: MMD-OPT-based denoiser



$$\text{MMD-OPT}(S_{\mathcal{C}}, g_{\boldsymbol{\theta}}(S_{\text{noise}}))$$

$$\mathcal{L}_{\text{ce}}(\widehat{h_{\mathcal{C}}^{*}}(g_{\boldsymbol{\theta}}(S_{\text{noise}})), Y_{\mathcal{C}})$$

Objective: $$g_{\boldsymbol{\theta}^*} = \arg\min_{\boldsymbol{\theta}} \text{MMD-OPT}(S_{\mathcal{C}}, g_{\boldsymbol{\theta}}(S_{\text{noise}})) + \alpha \cdot \mathcal{L}_{\text{ce}}(\widehat{h_{\mathcal{C}}^{*}}(g_{\boldsymbol{\theta}}(S_{\text{noise}})), Y_{\mathcal{C}})$$

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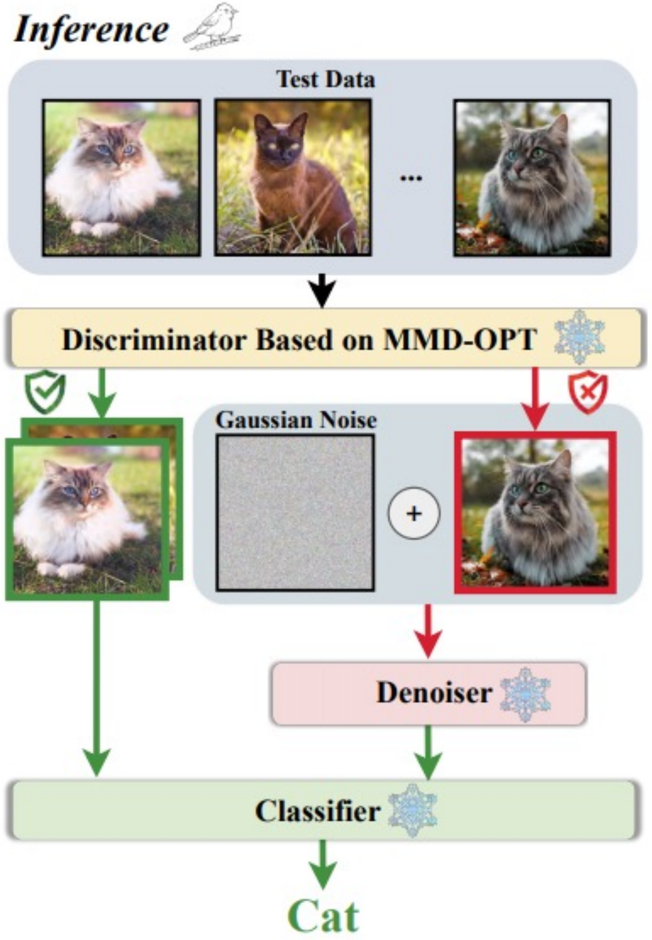
Second bird: MMD-OPT-based discriminator



$$\text{MMD-OPT}(S_{\mathcal{V}}, S_{\mathcal{T}}) = \widehat{\text{MMD}}_u^2(S_{\mathcal{V}}, S_{\mathcal{T}}; k_{\omega}^*)$$

optimized kernel

clean validation data

test data
(i.e., clean or adversarial)

0 → Classifier

1 → Denoiser → Classifier

One Stone, Two Birds: Enhancing Adversarial Defense Through the Lens of Distributional Discrepancy. In *ICML*, 2025.

Adaptive Attack based on PGD+EOT

Algorithm 3 Adaptive white-box PGD+EOT attack for DAD.

Input: clean data-label pairs $(S_\mathcal{C}, Y_\mathcal{C})$, optimized characteristic kernel k_ω^* by Algorithm 1, pre-trained classifier $\widehat{h_\mathcal{C}^*}$, denoiser g with parameters $\boldsymbol{\theta}$, maximum allowed perturbation ϵ, step size η, PGD iteration T, EOT iteration K;
Initialize adversarial data $S_\mathcal{A} \leftarrow S_\mathcal{C}$; $\mu \leftarrow 0$; $\sigma \leftarrow 0.25$; $\alpha \leftarrow 10^{-2}$; $t \leftarrow 0.05$;
for PGD iteration $1, \ldots, T$ **do**
  Initialize gradients over EOT $\mathcal{G}_{\mathrm{EOT}} \leftarrow \mathbf{0}$;
  Compute MMD-OPT$(S_\mathcal{C}, S_\mathcal{A})$ by Eq. (6);
  for EOT iteration $1, \ldots, K$ **do**
    if MMD-OPT$(S_\mathcal{C}, S_\mathcal{A}) < t$ **then**
      $\mathcal{G}_{\mathrm{EOT}} \leftarrow \mathcal{G}_{\mathrm{EOT}} + \nabla_{S_\mathcal{A}}(\text{MMD-OPT}(S_\mathcal{C}, S_\mathcal{A}) + \alpha \cdot \mathcal{L}_{\mathrm{ce}}(\widehat{h_\mathcal{C}^*}(S_\mathcal{A}), Y_\mathcal{C}))$;
    else
    else
      Generate Gaussian noise: $\mathbf{n} \sim \mathbb{N}(\mu, \sigma^2)$;
      $S_{\mathrm{noise}} \leftarrow S_\mathcal{A} + \mathbf{n}$;
      $\mathcal{G}_{\mathrm{EOT}} \leftarrow \mathcal{G}_{\mathrm{EOT}} + \nabla_{S_\mathcal{A}}(\text{MMD-OPT}(S_\mathcal{C}, S_\mathcal{A}) + \alpha \cdot \mathcal{L}_{\mathrm{ce}}(\widehat{h_\mathcal{C}^*}(g_{\boldsymbol{\theta}}(S_{\mathrm{noise}})), Y_\mathcal{C}))$;
    end if
  end for
  $\mathcal{G}_{\mathrm{EOT}} \leftarrow \frac{1}{K}\mathcal{G}_{\mathrm{EOT}}$;
  Update $S_\mathcal{A} \leftarrow \Pi_{\mathcal{B}_\epsilon(S_\mathcal{C})}(S_\mathcal{A} + \eta \cdot \mathrm{sign}(\mathcal{G}_{\mathrm{EOT}}))$;
end for
Output: $S_\mathcal{A}$

Aims to mislead MMD-OPT,
and then, mislead the denoiser and the classifier correspondingly

One Stone, Two Birds: Enhancing Adversarial Defense Through the Lens of Distributional Discrepancy. In *ICML*, 2025.

Main results: CIFAR-10

Type	Method	Clean	Robust
ℓ_∞ ($\epsilon = 8/255$)			
WRN-28-10			
AT	Gowal et al. (2021)	87.51	63.38
	Gowal et al. (2020)*	88.54	62.76
	Pang et al. (2022a)	88.62	61.04
AP	Yoon et al. (2021)	85.66	33.48
	Nie et al. (2022)	90.07	46.84
	Lee & Kim (2023)	90.16	55.82
Ours	DAD	**94.16 ± 0.08**	**67.53 ± 1.07**
WRN-70-16			
AT	Rebuffi et al. (2021)*	92.22	66.56
	Gowal et al. (2021)	88.75	66.10
	Gowal et al. (2020)*	91.10	65.87
AP	Yoon et al. (2021)	86.76	37.11
	Nie et al. (2022)	90.43	51.13
	Lee & Kim (2023)	90.53	56.88
Ours	DAD	**93.91 ± 0.11**	**67.68 ± 0.87**

Type	Method	Clean	Robust
ℓ_2 ($\epsilon = 0.5$)			
WRN-28-10			
AT	Rebuffi et al. (2021)*	91.79	78.80
	Augustin et al. (2020)†	93.96	78.79
	Sehwag et al. (2022)†	90.93	77.24
AP	Yoon et al. (2021)	85.66	73.32
	Nie et al. (2022)	91.41	79.45
	Lee & Kim (2023)	90.16	83.59
Ours	DAD	**94.16 ± 0.08**	**84.38 ± 0.81**
WRN-70-16			
AT	Rebuffi et al. (2021)*	**95.74**	82.32
	Gowal et al. (2020)*	94.74	80.53
	Rebuffi et al. (2021)	92.41	80.42
AP	Yoon et al. (2021)	86.76	75.66
	Nie et al. (2022)	92.15	82.97
	Lee & Kim (2023)	90.53	83.57
Ours	DAD	93.91 ± 0.11	**84.03 ± 0.75**

Main results: ImageNet-1K

ℓ_∞ $(\epsilon = 4/255)$			
Type	Method	Clean	Robust
RN-50			
AT	Salman et al. (2020a)	64.02	34.96
	Engstrom et al. (2019)	62.56	29.22
	Wong et al. (2020)	55.62	26.24
AP	Nie et al. (2022)	71.48	38.71
	Lee & Kim (2023)	70.74	42.15
Ours	DAD	**78.61 ± 0.04**	**53.85 ± 0.23**

Transferability

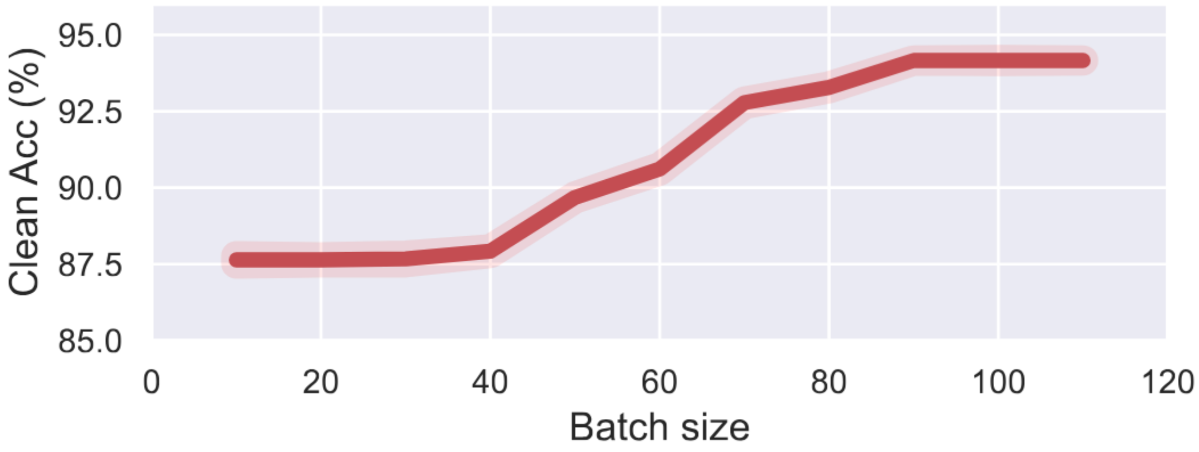
Trained on WRN-28-10					
Unseen Transfer Attack		WRN-70-16	RN-18	RN-50	Swin-T
PGD+EOT (ℓ_∞)	$\epsilon = 8/255$	80.84 ± 0.46	80.78 ± 0.60	81.47 ± 0.30	81.46 ± 0.29
	$\epsilon = 12/255$	80.26 ± 0.60	80.54 ± 0.45	80.98 ± 0.36	80.40 ± 0.41
C&W (ℓ_2)	$\epsilon = 0.5$	82.45 ± 0.19	91.30 ± 0.20	89.26 ± 0.11	93.45 ± 0.17
	$\epsilon = 1.0$	81.20 ± 0.39	90.37 ± 0.17	88.65 ± 0.22	93.41 ± 0.18

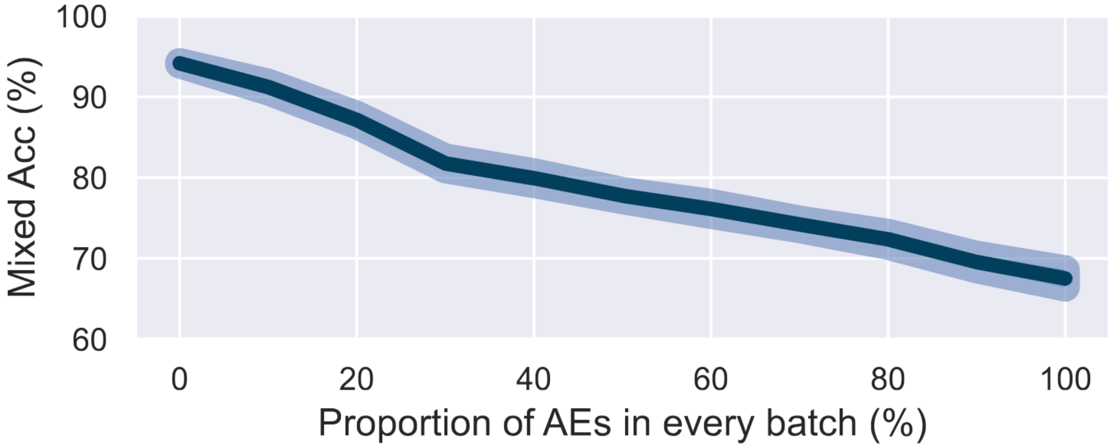
One Stone, Two Birds: Enhancing Adversarial Defense Through the Lens of Distributional Discrepancy. In *ICML*, 2025.

Strength of DAD

- **Strength 1:** DAD can largely preserve the original utility (i.e., clean accuracy of the classifier).
- **Strength 2:** Compared to DBP methods that reply on density estimation, learning distributional discrepancies is a simpler and more feasible task.
- **Strength 3:** DAD is efficient in both training and inferencing.

Limitations of DAD





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Thank You!