Trustworthy Machine Learning

Certified Adversarial Learning

Sangdon Park

POSTECH

Motivation

- Heuristic adversarial learning often fails against powerful adversaries with the <u>same</u> maximum perturbation ε.

CIFAR10

	Simple	Wide
Natural	92.7%	95.2%
FGSM	27.5%	32.7%
PGD	0.8%	3.5%

(a) Standard training

Simple	Wide
87.4%	90.3%
90.9%	95.1%
0.0%	0.0%

(b) FGSM training

Simple	Wide
79.4%	87.3%
51.7%	56.1%
43.7%	45.8%

(c) PGD training

  - ε-FGSM training and ε-FGSM attacks: 90.9% accuracy :)
  - ε-FGSM training and ε-PGD attacks: 0.0% accuracy :(

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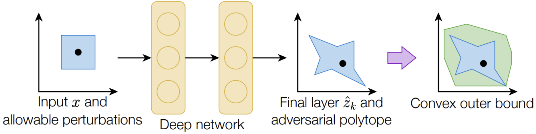
(c) PGD training

  - ε-FGSM training and ε-FGSM attacks: 90.9% accuracy :)
  - ε-FGSM training and ε-PGD attacks: 0.0% accuracy :(
- Can we learn a classifier robust to **any** small perturbations?

Certified Adversarial Learning

- Convex outer approximation [Kolter and Wong, 2017]



✓ Certified!

$$\max_{\|\delta\|_\infty \le \varepsilon} \ell(f, x+\delta, y) \le U(\varepsilon, f, x, y)$$

★ Essentially linear classification over overly approximated "convex polytope"-points

✗ Not scalable :(

Certified Adversarial Learning

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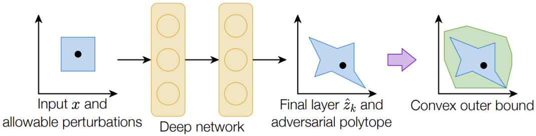

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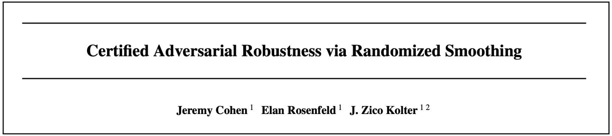
- Randomized smoothing: a post-hoc method



Certified Adversarial Robustness via Randomized Smoothing

Jeremy Cohen [1] Elan Rosenfeld [1] J. Zico Kolter [1 2]

  ✓ (Probably) Certified!

  ✓ Scalable!

A Goodness Definition: Robustness

"Hard" Robustness

$$\forall \delta \text{ s.t } \|\delta\|_p \leq \varepsilon,\ f(x+\delta) = f(x)$$

- $f : \mathcal{X} \to \mathcal{Y}$: a hard-classifier

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- The constraint on the perturbation δ can be more general.

A Goodness Definition: Robustness

"Hard" Robustness

$$\forall \delta \text{ s.t } \|\delta\|_p \leq \varepsilon, \; f(x+\delta) = f(x)$$

- $f : \mathcal{X} \to \mathcal{Y}$: a hard-classifier
- The constraint on the perturbation δ can be more general.
- It does not matter whether $f(x)$ is correct.

A Certified Method: Randomized Smoothing

Smoothed Classifier

$$g(x) \coloneqq \arg\max_{c \in \mathcal{Y}} \mathbb{P}\left\{ f(x+\delta) = c \right\} \quad \text{where} \quad \delta \sim \mathcal{N}(0, \sigma^2 I)$$

- $g : \mathcal{X} \to \mathcal{Y}$: a smoothed classifier
- σ is related to the maximum perturbation ε.
- Easier than convex outer approximation

Robustness Guarantee

Binary Classification

Theorem

Suppose that $\underline{p_A} \in (0.5, 1]$ *satisfies*

$$\mathbb{P}\left\{f(x+\delta) = c_A\right\} = p_A \geq \underline{p_A} \quad \textit{where} \quad \delta \sim \mathcal{N}(0, \sigma^2 I).$$

Then, we have $g(x+\delta) = c_A$ *if*

$$\|\delta\|_2 < \sigma \Phi^{-1}(\underline{p_A}).$$

- c_A: the most probable class when f classifies $x + \varepsilon$
- p_A: the chance that f classifies $x + \delta$ by c_A
- $\underline{p_A}$: the lower bound of p_A
- Φ^{-1}: the inverse of the standard Gaussian CDF

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- $\underline{p_A}$: the lower bound of p_A
- Φ^{-1}: the inverse of the standard Gaussian CDF
- Here, we assume that we can compute $\underline{p_A}$.
- We can compute the *data-dependent* maximum perturbation to be robust!

Robustness Guarantee: A Proof Sketch (1/3)

Binary Classification

- Fix a perturbation δ.
- From the definition of g, we have

$$\begin{aligned} g(x+\delta) &:= \arg\max_c \mathbb{P}\left\{f(x+\varepsilon+\delta)=c\right\} \quad \text{where} \quad \varepsilon \sim \mathcal{N}(0, \sigma^2 I) \\ &= \arg\max_c \mathbb{P}\left\{f(x+\varepsilon')=c\right\} \quad \text{where} \quad \varepsilon' \sim \mathcal{N}(\delta, \sigma^2 I) \\ &\stackrel{?}{=} c_A \end{aligned} \tag{1}$$

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- We wish to prove (1) for any classifier f under some condition. How?
  - f can be any classifier, which is not easy to analyze.
  - Consider a surrogate classifier that bounds the probability and is easier to analyze, *e.g.*,

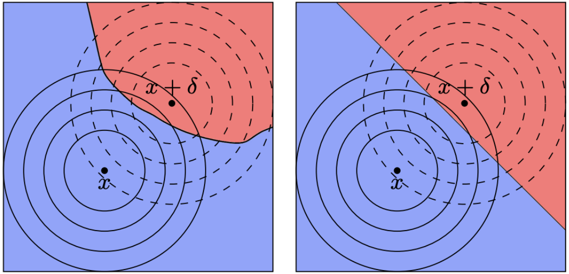
$$\mathbb{P}\left\{f(x+\varepsilon')=c_A\right\} \geq \min_{f':\mathbb{P}\{f'(x+\varepsilon)=c_A\}\geq \underline{p_A}} \mathbb{P}\left\{f'(x+\varepsilon')=c_A\right\} > \frac{1}{2} \quad \Longrightarrow \quad g(x+\delta)=c_A.$$

Robustness Guarantee: A Proof Sketch (2/3)

Binary Classification

- Interestingly, f^* is linear (due to the Neyman-Perason lemma), where

$$f^* = \arg \min_{f' : \mathbb{P}\{f'(x+\varepsilon)=c_A\} \geq \underline{p_A}} \mathbb{P}\left\{f'(x+\varepsilon') = c_A\right\}$$



  - There could be a non-linear classifier but we can find a corresponding linear classifier with the same mininum value.

Robustness Guarantee: A Proof Sketch (3/3)

Binary Classification

- We have a closed-form solution of f^*:

$$f^*(x') := \begin{cases} c_A & \text{if } \delta^T(x'-x) \le \sigma\|\delta\|_2\Phi^{-1}(\underline{p_A}) \\ c_B & \text{otherwise} \end{cases}.$$

- This (non-trivially) implies the following mininum value:

$$\min_{f':\mathbb{P}\{f'(x+\varepsilon)=c_A\}\ge\underline{p_A}} \mathbb{P}\left\{f'(x+\varepsilon')=c_A\right\} = \mathbb{P}\left\{f^*(x+\varepsilon')=c_A\right\} = \Phi\left(\Phi^{-1}(\underline{p_A}) - \frac{\|\delta\|_2}{\sigma}\right)$$

- The above probability should be larger than $\frac{1}{2}$, *i.e.*,

$$\Phi\left(\Phi^{-1}(\underline{p_A}) - \frac{\|\delta\|_2}{\sigma}\right) > \frac{1}{2} \quad \Longrightarrow \quad \|\delta\|_2 < \sigma\Phi^{-1}(\underline{p_A}).$$

Robustness Guarantee

Multi-class Classification

Theorem

Suppose that $\underline{p_A}, \overline{p_B} \in [0, 1]$ *satisfy*

$$\mathbb{P}\left\{f(x+\varepsilon) = c_A\right\} \geq \underline{p_A} \geq \overline{p_B} \geq \max_{c \neq c_A} \mathbb{P}\left\{f(x+\varepsilon) = c\right\}.$$

Then, we have $g(x+\delta) = c_A$ *for all* $\|\delta\|_2 < R$, *where*

$$R := \frac{\sigma}{2}\left(\Phi^{-1}(\underline{p_A}) - \Phi^{-1}(\overline{p_B})\right).$$

- c_A: the most probable label (with probability at least $\underline{p_A}$)
- $c_B := \arg\max_{c \neq c_A} \mathbb{P}\left\{f(x+\varepsilon) = c\right\}$: the second-most probable label (with probability at most $\overline{p_B}$)

Robustness Guarantee: An Alternative

Multi-class Classification

Theorem

Suppose that we have class A and B that satisfy

$$\max_{k} \mathbb{P}\left\{f_k(x+\varepsilon)\right\} = p_A \geq p_B = \max_{k \neq A} \mathbb{P}\left\{f_k(x+\varepsilon)\right\}.$$

Then, we have $g(x+\delta) = A$ for all $\|\delta\|_2 < R$, where

$$R := \frac{\sigma}{2}\left(\Phi^{-1}(p_A) - \Phi^{-1}(p_B)\right).$$

- Consider a soft classifier $f_k : \mathcal{X} \to [0,1]$ for class k
- A smoothed classifier $g_k(x) := \arg\max_k \mathbb{P}_\varepsilon\{f_k(x+\varepsilon)\}$

Robustness Guarantee: An Alternative Proof Sketch (1/2)

- Let $f_k : \mathbb{R}^n \to [0,1]$: a soft classifier for class k
- Let $\tilde{f}_k : \mathcal{X} \to [0,1]$: a smoothed classifier for class k, *i.e.*,

$$\tilde{f}_k(x) := (f_k * \mathcal{N}(0, \sigma I))(x) = \int_{\mathbb{R}^n} f_k(t) \frac{\exp\left(-\frac{1}{2\sigma^2}\|x-t\|^2\right)}{(2\pi\sigma^2)^n} dt = \mathbb{P}_\varepsilon\{f_k(x+\varepsilon)\}$$

  - The convolution of f_k and $\mathcal{N}(0, \sigma I)$, a.k.a. the Weierstrass transform of f_k

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  - The convolution of f_k and $\mathcal{N}(0, \sigma I)$, a.k.a. the Weierstrass transform of f_k
- Let p_A is the most-probable class probability assigned by the smoothded classifier $\tilde{f}_k$, *i.e.*,

$$p_A = \tilde{f}_A(x) \quad \text{where} \quad A = \arg\max_k \tilde{f}_k(x)$$

- Let p_B is the class probability by $\tilde{f}_k$ such that $A \neq B$ and less than p_A, *i.e.*,

$$p_B = \tilde{f}_B(x) \leq p_A.$$

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- Let Φ be a CDF of a Gaussian distribution, *i.e.*,

$$\Phi(a) := \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{a} \exp\left(-\frac{1}{2}s^2\right) \mathrm{d}s$$

Robustness Guarantee: An Alternative Proof Sketch (2/2)

Then, we have the robustness guarantee due to the following reasons:

- For any perturbation δ and any class k, we have

$$\left|\Phi^{-1}\left(\tilde{f}_k(x)\right) - \Phi^{-1}\left(\tilde{f}_k(x+\delta)\right)\right| \leq \frac{1}{\sigma}\|\delta\|_2.$$

  - $\Phi^{-1} \circ \tilde{f}$ is $\frac{1}{\sigma}$-Lipschitz (check out the paper)
- Consider any adversarial perturbation $\bar{\delta}$ that changes the classification result, *i.e.*,

$$\tilde{f}_A(x+\bar{\delta}) \leq \tilde{f}_B(x+\bar{\delta}) \quad \text{for some } B \neq A$$

- For $\bar{\delta}$, we have

$$\begin{aligned}
&\frac{1}{\sigma}\|\bar{\delta}\|_2 \geq \Phi^{-1}\left(\tilde{f}_A(x)\right) - \Phi^{-1}\left(\tilde{f}_A(x+\bar{\delta})\right) \text{ and } \frac{1}{\sigma}\|\bar{\delta}\|_2 \geq \Phi^{-1}\left(\tilde{f}_B(x+\bar{\delta})\right) - \Phi^{-1}\left(\tilde{f}_B(x)\right) \\
\Rightarrow &\frac{2}{\sigma}\|\bar{\delta}\|_2 \geq \left\{\Phi^{-1}\left(\tilde{f}_A(x)\right) - \Phi^{-1}\left(\tilde{f}_B(x)\right)\right\} + \left\{\Phi^{-1}\left(\tilde{f}_B(x+\bar{\delta})\right) - \Phi^{-1}\left(\tilde{f}_A(x+\bar{\delta})\right)\right\} \\
&\qquad\quad \geq \Phi^{-1}\left(\tilde{f}_A(x)\right) - \Phi^{-1}\left(\tilde{f}_B(x)\right) = \Phi^{-1}\left(p_A\right) - \Phi^{-1}\left(p_B\right)
\end{aligned}$$

Prediction

function PREDICT(f, σ, x, n, α)
  `counts` $\leftarrow$ SAMPLEUNDERNOISE(f, x, n, σ)
  $\hat{c}_A, \hat{c}_B \leftarrow$ top two indices in `counts`
  $n_A, n_B \leftarrow$ `counts`$[\hat{c}_A]$, `counts`$[\hat{c}_B]$
  if BINOMPVALUE($n_A, n_A + n_B, 0.5$) $\leq \alpha$ **return** $\hat{c}_A$
  else return ABSTAIN

- Recall the randomized smoothing method:

$$g(x) := \arg\max_{c \in \mathcal{Y}} \mathbb{P}\left\{f(x+\delta) = c\right\} \quad \text{where} \quad \delta \sim \mathcal{N}(0, \sigma^2 I)$$

  1. Draw n noisy perturbations $\delta_1, \ldots, \delta_n$.
  2. Empirically compute the most probable and the second most probably labels, *i.e.*, $\hat{c}_A$ and $\hat{c}_B$.
  3. If $\hat{c}_A$ is drawn from the binomial distribution with $p = 0.5$, return $\hat{c}_A$.

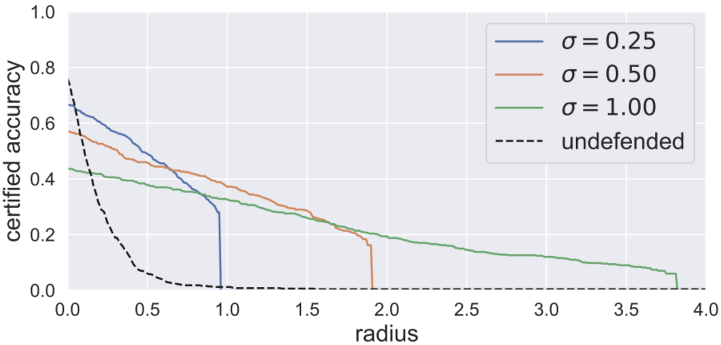
- Alternatively, you can use the (our-favorite) binomial tail bound.

Certification in Evaluation

```
# certify the robustness of g around x
function CERTIFY(f, σ, x, n_0, n, α)
    counts0 ← SAMPLEUNDERNOISE(f, x, n_0, σ)
    ĉ_A ← top index in counts0
    counts ← SAMPLEUNDERNOISE(f, x, n, σ)
    p_A ← LOWERCONFBOUND(counts[ĉ_A], n, 1 − α)
    if p_A > 1/2 return prediction ĉ_A and radius σ Φ^{-1}(p_A)
    else return ABSTAIN
```

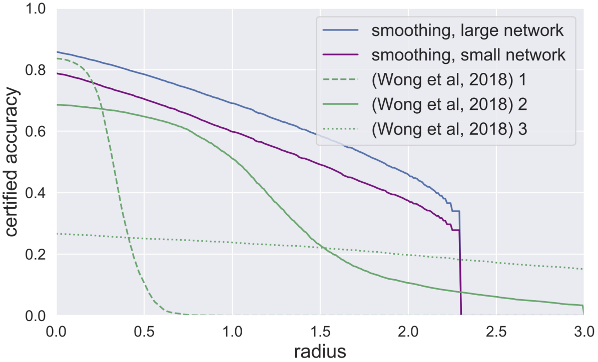
1. Compute $\underline{p_A}$ via the binomial tail bound.
2. Compute the robust radius, *i.e.*, $\sigma\Phi^{-1}(\underline{p_A})$.
3. If (a desired radius) $\leq \sigma\Phi^{-1}(\underline{p_A})$, then "certified".

Results: ImageNet



- Classifier: ResNet-50
- undefended: a classifier with heuristic adversarial training (using ℓ_2 adversarial attacks)
- perturbation: $\|\delta\|_2 \leq (\text{radius}) = (\text{maximum perturbation size})$

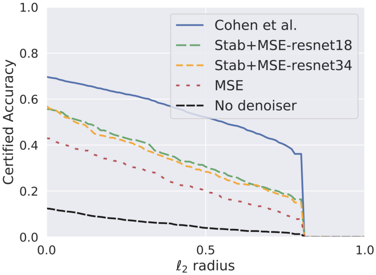
Results: Comparison



- (maybe) on MNIST
- Baseline: deterministic robustness guarantee
- randomized smoothing: high-probability guarantee

Limitation of Randomized Smoothing

- Randomized smoothing requires retraining (*e.g.*, Gaussian data augmentation).



  - Cohen et al.: Randomized smoothing with retraining
  - No denoiser: Randomized smoothing without retraining
- How to avoid retraining?

Denoise Gaussian Noise

**Denoised Smoothing:
A Provable Defense for Pretrained Classifiers**

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- A classifier randomized smoothing needs to be robust to Gaussian noise for better certified robustness.
- How about using denoised smoothing and then use the randomized smoothing?

Denoised Smoothing

Randomized Smoothing:

$$g(x) := \arg\max_{c \in \mathcal{Y}} \mathbb{P}\left\{f(x+\delta) = c\right\} \quad \text{where} \quad \delta \sim \mathcal{N}(0, \sigma^2 I)$$

- Applicable for any classifier f

Denoised Smoothing:

$$g(x) := \arg\max_{c \in \mathcal{Y}} \mathbb{P}\left\{f(\mathcal{D}(x+\delta)) = c\right\} \quad \text{where} \quad \delta \sim \mathcal{N}(0, \sigma^2 I)$$

- $\mathcal{D} : \mathcal{X} \to \mathcal{X}$: a denoiser that hopefully removes δ.
- Consider a NEW classifier $f \circ \mathcal{D}$ and then enjoy randomized smoothing.
- Retraining f is not required.

How to Train a Denoiser?

MSE objective:

$$L_{\mathsf{MSE}} := \mathop{\mathbb{E}}_{x,y,\delta} \|\mathcal{D}(x+\delta) - x\|_2^2$$

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✗ Does not consider the accuracy of a classifier.

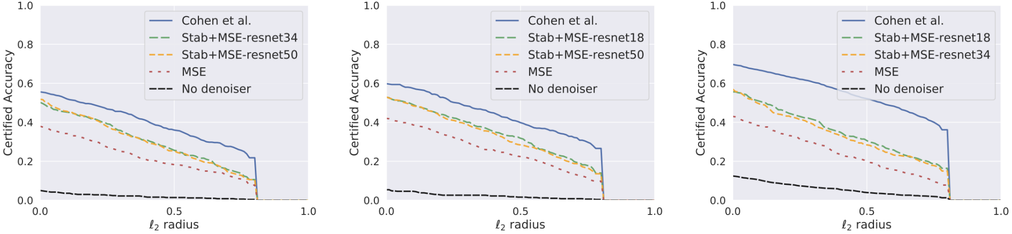
Stability objective:

$$L_{\mathsf{Stab}} := \mathop{\mathbb{E}}_{x,y,\delta} \ell_{CE}(F(\mathcal{D}(x+\delta)), f(x)) \quad \text{where} \quad \delta \sim \mathcal{N}(0, \sigma^2 I)$$

- $f : \mathcal{X} \to \mathcal{Y}$: a hard classifier
- $F : \mathcal{X} \to [0,1]^{|\mathcal{Y}|}$: a soft classifer

✓ Find a denoiser $\mathcal{D}$ that does not change predictions by the classifier f.

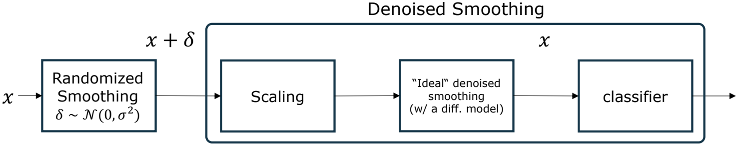
Results



(a) ResNet-18 (b) ResNet-34 (c) ResNet-50

- The denoised smoothing without retraining is quite similar to the randomized smoothing with retraining.
- But not outperform the retraining one. How can we train a better denoiser?

Diffusion Models as Denoisers



Assumptions:

- A diffusion model assumes the following noise model:

$$x_t := \sqrt{\alpha_t} x_0 + \sqrt{1 - \alpha_t} \cdot \mathcal{N}(0, \mathbf{I}),$$

  where x_0 is an initial example, t is a timestep, and α_t is any noise scheduler (monotonically decreasing in t).
    - Under this noise model, an ideal denoiser finds x_0 from x_t.

Method:

- Find t^* for randomized smoothing that fits to the noise model for a diffusion model, *i.e.*,

$$\text{find} \quad t \quad \text{subj. to} \quad x_0 + \mathcal{N}(0, \sigma^2 \mathbf{I}) \approx \sqrt{\alpha_t} x_0 + \sqrt{1 - \alpha_t} \cdot \mathcal{N}(0, \mathbf{I})$$

Conclusion

- Randomized smoothing provides a simple defense mechanism.
- Desnoised smoothing does not require to retrain a classifier (but still requires training the denoiser).
- Recently, the denoised smoothing was improved via denoising diffusion models [Carlini et al., 2023].

			Certified Accuracy at ε (%)				
Method	Off-the-shelf	Extra data	0.5	1.0	1.5	2.0	3.0
PixelDP (Lecuyer et al., 2019)	○	✗	$^{(33.0)}$16.0	-	-		
RS (Cohen et al., 2019)	○	✗	$^{(67.0)}$49.0	$^{(57.0)}$37.0	$^{(57.0)}$29.0	$^{(44.0)}$19.0	$^{(44.0)}$12.0
SmoothAdv (Salman et al., 2019)	○	✗	$^{(65.0)}$56.0	$^{(54.0)}$43.0	$^{(54.0)}$37.0	$^{(40.0)}$27.0	$^{(40.0)}$20.0
Consistency (Jeong & Shin, 2020)	○	✗	$^{(55.0)}$50.0	$^{(55.0)}$44.0	$^{(55.0)}$34.0	$^{(41.0)}$24.0	$^{(41.0)}$17.0
MACER (Zhai et al., 2020)	○	✗	$^{(68.0)}$57.0	$^{(64.0)}$43.0	$^{(64.0)}$31.0	$^{(48.0)}$25.0	$^{(48.0)}$14.0
Boosting (Horváth et al., 2022a)	○	✗	$^{(65.6)}$57.0	$^{(57.0)}$44.6	$^{(57.0)}$**38.4**	$^{(44.6)}$**28.6**	$^{(38.6)}$**21.2**
DRT (Yang et al., 2021)	○	✗	$^{(52.2)}$46.8	$^{(55.2)}$44.4	$^{(49.8)}$**39.8**	$^{(49.8)}$**30.4**	$^{(49.8)}$**23.4**
SmoothMix (Jeong et al., 2021)	○	✗	$^{(55.0)}$50.0	$^{(55.0)}$43.0	$^{(55.0)}$**38.0**	$^{(40.0)}$26.0	$^{(40.0)}$20.0
ACES (Horváth et al., 2022b)	◐	✗	$^{(63.8)}$54.0	$^{(57.2)}$42.2	$^{(55.6)}$35.6	$^{(39.8)}$25.6	$^{(44.0)}$19.8
Denoised (Salman et al., 2020)	◐	✗	$^{(60.0)}$33.0	$^{(38.0)}$14.0	$^{(38.0)}$6.0	-	-
Lee (Lee, 2021)	●	✗	41.0	24.0	11.0	-	-
Ours	●	✓	$^{(82.8)}$**71.1**	$^{(77.1)}$**54.3**	$^{(77.1)}$**38.1**	$^{(60.0)}$**29.5**	$^{(60.0)}$13.1

Reference I

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