Lipschitz Regularisation for Neural Networks in High Dimension

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- Introduction
- 2 CLIP: Test & Improvement

Lipschitz Regularisation for Neural Networks in High Dimension

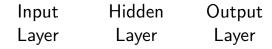
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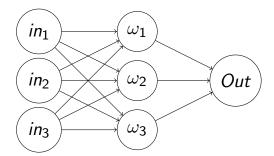


Figure. 1: Simplified neural network (one hidden layer).

```
We denote f_{\theta} our model where \theta = (\omega_1, \dots, \omega_w).
Denote \Gamma our dataset containing couple (x, y) \in \Gamma:
x \longrightarrow \text{input (from a set noted } \mathcal{X})
y \longrightarrow \text{output (from a set noted } \mathcal{Y})
```

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Neural Networks: How to train them?

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Denote \Gamma our dataset containing couple (x, y) \in \Gamma:
x \longrightarrow \text{input (from a set noted } \mathcal{X})
y \longrightarrow \text{output (from a set noted } \mathcal{Y})
Problem:
                                  \min_{\theta} \sum_{(x,y)\in\Gamma} \mathsf{loss}(f_{\theta}(x),y)
for example, loss could be : loss(f_{\theta}(x), y) = ||f_{\theta}(x) - y||^2
```

Neural Networks: Is it correct? Perfect?

Perfect? Obviously, not.

Overfitting:

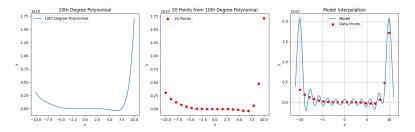


Figure. 2: Model interpolating a 10th degrees polynomial function : Overfitting example.

Neural Networks : Is it correct ? Perfect ?

Perfect ? Obviously, not.

Robustness:

Original Image. Label: ENSTA



Adversarial Image, Label: Polytechnique



Figure. 3: Adversarial attacks on a model leading to misclassification (Find code on https://github.com/Raphael-Bernas/).

- Introduction

Cheap Lipschitz Regularization (CLIP)

CLIP: Regularization

To regularize is to do an "intelligent training".

We introduce a new term reg to our theoretical training formula :

$$\min_{\theta} \sum_{(x,y) \in \Gamma} \mathsf{loss}(f_{\theta}(x), y) + \frac{\lambda}{\lambda} reg(f_{\theta}, \mathcal{X})$$

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 $\lambda >> 1$: then the model tends to be strongly regularized

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<u>ex :</u>

$$\min_{\theta} \left(\sum_{(x,y) \in \Gamma} \mathsf{loss}(f_{\theta}(x), y) + 100 * \max_{x \in \mathcal{X}} \lVert f_{\theta}(x) - 8 \rVert^2 \right)$$

Lipschitz constant of
$$f_{\theta}$$
: $Lip(f_{\theta}) = \sup_{(x,x') \in \mathcal{X}} \frac{\|f_{\theta}(x) - f_{\theta}(x')\|}{\|x - x'\|}$

CLIP: Lipschitz Constant

Lipschitz constant of
$$f_{\theta}$$
: $Lip(f_{\theta}) = \sup_{(x,x') \in \mathcal{X}} \frac{\|f_{\theta}(x) - f_{\theta}(x')\|}{\|x - x'\|}$

 $f_{ heta}$ is Lipschitz continuous if and only if $Lip(f_{ heta}) < +\infty$

- $\hookrightarrow f_{\theta}$ is continuous
- $\hookrightarrow f_{\theta}$ is almost everywhere differentiable (Rademacher Theorem)

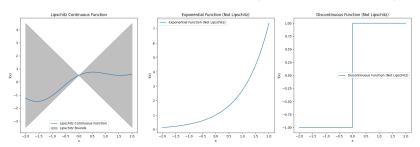


Figure. 4: Visualization of Lipschitz continuity.



CLIP: Lipschitz computation

Lipschitz regularization problem:

$$\min_{\theta} \sum_{(x,y) \in \Gamma} \mathsf{loss}(f_{\theta}(x),y) + \lambda \mathit{Lip}(f_{\theta})$$

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But computing a Lipschitz constant is NP-hard! [Sca18]

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But computing a Lipschitz constant is NP-hard! [Sca18]

Solution: Estimating a Lipschitz constant with cheap computational method [Bun22]

CLIP: Cheap Lipschitz

CLIP problem:

$$\min_{\theta} \sum_{(x,y) \in \Gamma} \mathsf{loss}(f_{\theta}(x),y) + \lambda \max_{(x,x') \in \mathcal{X}_{lip}} \frac{\|f_{\theta}(x) - f_{\theta}(x')\|}{\|x - x'\|}$$

CLIP: Cheap Lipschitz

CLIP problem:

$$\min_{\theta} \sum_{(x,y) \in \Gamma} \mathsf{loss}(f_{\theta}(x),y) + \lambda \max_{(x,x') \in \mathcal{X}_{\mathit{lip}}} \frac{\|f_{\theta}(x) - f_{\theta}(x')\|}{\|x - x'\|}$$

Where \mathcal{X}_{lip} verify :

$$\mathcal{X}_{lip}^{k+1} \leftarrow AdversarialUpdate(f_{\theta}, \mathcal{X}_{lip}^{k})$$

AdversarialUpdate : For all $({}^k x, {}^k x') \in \mathcal{X}^k_{lip}$

$$^{k+1}x \leftarrow^k x + \tau \nabla_x (Lip(^kx,^kx'))^2$$

$$^{k+1}x' \leftarrow^k x' + \tau \nabla_{x'} (Lip(^k x, ^k x'))^2$$



CLIP: Adversarial Update, how does it works?

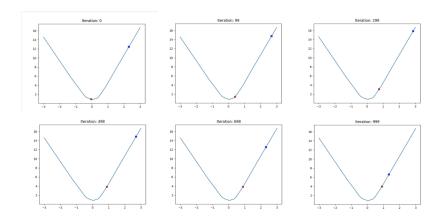


Figure. 5: Adversarial Update Evolution of \mathcal{X}_{lip} (Click here to see this evolution in video).

CLIP: At what cost?

Estimation precision: local extrema problem

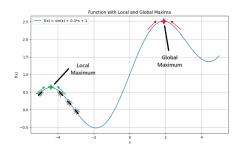


Figure. 6: Example of a function with global and local maxima, where the ant mistakenly reaches the local maximum.

CLIP: At what cost?

Estimation precision: local extrema problem

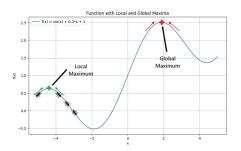


Figure. 6: Example of a function with global and local maxima, where the ant mistakenly reaches the local maximum.

Computation time : computing $\mathcal{X}_{\mathit{lip}}$ is still long





- 2 CLIP : Test & Improvement

Test: A polynomial approximation Improvement: Better, Faster, Stronger



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Test: A polynomial approximation

Improvement : Better, Faster, Stronger

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We define the following polynomial function :

$$P = \epsilon (0.5 + 0.01X + X^6)$$

Where ϵ is a scaling value.

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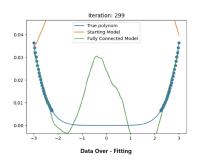
Then we define:

$$X = (x_1, \dots, x_N) \sim (\mathbb{U}([-3, -2] \cup [2, 3]))^N$$

Then the data set :

$$\Gamma = \{ (\mathbf{x}_i, P(\mathbf{x}_i)) : i \in [|1, N|] \}$$





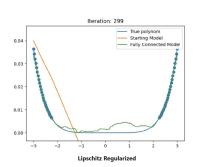


Figure. 7: DNN fitting polynomial function - Over-fitting VS lipschitz regularization (training video : with Lipschitz and without Lipschitz)

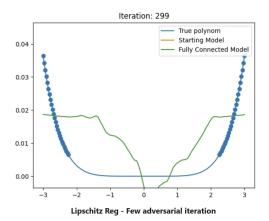


Figure. 8: DNN fitting polynomial function - lipschitz regularization with few X_{lip} update (training video : here)

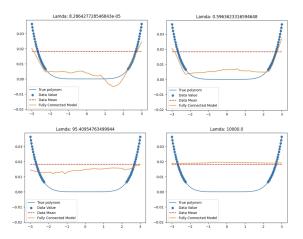


Figure. 9: Model evolution for different values of λ (Full evolution video : here)

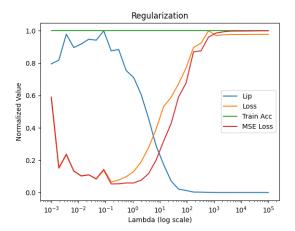


Figure. 10: Normalized Lipschitz constant, MSE Loss and train accuracy evolution for different values of λ

2 CLIP : Test & Improvement

Test: A polynomial approximation

Improvement: Better, Faster, Stronger

Improvement : Better & Faster

SGDM: Stochastic Gradient Descent Method

Basic CLIP:

$$\min_{\theta} \sum_{(x,y) \in \Gamma} \mathsf{loss}(f_{\theta}(x), y) + \lambda CLip(f_{\theta}, \mathcal{X}_{lip}) \longleftarrow SGDM$$

SGDM: Stochastic Gradient Descent Method

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Other possible gradient method:

NAGM: Nesterov Accelerated Gradient Method

Improvement : Better & Faster

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NAGM : Nesterov Accelerated Gradient Method

ADAM : Adaptive Moment Method ([Kin15])



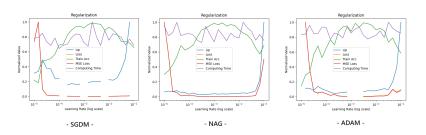


Figure. 11: Comparison of SGDM, NAG, ADAM results for log scaled learning rate - SGDM $time_{maximal}^{computation} = 0.0185 s$ - NAG $time_{maximal}^{computation} = 0.0173 s$ - ADAM $time_{maximal}^{computation} = 0.0176 s$ -



Warm-up Phase:

To improve CLIP efficiency, we propose adding a "warm-up" phase to the CLIP algorithm.

First Phase: [Pre-training] Train the model on the dataset Γ using only the regular loss (without regularization).

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Improvement : Stronger

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To improve CLIP efficiency, we propose adding a "warm-up" phase to the CLIP algorithm.

- First Phase: [Pre-training] Train the model on the dataset Γ using only the regular loss (without regularization).
- **Second Phase:** Stop the warm-up phase when the model's training accuracy reaches a predefined threshold α .
- **Third Phase:** [Training] Begin training the pre-trained model using the regularizer.

- 3 FLIP : Finite Lipschitz

- 3 FLIP : Finite Lipschitz Finite Computation for Lipschitz Total Variation Property

FLIP: Max & Sum

We compute:

$$MaxLip(f_{\theta}) = \max_{(x,x') \in \mathcal{X}_{lip}} \frac{\|f_{\theta}(x) - f_{\theta}(x')\|}{\|x - x'\|}$$

But to do so, we need to compute $\forall (x,x') \in \mathcal{X}_{lip}, \ \frac{\|f_{\theta}(x)-f_{\theta}(x')\|}{\|x-x'\|}$

- → Information loss...
- → Computationally expensive...



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- → Information loss...
- → Computationally expensive...

We introduce:

$$SumLip(f_{\theta}) = \frac{1}{|\mathcal{X}_{lip}|} \sum_{(x,x') \in \mathcal{X}_{lip}} \frac{\|f_{\theta}(x) - f_{\theta}(x')\|}{\|x - x'\|}$$



Definition: (Local Lipschitz constant) For $\epsilon > 0$ and $x \in \mathcal{X}$, we define $Lip_{\epsilon}^{loc}(f_{\theta},x) = \sup_{x_1,x_2 \in \mathcal{B}_{\epsilon}(x)} \frac{||f_{\theta}(x_1) - f_{\theta}(x_2)||}{||x_1 - x_2||}$ where : $\mathcal{B}_{\epsilon}(x) = \{ x' \in \mathcal{X}, \| x' - x \| \le \epsilon \}.$

FLIP: From Sum FLIP to Total Variation (TV)

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Remark:
$$(x, x') \in \mathcal{X}_{lip}$$
, $\frac{\|f_{\theta}(x) - f_{\theta}(x')\|}{\|x - x'\|} \approx Lip_{\epsilon}^{loc}(f_{\theta}, x)$

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Property: (Local Lipschitz to gradient) a.e $x \in \mathcal{X}$, $\lim_{\epsilon \to 0} Lip_{\epsilon}^{loc}(f, x) = \|\nabla f(x)\|_*$, where : $\|\cdot\|_* = \sup_{h \in \mathcal{B}_1(0)} \|\cdot h\|$.



$$\frac{1}{|\mathcal{X}_{lip}|} \sum_{(x,x') \in \mathcal{X}_{lip}} \frac{\|f_{\theta}(x) - f_{\theta}(x')\|}{\|x - x'\|} \xrightarrow{\bullet \bullet} \frac{1}{|\Gamma_{\mathcal{X}}|} \sum_{x \in \Gamma_{\mathcal{X}}} Lip_{\epsilon}^{loc}(f_{\theta}, x)$$

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$$\xrightarrow{\epsilon \to 0} \frac{1}{|\Gamma_{\mathcal{X}}|} \sum_{x \in \Gamma_{\mathcal{X}}} \|\nabla f_{\theta}(x)\|_{*}$$

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Introducing TV regularization [Rud92] :

$$\min_{\theta} \sum_{(x,y)\in\Gamma} \mathsf{loss}(f_{\theta}(x),y) + \lambda \int_{\mathcal{X}} \|\nabla f_{\theta}(x)\|_2 dx.$$

- → Not used for NN (but for image processing)
- → Norm used is Euclidean norm



With Norm Equivalence Theorem¹ & Setting for exemple \mathcal{X} as: $\mathcal{X} = \{x \in \mathbb{R}^m, \|x\| < 1 + \sup \|x_{\gamma}\|\}$ $x_{\gamma} \in \Gamma_{\mathcal{X}}$

$$SumLip(f_{\theta}) \longrightarrow \int_{\mathcal{X}} \|\nabla f_{\theta}(x)\|_* dx$$

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FLIP: TV Regularization

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$$SumLip(f_{\theta}) \longrightarrow \int_{\mathcal{X}} \|\nabla f_{\theta}(x)\|_{*} dx$$

$$\longrightarrow \int_{\mathcal{X}} \lim_{\epsilon \to 0} Lip_{\epsilon}^{loc}(f_{\theta}, x) dx$$

Under peculiar assumptions, Lebesgue Dominated Convergence Theorem :

$$\int_{\mathcal{X}} \lim_{\epsilon \to 0} \operatorname{Lip}_{\epsilon}^{loc}(f_{\theta}, x) \, dx = \lim_{\epsilon \to 0} \int_{\mathcal{X}} \operatorname{Lip}_{\epsilon}^{loc}(f_{\theta}, x) \, dx$$

FLIP: Cheap computation for TV

Our computed TV regularizer use cheap Lipschitz:

$$\forall B \subset \Gamma, \quad pTV_{reg}(f_{\theta}, B, \epsilon_{k}) = \sum_{(x, y) \in B} \max_{\substack{(x_{1}, x_{2}) \in \mathcal{X}_{lip} \\ s.t \ ||x - x_{1, 2}|| \le \epsilon_{k}}} \frac{||f_{\theta}(x_{1}) - f_{\theta}(x_{2})||}{||x_{1} - x_{2}||}$$

With $\epsilon_k \longrightarrow 0$ where k denotes each epochs of our training. $k \rightarrow +\infty$



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Let see what it looks like...

FLIP: Projected Finite Lipschitz Total Variation

```
for epoch e = 1 to E do
        for minibatch B \subset \Gamma do
                \mathcal{X}_{lin} \leftarrow B
                for (x_1, x_2) \in \mathcal{X}_{lin} do
                       x \leftarrow x_1
                      x_1 \leftarrow x_1 + \tau \nabla_{x_1} (Lip(x_1, x_2))^2
                      x_2 \leftarrow x_2 + \tau \nabla_{x_2} (Lip(x_1, x_2))^2
                      x_1; x_2 \leftarrow x + \epsilon \frac{(x_1 - x)}{\|x_2 - x\|}; x + \epsilon \frac{(x_2 - x)}{\|x_2 - x\|}
                end
                \theta \leftarrow \text{SGDM}_{\eta,\gamma} \left( \frac{1}{|B|} \sum_{(x,y) \in B} loss(f_{\theta}(x), y) + \lambda \sum_{(x_1,x_2) \in \mathcal{X}_{bo}} Lip(f_{\theta}, (x_1, x_2)) \right)
                accuracy \leftarrow accuracy + \frac{1}{|B|} \sum_{(x,y) \in B} \mathbf{1}(x,y)_{\{f_{\theta}(x)=y\}}
                if accuracy > \alpha then
                       \lambda \leftarrow \lambda + d\lambda
                end
                else
                       \lambda \leftarrow \lambda - d\lambda
               end
        end
        \epsilon \leftarrow \epsilon \times 0.9
end
```

Input:

Training data Γ , learning rate η , momentum γ , regularization parameter λ , threshold α , update step $d\lambda$, initial ball ray ϵ , total epochs E.

Output:

Trained model parameters θ .

- 3 FLIP : Finite Lipschitz Total Variation Property

• **Assumption 1**: Our *Loss* function is proper

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- **Assumption 2 :** Our NN f_{θ} is Lipschitz continuous and continous upon θ

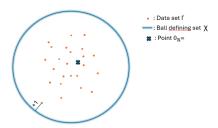
TV : Assumptions

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Lipschitz Regularisation for Neural Networks in High Dimension

TV : Solution existence

Under Assumption 1-4.

Our problem admit a finite solution :

$$\exists \theta, \ \sum_{(x,y)\in\Gamma} \mathsf{loss}(f_{\theta}(x),y) + \lambda \int_{\mathcal{X}} \lim_{\epsilon \to 0} \mathit{Lip}_{\epsilon}^{loc}(f_{\theta},x) \, dx < +\infty.$$

11 1 4 2 4 4

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And we have Lemma:

$$\theta \mapsto \int_{\mathcal{X}} \lim_{\epsilon \to 0} Lip_{\epsilon}^{loc}(f_{\theta}, x) dx$$
 is lower semi-continuous.

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Thus: Existence Theorem:

$$\min_{\theta} \sum_{(x,y) \in \Gamma} \mathsf{loss}(f_{\theta}(x),y) + \lambda \int_{\mathcal{X}} \lim_{\epsilon \to 0} \mathit{Lip}_{\epsilon}^{loc}(f_{\theta},x) \, dx \ \ \textit{admit a solution}$$



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Property (A limit for infinite λ): There exist θ_{∞}^* a limit: $\theta_{\lambda_n}^* \longrightarrow \theta_{\infty}^*$ such that TV-Problem with λ_n is solved by $f_{\theta_{\lambda_n}^*}$ and $\lambda_n \to +\infty$ f_{θ^*} is constant.

TV : Properties

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Property (Infinite limit constant value): We have that

$$\begin{split} f_{\theta_{\infty}^*} &= \underset{y_{\theta} \in \mathcal{Y}_{\Theta}}{\text{arg min}} \left\{ \sum_{(x,y) \in \Gamma} \mathsf{loss}(y_{\theta},y) \right\}, \text{ where } \\ \mathcal{Y}_{\Theta} &= \{ y \in \mathcal{Y} \mid \exists \theta \in \Theta, \ \forall x \in \mathcal{X}, \ f_{\theta}(x) = y \}. \end{split}$$

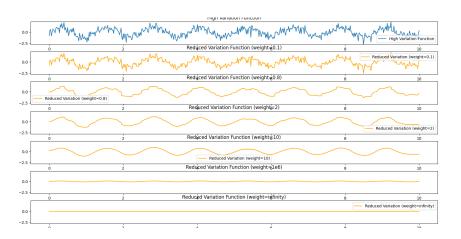


Figure. 12: Illustration of TV regularization with an increasing weight



With our algorithm we solve :

$$\min_{\theta} \sum_{(x,y) \in \Gamma} \mathsf{loss}(f_{\theta}(x),y) + \int_{\mathcal{X}} \mathsf{Lip}^{loc}_{\epsilon}(f_{\theta},x) \, dx$$

for different $\epsilon \longrightarrow 0$. But...

TV: Algorithm Validity

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Does it solve:

$$\min_{\theta} \sum_{(x,y)\in\Gamma} \mathsf{loss}(f_{\theta}(x),y) + \int_{\mathcal{X}} \lim_{\epsilon \to 0} \mathsf{Lip}_{\epsilon}^{\mathsf{loc}}(f_{\theta},x) \, dx$$

Using [Shi24] we can prove in (1, p)-Sobolev spaces that :

$$\int_{\mathcal{X}} \left(Lip_{\epsilon}^{loc}(f_{\theta}, x) \right)^{p} dx \xrightarrow{\gamma} \int_{\mathcal{X}} \lim_{\epsilon \to 0} \left(Lip_{\epsilon}^{loc}(f_{\theta}, x) \right)^{p} dx$$

 γ -convergence is a weaker convergence that permits to show minimizer convergence.

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Not for all $p \in \mathbb{N}$... Issue :

 $f_{\theta}(x)$ impossible in Sobolev spaces for p < n.

→ Need Sobolev Embedding Theorem in continuous function which is true for $p \ge n$.

(Reminder : we are set in \mathbb{R}^n)



But for MNIST images n = 784 and for high quality images n easily explode...

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For such n, if $p \ge n$ we are computationally near $p = +\infty$ which is basically computing a Lipschitz constant.

TV : Gamma convergence

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For such n, if $p \ge n$ we are computationally near $p = +\infty$ which is basically computing a Lipschitz constant.

But using Sobolev Embedding Theorem just for continuity here is **OVERKILL!**

Thus, we need to change our space!

The article direction in which we are going :

Using Barron spaces

 \hookrightarrow Neural Networks spaces



- 4 Conclusion

- 4 Conclusion Results

Results: Adversarial Attacks

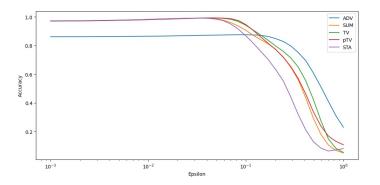


Figure. 13: Comparison of accuracy against FGSM adversarial attacks for different training methods.

Find the code for those experiments here: https://github.com/TimRoith/CLIP



Results: Adversarial Attacks

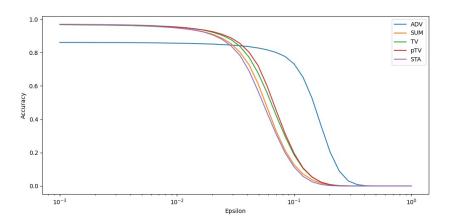


Figure. 14: Comparison of accuracy against PGD adversarial attacks for different training methods.



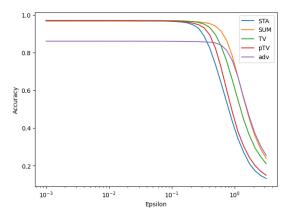


Figure. 15: Comparison of accuracy against Gaussian noise for different training methods.

Estimator	Train Accuracy	Computation Time (s)
SUM FLIP	0.979	126
ADV FGSM	0.837	116
TV	0.981	95
pTV	0.978	94
STA	0.979	54

Table. 1: Performance comparison of different training methods (On DESY server hardware: AMD EPYC 7402).

Conclusion 000000000

- 4 Conclusion To conclude

Exploration of robust training methods - Key Findings:



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- Validation of CLIP algorithm: Ensured stability and efficiency on 1D problems before scaling.
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- Theoretical Advances: Studied theoretical behavior of TV. Utilized γ -convergence to verify correctness of our algorithm.
- Empirical Results: TV-based methods demonstrated superior robustness under FGSM/PGD attacks and Gaussian noise compared to SUM FLIP and even sometime compared to adversarial training.



Exploration of robust training methods - Future Directions:

- Refine algorithms for more accurate TV estimation.
- Extend theoretical analysis for FLIP regularizers.
- Apply to complex, real-world datasets to test scalability.



- Introduction
- 2 CLIP: Test & Improvement
- 3 FLIP : Finite Lipschitz
- 4 Conclusion
- 6 References

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