Theoretically Principled Trade-off between Robustness and Accuracy





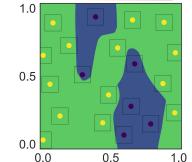
Notations

A sample $x \in \mathcal{X} \subseteq \mathbb{R}^d$ and label $y \in \{+1, -1\}$,

 $\mathbb{B}(x,\epsilon) = \{x' \in \mathcal{X} : |x' - x| \le \epsilon\}$ is the neighborhood of *x*.

|x| is the norm, e.g., $|x|_{\infty}$, $|x|_{2}$.





classifier

ion–linear

 $f: \mathcal{X} \to \mathbb{R}$, a score function, maps an instance to a confidence value (being positive). $sign(f(\cdot))$ is the associated binary classifier, where $sign(\cdot)$ is the sign of input, and sign(0) = 1. $DB(f) = \{x \in \mathcal{X}: f(x) = 0\}$ is the decision boundary of f. $\mathbb{B}(DB(f), \epsilon) = \{x \in \mathcal{X}: \exists x' \in \mathbb{B}(x, \epsilon) \text{ s.t. } f(x)f(x') \leq 0\}$ is the neighborhood of decision boundary.

For a given function $\psi(u)$, $\psi^*(v) \coloneqq \sup_{u} \{u^T v - \psi(u)\}$ is the conjugate function of ψ . ψ^{**} is the bi-conjugate, and ψ^{-1} is the inverse function.

1{*event*} is the indicator function indicating if *event* happens.

Notations



 $\mathbb{B}(x,\epsilon) = \{x' \in \mathcal{X} : |x' - x| \le \epsilon\} \text{ is the neighborhood of } x.$ $\mathbb{B}(\mathrm{DB}(f),\epsilon) = \{x \in \mathcal{X} : \exists x' \in \mathbb{B}(x,\epsilon) \text{ s.t. } f(x)f(x') \le 0\} \text{ is the neighborhood of decision boundary.}$

Assume that the data are drawn from an unknown distribution $(X, Y) \sim D$

The robust (classification) error under ϵ perturbation:

$$\mathcal{R}_{\operatorname{rob}}(f) \coloneqq \mathbb{E}_{(X,Y) \sim \mathcal{D}} \mathbb{1}\{\exists X' \in \mathbb{B}(X,\epsilon) \text{ s.t. } f(X')Y \leq 0\}$$

The natural (classification) error:

$$\mathcal{R}_{nat}(f) \coloneqq \mathbb{E}_{(X,Y)\sim\mathcal{D}} \mathbb{1}\{f(X)| Y \leq 0\}$$

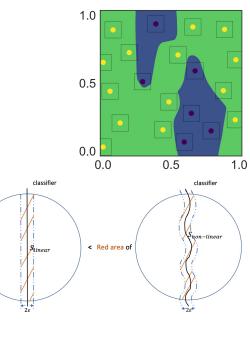
Clearly, $\mathcal{R}_{rob}(f) \ge \mathcal{R}_{nat}(f)$ for all f, and the equality holds when $\epsilon = 0$.

The boundary error:

$$\mathcal{R}_{\mathrm{bdy}}(f) \coloneqq \mathbb{E}_{(X,Y)\sim\mathcal{D}} \mathbb{1}\{X \in \mathbb{B}(\mathrm{DB}(f),\epsilon), f(X)Y > 0\}$$

Red area of

And $\mathcal{R}_{rob}(f) = \mathcal{R}_{nat}(f) + \mathcal{R}_{bdy}(f)$



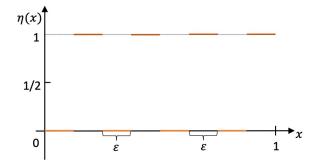
Toy example



The trade-off between natural and robust errors: training robust models may lead to a reduction of standard accuracy.

Assume that
$$\eta(x) \coloneqq \Pr(Y = 1 | X = x) = \begin{cases} 0, \ x \in [2k\epsilon, (2k+1)\epsilon), \\ 1, \ x \in ((2k+1)\epsilon, (2k+1)\epsilon]. \end{cases}$$
 where $x \sim U[0,1]$

Bayes optimal classifier: $sign(2\eta(x) - 1)$ All-one classifier: 1 (always outputs "positive")



	Bayes Optimal Classifier	All-One Classifier
$\mathcal{R}_{\mathrm{nat}}$	0 (optimal)	1/2
$\mathcal{R}_{\mathrm{bdy}}$	1	0
$\mathcal{R}_{ m rob}$	1	1/2 (optimal)

Toy example



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The Bayes optimal classifier: $sign(2\eta(x) - 1)$

The all-one classifier: 1 (always outputs "positive")

	Bayes Optimal Classifier	All-One Classifier
$\mathcal{R}_{\mathrm{nat}}$	0 (optimal)	1/2
$\mathcal{R}_{ ext{bdy}}$	1	0
$\mathcal{R}_{ m rob}$	1	1/2 (optimal)

• For the natural error: $\mathcal{R}_{nat}(f) \coloneqq \mathbb{E}_{(X,Y)\sim \mathcal{D}} \mathbb{1}\{f(X) | Y \leq 0\}$:

It is obvious that $\mathcal{R}_{nat}(f) = 0$ for Bayes classifier, and $\mathcal{R}_{nat}(f) = 1/2$ for all-one classifier.

• For the boundary error $\mathcal{R}_{bdy}(f) \coloneqq \mathbb{E}_{(X,Y)\sim \mathcal{D}} \mathbb{1}\{X \in \mathbb{B}(\mathrm{DB}(f), \epsilon), f(X)Y > 0\}$:

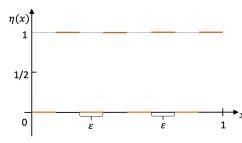
For Bayes classifier, we can always find a perturbation resulting in the right prediction, since the interval is ϵ .

For all-one classifier, DB(f) (if any) is not within [0,1], and thus the event never happens.

• For the robust error $\mathcal{R}_{rob}(f) \coloneqq \mathbb{E}_{(X,Y)\sim \mathcal{D}} \mathbb{1}\{\exists X' \in \mathbb{B}(X,\epsilon) \text{ s.t. } f(X')Y \leq 0\}$:

For Bayes classifier, we can always find a perturbation to flip the prediction, since the interval is ϵ . For all-one classifier, since f(X) = 1, $\forall X$, we have 1/2 change to obtain negative sample (Y = -1). Or we can compute it by $\mathcal{R}_{rob}(f) = \mathcal{R}_{nat}(f) + \mathcal{R}_{bdy}(f)$.

In most of existing works, we can assign different weights on both errors $(\mathcal{R}_{nat} + \mathcal{R}_{bdy})$ to balance them. In this paper, the authors try to devise tight differentiable upper bounds on both terms, as both involve 0-1 loss functions.



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0-1 loss function is intractable -> tractable surrogate loss $\mathcal{R}_{\phi}(f) \coloneqq \mathbb{E}_{(X,Y)\sim \mathcal{D}}\phi(f(X)Y)$.

Define conditional ϕ -risk:

For $\eta \in [0,1]$, $H(\eta) \coloneqq \inf_{\alpha \in \mathbb{R}} C_{\eta}(\alpha) \coloneqq \inf_{\alpha \in \mathbb{R}} (\eta \phi(\alpha) + (1-\eta)\phi(-\alpha))$, and define $H^{-}(\eta) \coloneqq \inf_{\alpha:\alpha(2\eta-1)\leq 0} C_{\eta}(\alpha) \coloneqq \inf_{\alpha:\alpha(2\eta-1)\leq 0} (\eta \phi(\alpha) + (1-\eta)\phi(-\alpha))$.

Assumption on ϕ : it is classification-calibrated: if $H^-(\eta) > H(\eta)$ for any $\eta \neq 1/2$.

Intuition:

 $\eta(x) \coloneqq \Pr(Y = 1 | X = x)$ and α is the probability of positive class predicted by f. $H(\eta) = \min_{f} \mathcal{R}_{nat}(f),$ $H^{-}(\eta) = \min_{f} \mathcal{R}_{nat}(f),$ s.t. f is inconsistent with Bayes optimal classifier



The functional transform of classification-calibrated loss ϕ :

Define $\tilde{\psi}(\theta) = H^{-}\left(\frac{1+\theta}{2}\right) - H\left(\frac{1+\theta}{2}\right)$ and $\psi: [0,1] \to [0,\infty)$ by $\psi = \tilde{\psi}^{**}$. (ψ^{*} is the conjugate function of ψ).

 $\psi(\theta)$ is the largest convex lower bound on $\tilde{\psi}(\theta) = H^{-}\left(\frac{1+\theta}{2}\right) - H\left(\frac{1+\theta}{2}\right)$

 $\tilde{\psi}(\theta)$ characterizes how close the surrogate loss ϕ is to the class of non-classification-calibrated losses.

Property of classification-calibrated loss:

For classification-calibrated surrogate loss ϕ , ψ is non-decreasing, continuous, convex on [0,1] and $\psi(0) = 0$.



Upper bound:

Let $\mathcal{R}_{\phi}(f) \coloneqq \mathbb{E}\phi(f(X)Y)$ and $\mathcal{R}_{\phi}^{*}(f)$, for non-negative classification-calibrated loss ϕ with $\phi(0) \ge 1$, any measurable $f: \mathcal{X} \to \mathbb{R}$, any probability distribution on $\mathcal{X} \times \{\pm 1\}$, and any $\lambda > 0$, we have:

$$\begin{aligned} \mathcal{R}_{\rm rob}(f) - \mathcal{R}_{\rm nat}^* &\leq \psi^{-1} \big(\mathcal{R}_{\phi}(f) - \mathcal{R}_{\phi}^* \big) + \Pr[\mathbf{X} \in \mathbb{B}({\rm DB}(f), \epsilon), f(\mathbf{X})Y > 0] \\ &\leq \psi^{-1} \big(\mathcal{R}_{\phi}(f) - \mathcal{R}_{\phi}^* \big) + \mathbb{E} \max_{\mathbf{X}' \in \mathbb{B}(\mathbf{X}, \epsilon)} \phi(f(\mathbf{X}')f(\mathbf{X})/\lambda) \end{aligned}$$

The models are vulnerable to small adversarial attacks because the probability that data lie around the decision boundary of the model is large.



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Proof:

The first inequality holds since ϕ is a classification-calibrated loss^[1] and $\mathcal{R}_{bdy} = \Pr[\mathbf{X} \in \mathbb{B}(DB(f), \epsilon), f(\mathbf{X})Y > 0]$:

$$\begin{aligned} \mathcal{R}_{\rm rob}(f) &= \mathcal{R}_{\rm nat}(f) + \mathcal{R}_{\rm bdy}(f) \\ \mathcal{R}_{\rm rob}(f) - \mathcal{R}_{\rm nat}^* &= \mathcal{R}_{\rm nat}(f) - \mathcal{R}_{\rm nat}^* + \mathcal{R}_{\rm bdy}(f) \leq \psi^{-1} \big(\mathcal{R}_{\phi}(f) - \mathcal{R}_{\phi}^* \big) + \mathcal{R}_{\rm bdy}(f) \end{aligned}$$

Now we consider the second inequality:

$$\Pr[\mathbf{X} \in \mathbb{B}(\mathrm{DB}(f), \epsilon), f(\mathbf{X})Y > 0] \le \Pr[\mathbf{X} \in \mathbb{B}(\mathrm{DB}(f), \epsilon)]$$
$$= \mathbb{E} \max_{\mathbf{X}' \in \mathbb{B}(\mathbf{X}, \epsilon)} 1\{f(\mathbf{X}') \neq f(\mathbf{X})\}$$
$$= \mathbb{E} \max_{\mathbf{X}' \in \mathbb{B}(\mathbf{X}, \epsilon)} 1\{f(\mathbf{X}')f(\mathbf{X})/\lambda < 0\}$$
$$\le \mathbb{E} \max_{\mathbf{X}' \in \mathbb{B}(\mathbf{X}, \epsilon)} \phi(f(\mathbf{X}')f(\mathbf{X})/\lambda)$$

[1] Bartlett, Peter L., Michael I. Jordan, and Jon D. McAuliffe. "Convexity, classification, and risk bounds." Journal of the American Statistical Association 2006.



Lower bound:

Suppose that $|\mathcal{X}| \ge 2$. For non-negative classification-calibrated loss ϕ with $\phi(x) \to 0$ as $x \to +\infty$, and any $\xi > 0$, any $\theta \in [0,1]$. There exists a probability distribution on $\mathcal{X} \times \{\pm 1\}$, a function $f: \mathbb{R}^d \to \mathbb{R}$ and a regularization $\lambda > 0$ such that $\mathcal{R}_{rob}(f) - \mathcal{R}_{nat}^* = \theta$ and:

$$\psi\left(\theta - \mathbb{E}\max_{X' \in \mathbb{B}(X,\epsilon)} \phi(f(X')f(X)/\lambda)\right) \le \mathcal{R}_{\phi}(f) - \mathcal{R}_{\phi}^* \le \psi\left(\theta - \mathbb{E}\max_{X' \in \mathbb{B}(X,\epsilon)} \phi(f(X')f(X)/\lambda)\right) + \xi$$

Under the extra conditions on loss functions $\lim_{x\to+\infty} \phi(x) = 0$, the upper bound is tight.

The first inequality holds since ψ is non-decreasing, continuous, convex on [0,1] and

$$\mathcal{R}_{\rm rob}(f) - \mathcal{R}_{\rm nat}^* \le \psi^{-1} \big(\mathcal{R}_{\phi}(f) - \mathcal{R}_{\phi}^* \big) + \mathbb{E} \max_{X' \in \mathbb{B}(X,\epsilon)} \phi(f(X')f(X)/\lambda)$$



Based on previous theorems, we consider a new surrogate loss:

$$\min_{f} \mathbb{E} \left\{ \phi(f(\mathbf{X})Y) + \max_{\mathbf{X}' \in \mathbb{B}(\mathbf{X},\epsilon)} \phi(f(\mathbf{X})f(\mathbf{X}')/\lambda) \right\}$$

The first term, $\phi(f(X)Y)$, minimizes the natural error.

The second regularization term, $\max_{X' \in \mathbb{B}(X,\epsilon)} \phi(f(X)f(X')/\lambda)$, minimizes the difference between the predictions of natural example and the adversarial example. Thus, it stands for the "robustness".

 λ can balance the importance of natural and robust errors.

(It tends to be Bayes optimal classifier when $\lambda \to +\infty$ and all-one classifier when $\lambda \to 0$.)

We can easily extend it to multi-class tasks by replacing ϕ with a multi-class calibrated loss $\mathcal{L}(\cdot, \cdot)$:

$$\min_{f} \mathbb{E}\left\{ \mathcal{L}(f(\boldsymbol{X}), Y) + \max_{\boldsymbol{X}' \in \mathbb{B}(\boldsymbol{X}, \epsilon)} \mathcal{L}(f(\boldsymbol{X}), f(\boldsymbol{X}')) / \lambda \right\}$$

In most of existing works:

$$\min_{f} \mathbb{E} \left\{ \max_{\mathbf{X}' \in \mathbb{B}(\mathbf{X}, \epsilon)} \phi(f(\mathbf{X}')Y) \right\}$$

is served as the upper bound of $\mathcal{R}_{rob}(f)$. However, it may not be the *tight* upper bound and may not capture the trade-off between natural and robust errors.

Adversarial training by TRADES



Line 5: x_i is global minimizer to $g(x') \coloneqq \mathcal{L}(f(x_i), f(x'))$, thus, initialize x'_i by adding small perturbation.

Line 7: solve $\max_{X' \in \mathbb{B}(X,\epsilon)} \mathcal{L}(f(X), f(X'))/\lambda$ by projected gradient descent.

Line 10: gradient descent for the objective function $\min_{f} \mathbb{E} \left\{ \mathcal{L}(f(\mathbf{X}), Y) + \max_{\mathbf{X}' \in \mathbb{B}(\mathbf{X}, \epsilon)} \mathcal{L}(f(\mathbf{X}), f(\mathbf{X}')) / \lambda \right\}$ Algorithm 1 Adversarial training by TRADES

- **input** Step sizes η_1 and η_2 , batch size m, number of iterations K in inner optimization, network architecture parametrized by θ
- **output** Robust network f_{θ}
 - 1: Randomly initialize network f_{θ} , or initialize network with pre-trained configuration
 - 2: repeat
 - 3: Read mini-batch $B = \{x_1, ..., x_m\}$ from training set
- 4: for i = 1, ..., m (in parallel) do
- 5: $x'_i \leftarrow x_i + 0.001 \cdot \mathcal{N}(\mathbf{0}, \mathbf{I})$, where $\mathcal{N}(\mathbf{0}, \mathbf{I})$ is the Gaussian distribution with zero mean and identity variance
- 6: **for** k = 1, ..., K **do**

7:
$$x'_i \leftarrow \Pi_{\mathbb{B}(x_i,\epsilon)}(\eta_1 \operatorname{sign}(\nabla_{x'_i} \mathcal{L}(f_{\theta}(x_i), f_{\theta}(x'_i))) + x'_i)$$
, where Π is the projection operator

8: **end for**

9: end for

10:
$$\theta \leftarrow \theta - \eta_2 \sum_{i=1}^m \nabla_{\theta} [\mathcal{L}(f_{\theta}(\boldsymbol{x}_i), \boldsymbol{y}_i) + \mathcal{L}(f_{\theta}(\boldsymbol{x}_i), f_{\theta}(\boldsymbol{x}'_i))/\lambda]/m$$

11: **until** training converged

Experiments



Verify the tightness of upper bound.

$$\Delta_{LHS} = \mathcal{R}_{\rm rob}(f) - \mathcal{R}_{\rm nat}^* \le \psi^{-1} \left(\mathcal{R}_{\phi}(f) - \mathcal{R}_{\phi}^* \right) + \mathbb{E} \max_{X' \in \mathbb{B}(X,\epsilon)} \phi(f(X')f(X)/\lambda) = \Delta_{RHS}$$

Train a classifier with natural training method to estimate $\mathcal{R}^*_{\mathrm{nat}} = 0\%$ and $\mathcal{R}^*_{\phi} = 0.0$

Find the classifier f by $\min_{f} \mathbb{E} \left\{ \phi(f(X)Y) + \max_{X' \in \mathbb{B}(X,\epsilon)} \phi(f(X)f(X')/\lambda) \right\}$ and approximate \mathcal{R}_{rob} and \mathcal{R}_{ϕ} . Estimate $\mathbb{E} \max_{X' \in \mathbb{B}(X,\epsilon)} \phi(f(X')f(X)/\lambda)$ by FGSM.

(The expectation is estimated in the test set.)

λ	$\mathcal{A}_{ m rob}(f)~(\%)$	$\mathcal{R}_{\phi}(f)$	$\Delta = \Delta_{\rm RHS} - \Delta_{\rm LHS}$
2.0	99.43	0.0006728	0.006708
3.0	99.41	0.0004067	0.005914
4.0	99.37	0.0003746	0.006757
5.0	99.34	0.0003430	0.005860

Experiments



Robust accuracy $\mathcal{A}_{rob}(f) = 1 - \mathcal{R}_{rob}(f)$, and $\mathcal{A}_{nat}(f) = 1 - \mathcal{R}_{nat}(f)$ Sensitivity of λ

$1/\lambda$	$\mathcal{A}_{ m rob}(f)~(\%)$ on MNIST	$\mathcal{A}_{\mathrm{nat}}(f)$ (%) on MNIST	$\mathcal{A}_{\mathrm{rob}}(f)$ (%) on CIFAR10	$\mathcal{A}_{\mathrm{nat}}(f)$ (%) on CIFAR10
1.0	94.75 ± 0.0712	99.28 ± 0.0125	44.68 ± 0.3088	87.01 ± 0.2819
2.0	95.45 ± 0.0883	99.29 ± 0.0262	48.22 ± 0.0740	85.22 ± 0.0543
3.0	95.57 ± 0.0262	99.24 ± 0.0216	49.67 ± 0.3179	83.82 ± 0.4050
4.0	95.65 ± 0.0340	99.16 ± 0.0205	50.25 ± 0.1883	82.90 ± 0.2217
5.0	95.65 ± 0.1851	99.16 ± 0.0403	50.64 ± 0.3336	81.72 ± 0.0286

Experiments



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		Defense	Defense type	Under which attack	Dataset	Distance	$\mathcal{A}_{\mathrm{nat}}(f)$	$\mathcal{A}_{ m rob}(f)$
$\min_{f} \mathbb{E} \left\{ \max_{X' \in \mathbb{B}(X,\epsilon)} \phi \right.$		Buckman et al. (2018)	gradient mask	Athalye et al. (2018)	CIFAR10	$0.031 \ (\ell_{\infty})$	-	0%
		Ma et al. (2018)	gradient mask	Athalye et al. (2018)	CIFAR10	$0.031 \ (\ell_{\infty})$	-	5%
		Dhillon et al. (2018)	gradient mask	Athalye et al. (2018)	CIFAR10	$0.031 \ (\ell_{\infty})$	-	0%
		Song et al. (2018)	gradient mask	Athalye et al. (2018)	CIFAR10	$0.031 \ (\ell_{\infty})$	-	9%
	$\max \phi(f(\mathbf{Y}')V))$	Na et al. (2017)	gradient mask	Athalye et al. (2018)	CIFAR10	$0.015(\ell_{\infty})$	-	15%
	$X' \in \mathbb{B}(X,\epsilon)$	Wong et al. (2018)	robust opt.	FGSM ²⁰ (PGD)	CIFAR10	$0.031 (\ell_{\infty})$	27.07%	23.54%
		Madry et al. (2018)	robust opt.	FGSM ²⁰ (PGD)	CIFAR10	$0.031 (\ell_{\infty})$	87.30%	47.04%
		Zheng et al. (2016)	regularization	FGSM ²⁰ (PGD)	CIFAR10	$0.031~(\ell_{\infty})$	94.64%	0.15%
		Kurakin et al. (2017)	regularization	FGSM ²⁰ (PGD)	CIFAR10	$0.031 (\ell_{\infty})$	85.25%	45.89%
		Ross & Doshi-Velez (2017)	regularization	FGSM ²⁰ (PGD)	CIFAR10	$0.031 \ (\ell_{\infty})$	95.34%	0%
		TRADES $(1/\lambda = 1.0)$	regularization	FGSM ²⁰ (PGD)	CIFAR10	$0.031 (\ell_{\infty})$	88.64%	49.14%
		TRADES $(1/\lambda = 6.0)$	regularization	FGSM ²⁰ (PGD)	CIFAR10	$0.031 (\ell_{\infty})$	84.92%	56.61%
		TRADES $(1/\lambda = 1.0)$	regularization	DeepFool (ℓ_{∞})	CIFAR10	$0.031 \ (\ell_{\infty})$	88.64%	59.10%
		TRADES $(1/\lambda = 6.0)$	regularization	DeepFool (ℓ_{∞})	CIFAR10	$0.031 \ (\ell_{\infty})$	84.92%	61.38%
		TRADES $(1/\lambda = 1.0)$	regularization	LBFGSAttack	CIFAR10	$0.031 \ (\ell_{\infty})$	88.64%	84.41%
		TRADES $(1/\lambda = 6.0)$	regularization	LBFGSAttack	CIFAR10	$0.031~(\ell_{\infty})$	84.92%	81.58%
		TRADES $(1/\lambda = 1.0)$	regularization	MI-FGSM	CIFAR10	$0.031 \ (\ell_{\infty})$	88.64%	51.26%
		TRADES $(1/\lambda = 6.0)$	regularization	MI-FGSM	CIFAR10	$0.031 \ (\ell_{\infty})$	84.92%	57.95%
		TRADES $(1/\lambda = 1.0)$	regularization	C&W	CIFAR10	$0.031 \ (\ell_{\infty})$	88.64%	84.03%
		TRADES $(1/\lambda = 6.0)$	regularization	C&W	CIFAR10	$0.031 \ (\ell_{\infty})$	84.92%	81.24%
		Samangouei et al. (2018)	gradient mask	Athalye et al. (2018)	MNIST	$0.005(\ell_2)$	-	55%
		Madry et al. (2018)	robust opt.	FGSM ⁴⁰ (PGD)	MNIST	$0.3(\ell_\infty)$	99.36%	96.01%
		TRADES (1/ λ = 6.0)	regularization	FGSM ⁴⁰ (PGD)	MNIST	$0.3(\ell_\infty)$	99.48%	96.07%
		TRADES $(1/\lambda = 6.0)$	regularization	C&W	MNIST	$0.005(\ell_2)$	99.48%	99.46%

Thank you

