

Florian Vincent – ICSP 2025

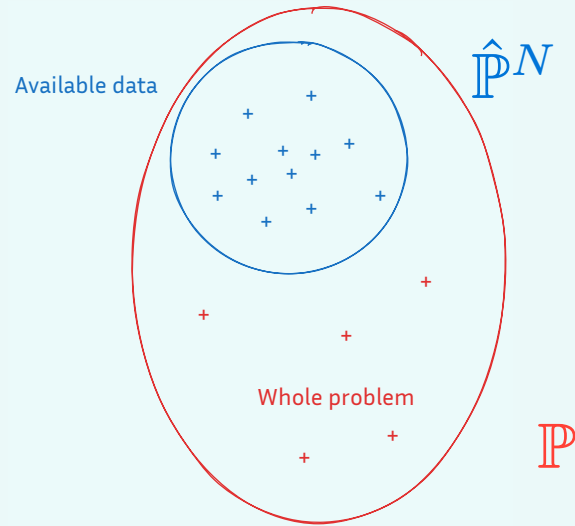
Solving Wasserstein distributionally robust classification by regularization



- Reference data: N points (finite) $\xi_1 \dots \xi_N$

$$\hat{\mathbb{P}}^N = \frac{1}{N} \sum_{\xi_i} \delta_{\xi_i}$$

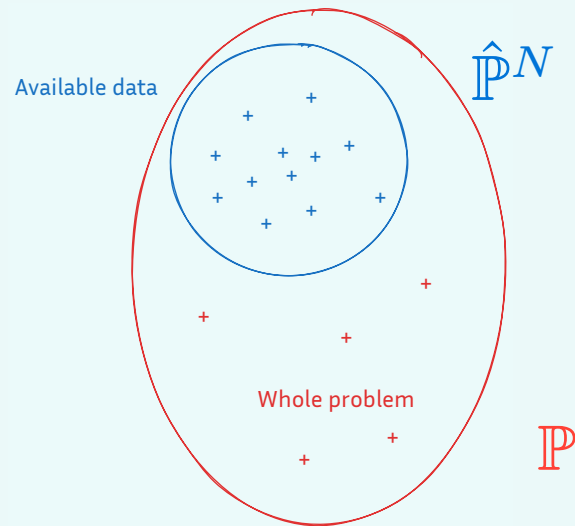
- Parameterized loss: $L_\theta \rightsquigarrow$ find θ
(e.g. θ are weights in an ANN)



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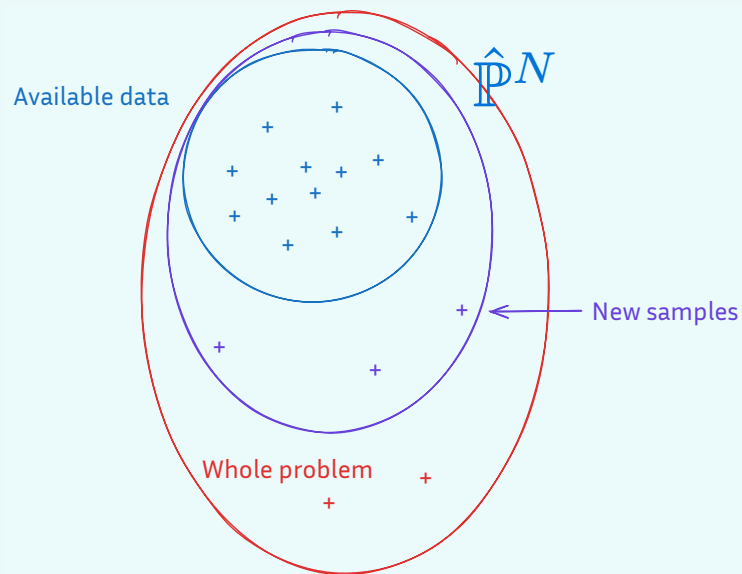
- Parameterized loss: $L_\theta \rightsquigarrow$ find θ
(e.g. θ are weights in an ANN)



- Learning:
 - Supervised: $(\xi_{\text{input}}, \xi_{\text{target}})$
 - Unsupervised: (ξ_{data})
- Operations research:
 - data-oriented: (ξ_{data})

Shift in the data

Various techniques exist, mainly in specific cases.



Distributional robustness:

Wide topic with rich diversity of methods cf
(This Session, July 2025)

(Wasserstein) Distributional robustness:












Entire zoos of examples formulated as convex programs
(Mohajerin Esfahani & Kuhn, 2018)

Extensive theoretical analysis
(Kuhn et al., 2019)

(New!) Sinkhorn regularisation of Wasserstein transport
(Wang et al., 2023)+(Azizian et al., 2023)

Data with distribution shift

E.g.: iWildsCam dataset

Train			Test (OOD)
$d = \text{Location 1}$	$d = \text{Location 2}$	$d = \text{Location 245}$	$d = \text{Location 246}$
 Vulturine Guinea fowl	 African Bush Elephant	 ...	 Wild Horse ...
 Cow	 Cow	 Southern Pig-Tailed Macaque	 Great Curassow
Test (ID)			
$d = \text{Location 1}$	$d = \text{Location 2}$	$d = \text{Location 245}$	
 Giraffe	 Impala	 Sun Bear	

$\hat{\mathbb{P}}^N$

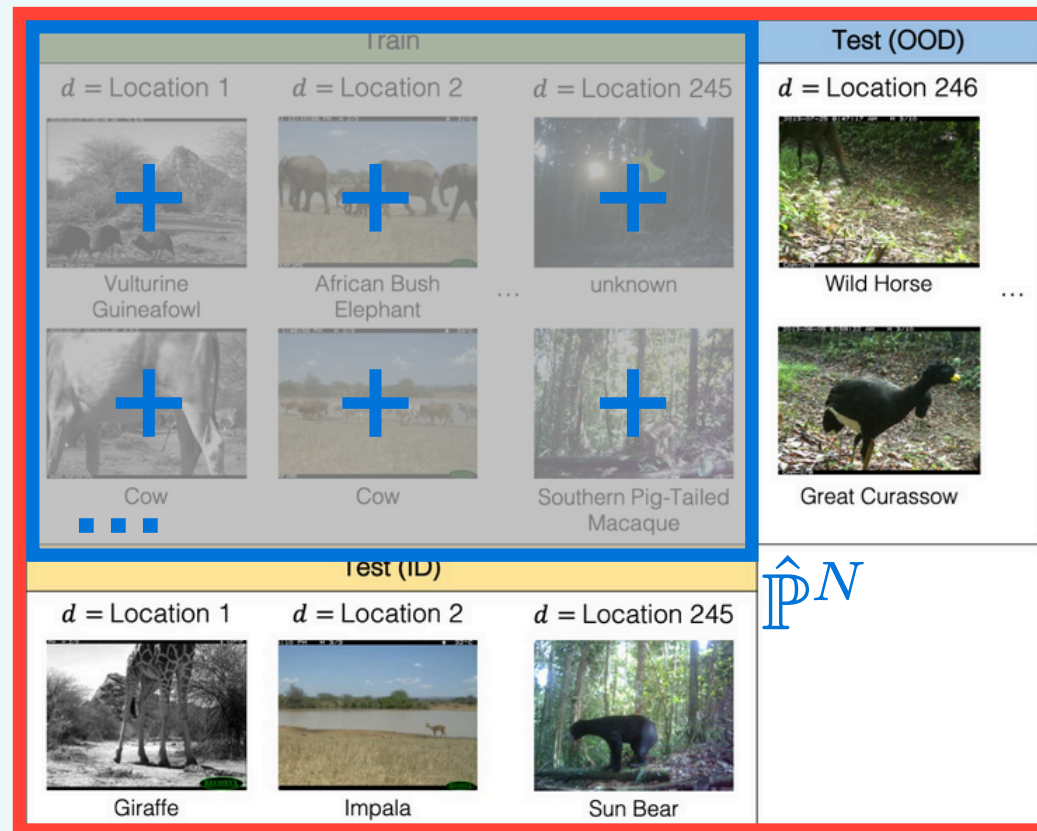
\mathbb{P}

Data with distribution shift

E.g.: iWildsCam dataset

Empirical risk minimization
(ERM):

$$\min_{\theta} \frac{1}{N} \sum_{\xi \sim \hat{\mathbb{P}}^N} [L_{\theta}(\xi)]$$



\mathbb{P}

(Distributional) Robustness

ERM

$$\min_{\theta} \frac{1}{N} \sum_{i=1}^N L_{\theta}(\xi_i)$$

Fit on dataset is
not enough to
protect against
shifts

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Robustify

$$\min_{\theta} \mathbb{E}_{\zeta \sim \mathbb{Q}} L_{\theta}(\zeta)$$

With \mathbb{Q} a “wider”
distribution

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Worst case

$$\min_{\theta} \sup_{\mathcal{Q}} \mathbb{E}_{\zeta \sim \mathcal{Q}} L_{\theta}(\zeta)$$

With the worst \mathcal{Q} !
But among
which?

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Define uncertainty

$$\min_{\theta} \sup_{\mathcal{Q} \approx \hat{\mathbb{P}}^N} \mathbb{E}_{\zeta \sim \mathcal{Q}} L_{\theta}(\zeta)$$

With \mathcal{Q} the worst,
“close to” $\hat{\mathbb{P}}^N$.

(Distributional) Robustness

ERM

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In this talk:
Wasserstein

W-DRO

Maximize over Wasserstein neighborhood of radius ρ (Mohajerin Esfahani & Kuhn, 2018).

(Primal)

$$\min_{\theta} \sup_{\substack{W_c(\hat{\mathbb{P}}^N, \mathbb{Q}) \leq \rho}} \mathbb{E}_{\zeta \sim \mathbb{Q}}[L_{\theta}(\zeta)]$$

(Dual)

$$\min_{\theta, \lambda \geq 0} \frac{1}{N} \sum_{\xi_i \sim \hat{\mathbb{P}}^N} \sup_{\zeta} \left\{ \underbrace{L_{\theta}(\zeta)}_{\text{objective}} + \lambda \underbrace{(\rho - c(\xi_i, \zeta))}_{\text{constraint (dualized)}} \right\}$$

W-DRO

Maximize over Wasserstein neighborhood of radius ρ (Mohajerin Esfahani & Kuhn, 2018).

(Primal)

$$\min_{\theta} \sup_{\substack{W_c(\hat{\mathbb{P}}^N, \mathbb{Q}) \leq \rho}} \mathbb{E}_{\zeta \sim \mathbb{Q}}[L_{\theta}(\zeta)]$$

(Dual)

$$\min_{\theta, \lambda \geq 0} \lambda \rho + \frac{1}{N} \sum_{\xi_i \sim \hat{\mathbb{P}}^N} \sup_{\zeta} \underbrace{\{L_{\theta}(\zeta) - \lambda c(\xi_i, \zeta)\}}_{\substack{\uparrow \\ c\text{-transform of } L_{\theta}}}$$

What about the sup?

$$\sup_{\zeta} \{L_{\theta}(\zeta) - \lambda \mathbf{c}(\zeta, \boldsymbol{\xi})\}$$

- $L_{\theta}(\zeta) - \lambda \mathbf{c}(\zeta, \boldsymbol{\xi})$ may be non-concave...
⇒ high difficulty
- Worked out in some cases (through disciplined programming): see [\(Mohajerin Esfahani & Kuhn, 2018\)](#), e.g.:
 - linear/logistic regression,
 - SVM,
 - portfolio optimization,
 - piecewise affine losses

What about the sup?

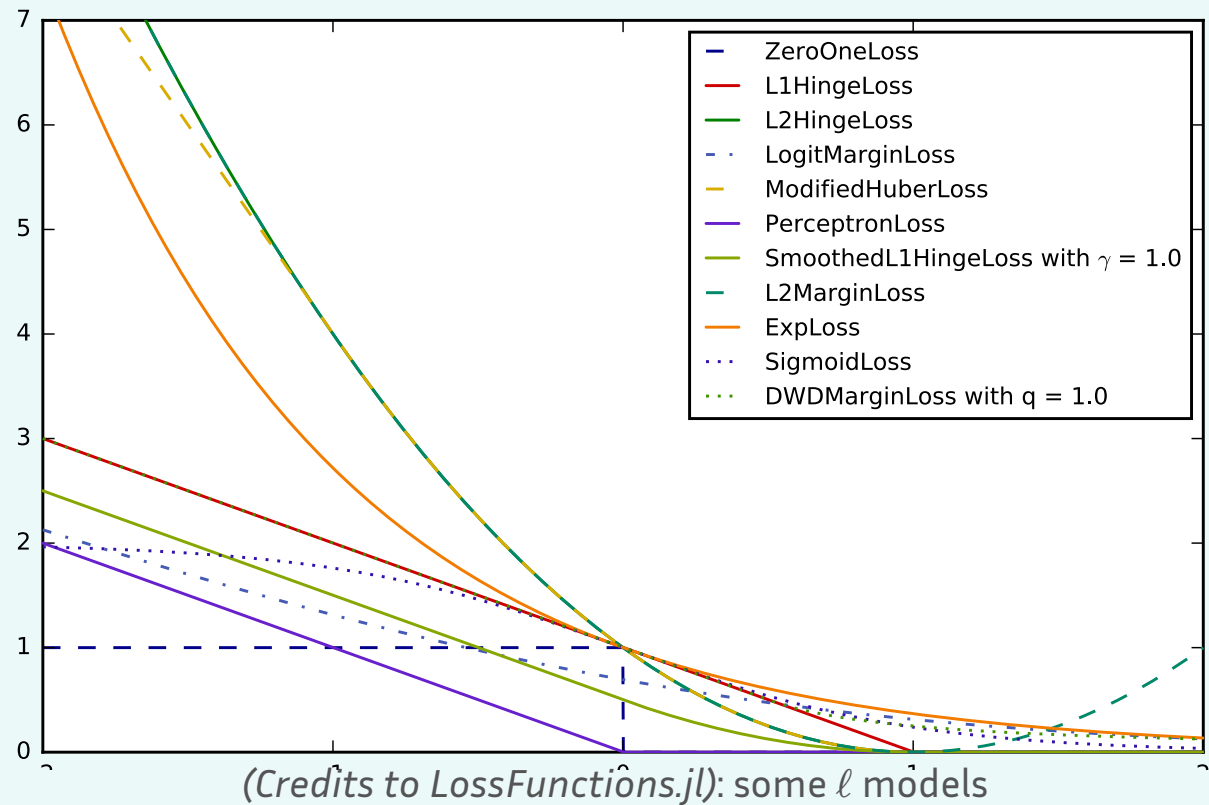
$$\sup_{\zeta} \{L_{\theta}(\zeta) - \lambda \mathbf{c}(\zeta, \xi)\}$$

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 - linear/**logistic regression**,
 - SVM,
 - portfolio optimization,
 - piecewise affine losses

The case of linear classification

Linear model:

$$\begin{cases} \boldsymbol{\xi} \in \mathbb{R}^d \\ L_{\boldsymbol{\theta}}(\boldsymbol{\xi}) := \ell(\boldsymbol{\theta}^T \boldsymbol{\xi}) \end{cases}$$



The case of linear classification

Theorem 1: [Shafieezadeh Abadeh et al. (2015)]

The WDRO problem for classification, with $c(\xi, \zeta) = \|\zeta - \xi\|_2$ can be written:

$$\min_{\theta} \text{Lip}(\ell) \rho \|\theta\|_2 + \frac{1}{N} \sum_{\xi_i \sim \hat{\mathbb{P}}^N} L_{\theta}(\xi_i)$$

For $c(\xi, \zeta) = \|\zeta - \xi\|$

- Soft margin: $\log(1 + e^{-y\theta^T x})$ ✓
- Hinge: $\max\{0, 1 - y\theta^T x\}$ ✓
- ...

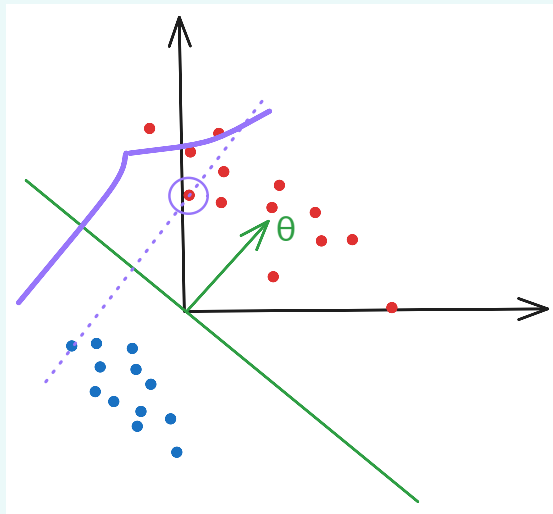
for $c(\xi, \zeta) = \|\zeta - \xi\|^2$

- L2-hinge: $\max\{0, (1 - y\theta^T x)^2\}$ ✓
- ...

The case of linear classification

This relies on a simple assumption (idea from [Gao & Kleywegt, 2023](#)):

The loss must behave like the costs in “worst case region”



- Well classified samples: $-\theta^T \xi \geq 0$, region where ℓ is small
- Misclassified samples: $-\theta^T \xi < 0$, region where ℓ grows.

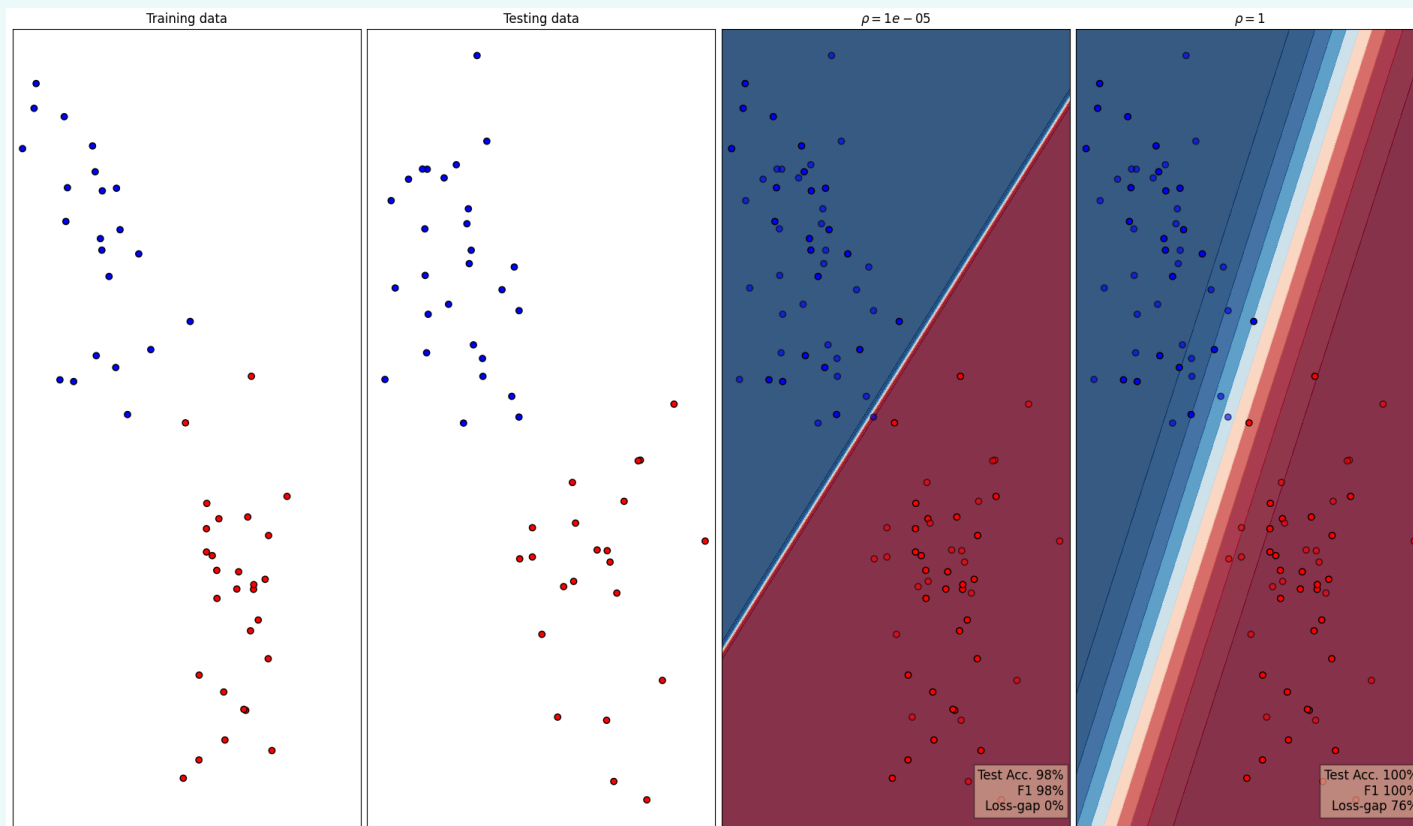
We know where the $\sup_{\zeta} \{\ell(\theta^T \zeta) - \lambda \|\zeta - \xi\|_2\}$ is in this case, so we can test numerically.

Toy example: linear classification #1

Simple balanced
separable dataset,

for $\rho = 10^{-5}$ vs 1:

- gained accuracy
- lower test loss (**-78%**)
- wider margin.

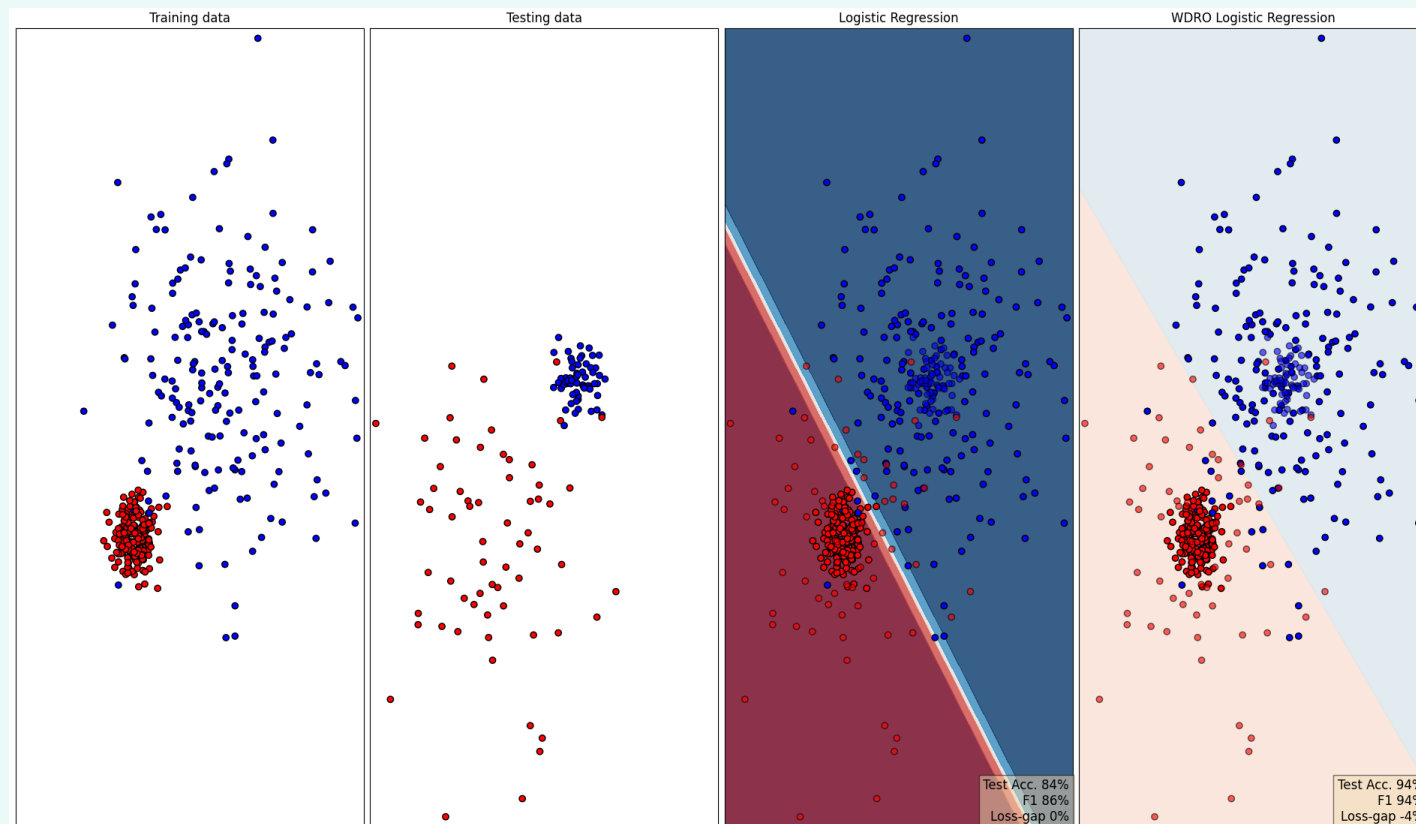


Toy example: linear classification #1

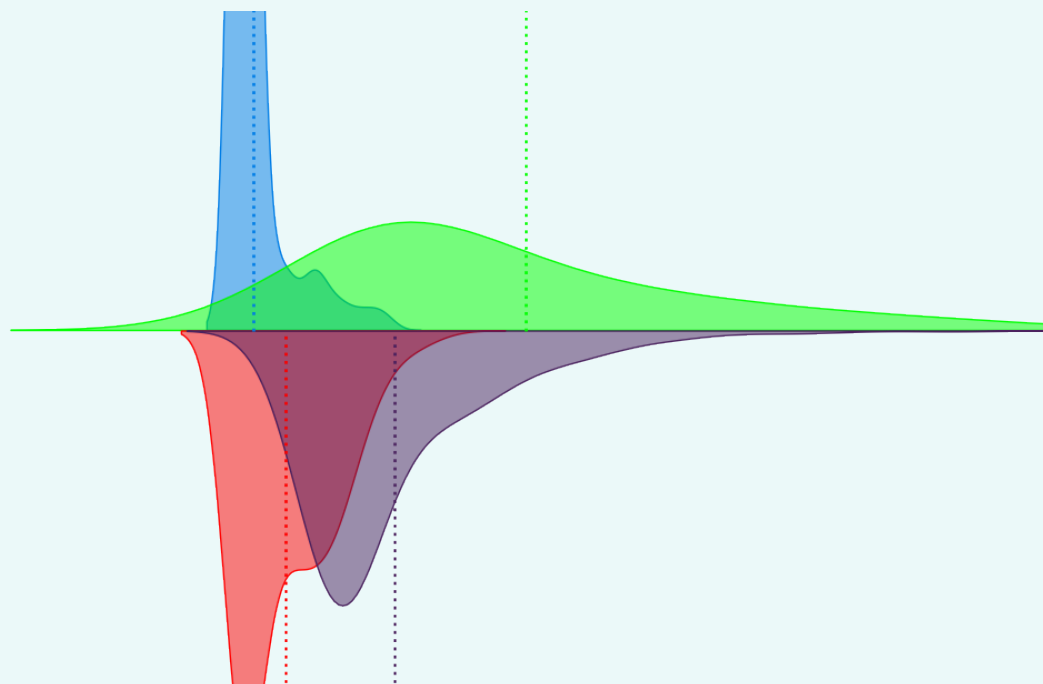
Swap variances

Hence distribution **shift** !

⇒ ~ 10% accuracy gain
w.r.t. non-robust (ERM)



Toy example: linear classification #2



Train 1000 models
on random data:



- ERM training losses
- ERM test losses
- DRO training losses
- DRO test losses

x-axis: average loss on the dataset, y-axis: frequency

General case

$$\sup_{\zeta} \{L_{\theta}(\zeta) - \lambda \, c(\xi, \zeta)\}$$

When the supremum:

- does not admit any closed form 
- and is intractable numerically 



Turn to smoothing the sup

Dual of regularized WDR0 problem – easier to solve for:

$$\min_{\theta, \lambda \geq 0} \lambda \rho + \frac{1}{N} \sum_{\xi_i \sim \hat{\mathbb{P}}^N} \epsilon \log \mathbb{E}_{\zeta \sim \mathcal{N}(\xi_i, \sigma^2)} \left[e^{\frac{L_{\theta}(\zeta) - \lambda c(\zeta, \xi_i)}{\epsilon}} \right]$$



(Azizian et al., 2023)

Close to other ideas:

- (Blanchet & Kang, 2020) : Smooth explicitly with unlabeled data points
- (Wang et al., 2023) : Sinkhorn regularization of the Wasserstein distance

E.g.: Smoothing the linear classification

Theorem 2: [Vincent et al. 2025]

With $c(\xi, \zeta) = \|\zeta - \xi\|_2^2$ and $K := \frac{1}{\epsilon} \in \mathbb{N}$ the regularized WDRO can be written:

$$\min_{\theta, \lambda \geq 0} \frac{1}{K} \left\{ \lambda \rho - \frac{1}{2} \log(1 + \lambda^d \sigma^{2d}) + \frac{1}{N} \sum_{\xi_i \sim \hat{\mathbb{P}}^N} \log \left[\sum_{k=1}^K \binom{K}{k} e^{Q_{\theta, \lambda}^{(k)}(\xi_i)} \right] \right\}$$

for a quadratic form: $Q_{\theta, \lambda}^{(k)}(\xi) = k \theta^T \xi - k^2 \frac{\sigma^2}{2(\lambda \sigma^2 + 1)} \|\theta\|_2^2$

→ Not simple ! **Tractable**, but less explicit than vanilla WDRO.

In general: smooth your own loss function

$$\epsilon \log \mathbb{E}_{\zeta \sim \mathcal{N}(\xi, \sigma^2)} \left[e^{\frac{L_{\theta}(\zeta) - \lambda c(\zeta, \xi)}{\epsilon}} \right]$$


- Smooth \Rightarrow you can optimize it, as you would L_{θ}
- Pick the hyperparameter ϵ depending on σ^2

Is it better?

	Pros	Cons
$\sup_{\zeta} L_{\theta}(\zeta) - \lambda \, c(\zeta, \xi)$	<ul style="list-style-type: none">▪ No hyperparameter	<ul style="list-style-type: none">▪ No closed form (in general)
$\epsilon \log \mathbb{E}_{\zeta \sim \mathcal{N}(\xi, \sigma^2)} \left[e^{\frac{L_{\theta}(\zeta) - \lambda \, c(\zeta, \xi)}{\epsilon}} \right]$	<ul style="list-style-type: none">▪ $\mathbb{E}_{\zeta \sim \mathcal{N}(\cdot, \sigma^2)}$ tractable by sampling (e.g. MC)	<ul style="list-style-type: none">▪ Pick ϵ and σ^2

Is it better?

$$\sup_{\zeta} L_{\theta}(\zeta) - \lambda \, c(\zeta, \xi)$$


$$\epsilon \log \mathbb{E}_{\zeta \sim \mathcal{N}(\xi, \sigma^2)} \left[e^{\frac{L_{\theta}(\zeta) - \lambda \, c(\zeta, \xi)}{\epsilon}} \right]$$

Pros

- No hyperparameter

- $\mathbb{E}_{\zeta \sim \mathcal{N}(\cdot, \sigma^2)}$ tractable by sampling (e.g. MC)

Cons

- No closed form (in general)

- Pick ϵ and σ^2

Our work: the SkWDR0 toolbox

Plan

A library for
your own
case:
SkWDR0

Experiments
(and real
world
data)

Insights on
what is
behind the
scene

Numerics

- Tackle with the smoothed sup
- Relevant default hyperparameters proposed

SkWDRO [Vincent et al. 2024]



- A python package:
 - \$ `pip install skwdro`
 - \$ `uv pip install skwdro`
 - \$ `mamba install flvincen:skwdro`
- PyTorch interface to solve smoothed problem for given ρ .

SkWDRO - PyTorch interface

(Try defaults)

```
def dualize_primal_loss(  
    loss_: nn.Module,  
    transform_: Optional[nn.Module],  
    rho: pt.Tensor,  
    xi_batchinit: pt.Tensor,  
    xi_labels_batchinit: Optional[pt.Tensor],  
    ) -> DualLoss:
```

This DualLoss torch Module can be optimized in the same way as the original loss.

SkWDRO - PyTorch interface

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    post_sample: bool=True,  
    cost_spec: Optional[str]=None,  
    n_samples: int=10,  
    seed: int=42,  
  
    *,  
    epsilon: Optional[float]=None,  
    sigma: Optional[float]=None,  
    l2reg: Optional[float]=None,  
    adapt: str="prodigy",  
    imp_samp: bool=True  
) -> DualLoss:
```

Lot of control
on the
hyperparameters

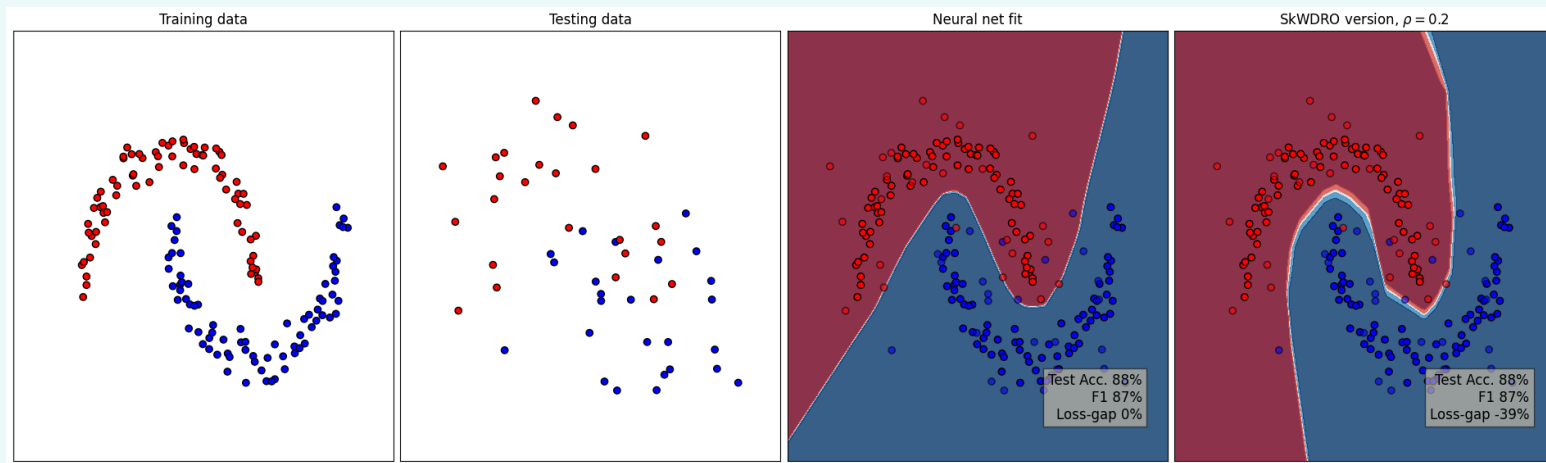
Toy example: classification #2

Non-convex
setting:
moons+noise

Train $\mathcal{N}\left(0, \begin{pmatrix} 2.5 \cdot 10^{-3} & 0 \\ 0 & 10^{-2} \end{pmatrix}\right)$












→

Test $\mathcal{N}\left(0, \begin{pmatrix} 10^{-2} & 0 \\ 0 & 2.5 \cdot 10^{-3} \end{pmatrix}\right)$



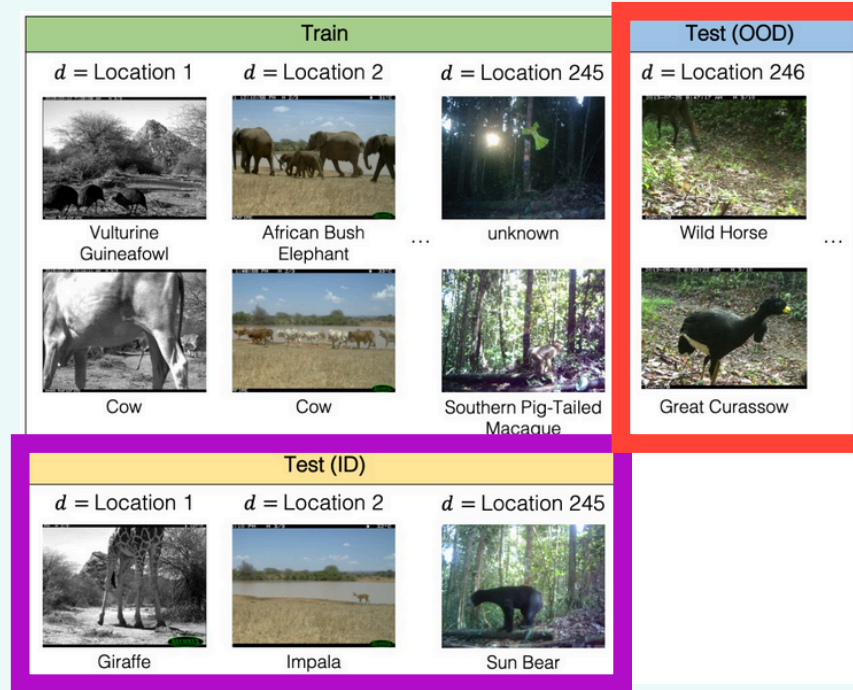
Test loss gets **39%** down, as the model gets conservative.

Back to the Wilds 🦁.

Train			Test (OOD)
$d = \text{Location 1}$	$d = \text{Location 2}$	$d = \text{Location 245}$	$d = \text{Location 246}$
			
Vulturine Guinea fowl	African Bush Elephant	...	Wild Horse
			
Cow	Cow	Southern Pig-Tailed Macaque	Great Curassow
Test (ID)			
$d = \text{Location 1}$	$d = \text{Location 2}$	$d = \text{Location 245}$	
			
Giraffe	Impala	Sun Bear	

Back to the Wilds 🦁.

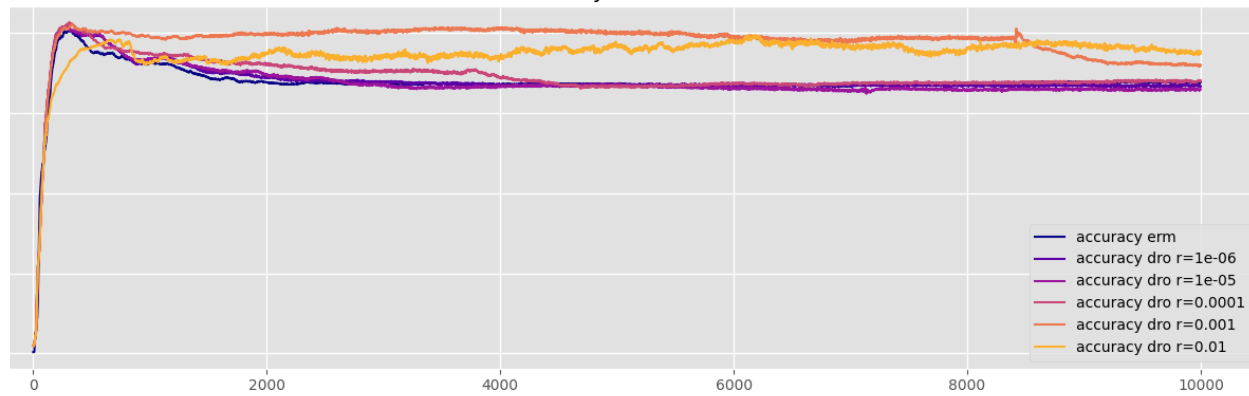
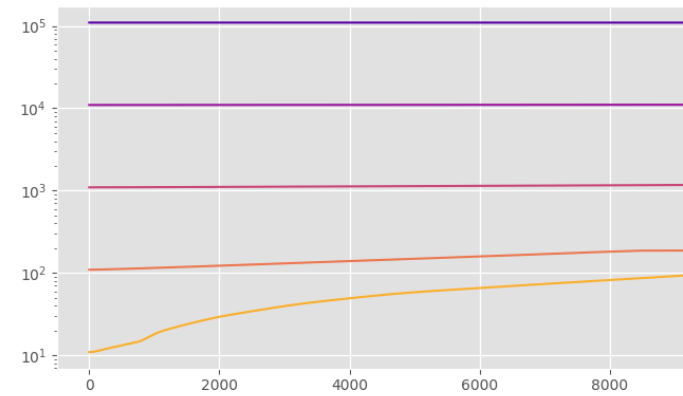
Track the
validation
loss during
training, with
test accuracy



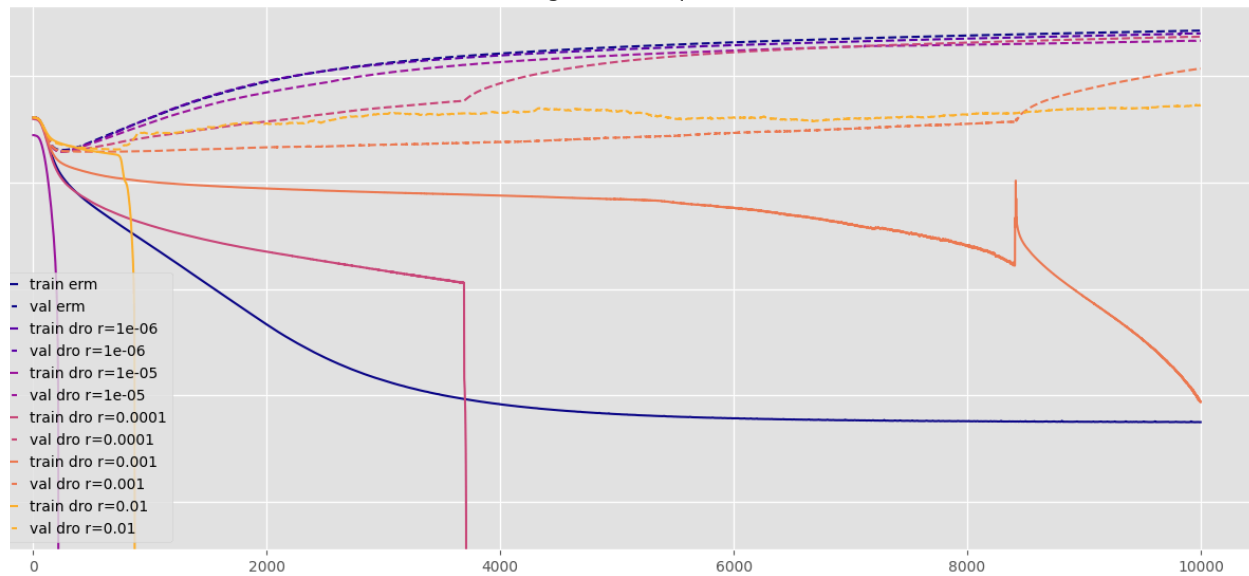
Setup:

- Data pre-treated with a resnet ($\Rightarrow d = 157$)
- 1 hidden layer neural-net ($d_h = 64$)
- $|\text{Train}| = 20000$
 $|\text{Val}| = |\text{Test}| = 5000$

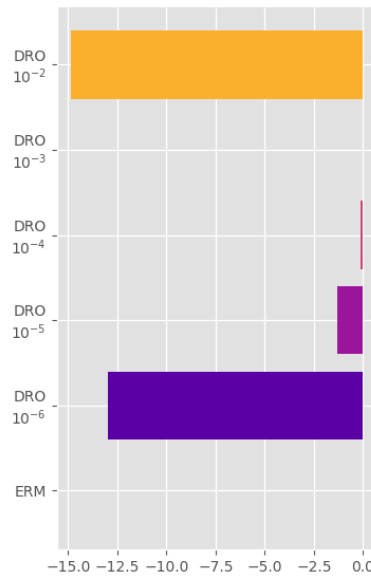
Accuracy on test set

 λ 

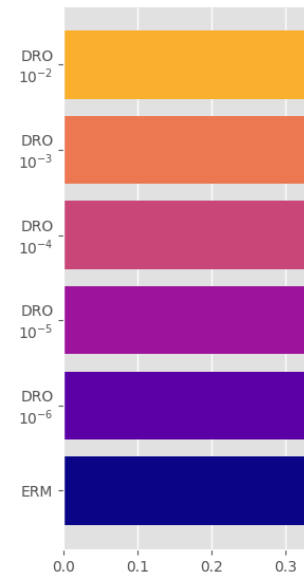
Training curve comparison



Last iterate train loss



Best iterate accuracy



Behind the scenes

- Clever sampling for the inner `logsumexp`
- Heuristics to set ϵ , Σ
- Numerically stable backward pass on the loss
- Heuristic to set starting λ
- User-friendly interfaces
- All-in-one API, no troubles to define the problem
- Test suite & documentation

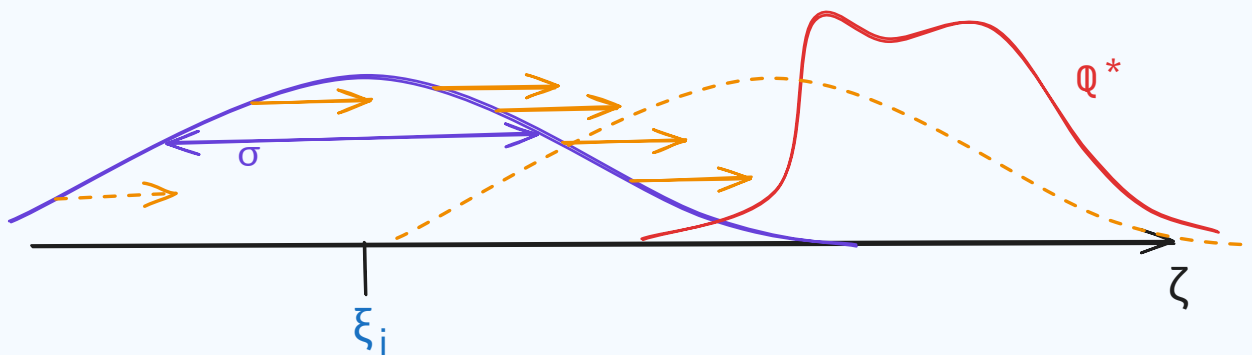
Behind the scenes

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- Heuristics to set ϵ , Σ
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- Heuristic to set starting λ
- User-friendly interfaces
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Clever sampling strategy

$$\epsilon \log \left(\mathbb{E}_{\zeta | \xi} \left[e^{\frac{1}{\epsilon} (L_{\theta} - \lambda c(\xi, \zeta))} \right] \right)$$

Importance sampling: push samples where they have more weights in $\mathbb{E}_{\zeta \sim \mathcal{N}(\xi, \sigma^2)}$.



Conclusion

Skwdro

A library that allows you to robustify your decision model written in PyTorch.

Take-away message

Big non-convex models are amenable to WDRO

Perspectives:

- Add constraints
- Scale up

Try it out!



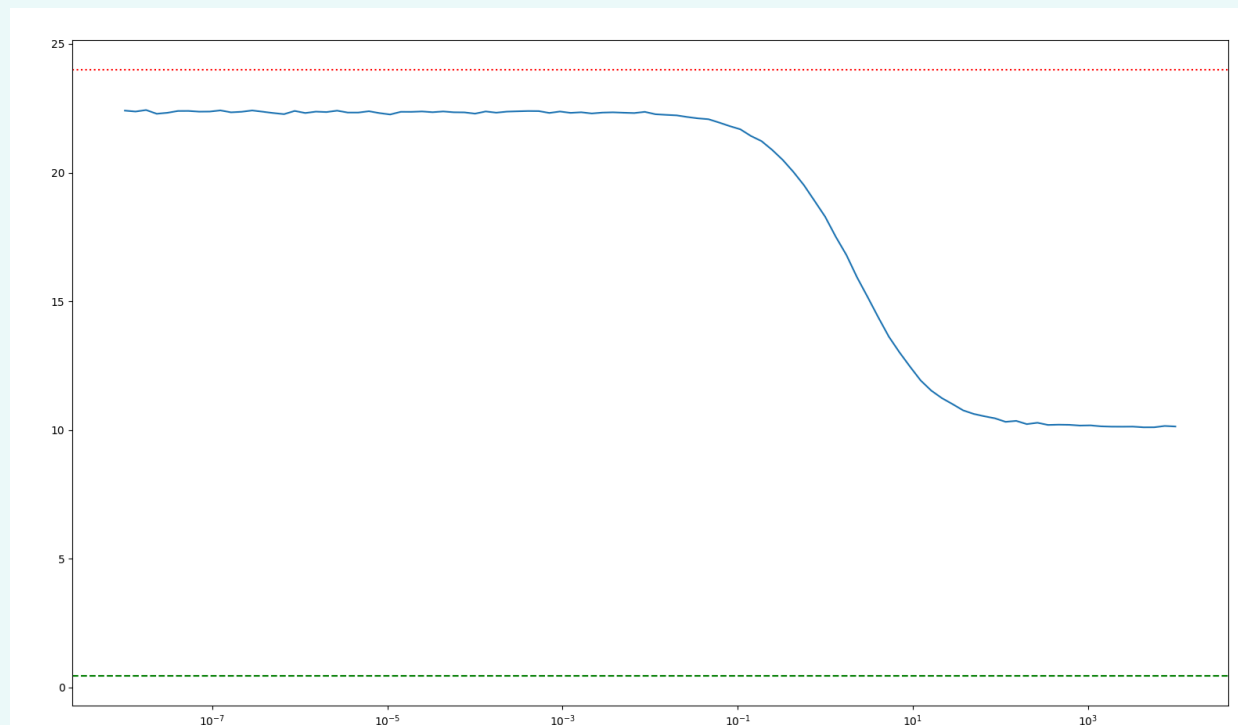
- [1] P. Mohajerin Esfahani and D. Kuhn, "Data-driven distributionally robust optimization using the Wasserstein metric: performance guarantees and tractable reformulations," *Mathematical Programming*, vol. 171, 2018.
- [2] D. Kuhn, P. M. Esfahani, V. A. Nguyen, and S. Shafieezadeh-Abadeh, "Wasserstein distributionally robust optimization: Theory and applications in machine learning," *Operations research & management science in the age of analytics*. Informs, 2019.
- [3] J. Wang, R. Gao, and Y. Xie, "Sinkhorn Distributionally Robust Optimization." 2023.
- [4] W. Azizian, F. Iutzeler, and J. Malick, "Regularization for Wasserstein distributionally robust optimization," *ESAIM: COCV*, 2023, doi: 10.1051/cocv/2023019.
- [5] S. Shafieezadeh Abadeh, P. M. Mohajerin Esfahani, and D. Kuhn, "Distributionally Robust Logistic Regression," in *Advances in Neural Information Processing Systems*, C. Cortes, N. Lawrence, D. Lee, M. Sugiyama, and R. Garnett, Eds., Curran Associates, Inc., 2015. [Online]. Available: https://proceedings.neurips.cc/paper_files/paper/2015/file/cc1aa436277138f61cda703991069eaf-Paper.pdf

- [6] R. Gao and A. Kleywegt, “Distributionally Robust Stochastic Optimization with Wasserstein Distance,” *Mathematics of Operations Research*, vol. 48, no. 2, pp. 603–655, 2023, doi: 10.1287/moor.2022.1275.
- [7] J. Blanchet and Y. Kang, “Semi-supervised Learning Based on Distributionally Robust Optimization,” Wiley, 2020, pp. 1–33. doi: 10.1002/9781119721871.ch1.
- [8] T. Le, “Unregularized limit of stochastic gradient method for Wasserstein distributionally robust optimization.” [Online]. Available: <https://arxiv.org/abs/2506.04948>

Hyperparameters

Numerical difficulties:

- **SkWDRO** is above **ERM**
- But it does not reach true **WDRO**



Regularized loss dependency on ϵ (logscale)

The Wasserstein distance

Wasserstein distance is inspired from Optimal Transport:

$$W_{\mathbf{c}}(\mathbb{A}, \mathbb{B}) := \inf_{\pi \mid \begin{cases} [\pi]_1 = \mathbb{A} \\ [\pi]_2 = \mathbb{B} \end{cases}} \{\mathbb{E}_{\pi}[\mathbf{c}]\}.$$

One may regularize this with entropy:

$$W_{\boldsymbol{\epsilon}, \mathbf{c}}(\mathbb{A}, \mathbb{B}) := \inf_{\pi \mid \begin{cases} [\pi]_1 = \mathbb{A} \\ [\pi]_2 = \mathbb{B} \end{cases}} \{\mathbb{E}_{\pi}[\mathbf{c}] + \boldsymbol{\epsilon} \text{KL}(\pi \parallel \pi_0)\}.$$

\Rightarrow need to pick $\boldsymbol{\epsilon}$ and π_0

Robustness

Maximize over “close” distribution.

$$\min_{\theta} \sup_{\mathbb{Q} \text{ "close to" } \hat{\mathbb{P}}^N} \mathbb{E}_{\zeta \sim \mathbb{Q}}[L_{\theta}(\zeta)]$$

Robustness

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Multiple possible
notions of neighborhood:

- KL divergence
- χ^2 -distance
- TV-distance
- ...

Focus on the Wasserstein distance:

$$W_c(\hat{\mathbb{P}}^N, \mathbb{Q}) := \inf_{\pi} \left\{ \mathbb{E}_{(\xi, \zeta) \sim \pi} [c(\xi, \zeta)] \mid [\pi]_1 = \hat{\mathbb{P}}^N, [\pi]_2 = \mathbb{Q} \right\}$$

- Today mostly $c(\zeta, \xi) = \|\zeta - \xi\|_2^2$ and $\|\zeta - \xi\|_2$

Convergence result:

Theorem (Le, 2025):

Gradients of (ϵ -Regularized WDRO) converge with $\epsilon \rightarrow 0$ and $M \rightarrow \infty$ to the Clarke differential of (WDRO).

$$\epsilon \frac{1}{N} \sum_{i=1}^N \log \frac{1}{M} \sum_{j=1}^M e^{\frac{L_{\theta}(\zeta_j) - \lambda c(\zeta_j, \xi_i)}{\epsilon}} \xrightarrow[\substack{\epsilon \rightarrow 0 \\ M \rightarrow \infty}]{} \frac{1}{N} \sum_{i=1}^N \sup_{\zeta} \{L_{\theta}(\zeta) - \lambda c(\zeta, \xi_i)\}$$

SkWDRO [Vincent et al. 2024]

CI	Test	TESTS PASSING
	Style	STYLE PASSING
	Doc	Workflow Doc
Doc	Readthedocs	READTHEDOCS
Checks	Code style	RUFF
	Types	MYPY CHECKED
	Build	BUILT BY RATTLE-BUILD
Install	Pip	PYTHON 2.7 3.5 3.6 3.7
	Conda	Anaconda.org 1.0.1
	Github	GITHUB
Cite		ARXIV 2410.21231

SkWDRO - Wasserstein Distributionally Robust Optimization

Model robustification with thin interface

"You can make pigs fly", [Kolter&Madry, 2018]

PYTHON **PYTORCH** **SCIKITLEARN** **LICENSE** **BSD 3-CLAUSE**

skwdro is a Python package that offers **WDRO versions** for a large range of estimators, either by extending **scikit-learn estimator** or by providing a wrapper for **pytorch modules**.

skwdro: a library for Wasserstein distributionally robust machine learning

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Abstract

We present **skwdro**, a Python library for training robust machine learning models. The library is based on distributionally robust optimization using optimal transport distances. For ease of use, it features both **scikit-learn** compatible estimators for popular objectives, as well as a wrapper for **PyTorch** modules, enabling researchers and practitioners to use it in a wide range of models with minimal code changes. Its implementation relies on an entropic smoothing of the original robust objective in order to ensure maximal model flexibility. The library is available at <https://github.com/iutzeler/skwdro>.

Keywords: Distributionally robust optim., distribution shifts, entropic regularization

A library

and a preprint

Our work: the SkWDR0 toolbox

Numerics

- Tackle with the smoothed sup
- Sound default hyperparameters proposed

Engineering

- Maintained library
- Documentation and examples
- **Friendly+idiomatic interfaces**