The Devil is in the Tails and other Stories of Interpolation

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with Tatsunori Hashimoto, Saminul Haque, Philip Long and Alexander Wang











(Zhang et al. 2016)

Deep networks generalize well even when





(Zhang et al. 2016)

Deep networks generalize well even when

data has misclassification noise





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Deep networks generalize well even when

data has misclassification noise

model is overparameterized





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Deep networks generalize well even when

data has misclassification noise

model is overparameterized

not regularized





(Zhang et al. 2016)

Deep networks generalize well even when

data has misclassification noise

model is overparameterized

not regularized

trained to zero training loss via SGD





(Belkin et al. 2018)



(Nakkiran et al. 2021)







Vignette I: Interpolating Classifiers under shift $P_{train} \neq P_{test}$



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y: blond hair 14%a: female

(low error)



y: dark hair 41%a: male



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Atypical groups (high error)



y: blond hair 1%a: male



Vignette I: Interpolating Classifiers under shift $P_{train} \neq P_{test}$



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• P_{train} is an imbalanced mixture of the groups

(low error)



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Vignette I: Interpolating Classifiers under shift $P_{train} \neq P_{test}$



- a: female
- P_{train} is an imbalanced mixture of the groups
- Ptest is an uniform mixture over all groups

Common groups (low error) ------.000 y: dark hair 41%

a: male

Atypical groups (high error)



y: blond hair 1%a: male



Is Interpolating at odds with Robustness?

Common groups (low error)

CelebA 162,770 training examples



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Atypical groups (high error)



y: blond hair a: male

1%



worst-group test	— average test
worst-group train	— average train

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(Sagawa et al. 2020)

Interpolating classifiers trained on the reweighted CE loss suffer high test error



Interpolation breaks Robustness Interventions

Training dynamics of a linear classifier with 2D toy data

Cross Entropy: No IW



Interpolation breaks Robustness Interventions

Training dynamics of a linear classifier with 2D toy data

Cross Entropy: No IW \bigcirc



Reweighting results in identical interpolating classifiers!

Is Reweighting Incompatible with Interpolation?

Vignette II: Training Sparse Models

Scaling model size has led to drastic improvements



ImageNet

Google Multilingual Corpus

(Huang et al. 2019)



Vignette II: Training Sparse Models







Vignette II: Training Sparse Models









Example: Large Language Models



Example: Large Language Models



To speed up inference and efficiency, sparse mixture-of-experts models

Example: Large Language Models





To speed up inference and efficiency, sparse mixture-of-experts models

However Sparsity can hurt test error

ResNet20 trained on CIFARI0

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	0.30				
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rain	0.10				
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(Chan et al. 2021)

However Sparsity can hurt test error



(Chan et al. 2021)

However Sparsity can hurt test error



(Chan et al. 2021)

Is Sparsity Incompatible with Interpolation?

Study these non-standard settings with linear models

Interpolation under Distribution Shift



Study these non-standard settings with linear models

Interpolation under Distribution Shift



Study these non-standard settings with linear models

Sparsity and Interpolation




Importance Weighting with Interpolating Classifiers

Consider a binary classification task with distribution shift

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Given data $(x_1, y_1), \dots, (x_n, y_n) \in \mathbb{R}^d \times \{-1, 1\} \sim \mathsf{P}_{\text{train}}$

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Goal: minimize test error $\mathbb{P}_{(x,y)} \sim \mathbb{P}_{\text{test}} \left[f_{\theta}(x) \neq y \right]$

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Goal: minimize test error $\mathbb{P}_{(x,y)} \sim \mathbb{P}_{\text{test}} \left[f_{\theta}(x) \neq y \right]$

Use gradient descent to minimize the *importance* weighted loss (Shimodaira 2000) $L(f(\theta)) = \sum w_i \log \left[1 + \exp(-y_i f_{\theta}(x))\right]$ i=1



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Train until interpolation: $L(f(\theta^{(t)})) \rightarrow 0$



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(Shimodaira 2000)

 $L(f(\theta)) = \sum w_i \log \left[1 + \exp(-y_i f_{\theta}(x))\right]$





Doesn't work



Cross Entropy: IW





Predicted Majority	•	Majority Class
Predicted Minority	$\mathbf{\Delta}$	Minority Class

Doesn't work



Cross Entropy: IW







Predicted Majority	•	Majority Class
Predicted Minority	$\boldsymbol{\bigtriangleup}$	Minority Class

Can we design interpolators that respond to weighting?



If gradient descent used to minimize

$$L(\theta) = \sum_{i=1}^{n} w_i \log_{\theta} \frac{1}{10}$$

Given linearly separable data $(x_1, y_1), \dots, (x_n, y_n) \in \mathbb{R}^d \times \{-1, 1\} \sim \mathsf{P}_{\mathsf{train}}$

 $\log \left| 1 + \exp(-y_i x_i^{\mathsf{T}} \theta) \right|$



If gradient descent used to minimize

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Given iterates $\theta^{(t+1)} = \theta^{(t)} - \eta \nabla L(\theta^{(t)})$ if η is small enough

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(Xu et al. 2019, Soudry et al. 2018, Ji and Telgarsky 2018)



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$$\frac{\theta^{(t)}}{\|\theta^{(t)}\|} \to \arg \max_{\|\theta\|_2 = 1} \left\{ \gamma : \|\theta\|_2 = 1 \right\}$$

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subject to $y_i x_i^{\mathsf{T}} \theta \ge \gamma, \forall i \in [n] \}$



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"maximum-margin classifier" θ_{MM}



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Intuition: Reweighting doesn't affect Exp-Tailed Losses

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Intuition: Reweighting does

Consider the reweighted objective L(

This is equivalent to creating a "new dataset" with w_i copies of sample i

 (x_i, y_i)

И

sn't affect Exp-Tailed Losses

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), ...,
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 $\overline{y_i}$ times

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The max-margin classifier for this new dataset is unchanged $\|\theta\|_2 = 1$

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 $(x_i, y_i), \dots, (x_i, y_i)$

 w_i times

 $\arg \max_{i} \left\{ \gamma : \text{ subject to } y_i x_i^{\mathsf{T}} \theta \ge \gamma, \forall i \in [n] \right\}$

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This is equivalent to creating a "new dataset" with w_i copies of sample i

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Prior implicit bias results implies $t \rightarrow \infty$ reweighting is ineffective (Soudry et al. 2018, Ji and Telgarsky 2018)

sn't affect Exp-Tailed Losses

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 w_i times

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Our Proposal: Switch losses $log(1 + exp(-yf_{\theta}(x))) \longrightarrow$





Our Proposal: Switch losses $log(1 + exp(-yf_{\theta}(x)))$





Predicted Majority Majority Class igodolMinority Class Predicted Minority Δ

Our Proposal: Switch losses $log(1 + exp(-yf_{\theta}(x)))$





We provably show it has the correct implicit bias

Predicted Majority Predicted Minority

Majority Class \bigcirc Minority Class Δ

Implicit bias for poly-tailed losses



Implicit bias for poly-tailed losses



If gradient descent used to minimize linearly separable $(x_1, y_1), \ldots, (x_n, y_n)$ $L(\theta) = \sum_{i=1}^{n} w_i \mathcal{C}(y_i x_i^{\mathsf{T}} \theta) \qquad \mathcal{C}(z) = \begin{cases} \frac{\log(1 + \exp(-z))}{\log(1 + \exp(-1))} & z \le 1\\ \frac{1}{z^{\alpha}} & z > 1 \end{cases}$

Implicit bias for poly-tailed losses If gradient descent used to minimize linearly separable $(x_1, y_1), \ldots, (x_n, y_n)$ Given iterates $\theta^{(t+1)} = \theta^{(t)} - \eta \nabla L(\theta^{(t)})$ if η is small enough

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- $L(\theta) = \sum_{i=1}^{n} w_i \ell(y_i x_i^{\mathsf{T}} \theta) \qquad \ell(z) = \begin{cases} \frac{\log(1 + \exp(-z))}{\log(1 + \exp(-1))} & z \le 1\\ \frac{1}{z^{\alpha}} & z > 1 \end{cases}$

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- Maximizes a sum of weighted margins

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Builds on results by Ji et al. 2020

Maximizes a sum of weighted margins



But what about the test performance?

But what about the test performance?

Does maximizing the weighted margin translate into robust test accuracy?



But what about the test performance?

What's coming up...

Does maximizing the weighted margin translate into robust test accuracy?


But what about the test performance?

What's coming up...

I. Setting where the poly-tailed classifier achieves minimax accuracy

Does maximizing the weighted margin translate into robust test accuracy?



But what about the test performance?

What's coming up...

I. Setting where the poly-tailed classifier achieves minimax accuracy

2. A lower bound that shows that the max-margin classifier fails

Does maximizing the weighted margin translate into robust test accuracy?



Want to study the generalization error in the overparameterized regime with distribution shift



(majority class, +1) $\mathscr{P}(x \sim \mathsf{N}(\mu_1, I))$ (or any subgaussian dist.) μ_1 \mathcal{N}

(minority class, -1)





Want to study the generalization error in the overparameterized regime with distribution shift

Skewed data with $|\mathcal{P}| \ge |\mathcal{N}|$, with



$$h \tau = \frac{|\mathcal{P}|}{|\mathcal{N}|}$$

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Assumptions on the data

- $n \ge C \log(1/\delta)$
- $\|\mu\|^2 \ge Cn^2 \log(n/\delta)$
- $d \ge Cn \|\mu\|^2$ (high dim. setting)



$$h \tau = \frac{|\mathcal{P}|}{|\mathcal{N}|}$$

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(minority class, -1)

Set weights as
$$w_i = \begin{cases} 1 & \text{if } i \in \mathscr{P} \\ w > 1 & \text{if } i \in \mathscr{N} \end{cases}$$







for any $\delta < 1/C$, if the weight





Theorem: There exists a constant c such that for all large enough C,

for any $\delta < 1/C$, if the weight $\frac{\tau^3}{2} \le w \le 2\tau^3$





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then with probability at least $1-\delta$





 $\mathsf{TestError}(\theta_1) \le \exp\left(-\frac{c \|\mathcal{N}\| \|\mu\|^4}{d}\right).$

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Theorem: There exists a constant c such that for all large enough C, for any $\delta < 1/C$, if the weight $\frac{\tau^3}{2} \le w \le 2\tau^3$

then with probability at least $1-\delta$ $\mathsf{TestError}(\theta_1) \le \exp\left(-\frac{c \,|\,\mathcal{N}\,|\,\|\mu\|^4}{d}\right) \to 0 \text{ if } \frac{\sqrt{|\,\mathcal{N}\,|\,}\|\mu\|^2}{\sqrt{d}} \to \infty$

Further, if the imbalance au is sufficiently large then w.p. at least $1-\delta$ $\text{TestError}(\theta_{\text{MM}}) \ge -\frac{1}{Q}$.





Giraud and Verzelen 2019)



Separation between poly-tailed and exp-tailed classifiers Example setting: • $\|\mu\|^2 = d^{\frac{1}{2} + \frac{1}{40}}$ $\bullet |\mathcal{N}| = d^{\frac{1}{5}}$ • $\tau = d^{\frac{3}{20}}$



Separation between poly-tailed and exp-tailed classifiers Example setting: • $\|\mu\|^2 = d^{\frac{1}{2} + \frac{1}{40}}$ $\bullet |\mathcal{N}| = d^{\frac{1}{5}}$ • $\tau = d^{\frac{3}{20}}$

$\text{TestError}(\theta_{\text{MM}}) \ge \frac{1}{8} \ge \text{TestError}(\theta_1) \to 0$ As $d \to \infty$ (w.h.p.) (IW exp-tailed classifier) (IW poly-tailed classifier)



Separation between poly-tailed and exp-tailed classifiers Example setting: • $\|\mu\|^2 = d^{\frac{1}{2} + \frac{1}{40}}$ $\bullet |\mathcal{N}| = d^{\frac{1}{5}}$ • $\tau = d^{\frac{3}{20}}$

As $d \to \infty$ TestError(θ_{MM}) $\ge \frac{1}{8} \ge \text{TestError}(\theta_1) \to 0$ (w.h.p.) (IW exp-tailed classifier) (IW poly-tailed classifier)

Importance weighted poly-tailed classifier provably generalizes better



for any $\delta < 1/C$, if the weight $\frac{\tau^3}{2} \le w \le 2\tau^3$

then with probability at least $1-\delta$



Theorem: There exists a constant c such that for all large enough C, $\mathsf{TestError}(\theta_1) \le \exp\left(-\frac{c \|\mathcal{N}\| \|\mu\|^4}{d}\right).$ Further, if the imbalance τ is sufficiently large then w.p. at least $1-\delta$ $\operatorname{TestError}(\theta_{MM}) \geq -\frac{1}{Q}$.





This choice is unusual since the resulting loss is biased





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Classical choice $w = \tau$ leads to unbiased training loss





This choice is unusual since the resulting loss is biased

Classical choice $w = \tau$ leads to unbiased training loss

Nothing special about au^3 ,



, if
$$L(z) \sim \frac{1}{z^{\alpha}}$$
, then $w \asymp \tau^{\frac{\alpha(\alpha+2)}{\alpha^2+\alpha-1}}$

Exponentiate the weights and train on biased loss







Exponentiate the weights and train on biased loss









Exponentiate the weights and train on biased loss









Exponentiate the weights and train on biased loss max. margin & no IW Test Error vs. Imbalance Ratio (τ) 10 w = 1 $w = \tau$ 8 Test Error (%) $w = \tau^3$ Max-margin 6 4 20 6 2 8 10 124 Imbalance Ratio (τ)













































In the overparameterized regime, exponentiating weights help!







Proof Idea: Lower Bound the Normalized Margin



 μ_1

Proof Idea: Lower Bound the Normalized Margin

Step I: By Hoeffding's inequality



 μ_1

Proof Idea: Lower Bound the Normalized Margin Step I: By Hoeffding's inequality $\text{TestError}(\theta^{(\infty)}) \leq \frac{1}{2} \left| \exp\left(-\frac{\langle \theta^{(\infty)}, \mu_1 \rangle^2}{\|\theta^{(\infty)}\|^2}\right) + \exp\left(-\frac{\langle \theta^{(\infty)}, \mu_2 \rangle^2}{\|\theta^{(\infty)}\|^2}\right) \right|$



Proof Idea: Lower Bound the Normalized Margin Step I: By Hoeffding's inequality $\text{TestError}(\theta^{(\infty)}) \le \frac{1}{2} \text{ exp}$

Step 2: Bound on the normalized margins by tracking iterates of GD

$$\left(-\frac{\langle\theta^{(\infty)},\mu_1\rangle^2}{\|\theta^{(\infty)}\|^2}\right) + \exp\left(-\frac{\langle\theta^{(\infty)},\mu_2\rangle^2}{\|\theta^{(\infty)}\|^2}\right)$$


Proof Idea: Lower Bound the Normalized Margin Step I: By Hoeffding's inequality TestError($\theta^{(\infty)}$) $\leq \frac{1}{2} \exp(\frac{1}{2})$

Step 2: Bound on the normalized margins by tracking iterates of GD $\frac{\langle \mu_2, \theta^{(t+1)} \rangle}{\|\theta^{(t+1)}\|} \gtrsim \frac{\|\mathcal{N}\| \|\mu\|^2}{\sqrt{d}} \left[\sum_{s=0}^t \frac{\sum_{i \in \mathcal{N}} w(\ell_i^{(s)})^2 - \frac{1}{\|\mu\|} \sum_{j \in \mathcal{P}} (\ell_j^{(s)})^2}{\sum_{k=1}^n w_i (\ell_k^{(s)})^2} \right]$

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Interpolating models



Interpolating models



Interpolating models



30

Interpolating models





Interpolating models







Interpolating models









Interpolating models







Interpolating models



Polynomial Losses + exponentiated weights improve performance for NNs

Performance improves even when regularization is used







Subsampled CelebA



Reweighted poly-loss is competitive current best reweighting methods



Reweighted poly-loss is competitive current best reweighting methods

Also possible to plug into sophisticated DRO methods and see improvements





• Robustness interventions behave differently in the interpolation regime

Cross Entropy: No IW

Cross Entropy: IW





Poly-tailed Loss: No IW

Poly-tailed Loss: IW





Robustness interventions behave differently in the interpolation regime



• Careful theoretical analysis leads us to new non-intuitive interventions



Poly-tailed Loss: No IW

Poly-tailed Loss: IW



Talk Outline

Interpolation under Distribution Shift



Study these non-standard settings with linear models

Sparsity and Interpolation





Talk Outline

Study these non-standard settings with linear models

Sparsity and Interpolation





Is sparsity incompatible with interpolation?



Sparsity seems to hurt the test error

(Chan et al. 2021)



Given *n* datapoints, $(x_1, y_1), ..., (x_n, y_n)$





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 $I. x_i \in \mathbb{R}^d$, with d > n





Given *n* datapoints, $(x_1, y_1), ..., (x_n, y_n)$

 $1. x_i \in \mathbb{R}^d$, with d > n

2. $y_i = \langle x_i, \theta^* \rangle + \xi_i$, where θ^* is k-sparse



Given *n* datapoints, $(x_1, y_1), ..., (x_n, y_n)$

 $|x_i \in \mathbb{R}^d$, with d > n2. $y_i = \langle x_i, \theta^* \rangle + \xi_i$, where θ^* is k-sparse



Is there an interpolant that leverages this underlying sparsity?

Q: How does the excess risk of a sparse interpolator behave?



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Example: the minimum ℓ_1 -norm interpolant is defined as



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Sparsity in Linear Regression Q: How does the excess risk of a sparse interpolator behave? $\theta_{\mathcal{C}_1} \in \arg\min_{\theta \in \mathbb{R}^d} \|\theta\|_1, \text{ such that } \mathbf{y} = X\theta$ θ_{ℓ_1} (Basis Pursuit) is known to promote sparsity

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Sparsity in Linear Regression Q: How does the excess risk of a sparse interpolator behave? $\theta_{\mathcal{C}_1} \in \arg\min_{\theta \in \mathbb{R}^d} \|\theta\|_1, \text{ such that } \mathbf{y} = X\theta$ θ_{ℓ_1} (Basis Pursuit) is known to promote sparsity

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We show that sparsity is *incompatible* with interpolation by a lower bound

- **Example:** the minimum ℓ_1 -norm interpolant is defined as



Construction for the Lower bound

Given *n* datapoints, $(x_1, y_1), \ldots, (x_n, y_n)$, where $x_i \in \mathbb{R}^d$ and $y_i = \langle x_i, \theta^* \rangle + \xi_i$

Under the following assumptions:

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$$(k, \varepsilon) \text{ Model}$$
$$\lambda_{1} = \dots = \lambda_{k} = 1$$
$$\lambda_{k+1} = \dots = \lambda_{d} = \epsilon$$
$$\Sigma = \begin{bmatrix} I_{k \times k} & 0\\ 0 & \varepsilon \cdot I_{d-k \times d-k} \end{bmatrix}$$



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2) if
$$og^{2}(1/\delta) + k^{1+c}$$

$$\theta^{\star}\|_{\Sigma}^{2} \gtrsim \frac{\sigma^{2}n}{s \log^{2}(d/s)}$$

(Similar bound in the isotropic case by Muthukumar et al. 2020)



Risk is larger for Sparser Models



 $R(\theta) \gtrsim \frac{\sigma^2 n}{s \log^2(d/s)}$

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k <



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Sparsity Level (s)



Risk is larger for Sparser Models

 $R(\theta) \gtrsim \frac{\sigma^2 n}{1}$

Spars





$$s \log^2(d/s)$$

$R(\theta)$





Basis pursuit outputs *n*-sparse model a.s.





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 $(\theta_{\ell_1} = \arg\min_{\theta \in \mathbb{R}^d} \|\theta\|_1, \text{ s.t. } \mathbf{y} = X\theta)$













Basis pursuite o $k = \sqrt{n}$ -sp • $d = n^2$ • $\varepsilon = 1/n^2$ • $\sigma^2 = ||\theta^*||^2 = 1$





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Sparse Min. ℓ_1 -norm (BP)





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Sparse Min. ℓ_1 -norm (BP)

Exponential Slowdown!





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Sparse Min. ℓ_1 -norm (BP)

Exponential Slowdown!

Nearly matching upper bounds (Koehler et al., Wang et al., Li and Wei 2021, Donhauser et al. 2021)



Intuition



Energy of the noise scales as $\|\mathbf{y}\|^2 \ge \sigma^2 n$



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Dense interpolators like the OLS can spread this over d directions



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$$\mathbf{y} = X\boldsymbol{\theta} = \begin{bmatrix} x_{11} & \cdots \\ x_{21} & \cdots \\ \vdots & \cdots \\ x_{n1} & \cdots \end{bmatrix}$$

x_{1k}	<i>x</i> _{1<i>k</i>+1}	• • •	x_{1d}	$\left\lceil \theta_{1} \right\rceil$
x_{2k}	x_{2k+1}	• • •	x_{2d}	θ_2
•	•	• • •	•	•
x_{nk}	x_{nk+1}	• • •	x_{nd}	θ_d

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Including many *unimportant* directions

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Including many *unimportant* directions

However, sparse estimators like BP can only spread it over s directions

x_{1k}	x_{1k+1}	• • •	x_{1d}	$ \theta_1 $
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I. Importance Weighting with Interpolators





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- Robustness interventions behave differently in the interpolation regime





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Summary and Future Directions

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2. Sparsity and Interpolation







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Summary and Future Directions

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- Are other properties are aligned/misaligned with generalization?
- Can we analyze NNs and also understand if sparsity is harmful?



